Mathematics for Physicists: Introductory Concepts and Methods

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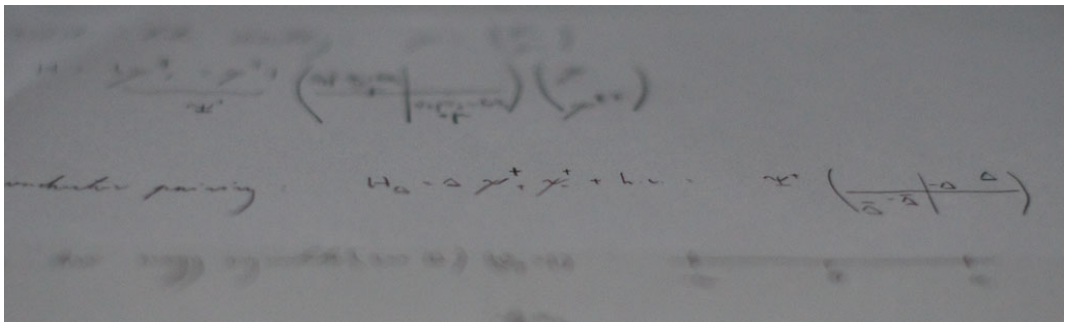

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Changes relative to the version from 22.10.2017:
Revisions in chapters L1-L5, C1-C4

Contents

Preface

The miracle of the appropriateness of the language of mathematics for the formulation of the laws of physics is a wonderful gift which we neither understand nor deserve. Eugene Paul Wigner

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This text is an introduction to mathematics for beginner physics students. Perhaps the first question to ask is in what sense it differs from the large number of existing books on the subject. The short answer is that it presents **the concepts and the methods** of mathematics in unison and on equal footing.

In contrast, traditional approaches mainly emphasize **the training of methods**. For example, standard courses on 'Mathematical methods for physicists' provide practical recipes for the algebraic manipulation of vectors, the diagonalization of matrices, the computation of Fourier transforms, or the solution of differential equations. This pragmatic approach is motivated by the fact that a wide assortment of mathematical methods are required early on in physics courses and that students have to learn them as quickly as possible.

Conceptual mathematical thinking, on the other hand, will emphasize *connections* betweens vectors, matrices, Fourier transforms, and differential equations. Although these links are very important to physics (in quantum mechanics, for example) they remain opaque in teaching that is entirely methodological. Appreciating this shortcoming many physics curriculae include lecture courses in pure mathematics — who would be better authorized to teach mathematical concepts than mathematicians themselves? However, a downside of such outsourcing is that mathematical teaching emphasizes concepts somewhat different from those which are most relevant to physics. For example, the chain of connections alluded to above is not addressed in standard mathematics courses.

In this book, we aim to present concepts and methods of mathematics for physicists in an integrated manner. Importantly, this approach will not be more 'formal' or less intuitive than what is standard in physics. Perhaps the main difference is that somewhat more attention is paid to the discussion of mathematical structures, and that this is done with a 'loving eye'. Let us illustrate this point with the example of *vectors.* When vectors are introduced early in the curriculum, emphasis is usually put on three-dimensional vectors, described in terms of components and visualized in terms of arrows. This picture is familiar to many students from high school, and it is sufficient to follow introductory mechanics courses in university. However, only one year later, quantum mechanics becomes part of the agenda. The mathematics of quantum mechanics is all about vectors, but now they live in a more abstract (Hilbert) space which is hard to visualize. This can be confusing for students who

have been conditioned to thinking of vectors as arrows in three-dimensional space. The problem is avoided by emphasizing the full meaning of vector spaces from the very beginning. This generalized approach will cover many different realizations of vector spaces in physics. From the beginning, it draws from a larger class of examples, including those which later appear in quantum mechanics. In this way the role played by vectors in physics becomes more tangible (and arguably less frightening) than in approaches fixated on only one realization. At any rate, our own teaching experience has shown that a conceptual introduction to vector spaces is well received by beginners and makes it a lot easier to cope with the linear algebra of quantum theory later on.

On a related note, the physics community has the habit to regard every object comprising components as either a vector or a matrix. In reality, however, only a fraction of the index-carrying objects encountered in physics are genuine vectors or matrices.[1] Equally relevant elements of linear algebra include dual vectors, bilinear forms, alternating forms, or tensors. Depending on the field one is working in, the 'everything–is–a–vector' attitude can be either tolerable or a source of confusion. The latter is the case in well established fields as particle physics and relativity, and increasingly in emerging areas such as quantum information or topological condensed matter physics. Linear algebra as introduced in this text naturally accommodates non-vectorial objects and the instances where these appear become more frequent as we go along. It happens first when we discuss the cross product of vectors, next when the metric of vector spaces is introduced and extensively in our discussion of tensor algebra. The advanced parts of the text contain a self contained introduction to differential forms and illustrate the potency of this language on the physical example of electromagnetism. In all this, we have paid careful attention not to 'sever the communication lines' to traditional teaching approaches; in this text, the extended view of linear algebra is an option, not a must, and the standard form of vector calculus always remains in sight.

Does an increased emphasis on concepts increase the teaching load or come at the expense of methodological training? The answer is an emphatic 'no'. This book is based on a course that has been taught more than ten times (at LMU Munich and Cologne university) to beginner students in their first semester at university. We affirm that mathematical methods are introduced at a pace compatible with standard physics curricula and at load levels manageable for average students. In fact, the concept-oriented approach turned out to be a pedagogical asset, quite the opposite of an 'abstract burden'. It supports the student's performance, including on the methodological level, because they have a deepened understanding of what they are doing. Where our choice of contents or notation differs from that standard in the physics culture, we explain the traditional views in parallel. For example, we do discuss why the magnetic field is not a genuine vector but a differential two-form. However, we also explain why it may be described as a vector, and point out potential pitfalls with this description.

The book is organized into **three parts** on **linear algebra** (L), **calculus** (C) (also known as analysis), and **vector calculus** (V), respectively. Starting at high school level, each part covers the material required in a standard bachelor curriculum and reaches out somewhat

[1] A prominent example is the magnetic field. Unlike conventional vectors, a magnetic field 'vector' does not change sign under a reflection of space. It therefore cannot be a true vector, which always causes confusion in teaching.

beyond that.[2] At the same time the writing style gradually changes from moderately paced and colloquial at the beginning to somewhat more concise and 'scientific' towards the final chapters. Due to its modular structure the text should work well as a reference covering all elements of linear algebra, calculus and vector calculus encountered in a Bachelor physics curriculum.

The individual parts include a wide range of material and should not be read in strict succession. Specifically, later chapters generally rely on interconnections between linear algebra, calculus and vector calculus (where this happens we indicate the required material in a preamble). Perhaps a good way to enter the subject is to first read a few sections of part L and C each and then move into V. This approach, alternating between subjects, actually helps to stay organized and appreciate the individual characteristics of each field as much as the connections between them. While it is perfectly fine for first time readers to choose a preferred reading order themselves, Tables 1 and xx suggest **reading roadmaps**, based on the order in the material has been taught in a one-semester course at LMU Munich and a two-semester course at Cologne, respectively.

About a third of the book is devoted to **problems**. The tackling of these problems, more than 200 in number, should be considered an integral part of learning the material. Each *odd*-numbered problem includes a detailed solution which may be consulted if necessary. The subsequent *even*-numbered problem are of similar structure but should be solved without guidance. (A solution manual for the even-numbered problems can be obtained from the authors on request.) All exercises have been given to students of the LMU and Cologne lecture courses and should provide a impression of what to expect in a 'real' physics curriculum. In addition to the problems we have included a small number of more expansive 'case studies'. The **case studies** are meant to give the reader an impression of how different concepts and methods interrelate in the solution of real physics problems. For example, a case study on computer tomography discusses how elementary geometry, line integration and Fourier transform can be combined to extract three-dimensional images from recorded absorption data, etc. Finally, the text includes a large number of **info sections** where we suggest an alternative view of a subject, or provide background material we consider interesting and worth knowing. If time is short, these sections can be skipped. However they are all there for a reason and reading them at some later time may be worthwhile.

A final word for non-native **English** speakers: although we are non-natives ourselves (many grammatical and stylistic issues in the text testify to that) we preferred to use English in the lecture notes on which this text is based. English is the lingua franca of the science world and it is important to become fluent in it at the earliest possible stage. Besides, we have observed that even students who do not speak English well usually find it easy to read formula-heavy texts — formulas appear to serve as anchor points aiding the navigation of text passages — and in this way quickly advance their language skills. For the convenience of international readers we have included translations of keywords whose meaning is not self evident[3] in the

[2] For experts: the final chapters deal with multilinear algebra, complex calculus, and differential forms, respectively.

[3] For example, German readers will have guessed that 'vector' translates to 'Vektor', but that 'angular momentum' means 'Drehimpuls' may be not so obvious.

index.

	L	C	V	Topic
1	1			Basic concepts: sets, maps, groups, fields, complex numbers
2		1,2		Differentiation and integration of 1-dimensional functions
3	2			Vector spaces: definition, examples, basis
4	3			Euclidean spaces: inner product, norm, orthogonality, metric
5	4			Vector product: Levi-Civita symbol, various identities
6			1	Curves, line integrals
7		3,4.1		Partial derivatives; Multi-dimensional integration (Cartesian)
8			2	Curvilinear coordinates (polar, cylindrical, spherical)
9		4.2		Multidimensional integration in curvilinear coordinates
10			3.1	Scalar fields, gradient
11			3.2	Vector fields: gradient fields
12	5.1-3			Linear maps, matrices, matrix multiplication
13	5.4-6			Inverse of a linear map, basis transformations
14	6			Determinants: definition, properties
15	7			Diagonalization: eigenvalues, eigenvectors
16	8,9			Orthogonal, unitary, symmetric and Hermitician matrices
17		5.1-3		Taylor series: definition, standard examples (exp, sine, cosine)
18		7.1-3		Differential equations: typology, linear first-order equations
19		7.4-6		Systems of first-order differential equations
20		5.4-5		Perturbation expansions; higher-dimensional Taylor series
21		6.1-2		Fourier calculus: Dirac delta function, Fourier series
22		6.3-4		Fourier series for periodic functions, convolution theorem
23		7.6-8		n-th order differential equations; linearization, fixed points
24		6.3		Fourier transforms
25		6.4		Fourier transform applications
26		4.3	3.3	Integration in arbitrary dimensions; flux integrals of vector fields
27			3.3	Divergence of vector fields, Gauss' theorem
28			3.4	Circulation of vector fields, Stokes' theorem

Table 1: Outline of a one-semester course based on this text. Each row refers to a 90 min. lecture.

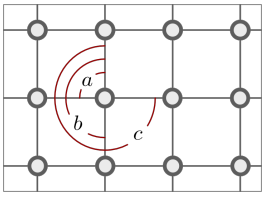
L

Linear Algebra

The first part of this book is an introduction to linear algebra, the mathematical discipline of structures that are, in a sense to be discussed, 'straight'. No previous knowledge of the subject is assumed. We start with an introduction to various basic structures in mathematics: sets, groups, fields, different types of 'numbers', and finally vectors. This is followed by a discussion of elementary geometric operations involving vectors, the computation of lengths, angles, areas, volumes, etc. We then explain how to describe relations between vectorial objects via so-called linear maps, how to represent linear maps in terms of matrices, and how to work with these operations in practice. Part L concludes with two chapters on advanced material. The first introduces the interpretation of functions as vectors (a view of essential importance to quantum mechanics). In the second, we discuss linear algebra in vector spaces containing a high level of intrinsic structure, so-called tensor spaces, which appear in disciplines such as relativity theory, fluid mechanics, or quantum information theory.

L1 Mathematics before numbers

Many people believe that 'numbers' are the most basic elements of mathematics. This, however, is an outside view which does not reflect the way mathematics herself thinks about numbers. Numbers can be added, subtracted, multiplied and divided by, which means that they possess considerable degree of complexity.[1] Metaphorically speaking, they are high up in the evolutionary tree of mathematics, and beneath them, there exists numerous structures of lesser complexity. Much like a basic understanding of evolutionary heritage is important in understanding live — reptiles, vs. mammals, vs. birds, etc. — the evolutionary ancestry of numbers is an key element in the understanding of mathematics, and physics. We take this as motivation to start with a synopsis of various pre-numerical structures which we will later see play a fundamental role throughout the entire text.



EXAMPLE Consider a two-dimensional square lattice that is invariant under rotations by 90 degrees (deg) (i.e. if you rotate the lattice by 90 deg[2] it looks the same as before, see figure). Then rotations by 0, 90, 180 or 270 deg are '**symmetry operations**' that map the lattice onto itself. Let us denote these operations by e, a, b and c, respectively. Two successive rotations by 90 deg are equivalent to one by 180 deg, a fact we may express as $a \cdot a = b$. Similarly, $b \cdot b = e$ (viewing a 360 deg rotation equivalent to one by 0 deg). These operations are examples of mathematical objects which can be 'combined' with each other, but not 'divided' by one another. Together, they form a pre-number structure, soon to be identified as a 'group'. Generic groups have less structure than numbers and yet are very important in physics.

[1] At the end of the nineteenth century mathematicians became increasingly aware of gaps in the logical foundations of their science. It became understood that the self-consistent definition even of natural numbers (1,2,3,...) was more complex than was previously thought. For an excellent account of the ensuing crisis of mathematics, including its social dimensions, we refer to the graphic novel *Logicomix*, A. Doxiadis, Bloomsbury Publishing, 2009.

[2] In this text we use the standard abbreviation 'deg' for degrees.

L1.1 Sets and maps

When we work with a complex systems of objects of *any* kind we better have ways to categorize and store them. At the very least, we need containers capable of storing objects (think of the situation in a repair shop). On top of that one may want to establish connections between the objects of different containers (such as a table indicating what screw in the screw-box matches what screwdriver in the screwdriver rack.) In the terminology of mathematics, containers are called 'sets', and the connections between them are established by 'maps'. In this section we define these two fundamental structures and introduce various concepts pertaining to them.

Sets

Perhaps the most basic mathematical structure is that of a **set**. (The question whether there are categories even more fundamental than sets is in fact a subject of current research.) As indicated above, one may think of a set as a container holding objects. In mathematical terminology, the objects contained in a set are called its **elements**. Unlike the containers in a repair shop, mathematical sets are not 'physical' but simply serve to group objects according to certain categories (which implies that one object may be an element of different sets). For example, consider the set of all your relatives. Your mother is an element of that set, and at the same time one of the much larger set of all females on the planet, etc. More formally, the notation $a \in A$ indicates that a is an element of the set A, and $A = \{a, b, c, \dots\}$ to denote the full set.

INFO Be careful to be exercise **precision in matters of notation**. For example, denoting a set by $(a, b, c, \dots)$ would be incompatible with the standard curly bracket format $\{a, b, c, \dots\}$ and an abuse of notation. Insistence on clean notation has nothing to do with pedantry and serves multiple important purposes. For example, the notation $B = \{1, 2, 3\}$ is understood by every mathematically educated person on the planet meaning that standardized mathematical notation makes for the most international idiom there is. At the same time, uncertainties in matters of notation often indicate a lack of understanding of a concept. For example, $a \in \{a\}$ is correct notation indicating that a is an element of the set $\{a\}$ containing just this one element. However, it would be incorrect to write $a = \{a\}$. The element a and the one-element set $\{a\}$ are different objects. The feeling of uncertainty in matters of notation is a sure and general indicator of a problem in ones understanding and should always be considered a warning sign — stop and rethink.

The definition of sets and elements motivates a number of generally useful secondary definitions:

- ▷ An **empty set** is a set containing no elements at all and denoted by $A = \{\}$, or $A = \emptyset$.
- ▷ A **subset** of A, denoted by $B \subset A$, contains some of the elements of A, for example, $\{a, b\} \subset \{a, b, c, d\}$. The notation $B \subseteq A$ indicates that the subset B may actually be equal to A. On the other hand, $B \subsetneq A$ means that this is certainly not the case.

- The **union** of two sets is denoted by $\cup$, for example, $\{a,b,c\} \cup \{c,d\} = \{a,b,c,d\}$. The **intersection** is denoted by $\cap$, for example, $\{a,b,c\} \cap \{c,d\} = \{c\}$.
- The removal of a subset $B \subset A$ from a set A results in the **difference set**, denoted by $A \backslash B$. For example, $\{a,b,c,d\} \backslash \{c\} = \{a,b,d\}$.
- We will often define sets by **conditional rules** and the standard notation for this is set $=$ $\{\text{elements} \,|\, \text{rule}\}$. For example, with $A = \{1,2,3,4,5,6,7,8,9,10\}$ the set of all even integers up to 10 could be defined as $B = \{a \in A \,|\, a/2 \in A\} = \{2,4,6,8,10\}$.
- Given two sets A and B, the **Cartesian product** as[3]

$$A \times B \equiv \{(a,b) \,|\, a \in A, b \in B\}, \tag{L1}$$

  is a set containing all pairs (a,b) formed by elements of A and B.

The number of elements of a set is called its **cardinality**. The cardinality can be finite (the set of all your relatives) or infinite (the set of all natural numbers). Among the infinite sets one distinguishes between 'countable' and 'uncountable' sets. A set is **countable** if one can come up with a way to number its elements. For example, the set of even integers $A = \{0,2,4,\dots\}$ is countable. The real numbers (cf. section L1.3) form an uncountable set.

It is often useful to organize sets in **equivalence classes** expressing the equality $a \sim b$ of two elements relative to a certain criterion, R. For example, let A be the set of relatives and let the distinguishing criterion, R, be their sex. The notation Victoria $\sim$ Erna then indicates that the two relatives are equivalent in the sense that they are female. An equivalence relation has the following defining properties:

- **reflexivity**: $a \sim a$, every element is equivalent to itself.
- **symmetry**: $a \sim b$ implies $b \sim a$ and vice versa.
- **transitivity**: $a \sim b$ and $b \sim c$ implies $a \sim c$.

The subset of all elements equivalent to a given reference element a is called an **equivalence class** and denoted $[a] \subset A$. In the example of relatives and their sex, there are two such subsets, for example $A = [\text{Herbert}] \cup [\text{Erna}]$. The label used for of an equivalence class is not unique; for example, one might relabel $[\text{Erna}] = [\text{Victoria}]$. The set of all equivalence classes relative to a relation R is called its **quotient set** and is denoted by A/R. In the example of relatives (A) and their sex (R), the quotient set $A/R = \{[\text{Herbert}], [\text{Victoria}]\}$ would have two elements, the class of males and that of females.

EXAMPLE Consider the set of integers, and pick some integer q. Now view any two integers as **equivalent if they have the same remainder under division by** q. For example, $q = 4$ defines $0 \sim 4 \sim 8$, $1 \sim 5 \sim 9$. In this case there are four equivalence classes, denotable by $[0]$, $[1]$, $[2]$ and $[3]$. In general, the remainder of p divided by q is denoted by $p \bmod q$ (spoken 'p-modulo-q', or just

[3] We follow a widespread convention whereby $\square \equiv \triangle$ means '$\square$ is defined by $\triangle$'. In the German literature, the alternative notation $\square := \triangle$ is frequently used.

'p-mod-q'), e.g., $8 \bmod 4 = 0$, $6 \bmod 4 = 2$, or $-5 \bmod 4 = 3$ (by definition, remainders are taken to be positive). The equivalence class of all integers with the same remainder r under division by q is the set $[r] = \{p \in \mathbb{Z} | p \bmod q = r\}$. There are q such equivalence classes, and the set of these classes is denoted by $\mathbb{Z}_q \equiv \mathbb{Z}/q\mathbb{Z} = \{[0], [1], \ldots, [q-1]\}$.

Maps

Consider two sets, A and B, plus a rule, F, assigning to each element a of A an element b of B. Such a rule, written as $F(a) \equiv b \in B$, is called a **map**. In mathematics and physics, maps are specified by the following standard notation:

$$F : A \to B, \qquad a \mapsto F(a). \tag{L2}$$

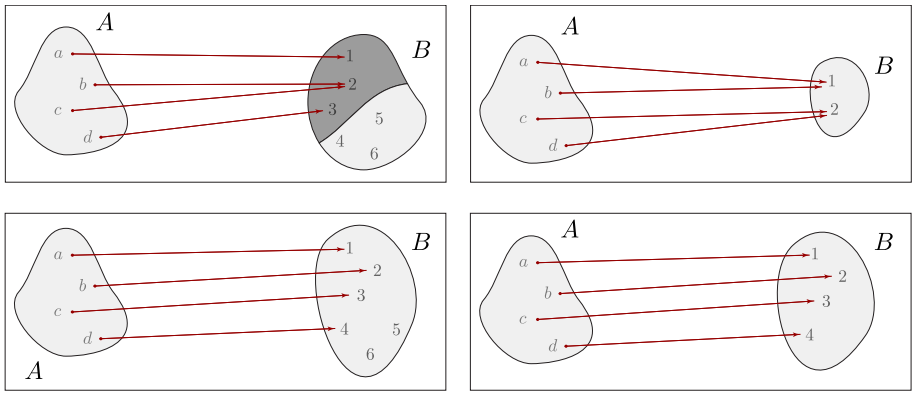


Figure L1: Different types of maps. Top left: a generic map, top right: surjective map, bottom left: injective map, bottom right: bijective map.

The set A is called the **domain** of the map and B is its **codomain**.[4] An element $a \in A$ fed into the map is called an **argument** and $F(a)$ is its **image (element)**. Note that different types of arrows are used for 'domain $\to$ codomain' and 'argument $\mapsto$ image'.

The **image** of A under F, denoted by $F(A)$, is the set containing all image elements of F: $F(A) = \{F(a) | a \in A\} \subseteq B$ (cf. dark shaded area in the first panel of Fig. L1). A map is called **surjective** (second panel) if its image covers all of B, $F(A) = B$, i.e. if any element of the codomain is the image of *at least* one element of the domain. It is called **injective** (third panel) if every element of the codomain is the image of *at most* one element of the domain. The map is **bijective** if it is both surjective and injective (fourth panel), i.e. if every element $b \in B$ of the codomain is the image of *exactly* one element $a \in A$ of the domain. Bijective maps establish an unambiguous relation between the elements of the sets A and B. The one-to-one nature of this assignment means that it can be inverted: there exists an **inverse map**, $F^{-1} : B \to A$ such that $F^{-1}(F(a)) = a$ for every $a \in A$.

[4] The designation 'codomain' is standard in mathematics, but not in physics. Oddly, physics does not seem to have an established designation for the 'target set' of a map.

Given two maps, $F : A \to B$ and $G : B \to C$, their **composition** is defined by substituting the image element of the first as an argument into the second:

$$G \circ F : A \to C, \qquad a \mapsto G(F(a)). \tag{L3}$$

For example, the above statement about bijective maps means that the composition of a bijective map F with its inverse, F^{-1}, yields the identity map: $F^{-1} \circ F : A \to A$, with $a \mapsto F^{-1}(F(a)) = a$.

Finally, a map F defined on a Cartesian product set, $A \times B$, is denoted as

$$F : A \times B \to C, \qquad (a, b) \mapsto c = F(a, b).$$

This map assigns to every pair (a, b) an element of C. For example, the shape of a sand dune can be described by a map, $h : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$, $(x, y) \mapsto h(x, y)$, where for each point (x, y) in the plane, the function $h(x, y)$ gives the height of the dune above that point.

L1.2 Groups

Sets as such are just passive containers storing elements. Often, however, the elements of a set are introduced with the purpose of doing something with them. As an example, consider the set of 90 deg rotations, $R \equiv \{e, a, b, c\}$, introduced on p. 2. A two-fold rotation by 180 deg is equivalent to a non-rotation and this fact may be described as $b \cdot b = e$. Or we may say that $a \cdot b = c$, meaning that a 90 degree rotation following one by 180 degrees equals one by 270 degrees, etc. In this section, we define groups as the simplest category of sets endowed with an 'active' operation on their elements.

Definition of groups

The minimal structure[5] which brings a set to life in terms of operations between its elements is called a **group**. Let A be a set and consider an **operation**, '$\cdot$', (equivalently called **group law** or **composition rule**) assigning to every pair of elements a and b in A another element, $a \cdot b$: $\cdot$

$$\cdot : A \times A \to A, \qquad (a, b) \mapsto a \cdot b. \tag{L4}$$

This map defines a group operation provided that the following four **group axioms** are satisfied:[6]

[5] This statement is not fully accurate. There is a structure even more basic than a group, the **semigroup**. A semigroup need not have a neutral element, nor inverse elements to each element. In physics, semigroups play a less prominent role than groups, hence we will not discuss them further.

[6] Mathematicians often formulate statements of this type in a more compact notation. Frequently used symbols include $\forall$, abbreviating **for all**, and $\exists$, for **there exists**. Expressed in terms of these, the group axioms read: (i) $\forall a, b \in A$, $a \cdot b \in A$. (ii) $\forall a, b, c \in A$, $a \cdot (b \cdot c) = (a \cdot b) \cdot c$. (iii) $\exists e \in A$ such that $\forall a \in A$, $a \cdot e = e \cdot a = a$. (iv) $\forall a \in A, \exists b \in A$ such that $a \cdot b = b \cdot a = e$. Although this notation is less frequently used in physics texts, it is very convenient and we will use it at times.

(i) **Closure**: for all a and b in A the result of the operation $a \cdot b$ is again in A. (Although this condition is already implied by the definition L4, it is generally counted as one of the group axioms.)
(ii) **Associativity**: for all a, b and c in A we have $(a \cdot b) \cdot c = a \cdot (b \cdot c)$.
(iii) **neutral element**: there exists an element e in A such that for every a in A, the equation $e \cdot a = a \cdot e = a$ holds. Depending on context, the neutral element is also called identity element or null element.
(iv) **Inverse element**: For each a in A there exists an element b in A such that $a \cdot b = b \cdot a = e$.

Under these conditions, A and '$\cdot$' define a group as $G \equiv (A, \cdot)$. A group should always be considered a double comprising a set, and an operation. It is important to treat the operation as an integral part of the group definition: there are numerous examples of sets, A, which admit two different group operations, '$\cdot$' and '$*$'. The doubles $G = (A, \cdot)$ and $G' = (A, *)$ then are different groups. We finally note that in some cases it can be more natural to denote the group operation by different symbols '$+, *, \ldots$'.

Nils Henrik Abel (1802–1829)

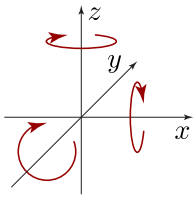
Norwegian mathematician who made breakthrough contributions to various fields of mathematics before dying at young age. Abel is considered the inventor (independently with Galois) of group theory. He also worked on various types of special functions, and on the solution theory of algebraic equations.

EXAMPLE Here are a few first examples of groups.

- ▷ The simplest group of all, $G = (\{e\}, \cdot)$, contains just one element, its neutral element. Nothing much to discuss.
- ▷ The introductory example of 90 deg rotations, $R \equiv \{e, a, b, c\}$, defines a group of cardinality four. Its neutral element is e and for each element we have an inverse, for example $a \cdot c = e$. (Set up a 'multiplication table' specifying the group operation for all elements of $R \times R$.) The *same* group, i.e. a set of four elements with the same group law, can be realized in different contexts. For example, for the quotient set $\mathbb{Z}_4 = \{[0], [1], [2], [3]\}$ defined on p. 4, a group operation may be defined as 'addition modulo 4'. This means that the addition of a number with remainder $1 \bmod 4$ to one with remainder $3 \bmod 4$, yields one with remainder $0 \bmod 4$, for example $[1] + [3] = [0]$. Set up the full group operation table for this group and show that it is identical to that of the group of 90 deg rotations discussed previously. This implies that $(\mathbb{Z}_4, +)$ and $(R, \cdot)$ define the same group. Explain in intuitive terms why this is so. The concept of different realizations of the same group is very important in both physics and mathematics. We will see many more examples of such correspondences throughout the text. (→ L1.2.2)
- ▷ The simplest nontrivial group, which nevertheless has many important applications, contains just two elements, $\mathbb{Z}_2 = \{e, a\}$, with $a \cdot a = e$. This group can be realized by rotations by 180 deg, or as the group of integers $\bmod 2$ (→ L1.2.1). The group $(\mathbb{Z}_2, \cdot)$ plays a very important role in modern physics. For example, in information science, $\mathbb{Z}_2$ is the mathematical structure used to describe '**bits**', objects that can assume only one of two values, 'on' and 'off', or '0' and '1'.

- ▷ The integers, $\mathbb{Z} \equiv \{\dots, -2, -1, 0, 1, 2, \dots\}$, with group operation '+' ='addition' (e.g. $2+4=6$) are an example of a group of infinite cardinality. $(\mathbb{Z}, +)$ has neutral element 0 and the inverse of a is $-a$, i.e. $a+(-a)=0$. Why are the integers $(\mathbb{Z}, \cdot)$ with multiplicative composition $(2\cdot 3=6)$ *not* a group?

- ▷ Other important examples of discrete groups include the translation group on a lattice (→ L1.2.3-4) and the group of permutations of n objects to be discussed in more detail in the next subsection.



If the group operation is **commutative** in the sense that it satisfies $a \cdot b = b \cdot a$ for all elements the group is called an **abelian group**. All examples mentioned so far have this property. **Non-Abelian groups** possess at least some elements for which $a \cdot b \neq b \cdot a$. An important example is the group formed by all **rotations of three-dimensional space**. This group can be given a concrete realization by fixing three perpendicular coordinate axes in space. In other words, R, can then be represented as a succession of rotations around the coordinate axes (see figure) and the set of all these rotations forms a group where the group operation is the successive application of rotations. For example, $R_2 \cdot R_1$ is the rotation obtained performing R_1 and R_2 in succession. This concatenation is not commutative. For example, a rotation first around the x-axis and then around the z axis is different from the operation in reverse order.

INFO Groups play an important role in **physics**. This is because many classes of physical operations effectively carry a group structure. Simple examples include **rotations** or **translations** in space or time. These operations define groups because they can be applied in succession ('composed'), are associative, possess a neutral element (nothing is done), and can be inverted (undone). The translation and rotation groups play crucial roles in the description of momentum and angular momentum, both in classical and quantum mechanics. While continuous translations and rotations define groups of infinite cardinality, the physics of crystalline structures is frequently described in terms of finite restrictions. We mentioned the group $\mathbb{Z}_4$ of rotations by 90 deg around one axis as an example. In the late 1960's, group theory became important as a cornerstone of the **standard model** describing the fundamental structure of matter in terms of quarks and other elementary particles.

Despite the deceptive simplicity of the group axioms, the theory of groups is of great depth and beauty, and it remains a field of active research in modern mathematics.

Group homomorphism

Above, we have seen that the same group structure can be 'realized' in different ways. For example, the group $\mathbb{Z}_2$ can be realized as the group of rotations by 180 deg, or as addition in $\mathbb{Z}$ mod 2. Identifications of this type frequently appear in physics and mathematics, and it is worthwhile to formulate them in a precise language. To this end, consider two groups, $(G, \cdot)$ and $(H, \bullet)$ with *a priori* independent group operations. Let $\psi : G \to H$ be a map from G to H. If this map is such that for all $a, b \in G$ the equality $\psi(a \cdot b) = \psi(a) \bullet \psi(b)$

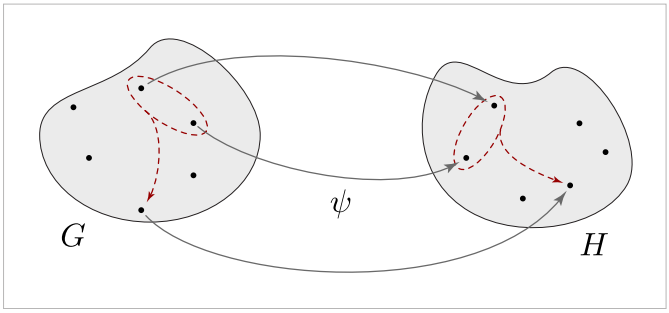


Figure L2: The concept of a group homomorphism: a map between two groups that is compatible with the group operations (dashed) in that the image of the composition of two elements in the domain group (left) equals the composition of the image elements in the target group.

holds, then ψ is called a **group homomorphism** (cf. Fig. L2). The defining feature of a group homomorphism is its compatibility with the group law. As an example consider $G = H = (\mathbb{Z}, +)$. Now assign to each integer its double, $n \mapsto \psi(n) = 2n$. This map is a group homomorphism because $\psi(n+m) = 2(n+m) = 2n+2m = \psi(n)+\psi(m)$. However, the map ϕ assigning to each integer its square, $n \mapsto \phi(n) = n^2$, is not a group homomorphism, because $\phi(1)+\phi(2) = 1+2^2 \neq \phi(1+2) = \phi(3) = 3^2$. As another example, consider the map $\psi : \mathbb{Z} \to \mathbb{Z}_2$, $n \mapsto \psi(n) = n \bmod 2$, assigning the number 0 or 1 to the integers, depending on whether n is even or odd. This is a homomorphism between the infinite group $(\mathbb{Z}, +)$ and the two-element group $\mathbb{Z}_2$.

A perfect identification between two groups G and H is obtained if there exists a *bijective* homomorphism between the two, a so-called a **group isomorphism**. In this case, we write $G \cong H$. Mathematicians tend to not even distinguish between isomorphic groups, a view that can be confusing to physicists. The identification $\mathbb{Z}_2 \cong (\mathbb{Z} \bmod 2) \cong$ (rotations group by 180 deg) discussed above is a group isomorphism.

EXERCISE Consider the set $\mathbb{Z}_n \equiv (\mathbb{Z} \bmod n, +)$, $n \in \mathbb{Z}$. Show that it defines a group of cardinality n. Show that $\mathbb{Z}_n$ is isomorphic to the group of rotations by $360/n$ deg around a fixed axis. (→ L1.2.2)

Permutation group

The permutations of n objects define one of the most important finite groups, the permutation group, S_n. Consider n arbitrary but distinguishable objects. For definiteness it may be useful to think of a set of n billiard balls (see Fig. L3 for $n = 4$). A **permutation** is a rearrangement of these objects into a different order. For example, the reordering of four objects indicated in the left panel of the figure leads to the new arrangement shown in the middle. There are n–**factorial**, $n! \equiv n(n-1)(n-2)\dots 1$ different arrangements or permutations,[7]

[7] One way to understand this number is to notice that the first of n objects can be put in any of n places. This leaves $n-1$ options for the second object (one position is already occupied by the first object), $n-2$

and we consider the set, S_n, of cardinality $n!$ containing all of them.

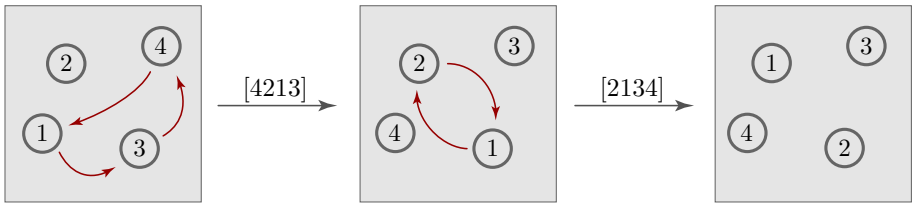


Figure L3: Two permutations of four objects performed in succession.

Rearrangements can be iterated. For example, the exchange in the middle panel of the figure leads to the final arrangement shown in the right panel. The group composition in S_n is this iteration of permutations. Evidently, there is a trivial permutation (the one that leaves sequences unaltered), the composition of permutations is associative, and each permutation can be undone, such that there exists an inverse. This shows that S_n forms a group, the **permutation group**, or **symmetric group** of n objects. It is easy to verify that the permutation group is non-abelian. (Invent examples of perturbations proving the point.)

Although the permutation group is easily defined, its mathematical structure is rather rich. (For example, the solution of Rubik's cube amounts to a permutation of the 54 differently colored squares covering the six faces of the cube, and the solution algorithms reflect the mathematics of the permutation group S_{54}.) Below, we will frequently work with permutations and it will be useful to have a good notation for them. One popular labeling system denotes the permutation shown in the left part of the figure by $[4213]$. This notation logs the final configuration of the objects after a permutation $(1,2,3,4) \mapsto (4,2,1,3)$ as a list in angular brackets. The second permutation is thus denoted as $[2134]$, and the composition of the two becomes $[2134] \cdot [4213] = [4123]$.

EXERCISE Check that the permutation group of 3 objects can be represented as (→ L1.2.5)

$$S_3 = \{[123], [213], [321], [231], [312], [132]\}.$$

Alternatively, a permutation may be identified with a map $P : \mathbb{N}_n \to \mathbb{N}_n, j \mapsto P(j)$, where $\mathbb{N}_n = \{1, 2, \ldots, n\}$ is the set of n integers, and $P(j) \in \mathbb{N}_n$ the number to which j is permuted. Sometimes, the shorthand notation $Pj \equiv P(j)$ is used instead. In this language, $[4213]$ is represented as $P1 = 4$, $P2 = 2$, $P3 = 1$, $P4 = 3$.

Note that each permutation can be reduced to a product of **pair permutations**, i.e. permutations which exchange just two objects at a time. This statement is easy to understand: any re-ordering of n objects can be achieved manually (with one's own two hands) by sequentially swapping pairs of objects. For example, the permutation $[4213]$ of the figure can be

for the third, etc. The total number of rearrangements is obtained as the product of the number of options for object no.1,2,..., i.e. $n(n-1)\cdots = n!$.

effected by first exchanging $1 \leftrightarrow 3$, and then $3 \leftrightarrow 4$. For any permutation $P \in S_n$ we then have two options:[8] the number of pair permutations needed to arrive at P may be even or odd (determine the even/odd attribute for the six permutations of S_3). In the former/latter case, we call P an **even/odd permutation** and define

$$\mathrm{sgn}(P) = \begin{cases} +1, & P \text{ even}, \\ -1, & P \text{ odd}. \end{cases} \tag{L5}$$

as the **signum** of a permutation. (→ L1.2.6)

EXERCISE Define a map $S_n \to \mathbb{Z}_2, P \mapsto \mathrm{sgn}(P)$, where $\mathrm{sgn}(P) = \pm 1$ are identified with the two elements of $\mathbb{Z}_2 = \{+1, -1\}$. Show that this is a group homomorphism, between S_n and $\mathbb{Z}_2$, i.e. that $\mathrm{sgn}(P \cdot Q) = \mathrm{sgn}(P) \cdot \mathrm{sgn}(Q)$ where the multiplication on the right is that of numbers ± 1. Understand this as the educated formulation of the statement that the product of two odd permutations is even, that of an even and an odd is odd, etc.

In this text, the signum of permutations will appear frequently and once more it will be important to have a good notation. A convenient way to track this quantity is provided by the **Levi-Civita tensor**, $\epsilon^{j_1 j_2 \ldots j_n}_{i_1, i_2, \ldots, i_n} = \pm 1$. It is defined as the signum of the permutation $P(i_l) = j_l$ permuting the sequence of symbols $(i_1, i_2, \ldots, i_n)$ into $(j_1, j_2, \ldots, j_n)$. For example, $\epsilon^{321}_{231} = -1$, because a single pair permutation transmutes $(2, 3, 1)$ into $(3, 2, 1)$. For the same reason, the Levi-Civita tensor is **fully antisymmetric** under the exchange of any two indices, e.g. $\epsilon^{4321}_{2341} = -\epsilon^{4321}_{3241}$.

In applications one often has situations where one of the involved permutations is the ordered one, $(i_1, i_2, \ldots i_n) = (1, 2, \ldots, n)$. In such cases, it is customary to suppress the ordered sequence in the notation and just write $\epsilon^{j_1 j_2 \ldots j_n} \equiv \epsilon^{j_1 j_2 \ldots j_n}_{12 \ldots n}$, and similarly $\epsilon_{i_1 i_2 \ldots i_n} \equiv \epsilon^{12 \ldots n}_{i_1 i_2 \ldots i_n}$. For example, $\epsilon_{321} = 1$ because reordering $(1, 2, 3)$ to $(3, 2, 1)$ requires two pair permutations. These tensors are fully antisymmetric too, e.g. $\epsilon_{213} = -\epsilon_{231}$.

The Levi-Civita symbol is often used in contexts where two or more of its indices can be equal. In that case, its value is defined to be zero, e.g. $\epsilon_{112} = 0$, to ensure consistency with its antisymmetry property: ϵ_{iij} must both change sign and remain unchanged when its first two indices are interchanged, which is possible only if it vanishes.

L1.3 Fields

Numbers are mathematical objects that can be added, subtracted, multiplied, and divided. Seen as composition rules, **multiplication**, $a \cdot b$, and **addition**, $a + b$, have several features in common (associativity, commutativity, neutral element exists, inverse elements exist). A set for which both addition *and* multiplication is defined as separate operations is called a

[8] Notice that the even/odd attribute is not entirely innocent: there are different ways of realizing a given P by a sequence of pair permutations. However, the 'parity', i.e. the even- or oddness of the number of pair permutations, is an invariant. This makes the function sgn well defined.

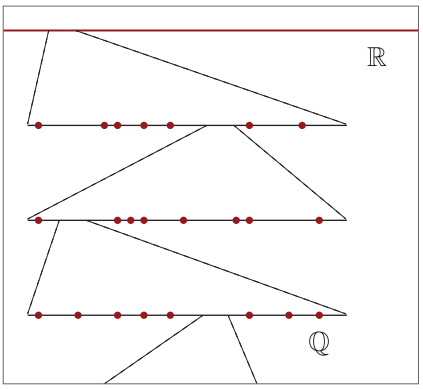
(number) **field**. Referring to lecture courses in mathematics for a more rigorous approach, we here introduce the concept of fields in a quick and informal manner: a field is a triple, $F \equiv (A, +, \cdot)$, comprising a set A and *two* composition rules, addition and multiplication. Addition and multiplication each define their own *abelian* group structure, the neutral elements being denoted by 0 and 1, respectively, i.e. $a + 0 = a$ and $a \cdot 1 = a$.

The inverse element of a under addition is denoted by $-a$, i.e. $a + (-a) = 0$, and the addition of the inverse is called **subtraction**. Likewise, the inverse element of a under multiplication is called a^{-1}, and multiplication by the inverse is called **division** (alternatively denoted by $b \cdot a^{-1} \equiv b/a \equiv \frac{b}{a}$). The group structures defined by addition and multiplication are independent, except for two points: (i) the neutral element of addition, 0, does not have a multiplicative inverse. In other words, 0^{-1} does not exist and 'division' by zero is not allowed. (ii) Multiplication is distributive over addition in the sense that $a \cdot (b + c) = a \cdot b + a \cdot c$.

It is possible to construct fields with a finite number of elements, the so-called **Gallois fields** (→ L1.3.7). However, most fields of relevance to physics are infinite, and the most important ones — the rational, the real, and the complex numbers — are introduced below.

Rational and real numbers

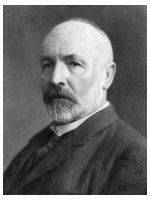
The integers, $\mathbb{Z}$, do *not* form a field because the operation of multiplication does not have an inverse in $\mathbb{Z}$. For example, the multiplicative inverse of $3 \in \mathbb{Z}$, does not exist in $\mathbb{Z}$. There is no integer number that can be multiplied with three to obtain unity.[9]



The most elementary example of an infinite field are the **rational numbers**, $\mathbb{Q} \equiv \{\frac{q}{p} | q, p \in \mathbb{Z}, p \neq 0\}$, i.e. the set of all ratios of integers. The rational numbers $\mathbb{Q} \subset \mathbb{R}$ are contained in a larger number field, the **real numbers**. Heuristically, the set of real numbers may be imagined as a continuous line extending from $-\infty$ to $+\infty$. Each rational number can be positioned on a continuous line of numbers which explains the 'embedding' of the rationals in the reals. However, the ray of real numbers also contains **irrational numbers**, $r \notin \mathbb{Q}$. Irrational numbers may be approximated to arbitrary precision by rational numbers but are not rational themselves. For example, $\sqrt{2}$ has rational approximations as $\sqrt{2} \simeq 1.4142 = \frac{14142}{10000}$, etc., but $\sqrt{2}$ itself can not be written as a ratio of two fixed integers and therefore is not rational. In mathematics courses one learns how the reals can be defined as the union of the rational numbers with the set of all limits of rational numbers (for example, $\sqrt{2}$ can be viewed the limit of an infinitely refined approximation in terms of rational fractions). However, we do not discuss this formalization here.

[9] In passing we note that a structure allowing addition, multiplication, subtraction but not division is called a **ring**.

Georg Ferdinand Ludwig Philipp Cantor (1845–1918)



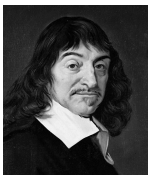
German mathematician who did pioneering work in set and number theory. Cantor proved that there are 'more' real numbers than integer numbers. His work raised questions of philosophical significance and eventually triggered a crisis in the understanding of the logical foundations of mathematics.

The understanding of the reals as a continuous 'line' implies that there are more real numbers than rational numbers. The precise understanding of what is meant by 'more' is far from trivial. Pioneering work by Georg Cantor on the comparison of infinite sets of different size (1874) showed where the conceptual problems lie and caused consternation among his contemporaries. However, the intuitive picture is that the rationals form a subset of infinitely many points embedded into the continuous line of the reals. The 'discreteness' of these points means one can come up with an intricate numbering numbering scheme that lists them all; much like the integer numbers, the rationals form a **countable set** as defined on on p. 4. Between any two rational numbers there are gaps corresponding to irrational numbers (see figure, where each dot represents a rational number). Although, the set of rationals is 'dense' in the reals, in the sense that any real number can be rationally approximated to any desired accuracy, there is no way to count the real numbers lying between them; the reals are uncountable in the sense of the definition of p. 4. For a more substantial discussion of these aspects we refer to lecture courses in mathematics.

The complex numbers

The set of real numbers is large enough to accommodate operations which cannot be performed in the rationals, such as taking of the square root of 2. In this sense, they represent a 'closure' of the rational numbers. However, there are operations with respect to which the real numbers lack closure themselves. We all know that the square root of a negative number, such as $\sqrt{-1}$, is not a real number. Similarly, some real polynomials can be factored as $x^2-1=(x-1)(x+1)$ where the factors specify the zeros of the polynomial. However, x^2+1 cannot be factorized into a product of two real factors. Somehow, it does not feel 'right' that similar polynomials behave so strikingly different.

René Descartes
(1596 - 1650)



French philosopher and mathematician. Descartes is not only considered the founding father of modern western philosophy but also made important contributions to mathematics. The *Cartesian* coordinate system is named after him and he is considered the inventor of analytical geometry, the bridge between algebra and geometry.

INFO Complex numbers were introduced and used long before they were understood conceptually. Their first appearances can be traced to early studies of geometric objects in the ancient world. Complex numbers became an element of mainstream mathematics in the early 17th century when mathematicians worked on the solution theory of algebraic equations. The term **imaginary numbers** was coined by Descartes in 1637, who wrote "sometimes only imaginary, that is one can imagine as many as I said in each equation, but sometimes there exists no quantity that matches that which we imagine." The confused wording of this sentence suggests that Descartes was ill at ease with objects that were apparently quite useful, but hard to conceptualize within 17th century mathematics. It took almost three hundred more years before the modern theory of number fields was invented, and a sound conceptual framework for complex numbers came to existence. In the meantime, numerous mathematicians — Euler, Gauss, Abel, Jacobi, Cauchy, Riemann, and various others more — contributed the the applied theory of complex numbers. Interested readers are encouraged to study these developments and sense the difficulties mathematicians had in working with an irresistibly interesting, yet hard to grasp concept.

The complex numbers are an extension of the real numbers large enough to accommodate all algebraic operations commonly associated with 'numbers'. In the following we sketch the extension from real to complex numbers in a language adjusted to the modern theory of fields. We start by giving $\sqrt{-1}$ a name,

$$\sqrt{-1} \equiv \mathrm{i}, \tag{L6}$$

where i is called the **imaginary unit**. If we accept the existence of this object as a valid mathematical 'number', the problem of taking the square root of negative reals is solved:

$$r > 0: \qquad \sqrt{-r} = \sqrt{-1}\sqrt{r} = \mathrm{i}\sqrt{r}.$$

By squaring (L6) we also know that $\mathrm{i}^2 = -1$. Now let us define the set,

$$\mathbb{C} \equiv \{z = x + \mathrm{i}y \,|\, x, y \in \mathbb{R}\}, \tag{L7}$$

and call it the 'complex numbers'. We call $x \equiv \mathrm{Re}(z)$ and $y \equiv \mathrm{Im}(z)$ the **real part** and the **imaginary part** of the complex number z, respectively. If one of these vanishes the notation is simplified by writing $0 + \mathrm{i}y \equiv \mathrm{i}y$ or $x + \mathrm{i}0 \equiv x$. Thus, real numbers are complex numbers with vanishing imaginary part, implying the embedding $\mathbb{R} \subset \mathbb{C}$.

Next, define the **addition and multiplication** of complex numbers, as

$$z + z' = (x + \mathrm{i}y) + (x' + \mathrm{i}y') \equiv (x + x') + \mathrm{i}(y + y'), \tag{L8}$$

$$zz' = (x+\mathrm{i}y)(x'+\mathrm{i}y') \equiv (xx' + \mathrm{i}xy' + \mathrm{i}yx' + \mathrm{i}^2yy') = (xx' - yy') + \mathrm{i}(xy' + yx').$$

These definitions are such that i behaves as an 'ordinary' number, except for the identification $\mathrm{i}^2 = -1$. Addition and multiplication are closed in $\mathbb{C}$, i.e. both the sum and product of two complex numbers again produce a complex number. This means that we are on the way towards constructing a number *field*.

Indeed, it is straightforward to show that $(\mathbb{C}, +)$ forms an additive group (do it!). A little more work is required to show that multiplication defines a group structure, too. We first need to know how to construct the inverse of a given complex number, $z = x + \mathrm{i}y \in \mathbb{C}$. To this end, the **complex conjugate**, $\bar{z}$,[10] of z is defined as the complex number obtained by inverting the imaginary part of z,

$$\boxed{\bar{z} \equiv x - \mathrm{i}y.}$$

Eq. (L8) then yields

$$z\bar{z} = x^2 + y^2 \tag{L9}$$

meaning that $z\bar{z}$ is real. If z is nonzero, $x^2 + y^2 \neq 0$ and the result can be used to construct the inverse of z. We know that $z\bar{z}/(z\bar{z}) = 1$, which means that the inverse of z is given by

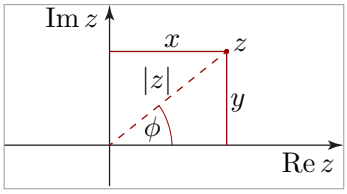
$$z^{-1} = \frac{\bar{z}}{z\bar{z}} \overset{(L9)}{=} \frac{x - \mathrm{i}y}{x^2 + y^2} \in \mathbb{C}. \tag{L10}$$

This expression is 'explicit' in the sense that for any $z = x + \mathrm{i}y$ the inverse is obtained as a rational function of x and y.

When encountered for the first time, these definitions may feel alien. However, complex numbers are as easy to handle as real ones. Just keep the rule $\mathrm{i}^2 = -1$ in mind and otherwise compute products as usual, for example,

$$(2 + 3\mathrm{i})(1 + 2\mathrm{i}) = -4 + 7\mathrm{i}, \qquad \mathrm{i}(4 + 6\mathrm{i}) = -6 + 4\mathrm{i}.$$

Practice computations with complex numbers by doing problems L1.3.1-4.



It is often useful to represent the complex numbers as points in a two-dimensional **complex plane**. The complex plane plays a role analogous to the one-dimensional line representing the reals. In it, a complex number $z = x + \mathrm{i}y$ is represented by a point with coordinates (x, y), such that its real and imaginary parts define the abscissa and ordinate, x and y, respectively. The horizontal axis represents the real numbers, the vertical axis the purely imaginary ones, and generic complex numbers populate the plane. Note that z can also be written in the form

$$z = |z|(\cos\phi + \mathrm{i}\sin\phi), \tag{L11}$$

[10] The complex conjugate is equivalently denoted by an asterisk, $z^* \equiv \bar{z} \equiv x - \mathrm{i}y$.

which defines the **polar representation** of complex numbers . Here ϕ is the angle between the real axis and a line connecting the points $(0,0)$ and (x,y) in the complex plane, and $|z| \equiv \sqrt{z\bar{z}} = \sqrt{x^2+y^2}$ is the length of this line. Angle and length are called the **argument**, $\arg(z) = \phi$, and **modulus**, $\mathrm{mod} z = |z|$, of z, respectively. The argument of z is only defined modulo 2π, i.e. an argument $-\pi$ is equivalent to $+\pi$, where $\arg(z) \in [0, 2\pi)$[11] is the conventional choice for its range of values. The complex conjugate, $\bar{z} = x - \mathrm{i}y$, is represented by the reflection of (x,y) at the x-axis, $(x,-y)$. This implies $|\bar{z}| = |z|$ and $\arg(\bar{z}) = -\arg(z) \bmod 2\pi$.

EXERCISE Show that the product of two complex numbers, $z_j = |z_j|(\cos\phi_j + \mathrm{i}\sin\phi_j)$, with $j = 1, 2$, can be written as $z_1 z_2 = |z_1||z_2|\big(\cos(\phi_1+\phi_2) + \mathrm{i}\sin(\phi_1+\phi_2)\big)$. Illustrate this result with a sketch showing z_1, z_2 and $z_1 z_2$ in the complex plane. (→ L1.3.5-6)

Complex numbers are **powerful tools in physics and mathematics**: algebraic operations which are not globally defined on the real numbers — such as square roots, logarithms, trigonometric functions, etc. — do exist as complex functions. Polynomials of degree n always have n complex zeros and can be decomposed into n factors, for example, $z^2-1 = (z+1)(z-1)$ or $z^2+1 = (z+\mathrm{i})(z-\mathrm{i})$. Throughout this text we will encounter numerous applications where these and other features of the complex numbers are of importance. Generally speaking, one may say that complex numbers are more frequently used in the mathematics of physics than real numbers!

INFO To any two real or complex numbers one may assign a real value specifying the 'distance' between them. In the case of real numbers, $x, y \in \mathbb{R}$, this is the **norm** $|x-y| \in \mathbb{R}$, i.e. the **absolute value** of their difference. For two complex numbers, $z, w \in \mathbb{C}$, the **(complex) norm** $|z-w|$ is the modulus of their difference. Norm functions are important in different ways. Specifically, they are used to distinguish between different types of real intervals and domains in the complex plane.

For example, we call $U \in \mathbb{F} = \mathbb{R}, \mathbb{C}$ a **bounded subset** of $\mathbb{F}$ if there exists a positive real number r such that $\forall u, v \in U$, $|u-v| < r$. The extent of U is then finite in the sense that no two elements have a distance exceeding r. A subset U is called **open** if any point $u \in U$ is enclosed within a region of nonzero extent fully included in U itself. More formally, this means that there must exist a positive $\epsilon \in \mathbb{R}$ such that $\forall v \in \mathbb{F}$ with $|v-u| < \epsilon$, $v \in U$. Heuristically, one may imagine open sets as sets with soft boundaries.

The **openness of real intervals** is indicated by round brackets as in $(0,1) \equiv \{u \in \mathbb{R} \,|\, 0 < u < 1\}$. If the endpoints are included one obtains a **closed interval**, generally denoted by square brackets, $[0,1] \equiv \{u \in \mathbb{R} \,|\, 0 \leq u \leq 1\}$. (Closed intervals are not open because their end points do not contain neighborhoods fully contained in them.) The exclusion of just one endpoint, as in $[0,1) \equiv \{u \in \mathbb{R} \,|\, 0 \leq u < 1\}$, defines a **semi-open interval**.

More generally, the **closure**,, $\mathrm{cl}(U)$, of a set is defined as the union of the set and all of its limit points. A limit point of a set is a point for which every neighborhood contains at least one point

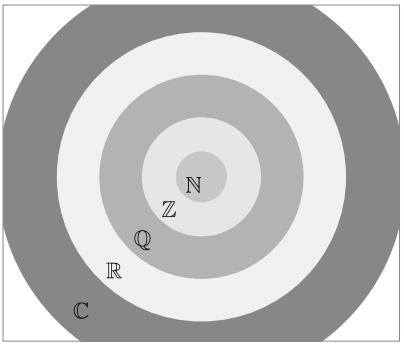
[11] Referring for a more detailed discussion to the info box below, we use notation in which $[a,b)$ is an interval with right boundary point excluded, $b \notin [a,b)$. However, the left boundary point is included, $a \in [a,b)$. The type of the brackets indicates which situation is realized. For example, $(0,1)$ contains neither 0 nor 1.

belonging to the set. For example, if the number 1 is not contained in $[0,1)$ but it is still one of its limit points. This can be seen by inspection of the sequence $1-1/n$. Every neighborhood of 1, no matter how small, contains elements of this sequence with sufficiently large n. This shows that $\mathrm{cl}([0,1)) = [0,1]$. As an example of an open set in the *complex* numbers consider the open disk $D \equiv \{z \in \mathbb{C} \,|\, |z| < 1\} \subset \mathbb{C}$. The circle $|z| = 1$, is not included in D but it is contained in the closure $\mathrm{cl}(D) = \{z \in \mathbb{C} \,|\, |z| \leq 1\}$.

More rigorous definitions of these terms are usually discussed in introductory mathematics courses. The more advanced discipline of mathematical **topology** addresses the extension of the concepts of openness, compactness, closure, etc. to sets more general than the number fields. While this is a very interesting subject, and not entirely irrelevant to physics, it is beyond the scope of the present text.

L1.4 Summary and outlook

In this chapter we have introduced various fundamental structures of mathematics, notably sets, maps, groups, and eventually fields. We gave several examples indicating that all these structures are tailored to specific tasks, both in mathematics and physics. For example, the set of lattice translations of a crystal — evidently a set of physical importance — realizes a group, and this classification is a powerful aid in the understanding of crystal structures.



At the end of this chapter we have arrived at a **hierarchy of numbers**, $\mathbb{N} \subset \mathbb{Z} \subset \mathbb{Q} \subset \mathbb{R} \subset \mathbb{C}$. Starting with $\mathbb{Q}$, these number sets are fields. Each new member of the hierarchy realizes a new level of structure and admits operations which its predecessor cannot accommodate, $\mathbb{Q}$ closes under division whereas $\mathbb{Z}$ does not, etc. We have seen how mathematics provides the proper structures to describe the algebraic features of all number sets: beginning with $\mathbb{Z}$ the numbers were groups, and beginning with $\mathbb{Q}$ fields. That this understanding is much more than a formality is seen from the historical fact that for hundreds of years the complex numbers remained somewhat of a mystery. The situation changed only after the concept of the number field had been introduced.

Given the supreme potency of the complex numbers one may wonder if the 'less powerful' numbers can be abandoned altogether. The answer is no, they remain universally useful. Generally speaking it is good practice to solve problems in terms of number sets just large enough to achieve what needs to be done. For example, we do not use real numbers to count the number of balls in a box, we use integers, etc.

We are now ready to advance to the next hierarchical level, the vector spaces. Where numbers have a 'norm' specifying their magnitude, vectors are objects of a given magnitude *and* direction. As we will see, this added feature makes them indispensable tools in the mathematical description of physics.

L2 Vector spaces

Many objects of physical interest can be described in terms of a single number. Examples include the temperature of a body, its mass or volume, the energy required to move a body, or the number of gas molecules in a container. Quantities of this type are called **scalars**. However, scalars do not suffice to describe even many daily-life situations. For example, if a person who got lost asks for guidance the answer generally includes a direction and a distance. The two pieces of information can be combined into a '**vector**' whose length and geometric orientation encode distance and direction respectively. Vectorial quantities play an important role in physics, and in this chapter we introduce their mathematics from a perspective broad enough to include types of vectors that cannot be visualized in easy geometric ways. Such 'non-visual' realizations are ubiquitous in physics — for example, they are key to the mathematical description of quantum mechanics and the theory of relativity — and the beauty of the overarching mathematical framework is that they can all be understood in a unified manner.

However, before turning to the general level, let us begin by introducing a concrete realization of a set of vectors. This example will anticipate the key mathematical structures of vectors and motivate the general definition of section L2.2.

L2.1 The standard vector space $\mathbb{R}^n$

In this section, we will define $\mathbb{R}^n$ as an important class of vector spaces. (Sets of vectors that are complete in a sense to be defined a little further down are called vector 'spaces'.) The spaces $\mathbb{R}^n$ can be looked at from two different perspectives: first they are vector spaces in their own right, second they provide a 'language' in which all other vector spaces can be described. This bridging functionality makes them important from both a fundamental and an applied perspective. However, before turning to a mathematical formulation of these statements, let us demonstrate the appearance of vectors and their relation to $\mathbb{R}^n$ on a daily life example.

A motivating example

Consider the layout of a kitchen as shown in Fig. L4. How can the information contained in the plan be described quantitatively? The first step must be the definition of a unit of length, such as centimeters or inches. Second, a system of coordinates has to be specified. The latter is defined by two axes along which distances are to be measured. In a rectangular

room, directions parallel to the walls would be a natural choice, cf. the axes labeled 1 and 2 in the figure. However the choice is arbitrary and the axes labeled 1 and 2' would define an alternative and equally valid coordinate system as well.

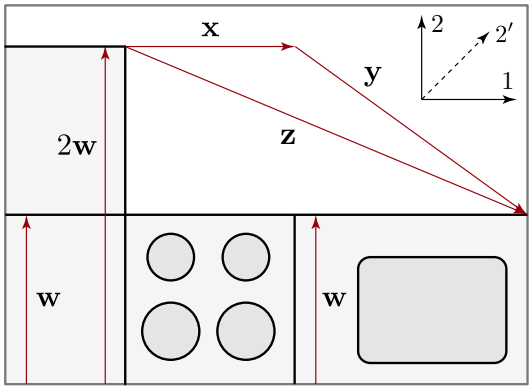


Figure L4: The layout of a kitchen described in terms of various vectors.

Given a coordinate system, a *vector* describing the position of two points relative to each other is specified through two numbers fixing the separation between the points in the coordinate directions. These numbers define the components of the vector in the chosen system of coordinates. For example, the vector labeled $\mathbf{x}$ in the figure describes points shifted relative to each other by 90cm in the 1-direction and 0cm in the 2-direction. For brevity, we write $\mathbf{x} = \left(\begin{smallmatrix} 90 \\ 0 \end{smallmatrix}\right)$. Likewise, $\mathbf{w} = \left(\begin{smallmatrix} 0 \\ 90 \end{smallmatrix}\right)$, $\mathbf{y} = \left(\begin{smallmatrix} 120 \\ -90 \end{smallmatrix}\right)$, etc. A vector may be graphically represented by an arrow connecting its two defining points. The length of the arrow measures the distance between the points and its direction their relative orientation. Note that the *same* arrow is obtained for any two points that have the same relative distance and orientation, irrespective of their actual location. For example, the arrow denoted by $\mathbf{w}$ in the figure describes the separation of any two points shifted relative to each other by 90cm in the 2-direction. We should think of a vector as an object that can be shifted (but not rotated or stretched) to any desired point of origin.

Two vectors can be concatenated to define a new vector. For example, the vector $\mathbf{z}$ in the figure is obtained by concatenation of $\mathbf{x}$ and $\mathbf{y}$ and denoted by $\mathbf{z} = \mathbf{x} + \mathbf{y}$. The two components of $\mathbf{z}$ are given by the sum of the components of $\mathbf{x}$ and $\mathbf{y}$, respectively, $\mathbf{z} = \left(\begin{smallmatrix} 90 \\ 0 \end{smallmatrix}\right) + \left(\begin{smallmatrix} 120 \\ -90 \end{smallmatrix}\right) = \left(\begin{smallmatrix} 210 \\ -90 \end{smallmatrix}\right)$. (Exercise: draw the vector $\mathbf{w} + \mathbf{x}$ and compute its components.) Similarly, a vector can be multiplied by a real number $a \in \mathbb{R}$ to change its length. For example, $2\mathbf{w} = \left(\begin{smallmatrix} 0 \\ 180 \end{smallmatrix}\right)$, is a vector with doubled components and thus corresponds to a vector of doubled length, as indicated in the figure. If $a < 0$, the direction of the vector is inverted, for example $-\mathbf{w}$ has the same length as $\mathbf{w}$ but points downwards.

EXERCISE Suppose we had decided to use the axes labeled 1 and $2'$ in Fig. L4 as coordinate axes. Assume that the angle between $2'$ and 1 is 45 deg. The component representations of the vectors $\mathbf{x}$, $\mathbf{y}$, $\mathbf{w}$, etc., change accordingly. Specifically, which of the following three representations of the

vector $\mathbf{w}$ is correct?

$$\text{(a)}\quad \mathbf{w} = 90\begin{pmatrix}0\\ \sqrt{2}\end{pmatrix}, \qquad \text{(b)}\quad \mathbf{w} = \begin{pmatrix}0\\ 45\end{pmatrix}, \qquad \text{(c)}\quad \mathbf{w} = 90\begin{pmatrix}-1\\ \sqrt{2}\end{pmatrix}. \tag{L12}$$

A systematic way to find the answer is to represent $\mathbf{w} = \mathbf{w}_1 + \mathbf{w}_{2'}$ as the sum of two vectors where $\mathbf{w}_1$ and $\mathbf{w}_{2'}$ point in the direction of 1 and $2'$, respectively. We then need to find out how long $\mathbf{w}_1$ and $\mathbf{w}_{2'}$ need to be if $\mathbf{w}$ has length 90? Compute the $(1, 2')$ coordinate representation of the other vectors shown in the figure.

The space of all two-component[1] vectors $\mathbf{x} = \binom{x^1}{x^2}$ is called $\mathbb{R}^2$ (spoken r-two). Our discussion above shows that there are different ways to look at vectors and their representation through elements of $\mathbb{R}^2$: (i) we can think of vectors as objects geometrically defined as classes of arrows in the plane. Arrows are unique up to translation. (ii) Once a system of coordinates has been chosen, each of these arrows is uniquely described through a two-component element of $\mathbb{R}^2$. However, keep in mind that the description changes if different coordinates are chosen. (iii) Elements of $\mathbb{R}^2$ are vectors in their own right in that the geometrically defined vector operations concatenation and stretching correspond to equivalent operations in $\mathbb{R}^2$. The example suggests that $\mathbb{R}^2$ is a 'reference' or standard vector space in terms of which vectors defined in different (geometric) ways can be described. However, the concrete numerical 'language' in which $\mathbb{R}^2$ represents a geometric vector depends on a choice of coordinates. The situation is not so different from human languages which describe the identical objects in different ways. However, before formulating the connection between component vectors to generic vectors (which have not been defined yet) in generality, let us extend the definition of $\mathbb{R}^2$ to to objects containing an arbitrary number of components.

Definition of $\mathbb{R}^n$

The definition of $\mathbb{R}^2$ affords an obvious generalization to vectors with an arbitrary number of components: we define the so-called **standard vector space** $\mathbb{R}^n$ as the set of all multicomponent objects,

$$\mathbb{R}^n \equiv \left\{ \mathbf{x} = \begin{pmatrix}x^1\\ x^2\\ \vdots\\ x^n\end{pmatrix} \middle| \, x^1, x^2, \ldots, x^n \in \mathbb{R} \right\}. \tag{L13}$$

The elements $\mathbf{x}$ of $\mathbb{R}^n$ are ***n*-component vectors**. In the introductory parts of this text, vectors will generally be denoted by boldface symbols, $\mathbf{x}, \mathbf{y}$, etc.[2] The components of a vector $\mathbf{x}$ are referred to by x^i, although the alternative notation $(\mathbf{x})^i$ will be occasionally used as well.

[1] The superscripts on x^1 and x^2 are indices (not powers of x!) distinguishing the first from the second component. The reason why we use superscripts rather than subscripts will be explained on p. 23.

[2] Since the boldface convention is inconvenient in handwriting, a variety of **alternative notations for vectors** exist: physicists and engineers often write $\vec{v}$. However, the repeated drawing of arrows costs time and more time-efficient alternative notations include $\vec{v}$, $\overline{v}$, or $\underline{v}$. Mathematicians often prefer an totally 'naked'

For example $(\mathbf{y})^1 = y^1 = 120$ in the kitchen example above. To save space we often use the in-line notation $\mathbf{x} = (x^1, \ldots, x^n)^T$, where '$T$' is spoken 'transpose'.[3] Finally, the number n is called the **dimension** of $\mathbb{R}^n$.

Much like a group is more than a simple set of elements (it is a set plus rules of composition), $\mathbb{R}^n$ is more than a just set of multicomponent objects: vectors can be added to each other and they can be multiplied by real numbers. As illustrated in our introductory discussion, the sum $\mathbf{z} = \mathbf{x} + \mathbf{y}$ of two vectors is the vector with components $z^i = x^i + y^i$. For example,

$$\begin{pmatrix} 1.5 \\ 2 \\ 0 \end{pmatrix} = \begin{pmatrix} 0.5 \\ -3 \\ 1 \end{pmatrix} + \begin{pmatrix} 1 \\ 5 \\ -1 \end{pmatrix}.$$

Likewise, the multiplication of a vector by a number is defined component-wise, i.e. the vector $a\mathbf{x}$ has components ax^i, for example

$$2 \begin{pmatrix} 1.5 \\ 2 \\ 0 \end{pmatrix} = \begin{pmatrix} 3 \\ 4 \\ 0 \end{pmatrix}.$$

Notice, however, that elements of $\mathbb{R}^n$ cannot be multiplied with each other,[4] nor divided by each other.

The vector space is $\mathbb{R}^n$ is just one example of many other vector spaces encountered in physics and mathematics. In the next two sections we define vector spaces in general terms and introduce a number of important spaces to be discussed in more depth later in the text.

L2.2 General definition of vector spaces

Above we introduced two different perspectives of vectors. The first was geometrical ('arrows'), the second algebraic in that it emphasized the operations that can be performed with vectors — addition and multiplication by numbers. In this section we upgrade the algebraic description to a definition of vector spaces in generality. The algebraic approach is motivated by its generality and the fact that the vectors relevant to physics often do not have a visual geometric interpretation. The situation resembles that with groups which, likewise, were defined by the operations defined for them. That approach, too, was motivated by the observation that identical algebraic properties describe a multitude of very different realizations of groups.

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notation as v. This is OK as long as it is made clear that $v \in V$ is a vector and *not* a number. We will use this notation in later chapters of the text when vectors belonging to different spaces are handled at the same time. However, whichever notation is chosen, consistency and clearly stated definitions are imperative. The convention $\underline{v}$ may be a good compromise between efficiency and explicitness.

[3] At this stage $\mathbf{x} = (x^1, \ldots, x^n)^T$ is just a space-saving alternative to the column notation (L13). The actual mathematical meaning of transposition is discussed later in Sec. L5.

[4] However, different types of vector 'multiplication' will be introduced below.

Vector space definition

Vectors are objects that can be added to each other and multiplied by elements of a number field $\mathbb{F}$. (So far, we discussed the case $\mathbb{F} = \mathbb{R}$). The corresponding formal definition reads as follows:

An $\mathbb{F}$-**vector space** is a triple, $(V, +, \cdot)$, consisting of a set, V, a **vector addition** rule,

$$+ \,:\, V \times V \to V, \qquad (\mathbf{v}, \mathbf{w}) \mapsto \mathbf{v} + \mathbf{w}, \tag{L14}$$

and a rule for **multiplication by scalars**,

$$\cdot \,:\, \mathbb{F} \times V \to V, \qquad (a, \mathbf{v}) \mapsto a \cdot \mathbf{v} \equiv a\mathbf{v}, \tag{L15}$$

such that the following **vector space axioms** hold: (i) the addition of vectors, $(V, +)$, defines an abelian group. The neutral element of addition, $\mathbf{0}$, is called null vector; the inverse element of a vector is called the negative vector, $-\mathbf{v}$. (ii) Scalar multiplication satisfies the following rules, $\forall a, b \in \mathbb{F}, \mathbf{v}, \mathbf{w} \in V$:

(a) $(a+b)\mathbf{v} = a\mathbf{v} + b\mathbf{v}$ (scalar multiplication by a sum of scalars is distributive),
(b) $a(\mathbf{v}+\mathbf{w}) = a\mathbf{v} + a\mathbf{w}$ (scalar multiplication of a sum of vectors is distributive),
(c) $(ab)\mathbf{v} = a(b\mathbf{v})$ (scalar multiplication by a product of scalars is associative),
(d) $1\mathbf{v} = \mathbf{v}$ (neutral element of $\mathbb{F}$ is neutral element of scalar multiplication).

(L16)

Comments:

- The first part of the definition, (L14), formalizes the addition of vectors. In the case of $\mathbb{R}^n$ the null vector is given by $\mathbf{0} = (0, \ldots, 0)^T$. We may think of it as an arrow shrunk to a point (and hence not pointing anywhere). The negative vector, $-\mathbf{v}$, can be imagined as a vector pointing in the direction opposite to $\mathbf{v}$, such that $\mathbf{v} + (-\mathbf{v}) = \mathbf{0}$. Equivalently, one may think of $-\mathbf{v}$ as $(-1)\mathbf{v}$ (multiplication of $\mathbf{v}$ by $-1 \in \mathbb{F}$). Axiom (a) above then states that $0\mathbf{v} = (1-1)\mathbf{v} = \mathbf{v} - \mathbf{v} = \mathbf{0}$. Addition of this object to another vector does not do anything.
- Relations (a) to (d) appear to be so obvious that they hardly seem worth mentioning. However they are required to ensure that the 'algebraic' properties of a vector space match the geometric understanding of directed objects ('arrows'). Without these specifications the definition would not be sharp enough to exclude 'weird spaces' outside the useful category of vector spaces.
- The definition does not make reference to vector components, nor to the 'dimension' of vectors. We conclude that these must be secondary characteristics deducible from the general definition.
- Given $a, b, c \in \mathbb{F}$ and $\mathbf{u}, \mathbf{v}, \mathbf{w} \in V$, the combination $a\mathbf{u} + b\mathbf{v}$ also lies in V. The same is true for $a\mathbf{u} + b\mathbf{v} + c\mathbf{w}$, etc. Expressions of this sort are called **linear combinations** of vectors.

▷ As mentioned previously, sets fulfilling the criteria above are generally called 'spaces', a space of functions, the space of matrices, etc.

The definition above introduces the concept of a vector in its most general form, including realizations where geometric visualizations are not natural. In practice, the question whether a given set is a vector space is always answered by checking the defining criteria above. Geometric visualizations can, but need not be involved. In some cases they can even be counterproductive.

Covariant notation

We conclude this section with some remarks on notation. Below, we will frequently consider sums $\mathbf{v}_1 a^1 + \mathbf{v}_2 a^2 + \dots$ of vectors $\mathbf{v}_1, \mathbf{v}_2, \dots$ with coefficients $a^1, a^2, \dots$. Notice that we write the coefficients, a^i, with superscript^i indices while the vectors, $\mathbf{v}_i$, carry subscript$_i$ indices. Superscript and subscript indices are called **contravariant indices** and **covariant indices**, respectively. Notation adopting this index positioning convention is called **covariant notation** and it will be used throughout this text. At this stage, this may seem to be a purely technical convention. However, as we progress we will see that the distinction between co- and contravariant objects becomes more and more important both from a physical and a mathematical perspective. (For a first motivation in this direction, see the info section below.) Anticipating this development, we use covariant notation from the very beginning. However, it should not go unnoted that this approach is not standard and that most introductory texts on linear algebra prefer and all–indices–downstairs notation.

INFO Vectors are members of a more general category of objects known as tensors (the topic of chapter L11). For example, *matrices*, which are perhaps familiar from high school and which will be discussed later in this chapter, also belong to this family of objects.

It is common practice in physics to treat every object that carries a single index (such as $\mathbf{x} \leftrightarrow \{x^i\}$) as if it were a vector. However, many of the 'vectors' routinely encountered in physics are actually not vectors, but objects of different structure known as **tensors**. Important examples of such tensors–in–disguise include electric and magnetic fields, mechanical forces and currents, and more. In cases where the non-vectorial nature of such quantities becomes too apparent to ignore, they are assigned special names, such as 'pseudo- vector' or 'axial vector', etc. However, physicists do not easily let go of the vector association as such. Depending on the research field one is working in, this practice can be either harmless or a potent source of confusion. The latter is the case in a growing number of disciplines including the theory of relativity, particle physics, topological condensed matter theory, quantum information theory, and others. It is probably fair to say that the only reason why the physics literature sticks to its all–is–vector culture is social inertia. The indiscriminate identification of single-component objects with vectors does not 'simplify' anything. On the contrary, it obscures connections that become clear within a more differentiated approach. On the other hand, a fully reformed approach which, for example, would describe a magnetic field as an alternating tensor of second degree rather than as a vector, might be too radical. Students trained in this way would not be able to communicate with colleagues speaking a more traditional language, so this is not a viable solution.

In this text, we aim to strike a middle ground. Tensor calculus and the ensuing interpretation of physical objects are explained in the advanced chapters L11 and V4 to V6 later in this text. However, from the beginning we will pay careful attention to the consistent positioning of co- and contravariant indices. This is done because **covariant notation is an important aid in discriminating between objects that are fundamentally vectors and others that are not.** Occasionally, we will run into trouble and realize that the use of covariant notation leads to inconsistent index positions. This is the way by which the notation signals that an object truly different from a vector has been encountered. Depending on the context, we will fix the situation right away or, on a few occasions, refer to a section of chapter L11 were the origin of the problem is explained.

L2.3 Vector spaces: examples

In the following we introduce a number of examples which all play an important role as vectors spaces in physics.

The standard vector spaces

We have already introduced $\mathbb{R}^n$ as the **standard vector space** defined over the real numbers, $\mathbb{F} = \mathbb{R}$. The alternative choice $\mathbb{F} = \mathbb{C}$ defines the **complex standard vector space** $\mathbb{C}^n$. This is the set of all vectors, $\mathbf{z} = (z^1, \ldots, z^n)^T$, with components $z^i \in \mathbb{C}$. At first sight $\mathbb{C}^n$ may seem to be 'more complicated' than $\mathbb{R}^n$ (inasmuch as complex numbers carry more structure than real numbers). However, we will see that the opposite is true and in many instances will prefer to work with $\mathbb{C}^n$.

EXERCISE Convince yourself that the standard vector spaces fulfills the vector space axioms.

Affine and Euclidean spaces

Consider infinite d-dimensional space, for example an infinite two-dimensional plane or the three-dimensional space we live in. The mathematical abstractions of these objects are called **affine spaces**, A. Elements $P \in A$ are called **points**.

Affine spaces are almost, but not quite, vector spaces. To understand the difference, notice that a vector space contains the neutral element of addition, $\mathbf{0}$, as its distinguished origin, or null-vector. By contrast, affine spaces are the mathematical formalization of idealized infinite space and therefore do not contain a 'special' point. To establish the connection between an affine space A and a vector space V of the same dimension one needs to pick an arbitrary reference point, $O \in A$, and identify it with the origin, $\mathbf{0} \in \mathbf{V}$. For example, if the focus is on describing our solar system (which lies in three-dimensional affine space) it would be natural to choose the center of the sun as a reference point. Each point $P \in A$ can then be identified with a vector, $\mathbf{v}$, representing the arrow from O to P, as illustrated in Fig. L5. If another point, $Q \in A$, is represented by the vector $\mathbf{w}$ then the linear combination $\mathbf{u} = \mathbf{w} - \mathbf{v}$

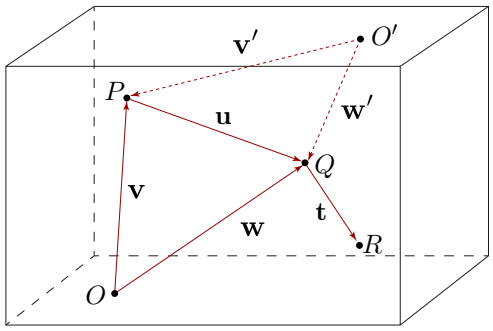


Figure L5: On the definition of affine space.

represents the arrow from P to Q.

Note that the points P and Q are independent of the choice of reference point, but the vectors representing them are not. If a different reference point O' is chosen then P and Q are described by different vectors $\mathbf{v}'$ and $\mathbf{w}'$, respectively. However, the vector representing the arrow from P to Q remains the same, $\mathbf{w}' - \mathbf{v}' = \mathbf{w} - \mathbf{v}$. As an example, take $P =$ (center of earth) and $Q =$ (center of Venus). The vectors representing P and Q depend on whether the centers of the sun or of Jupiter are chosen as reference points. However, the vector connecting the center of earth to that of Venus is independent of the choice of reference point.

The preceding description of affine spaces is made precise as follows: consider a set of **points**, $A = \{P, Q, \ldots, \}$ subject to the following three conditions: (i) there exists a vector space V such that to any ordered pair of points $(P, Q) \in A \times A$ a vector $\mathbf{u} \in V$ may be uniquely assigned. We call $\mathbf{u}$ the **difference vector** from P to Q. (ii) For any point $P \in A$ and any vector $\mathbf{u} \in V$ there exists a unique point $Q \in A$ such that $\mathbf{u}$ is the difference vector from P to Q. (iii) For any three points P, Q and $R \in A$, with difference vectors $\mathbf{u}$ from P to Q and $\mathbf{t}$ from Q to R, respectively, the difference vector from P to R is given by $\mathbf{u} + \mathbf{t}$. If these conditions are met, A is called an **affine space**. Once a point $O \in A$ has been chosen as reference point, A becomes identifiable with V and there is a bijection between points $P \in A$ and the difference vectors $\mathbf{v} \in V$ connecting O and P. This identification is sometimes written as $V = (A, O)$, and the correspondence between P and $\mathbf{v}$ as $P = O + \mathbf{v}$. For example, in this language criterion (iii) above assumes the form $P + \mathbf{u} + \mathbf{t} = Q + \mathbf{t} = R$.

In the particular case where $V = \mathbb{R}^d$ we call $A \equiv \mathbb{E}^d$ ***d*-dimensional Euclidean space**. This denotation hints at the fact that Euclidean space possesses structures that a generic affine space need not have: to vectors of $\mathbb{E}^d$ lengths and angles and other elements of Euclidean (!) geometry to be introduced in chapter L3 may be assigned. Both generic affine spaces and Euclidean spaces play important roles in physics. Their description in terms of vector spaces is so natural that the distinction between affine and vector spaces is easily forgotten. However, occasionally it has to be remembered to avoid confusion!

Function spaces

Let $f : I \to \mathbb{R}$, $t \mapsto f(t)$ be a function defined over a finite interval, I (cf. Fig. L6). The set containing all these functions is called $L^2(I)$.[5] Two functions, f, g may be added to each other to obtain a new function $f + g$ in the same set. That new function is defined as the superposition of f and g, $(f + g)(t) \equiv f(t) + g(t)$. Likewise, the product of a function with a number, $a \in \mathbb{R}$, defines another function, af, via $(af)(t) \equiv af(t)$. This shows that $L^2(I)$ is a vector space, and that one may think of the functions contained in it as vectors. Give yourself some time to let this message sink in! ($\to$ **??**)

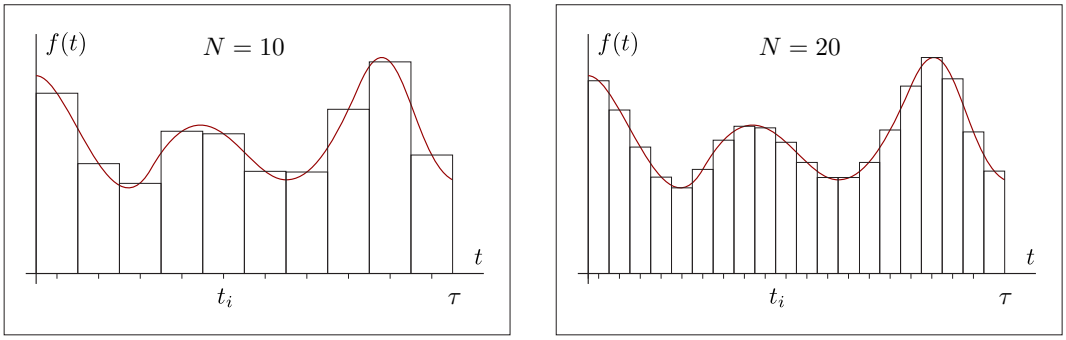


Figure L6: The discretization of a function in terms of N discrete values yields an N-component vector. The larger N, the more closely the discretized function approximates the continuous one.

To make the vectorial interpretation of functions more concrete, consider storing the signal $f(t)$ on a computer. This may be done by discretizing the time interval into a large number, N, of small intervals of width τ/N, each centered on a time t_i, $i = 1, \ldots, N$ (see Fig. L6). One then samples N representative readouts of the function, $f^i = f(t_i)$. These values define an N-dimensional vector, $\mathbf{f} \equiv (f^1, \ldots, f^N)$, which may be saved as a discrete approximation of the function. The number of components, N, may be increased to make the approximation of the 'continuous' function f as accurate as desired.[6]

Given two functions, f, g, with discrete representations, $\mathbf{f}, \mathbf{g}$, a discretized function, $\mathbf{f} + \mathbf{g}$, can be defined by addition of the individual function values: $(\mathbf{f} + \mathbf{g})^i = (\mathbf{f})^i + (\mathbf{g})^i$ (cf. Fig. L7, bottom right). Similarly, the discrete function $a\mathbf{f}$, $a \in \mathbb{R}$, may be defined by component-wise multiplication, $(a\mathbf{f})^i = a(\mathbf{f})^i$ (Fig. L7 top right). This construction shows that one may work with discretized functions just as with N-component vectors and that the set of N-step discretized functions is identical to $\mathbb{R}^N$.

Heuristically, $L^2(I)$ may be interpreted as the $N \to \infty$ limit of the discretization spaces $\mathbb{R}^N$, and functions are 'infinitely–high'-dimensional vectors with components $f(t) \leftrightarrow f^i = f(t_i)$. This view of functions is very important. It makes the connection between calculus and

[5] The notation $L^2(I)$ for the set of functions defined on I is standard in mathematics. Its definition requires one additional condition, namely 'square integrability' to be discussed in chapter L10. However, for the moment, this additional condition is not of relevance.

[6] For example if $f(t)$ represents an audio signal, sampling rates with $N = 44.100$ for a time interval of 1 second correspond to the resolution of standard CD recordings.

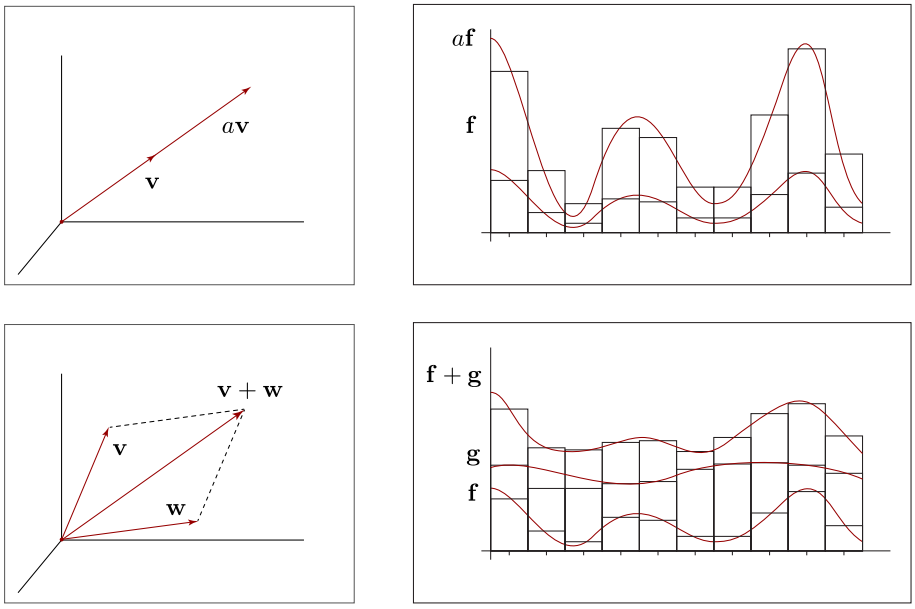


Figure L7: Visualization of vector multiplication and addition, respectively, for two-dimensional vectors in $\mathbb{E}^2$ (left), and discretized functions (right).

linear algebra tangible and plays an important role in various fields of physics.

EXAMPLE In the following we introduce a few more examples which may help in building familiarity with the concept of vector spaces:

- ▷ **Number fields as vector spaces**: for $n = 1$, the vector space $\mathbb{R}^n$ reduces to the real numbers, $\mathbb{R}^1 = \mathbb{R}$. (The set of vectors with just one real component is trivially equivalent to the real numbers.) Likewise, $\mathbb{Q}^1$ is a $\mathbb{Q}$-vector space (→ L2.4.1), and $\mathbb{C}^1$ is a $\mathbb{C}$-vector space. However, one may also think of $\mathbb{C}^1 \cong \mathbb{C}$ as an $\mathbb{R}$-vector space (→ L2.4.2): any complex number, z, can be multiplied by a real number, a, to yield another complex number az, and complex numbers can be added to each other. One may decompose $z = x + \mathrm{i}y$ into real and imaginary parts to uniquely describe it by a *pair* of real numbers, $z \leftrightarrow (x, y)^T$. This shows that $\mathbb{C} \cong \mathbb{R}^2$ can be identified with $\mathbb{R}^2$. The identification of $\mathbb{C}^2$ with the real vector space $\mathbb{R}^2$ is often useful in applications. For example, it is common practice to describe physical problems defined in two-dimensional space in a 'complex notation' in which each point is represented by a complex number. This is done because complex numbers are usually more convenient to work with than two-component vectors.

- ▷ Let $P_2 \equiv \{a_2x^2 + a_1x + a_0 | a_{0,1,2} \in \mathbb{R}\}$ denote the set of all **polynomials** in the variable x of degree 2. For two polynomials, $p(x) \equiv a_2x^2 + a_1x + a_0$ and $q(x) \equiv b_2x^2 + b_1x + b_0$, the sum, $(p + q)(x) = (a_2 + b_2)x^2 + (a_1 + b_1)x + (a_0 + b_0)$, is again a polynomial of degree two, and so is the product with a real number, $ap(x) = (aa_2)x^2 + (aa_1)x + (aa_0)$. This shows that P_2 is a vector space. Since each of these polynomials is uniquely identified by its three coefficients, $p \leftrightarrow (a_2, a_1, a_0)$ we have a bijection $P_2 \cong \mathbb{R}^3$. Exercise: think of generalizations to polynomials of arbitrary degree (→ L2.4.4), or to polynomials in more than one variable. For example, the polynomials of degree 2 in two variables, x and y, have the form $a_{22}x^2y^2 + a_{21}x^2y + a_{12}xy^2 +$

$a_{20}x^2 + a_{02}y^2 + a_{11}xy + a_{10}x + a_{01}y + a_{00}$, with real coefficients a_{ij}. How many components are required to uniquely describe the polynomials in two variables of maximal degree five?

▷ For some exotic examples of vector spaces with more contrived addition and multiplication rules see problems L2.4.5-6.

L2.4 Basis and dimension

A common property all vectors discussed above was that they could be represented through a list of components, $\mathbf{v} \leftrightarrow (v^1, \ldots, v^n)^T$. However, we also observed that the component representation was not unique. For example, the vector $\mathbf{x}$ in Fig. L4 has a representation $\mathbf{x} = (90, 0)^T$ if cm are used as a unit of length and the coordinate axes are oriented as indicated. It would change to $\mathbf{x} \simeq (35.4, 0)^T$ if inches were used, or to $\mathbf{x} \simeq (63.3, 63.3)$ if the coordinate axes were rotated by 45deg. However, irrespective of the chosen representation, *two* numbers are needed to describe it. The number of components required to specify a vector is a unique characteristic of each vector space,[7] called its *dimension*. Notice that the dimension is not mentioned in the fundamental definition of vector spaces given Sec. L2.2. This shows that it must be an attribute following from the vector space axioms. In the following we discuss how this happens.

Given a vector space V and a set S containing m of its vectors,

$$S \equiv \{\mathbf{v}_1, \ldots, \mathbf{v}_m\}, \quad \mathbf{v}_i \in V, \tag{L17}$$

the **linear span** (or **linear hull**) of S is defined as the set of linear combinations of the elements of S:

$$\mathrm{span}(S) \equiv \{\mathbf{v}_1 a^1 + \mathbf{v}_2 a^2 + \cdots + \mathbf{v}_m a^m \,|\, a^1, \ldots, a^m \in \mathbb{F}\}. \tag{L18}$$

For $\mathbf{u}, \mathbf{w} \in \mathrm{span}(S)$ the linear combination $a\mathbf{u} + b\mathbf{w}$, $a, b \in \mathbb{F}$ again lies in $\mathrm{span}(S)$, and this shows that $\mathrm{span}(S)$ is a vector space in itself.

We call a vector space, $W \subset V$, embedded in V a **subspace** of V. This includes the extremes $W = \{\mathbf{0}\}$ of the subspace containing just the null-vector, and the full space, $W = V$. At any rate, the linear hull, $\mathrm{span}(S)$, is a subspace of V, non-empty if S contains at least one non-vanishing vector. An interesting question to be addressed in the next sections is how large a sets of vectors has to be to include the full vector space in its span, $\mathrm{span}(S) = V$.

Linear independence

Suppose $S = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ has the property that one of its elements, say $\mathbf{v}_1$, can be represented as a linear combination of the others,

$$\mathbf{v}_1 = \mathbf{v}_2 b^2 + \cdots + \mathbf{v}_m b^m. \tag{L19}$$

[7] Readers to whom this sounds trivial may try to prove this statement. It is not as easy as one might think.

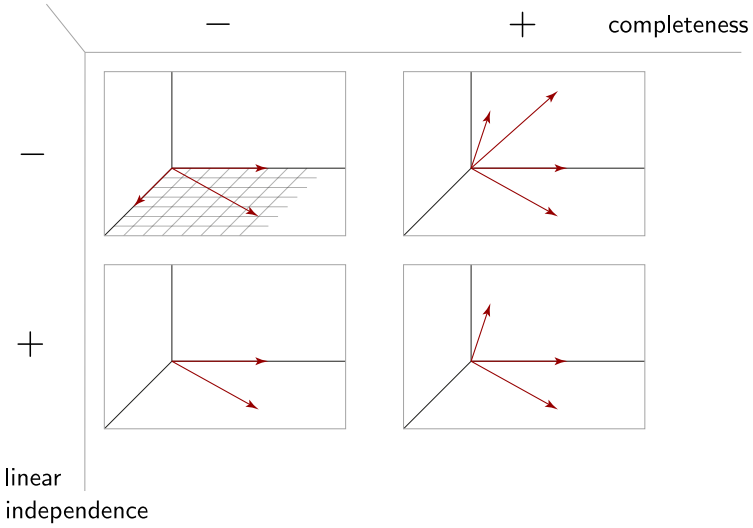


Figure L8: The concepts of linear independence and completeness, illustrated for the example $\mathbb{E}^3$.

In this case, the vectors defining S are called **linearly dependent vectors**, and S is called a **linearly dependent set**. Such sets contain redundancy in that some of their elements may be removed without diminishing the span. For example, with $S' \equiv S\backslash\{\mathbf{v}_1\}$ we have (why?)

$$\mathrm{span}(S) = \mathrm{span}(S'). \tag{L20}$$

The upper row of Fig. L8 shows linearly dependent sets containing three and four vectors of $\mathbb{E}^3$, respectively. Conversely, if none of the elements of S can be obtained by linear combination of the others, $\mathbf{v}_1$ to $\mathbf{v}_m$ are called **linearly independent** vectors.

For later reference we note that there is an alternative way to test linear independence: the vectors in S are linearly dependent if they can be linearly combined to form a non-trivial representation of the zero vector, $\mathbf{0}$, i.e. if there exist non-vanishing coefficients,

$$\{a^1, \ldots, a^m\} \neq \{0, \ldots, 0\}, \qquad \mathbf{v}_1 a^1 + \mathbf{v}_2 a^2 + \ldots \mathbf{v}_m a^m = \mathbf{0}\ . \tag{L21}$$

Why are the two conditions equivalent? If (L19) holds, then we have a representation $\mathbf{0} = -\mathbf{v}_1 + \mathbf{v}_2 b^2 + \cdots + \mathbf{v}_m b^m$. Conversely, if (L21) holds we may pick a non-vanishing coefficient, say a^1, to obtain the linear combination of $\mathbf{v}_1 = -\frac{1}{a^1}(\mathbf{v}_2 a^2 + \cdots + \mathbf{v}_n a^n)$ through the other vectors. This demonstrates linear dependence in the sense of Eq. (L19).

EXAMPLE Consider the vectors

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \mathbf{v}_2 = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \qquad \mathbf{v}_3 = \begin{pmatrix} -1 \\ -1 \end{pmatrix}\ . \tag{L22}$$

The set $S \equiv \{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ is linearly dependent because $\mathbf{v}_1 = -(\mathbf{v}_2 + 2\mathbf{v}_3)$. However, the set $S' = \{\mathbf{v}_1, \mathbf{v}_2\}$ is linearly independent, because $\mathbf{v}_1 a^1 + \mathbf{v}_2 a^2 = (a^1 + a^2, 2a^2)^T$, which equals $\mathbf{0}$ only if $a^1 = a^2 = 0$. Similarly, $S'' = \{\mathbf{v}_1, \mathbf{v}_3\}$ is linearly independent, as is $S''' = \{\mathbf{v}_2, \mathbf{v}_3\}$. (→ L2.5.1-2)

It is often useful to eliminate redundancy by working with linearly independent sets. This is done by removing redundant vectors of S until one arrives at a linearly independent set of reduced cardinality. That reduced set need not be unique, as shown by the example of S', S'' and S''' above. However, its span does not depend on which of the linearly dependent vectors are removed and S', S'' and S''' all span the same vector space.

Completeness

There is another important feature which the sets like (L17) may or may not have: a set $S = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ containing n vectors is called **complete** if

$$\mathrm{span}(S) = V. \tag{L23}$$

In this case, every vector $\mathbf{v} \in V$ can be written as a linear combination of the vectors $\mathbf{v}_i$. For example, the set $S = \{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ of Eq. (L22) is complete in $\mathbb{R}^2$ because any vector $\mathbf{v} = (a, b)^T$ can be represented as $\mathbf{v} = \mathbf{v}_1 a + \mathbf{v}_2 b + \mathbf{v}_3 b$. The reduced sets S', S'' and S''', too, are all complete in $\mathbb{R}^2$. Examples of sets complete in the Euclidean space $\mathbb{E}^3$ are shown in the second column of Fig. L8.

Basis

A set S that is both complete *and* linearly independent is called a **basis** of the vector space V. These properties guarantee (i) that each element $\mathbf{v} \in V$ can be expressed as a linear combination of basis elements (completeness),

$$\mathbf{v} = \mathbf{v}_1 a^1 + \mathbf{v}_2 a^2 + \cdots + \mathbf{v}_n a^n, \tag{L24}$$

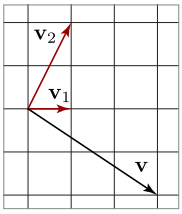
and (ii) that this linear combination is unique (linear independence). To understand how uniqueness follows from linear independence, suppose that $\mathbf{v}$ could also be represented in a different way, say $\mathbf{v} = \mathbf{v}_1 b^1 + \mathbf{v}_2 b^2 + \cdots + \mathbf{v}_n b^n$. Subtracting the second representation from the first, we obtain $\mathbf{0} = \mathbf{v} - \mathbf{v} = \mathbf{v}_1(a^1 - b^1) + \mathbf{v}_2(a^2 - b^2) + \cdots + \mathbf{v}_n(a^n - b^n)$. This is a representation of the null vector and so the assumed linear independence of the basis vectors requires that all coefficients must be zero, $b^j = a^j$. This in turn means that the two representations of $\mathbf{v}$ have to be identical. We call the representation of a vector in a given basis its **expansion**, and the corresponding coefficients the **expansion coefficients** with respect to that basis.

Each vector space has a basis. For given realizations of vector spaces this statement is usually straightforward to verify by the constructive specification of a basis. However, the general proof is not straightforward and will not be given here.[8] We also note that for a given

[8] Whereas the proof is relatively elementary for spaces with bases of finite cardinality, in the opposite case of **infinite-dimensional vector spaces** the situation is more involved. The function spaces $L^2(I)$ introduced above are examples of this type. Fortunately, the majority of vector spaces relevant to physics are finite dimensional, or can be made finite without significant loss of physical information. For example, we have discussed above how $L^2(I)$ can be approximated to any desired precision by an N-dimensional vector space $\mathbb{R}^N$.

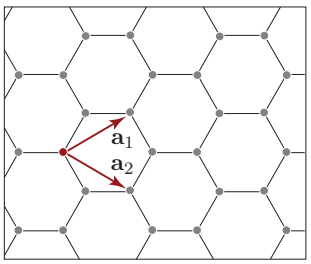
space there is infinite freedom in the choice of a basis. The expansion coefficients of vectors depend on this choice and therefore change under changes of basis. If vectors are regarded as invariant 'objects' one may think of their components as descriptions in a 'language' tied to a basis. Tools for the computation of vector expansion coefficients and their transformation under changes of bases will be introduced in section L5.6.

EXERCISE Show that the pair $\{\mathbf{v}_1, \mathbf{v}_2\}$ of vectors defined in Eq. (L22) defines a basis of $\mathbb{R}^2$. Draw the two basis vectors and an arbitrary other vector $\mathbf{v}$ of your choice. Compute its two expansion coefficients algebraically, and represent $\mathbf{v}$ graphically as a linear combination of $\mathbf{v}_1$ and $\mathbf{v}_2$. Repeat the exercise, to show that $\{\mathbf{v}_2, \mathbf{v}_3\}$, and $\{\mathbf{v}_1, \mathbf{v}_3\}$ are bases, too. Explain why the pair $\{\mathbf{e}_1, \mathbf{e}_2\}$ defined by $\mathbf{e}_1 = \mathbf{v}_1 = (1,0)^T$ and $\mathbf{e}_2 = (0,1)^T$ is a basis more convenient to work with than the others.



If the number n of elements of a basis is finite, it is unique. Any other basis then has the same number of elements, and n is called the **dimension** of the space. As an exercise, assume the existence of two bases of different cardinality n, m and show that the assumptions of linear independence and completeness leads to a contradiction.

INFO Many problems in **physics** are described in vector spaces whose dimensionality is different from the three dimensions of ambient space. For example, crystalline structures are often effectively two-dimensional. Einstein's theory of relativity adds 'time' to three-dimensional space, and is thus formulated in four-dimensional space-time. Functions describing physical phenomena can be discretized as N-dimensional vectors (with $N \gg 1$). Quantum mechanics is formulated in vector spaces whose dimension is determined by the number of particles under consideration. These and many more examples motivate the study of vector spaces of arbitrary dimensionality.



EXERCISE The microscopic structure of **graphite** is defined by stacked two-dimensional sheets of carbon.[9] The carbon atoms of each sheet form a regular hexagonal lattice, as shown in Fig. **??**. Choosing the position of an arbitrary carbon atom as a point of origin, the position of any other atom in the plane is described by a two-dimensional vector. Convince yourself that each of these vectors may be represented by a linear combination of two suitably chosen 'basis' vectors, e.g. the vectors denoted by $\mathbf{a}_1$ and $\mathbf{a}_2$ in the figure. Work out the linear combinations representing the positions of a few atoms of your choice. Try to derive a general formula specifying the position of all atoms as linear combinations of the basis vectors.

[9] As of 2005 it has become possible to isolate individual atomic layers of graphite. The ensuing two-dimensional crystalline material is known as **graphene**. For its discovery, A. Geim and K. Novoselov were awarded the 2010 Nobel prize in physics.

Einstein summation convention

Linear combinations such as $\mathbf{v}_1 a^1 + \mathbf{v}_2 a^2 + \cdots + \mathbf{v}_n a^n$ appear very frequently in the following and it is worthwhile to discuss a few notation conventions. First, note that the summation involves a contravariant (superscript) and a covariant (subscript) index. This structure by itself helps to avoid errors:

- ▷ An index summation always runs over a pair of co-and contravariant indices, e.g. $\mathbf{w} = \mathbf{v}_1 a^1 + \mathbf{v}_2 a^2 + \mathbf{v}_3 a^3$.
- ▷ An unsummed ('free') index always appears at the same position on both sides of an equation, e.g. $\mathbf{w}_i = \mathbf{v}_1 A^1{}_i + \mathbf{v}_2 A^2{}_i + \mathbf{v}_3 A^3{}_i$.

Violations of either of these rules usually indicate mistakes.

Expressions of the architecture $A_1 B^1 + A_2 B^2 + \cdots + A_n B^n$ appear so frequently that various abbreviating notations have been introduced:

$$A_1 B^1 + A_2 B^2 + \cdots + A_n B^n \equiv \sum_{i=1}^{n} A_i B^i \equiv \sum_i A_i B^i \equiv A_i B^i. \tag{L25}$$

In the third representation the upper and lower limits of the sum are implicit. In the last one we have introduced the **Einstein summation convention**, according to which indices occurring pairwise on one side of an equation are to be summed over. Such index pairs are called 'pairwise repeated indices' or 'dummy indices' and their summation is called a **contraction of indices**. The Einstein summation convention assumes that the summation range is specified by the context. For example, the Einstein representation of the argument formulated after Eq. (L24) reads: if $\mathbf{v} = \mathbf{v}_i a^i = \mathbf{v}_i b^i$ then $\mathbf{0} = \mathbf{v} - \mathbf{v} = \mathbf{v}_i (a^i - b^i)$, implying $a^i = b^i$. We will soon turn to using these abbreviated representations. However, to ease the transition they will be temporarily used in parallel with a more expansive representation (→ L2.5.3-**??**). We finally note that the convention to sum over pairwise occurring indices does not require covariant notation; texts writing all indices as subscripts frequently implement this rule as well. However as we will see in chapter L11, the Einstein convention has a deeper meaning which becomes visible only in covariant notation.

Vector space bases: examples

The concept of a basis is very important to the description of vector spaces. So much so that the choice of a suitable basis usually comes first in the work with a new vector space. Some spaces have a 'canonical' basis [10] and some do not. In the following we revisit the examples of Sec. L2.3 to illustrate this point.

- ▷ The natural basis, $\{\mathbf{e}_j | j = 1, \ldots, n\}$, of the **standard vector spaces** $\mathbb{R}^n$ and $\mathbb{C}^n$ contains the basis vectors

$$\mathbf{e}_j = (0, \ldots, 1, \ldots, 0)^T, \tag{L26}$$

[10] The attribute 'canonical' stands for 'natural' or 'standard' but does not have a mathematically precise definition.

where the 1 stands at position number j. (Verify linear independence and completeness of this set.) The components of the standard basis vectors may be alternatively specified as $(\mathbf{e}_j)^i = \delta^i{}_j$, where the **Kronecker delta** $\delta^i{}_j$ is defined by

$$\delta^i{}_j = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} . \tag{L27}$$

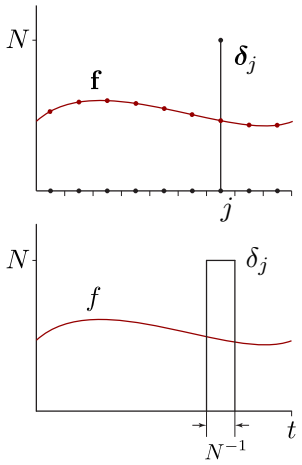
In the basis (L26), the expansion of a general vector $\mathbf{x} = (x^1, \ldots, x^n)^T$ assumes the form

$$\mathbf{x} = \mathbf{e}_1 x^1 + \mathbf{e}_2 x^2 + \cdots + \mathbf{e}_n x^n = \mathbf{e}_j x^j .$$

This shows that the components of an $\mathbb{R}^n$-vector and its expansion coefficients in the standard basis *coincide*. This is the defining feature of that basis.

▷ By contrast, the **Euclidean spaces**,[11] $\mathbb{E}^d$, do not favor particular directions over others and therefore do not possess a 'canonical' basis. However, in many cases the identity of a suitable basis is determined by the context. For example, the kitchen layout of Fig. L4 favors a basis of vectors $\mathbf{v}_i$, $i = 1, 2$ parallel to the walls of the room. The representation of generic vectors as $\mathbf{x} = 90\mathbf{v}_1$, or $2\mathbf{w} = 180\mathbf{v}_2$, then defines component representations as $\mathbf{x} = (90, 0)^T$, $2\mathbf{w} = (0, 180)^T$.

▷ The choice of a basis is particularly important in the case of **function spaces** such as $L^2(I)$. For definiteness, consider the N-dimensional space obtained by discretizing functions $f : [0, 1] \to \mathbb{R}$, $t \mapsto f(t)$ into N-component vectors, $\mathbf{f} = (f^1, \ldots, f^N)^T \in \mathbb{R}^N$, where $f^i = f(t_i)$. In this case it is preferable to work with basis vectors $\boldsymbol{\delta}_j = N\mathbf{e}_j$, i.e. the standard basis vectors $\{\mathbf{e}_j\}$ of $\mathbb{R}^N$ scaled by a factor of N. The basis vector $\boldsymbol{\delta}_j$ may be viewed as a 'discrete function', $\boldsymbol{\delta}_j : \{1, \ldots, N\} \to \mathbb{R}$, $i \mapsto (\boldsymbol{\delta}_j)^i$, vanishing for all values of i, except for $i = j$, where it equals N. We can think of $\boldsymbol{\delta}_j$ as a discretized version of a box-shaped function $\delta_j : [0, 1] \to \mathbb{R}$, $t \mapsto \delta_j(t)$, which equals zero everywhere except in an interval of width $1/N$ centered on time t_j, in which it takes the constant value N. A general function vector can now be expanded as



$$\mathbf{f} = \frac{1}{N}(\boldsymbol{\delta}_1 f^1 + \boldsymbol{\delta}_2 f^2 + \cdots + \boldsymbol{\delta}_N f^N) = \frac{1}{N}\,\boldsymbol{\delta}_j f^j . \tag{L28}$$

This shows how a discretized function can be expanded in terms of a 'standard basis'. However, it is less obvious what becomes of this strategy in the limit $N \to \infty$. We will address this question later in the text, see section C6.1 and chapter L10.

[11] Unless stated otherwise, we assume that a point of origin has been chosen so that $\mathbb{E}^d$ can be identified with a vector space.

EXERCISE Returning to the examples discussed on p. 27, consider $\mathbb{R}$ as a vector space, and show that the number $\{1\}$ (or any other set containing just one non-vanishing number) is a basis. Show that $\{1, \mathrm{i}\}$ defines a basis of $\mathbb{C}$ if it is interpreted as a two-dimensional $\mathbb{R}$-vector space. Why is $\{1, 2\}$ not a basis? Show that the set containing three polynomials $\{1, x, x^2\}$ forms a basis of the space of polynomials P_2. What would be a basis of the space of polynomials in two variables, x and y up to degree 2?

Subspaces

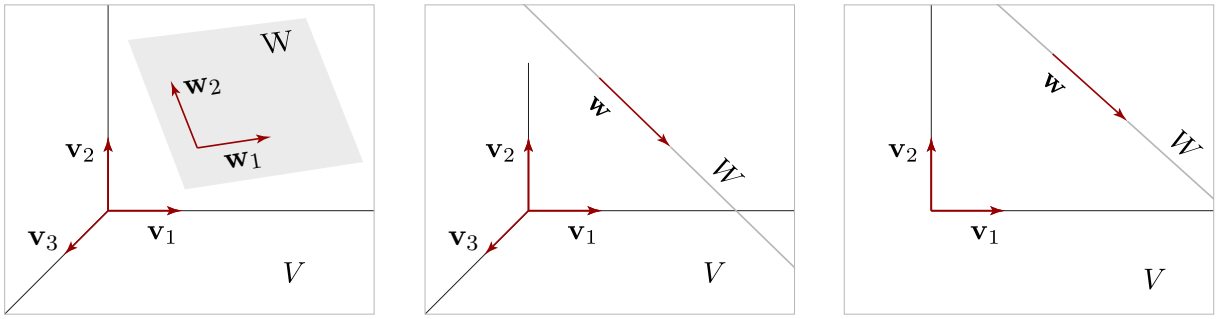


Figure L9: Left: a two-dimensional subspace (plane) in three-dimensional space. Center: a one-dimensional subspace (line) in three-dimensional space. Right: a one-dimensional subspace in two-dimensional space.

If the span W of a set of vectors in V is not complete, then $W \subsetneq V$ and W is called a true **true subspace** of V. For example, if $\mathbf{w}_1$ and $\mathbf{w}_2$ are linearly independent vectors in $\mathbb{R}^3$, then $W = \mathrm{span}(\{\mathbf{w}_1, \mathbf{w}_2\})$ is a two-dimensional subspace of three-dimensional space.

Subspaces of dimension one and two are called **lines** and **planes**, respectively. Examples include planes in three-dimensional space ($m = 2, n = 3$), lines in three-dimensional space ($m = 1, n = 3$), or lines in two-dimensional space ($m = 1, n = 2$), as illustrated in Fig. L9. Subspaces of higher dimension can no longer be visualized. For example, the space of polynomials of degree 2 is a three-dimensional subspace of the infinite-dimensional space $L^2(I)$.

As with vectors, subspaces are defined only up to parallel translation. For example, a parallel translation of the plane shown in Fig. L9, left, would still represent the same plane.

L2.5 Vector space isomorphism

REMARK In this section, connections between vectors of a general n-dimensional real space, V, and component vectors in $\mathbb{R}^n$ will be addressed. To distinguish the former from the latter, a caret notation $\hat{\mathbf{v}} \in V$ is used for general vectors. The component vector representing $\hat{\mathbf{v}}$ in $\mathbb{R}^n$ is denoted by the same symbol without caret, $\mathbf{v}$.

Once a basis $\{\mathbf{v}_i\}$ has been chosen, every vector $\hat{\mathbf{v}}$ of an n-dimensional vector space can be expanded as $\hat{\mathbf{v}} = \hat{\mathbf{v}}_1 v^1 + \hat{\mathbf{v}}_2 v^2 + \cdots + \hat{\mathbf{v}}_n v^n$. This expansion assigns to $\hat{\mathbf{v}}$ an n-tuple[12] of real numbers, v^1 to v^n, which together can be viewed as an element of $\mathbb{R}^n$. In other words, the basis defines a map

$$\phi_{\hat{\mathbf{v}}} : \to \mathbb{R}^n, \qquad \hat{\mathbf{v}} = \hat{\mathbf{v}}_i v^i \mapsto \phi_{\hat{\mathbf{v}}}(\hat{\mathbf{v}}) \equiv \begin{pmatrix} v^1 \\ \vdots \\ v^i \\ \vdots \\ v^n \end{pmatrix}, \tag{L29}$$

where the subscript in $\phi_{\hat{\mathbf{v}}}$ indicates that the map is specific to the basis $\{\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_n\}$. Under this map, the basis vectors $\hat{\mathbf{v}}_i$ themselves are assigned to the standard basis vectors of $\mathbb{R}^n$, $\phi_{\hat{\mathbf{v}}}(\hat{\mathbf{v}}_i) = \mathbf{e}_i$.

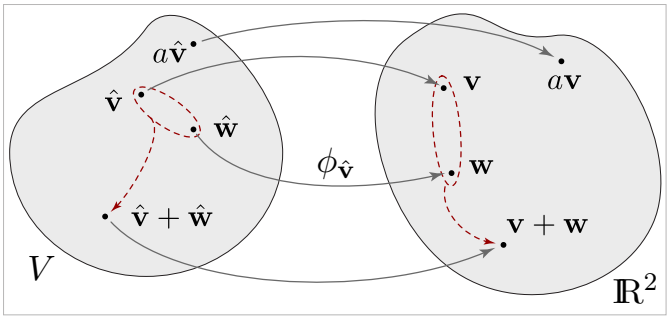


Figure L10: On the isomorphism between a general two-dimensional real vector space V and $\mathbb{R}^2$.

We saw above that for a given basis the assignment (vector) $\leftrightarrow$ (components) is unique. Every vector has a unique component representation and every set of components corresponds to a unique vector. This is another way of saying that the map $\phi_{\hat{\mathbf{v}}}$ is **bijective**. However, it is more than that: the sum of two vectors, $\hat{\mathbf{v}} + \hat{\mathbf{w}}$, is represented as $\hat{\mathbf{v}} + \hat{\mathbf{w}} = (\hat{\mathbf{v}}_i v^i) + (\hat{\mathbf{v}}_i w^i) = \hat{\mathbf{v}}_i (v^i + w^i)$ so that its components are given by the sum $v^i + w^i$ of the components of $\hat{\mathbf{v}}$ and $\hat{\mathbf{w}}$, respectively. The same fact may be expressed as $\phi_{\hat{\mathbf{v}}}(\hat{\mathbf{v}} + \hat{\mathbf{w}}) = \phi_{\hat{\mathbf{v}}}(\hat{\mathbf{v}}) + \phi_{\hat{\mathbf{v}}}(\hat{\mathbf{w}})$. Notice that the two '$+$' signs in this equation are defined in different vector spaces: on the left side it acts in V, on the right side in $\mathbb{R}^n$ (cf. Fig. L10). An analogous statement holds for scalar multiplication, $\phi_{\hat{\mathbf{v}}}(a\hat{\mathbf{v}}) = a\phi_{\hat{\mathbf{v}}}(\hat{\mathbf{v}})$.

In the language of section L1.2, $\phi_{\hat{\mathbf{v}}}$ defines a (bijective) **homomorphism** between the spaces $(V, +)$ and $(\mathbb{R}^n, +)$, i.e. it is an **isomorphism**. We have argued that the existence of an isomorphism between two spaces means that they are 'practically identical', $V \cong \mathbb{R}^n$. Since this link to $\mathbb{R}^n$ can be established for any n-dimensional vector space V, the former is justly called the 'standard' vector space. However, one always has to keep in mind that

[12] In mathematics an n-**tuple** is an ordered list of n-objects. For example $(1, 4, 2, 6)$ is a 4-tuple. It is ordered in the sense that it must be distinguished from the differently ordered list $(4, 1, 2, 6)$.

The isomorphism $V \cong \mathbb{R}^n$ is not canonical.

For a different basis, V-basis, $\{\hat{\mathbf{w}}_1, \ldots, \hat{\mathbf{w}}_n\}$ a different isomorphism, $\phi_{\hat{\mathbf{w}}}$ and a different component representation is obtained.

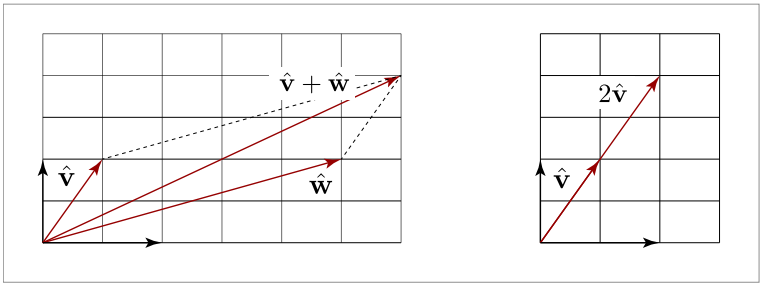


Figure L11: Figure illustrating the isomorphism between two-dimensional Euclidean space and $\mathbb{R}^2$. Geometrically defined vector addition/multiplication is compatible with the algebraic operation on $\mathbb{R}^2$-component representations.

EXAMPLE Fig. L11 illustrates the **isomorphism between two-dimensional Euclidean space and $\mathbb{R}^2$**. In Euclidean space, vector addition and scalar multiplication are geometric operations — the concatenation of vector–arrows and their stretching by scalar factors. These operations are compatible with the algebraic addition and scalar multiplication of the corresponding $\mathbb{R}^2$ component representations, irrespective of what basis is chosen. For example, in a basis defined by horizontal and vertical vectors of unit length, the geometric vectors $\hat{\mathbf{v}}$ and $\hat{\mathbf{w}}$ have the representations $\mathbf{v} = \binom{1}{2}$ and $\mathbf{w} = \binom{5}{2}$. Left: the geometric sum $\hat{\mathbf{v}} + \hat{\mathbf{w}}$ has components $\mathbf{v} + \mathbf{w} = \binom{6}{4}$. Right: the geometrically stretched vector $2\hat{\mathbf{v}}$ has components $2\mathbf{v} = \binom{2}{4}$. In either case, the same results are obtained by addition and multiplication in $\mathbb{R}^2$.

Thanks to the correspondence $V \cong \mathbb{R}^n$, vector calculations can be performed either in V or in $\mathbb{R}^n$. In the latter case one first assigns components to vectors, $\hat{\mathbf{v}}$, $\hat{\mathbf{w}}, \ldots$, does computations with the component representations, $\mathbf{v}$, $\mathbf{w}, \ldots$, and finally uses the inverse of the map $\phi_{\hat{\mathbf{v}}}$ to reassign V-vectors to $\mathbb{R}^n$-vectors. The correspondence between vectors and their components is so tight that the symbol $\phi_{\hat{\mathbf{v}}}$ is often omitted and a notation $\hat{\mathbf{v}} = (v^1, \ldots, v^n)^T$ is used. Although this is illegitimate (because it equates a vector in $\hat{\mathbf{v}} \in V$ with a vector $\mathbf{v} = (v^1, \ldots, v^n)^T \in \mathbb{R}^n$), the notation is ubiquitous and one just has to accept its presence. However, in this text we avoid it and keep using the caret to distinguish between vectors in V and their component representations in $\mathbb{R}^n$.

L2.6 Summary and outlook

In this chapter we introduced the important concept of vector spaces. Starting from a geometric motivation, we emphasized a view in which vectors where characterized by the operations defined on them — addition and scalar multiplication — and not so much through

concrete realizations. We argued that this more general approach was motivated by the frequent occurrence of vectors without visual representation in physics. Conversely it allows one to understand very different realizations of vectors in unified terms.

We saw that the general definition of vector spaces led to various secondary definitions, including that of the dimension of a vector space, linear dependence, completeness and that of a basis. Vector space bases were the key to the description of vectors through component representations, or elements of the standard space $\mathbb{R}^n$ (or $\mathbb{C}^n$). The existence of a unified $\mathbb{R}^n$ language is very important and it implies that the mathematics of $\mathbb{R}^n$ is a template describing all other vector spaces at once.

So far, we have not done much other than defining vector spaces. Building on this foundation there are two directions to move forward. The first is the definition of additional structures required to perform actual geometric operations with vectors, the measurement of lengths and angles, etc. The second will be the discussion of *maps* preserving the fundamental structures of vector spaces. We will discuss these two extensions in turn, beginning with the 'geometrization' of vector spaces.

L3 Euclidean geometry

REMARK In most of this chapter, we focus on the case $\mathbb{F} = \mathbb{R}$; section L3.4 considers $\mathbb{F} = \mathbb{C}$.

Euclid
Often referred to as the father of geometry. In his influential work *Elements* Euclid formulated the principles of Euclidean geometry (see below). Little is known about the date of his birth and death, and about his personal life. He was active around 300 BC.

In school, vectors are usually introduced as arrows of specified length and direction. The reason why these features have not been mentioned so far is that they are not included in the general definition of vector spaces. There are vector spaces for which the concept of length is not meaningful. Very often, however, it is, and to define it an additional structure known as the **Euclidean scalar product** is required. In section L3.1 we introduce a scalar product for the standard vector space $\mathbb{R}^n$ and discuss the ensuing geometric structures in section L3.2. Scalar products of generic $\mathbb{R}$-vector spaces will be introduced in section L3.3, and of generic $\mathbb{C}$-vector spaces in section L3.4.

INFO When introducing mathematical concepts it is generally good practice to progress stepwise from minimal structures to elements of higher structure. Such a hierarchical approach to, e.g., vector spaces is also useful from a physical perspective. Key physical theories like thermodynamics or classical mechanics rely on vector space structures such as completeness and linear independence, but not on the additional structure of a scalar product. For example, the so-called **phase space** of classical mechanics combines the d-dimensional coordinate vector, $\mathbf{q}$, of a point particle, and its **momentum**, $\mathbf{p}$, into a vector $\mathbf{x} = \binom{\mathbf{q}}{\mathbf{p}}$ of dimensionality $2d$. The space defined by such vectors does not possess a natural scalar product. (What would be the 'length' of a vector having coordinates and momenta as components?) In such contexts a scalar product would not only be superfluous but could even obscure physical contents.

L3.1 Scalar product of $\mathbb{R}^n$

Definition

A scalar product of a vector space is a function that takes two vectors as arguments to produce an ($\mathbb{F}$-valued) number. Let us begin by introducing a scalar product of the standard vector space, $\mathbb{R}^n$. Technically, this so-called **standard scalar product** of $\mathbb{R}^n$ is defined as[1]

$$\langle\ ,\ \rangle\ : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}\,, \qquad (\mathbf{v}, \mathbf{w}) \mapsto \langle \mathbf{v}, \mathbf{w}\rangle \equiv v^1 w^1 + v^2 w^2 + \cdots + v^n w^n\ . \tag{L30}$$

This map is bilinear map (linear in both its arguments). It assigns to each pair of vectors, $(\mathbf{v}, \mathbf{w})$, the number $\langle \mathbf{v}, \mathbf{w}\rangle$ defined on the right. Notice that the indices on the right occur in pairs that both sit *upstairs*. This definition thus does not conform to the conventions of covariant notation (see p. 32), which requires index pairs in sums to occur in co- and contravariant (downstair-upstairs) combinations. The notation thereby signifies that though the formula is correct as written, from a general point of view 'something is missing' from it. In section L3.3 we will uncover the missing object (a so-called 'metric'), but for the moment let us proceed with Eq. (L30) and explore its consequences.

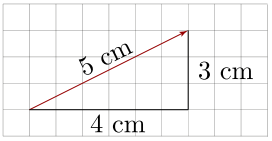
The scalar product Eq. (L30) has a number of important properties: it is

(i) **symmetric**: $\langle \mathbf{v}, \mathbf{w}\rangle = \langle \mathbf{w}, \mathbf{v}\rangle$,
(ii) **linear**: $\langle a\mathbf{v}, \mathbf{w}\rangle = a\langle \mathbf{v}, \mathbf{w}\rangle$ and
$\langle \mathbf{u} + \mathbf{v}, \mathbf{w}\rangle = \langle \mathbf{u}, \mathbf{w}\rangle + \langle \mathbf{v}, \mathbf{w}\rangle$, and
(iii) **positive definite**: $\langle \mathbf{v}, \mathbf{v}\rangle > 0$ for all $\mathbf{v} \neq \mathbf{0}$. (L31)

All geometric structures following from a scalar product rely solely on these three properties. This will become apparent in our discussion below, which makes repeated reference to (i-iii) but not to the specific formula (L30).

Given a scalar product, we can define the **norm of a vector** as

$$\|\mathbf{v}\| = \sqrt{\langle \mathbf{v}, \mathbf{v}\rangle}. \tag{L32}$$



[1] Other notations for the scalar product of $\mathbb{R}^n$ include $\mathbf{v}^T\mathbf{w}$ or $\mathbf{v}\cdot\mathbf{w}$. However, these ways of writing scalar products are specific to $\mathbb{R}^n$. We here prefer to use the general notation $\langle \mathbf{v}, \mathbf{w}\rangle$.

Pythagoras
(ca. 570-495 BC)

Greek philosopher and mathematician. He had great influence on the philosophical and religious teaching of the late 6th century BC. He is best known for his theorem relating the length of the three sides of a right-angled triangle.

In $\mathbb{R}^n$ with its standard scalar product this quantity is the **geometric length** of a vector.[2] To see this, consider $\mathbb{R}^2$ where $\| \binom{a}{b} \| = \sqrt{a^2+b^2}$ is the Pythagorean length familiar from school. It is left as an exercise to show that the generalization to higher dimensional space, e.g. $n = 3$, assigns to a vector its geometric length, i.e. the length one would obtain with the help of a ruler.

Given a scalar product, it can be used to introduce various features describing the geometry of vectors — 'angles', 'length', 'parallelity' and 'orthogonality', etc. These concepts are the subject of 'Euclidean geometry' and will be discussed next.

Euclidean geometry

Euclidean geometry Geometric concepts based on the definition of the scalar product (L30) are generally subsumed under the name 'Euclidean geometry'. Euclidean geometry can be understood graphically, i.e. in terms of geometric lengths, angles, etc., or 'algebraically' in terms of the criteria (i-iii). While the geometric formulation may be more intuitive, the advantage of the algebraic approach is that it extends to general vector spaces – function spaces, for example – in which no graphical interpretation exists.

The most fundamental relation of Euclidean geometry is the **Cauchy-Schwarz inequality**: $\forall \mathbf{v}, \mathbf{w} \in V$,

$$\boxed{|\langle \mathbf{v}, \mathbf{w} \rangle| \leq \|\mathbf{v}\| \|\mathbf{w}\|.} \tag{L33}$$

The proof of this inequality illustrates how nontrivial results may be derived from the general properties of the scalar product: For $\mathbf{w} = \mathbf{0}$ Eq. (L33) holds trivially. Suppose, then, $\mathbf{w} \neq 0$, define the number $a \equiv \langle \mathbf{v}, \mathbf{w} \rangle / \|\mathbf{w}\|^2$, and consider the vector $\mathbf{v} - a\mathbf{w}$. Since its norm is greater or equal to zero we have $0 \leq \langle \mathbf{v} - a\mathbf{w}, \mathbf{v} - a\mathbf{w} \rangle = \|\mathbf{v}\|^2 - 2a\langle \mathbf{v}, \mathbf{w} \rangle + a^2 \|\mathbf{w}\|^2 = \|\mathbf{v}\|^2 - (\langle \mathbf{v}, \mathbf{w} \rangle)^2 / \|\mathbf{w}\|^2$, where in the last step the definition of a was used. Multiply this inequality by $\|\mathbf{w}\|^2$, rearrange terms, and take the square root to arrive at Eq. (L33). For **colinear vectors**, i.e. for vectors 'pointing in parallel directions', $\mathbf{v} = b\mathbf{w}$ with $b \in \mathbb{R}$, the inequality becomes an equality.[3] However, if $\mathbf{u}$ and $\mathbf{v}$ are not colinear their scalar product is strictly smaller than the product of their norms, and the inequality (L33) quantifies the degree of 'misalignment'.

This interpretation motivates the definition of the **angle**, $\angle(\mathbf{v}, \mathbf{w})$, between two vectors as

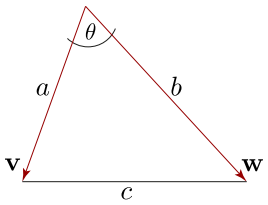
$$\angle(\mathbf{v}, \mathbf{w}) \equiv \arccos\left(\frac{\langle \mathbf{v}, \mathbf{w} \rangle}{\|\mathbf{v}\| \|\mathbf{w}\|} \right), \tag{L34}$$

[2] The more general denotation 'norm' is used also for vector spaces with scalar products for which (L32) does not have an interpretation as 'length'.

[3] If $\mathbf{v} = b\mathbf{w}$, then $\|\mathbf{v}\| = |b| \, \|\mathbf{w}\|$ and $\langle \mathbf{v}, \mathbf{w} \rangle = |b| \, \langle \mathbf{w}, \mathbf{w} \rangle = |b| \, \|\mathbf{w}\|^2 = \|\mathbf{v}\| \|\mathbf{w}\|$.

or the equivalent representation

$$\boxed{\langle \mathbf{v}, \mathbf{w} \rangle = \cos(\angle(\mathbf{v}, \mathbf{w}))\, \|\mathbf{v}\| \|\mathbf{w}\|.} \tag{L35}$$



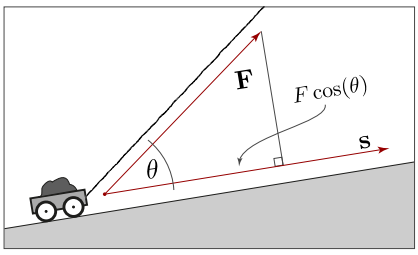
Before elucidating in what sense this is an 'angle' we note that the definition makes mathematical sense: from Eq. (L33) we know that $\langle \mathbf{v}, \mathbf{w} \rangle / \|\mathbf{v}\| \|\mathbf{w}\| \in [-1, 1]$, and so the inverse of the cos-function, arccos, can be applied to produce a value between 0 and π. These two values represent the extreme limits of complete alignment and anti-alignment, $\langle \mathbf{v}, \mathbf{w} \rangle = \pm \|\mathbf{v}\| \|\mathbf{w}\|$, respectively.
On this basis, let us now give the equation a geometric interpretation. Consider the triangle in $\mathbb{E}^2$ shown the figure. Its sides are defined by the vectors $\mathbf{v}$, $\mathbf{w}$ and $\mathbf{v} - \mathbf{w}$, with side lengths $a \equiv \|\mathbf{v}\|$, $b \equiv \|\mathbf{w}\|$ and $c \equiv \|\mathbf{v} - \mathbf{w}\|$, and the geometric angle enclosed by $\mathbf{v}$ and $\mathbf{w}$ is θ. *If* we identify the geometric angle with the one appearing in the Cauchy-Schwarz context, $\theta \equiv \angle(\mathbf{v}, \mathbf{w})$, Eq. (L35) can be written as $\langle \mathbf{v}, \mathbf{w} \rangle = ab \cos(\theta)$. Now consider the vector identity $\langle (\mathbf{v} - \mathbf{w}), (\mathbf{v} - \mathbf{w}) \rangle = \langle \mathbf{v}, \mathbf{v} \rangle + \langle \mathbf{w}, \mathbf{w} \rangle - 2\langle \mathbf{v}, \mathbf{w} \rangle$. With the above identifications, it assumes the form $c^2 = a^2 + b^2 - 2ab \cos(\theta)$, which is the familiar 'law of cosines'[4]

$$a^2 + b^2 - c^2 = 2ab \cos(\theta). \tag{L36}$$

In other words, the identification of the Cauchy-Schwarz angle of Eq. (L34) with the geometric angle follows from basic geometric considerations in the space $\mathbb{E}^2$. However, the definition (L34) holds more generally and can be used to quantify the mismatch between two vectors even in contexts where these vectors do not have a straightforward geometric interpretation.

INFO Scalar products play an important role in all areas of physics. As an example, consider **mechanical work**. If a constant force, $\mathbf{F}$, is applied to move an object along a straight line to induce a certain displacement, $\mathbf{s}$, the force performs work, W. Both force and displacement are vectorial quantities and the work done by the force is given by

$$W = \mathbf{F} \cdot \mathbf{s}\,. \tag{L37}$$



This equation can be read as the *definition* of force. The norm $F \equiv \|\mathbf{F}\|$ quantifies its magnitude, and the direction of $\mathbf{F}$ is the direction in which the force acts. Similarly, $s \equiv \|\mathbf{s}\|$ is the length of a displacement $\mathbf{s}$, whose direction may differ from that of $\mathbf{F}$ by an arbitrary angle, $\theta = \angle(\mathbf{F}, \mathbf{s})$ (see figure). Only the component of force parallel to $\mathbf{s}$, $F \cos\theta$, effectively performs work, and the total amount of work is proportional to the length of the displacement. This leads to $W = Fs \cos(\theta)$ which can be equivalently expressed as (L37). Notice that in experiment, Eq. (L37)

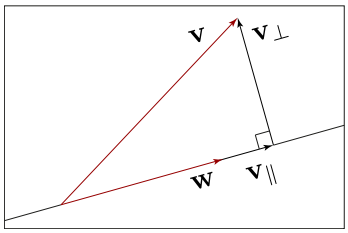
[4] The law of cosines, which holds for arbitrary triangles in $\mathbb{E}^2$, is usually taught in school. It may be proven by subdividing the triangle into two right-handed triangles and applying the Pythagorean theorem to each.

really *is* applied to define forces. For example, the Coulomb force acting on charged particles can be determined by displacing a test particle of a given charge in definite ways and measuring the required work. If this is done for sufficiently many displacements (how many?) a force vector is determined.

L3.2 Normalization and orthogonality

Scalar products can be used to define vectors of definite length. Specifically, we call a vector, $\hat{\mathbf{w}}$, **unit normalized** if $\|\hat{\mathbf{w}}\| = 1$, and indicate this feature by a caret ($\hat{}$).[5] For a given vector $\mathbf{w}$, the associated unit vector is obtained by **normalization**, i.e. division through its norm,

$$\hat{\mathbf{w}} \equiv \frac{\mathbf{w}}{\|\mathbf{w}\|}. \tag{L38}$$



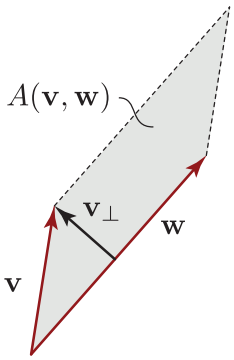
Two vectors $\mathbf{v}$ and $\mathbf{w}$ are called **orthogonal** if $\langle \mathbf{v}, \mathbf{w} \rangle = 0$ and this is indicated by $\mathbf{v} \perp \mathbf{w}$. If two vectors are **parallel** to each other (in the sense that the Cauchy-Schwarz inequality becomes an equality) we write $\mathbf{v} \parallel \mathbf{w}$. For given $\mathbf{w}$, any vector $\mathbf{v}$ can be decomposed as $\mathbf{v} = \mathbf{v}_\perp + \mathbf{v}_\parallel$, where the **projection**, $\mathbf{v}_\parallel$ (spoken 'v-parallel'), and the **orthogonal complement**, $\mathbf{v}_\perp$ (spoken 'v-perpendicular'), are parallel and orthogonal to $\mathbf{w}$, respectively (see figure).

To obtain an explicit formula for this decomposition we write the projection as $\mathbf{v}_\parallel = \hat{\mathbf{w}}\, a$. The coefficient a is determined by requiring that $\mathbf{v}_\perp = \mathbf{v} - \mathbf{v}_\parallel$ be orthogonal to $\hat{\mathbf{w}}$, i.e. that $0 = \langle \hat{\mathbf{w}}, \mathbf{v}_\perp \rangle = \langle \hat{\mathbf{w}}, \mathbf{v} \rangle - \langle \hat{\mathbf{w}}, \hat{\mathbf{w}} \rangle\, a$. Since $\langle \hat{\mathbf{w}}, \hat{\mathbf{w}} \rangle = 1$, we obtain $a = \langle \hat{\mathbf{w}}, \mathbf{v} \rangle$. Projection and orthogonal complement are therefore given by

$$\boxed{\begin{aligned} \mathbf{v}_\parallel &= \hat{\mathbf{w}}\, \langle \hat{\mathbf{w}}, \mathbf{v} \rangle, \\ \mathbf{v}_\perp &= \mathbf{v} - \hat{\mathbf{w}} \langle \hat{\mathbf{w}}, \mathbf{v} \rangle. \end{aligned}} \tag{L39}$$

Note that the projection can also be written as $\mathbf{v}_\parallel = \cos(\angle(\mathbf{v}, \mathbf{w}))\, \|\mathbf{v}\|\, \hat{\mathbf{w}}$. This follows from Eq. (L35) and is consistent with an elementary geometric construction. (→ L3.2.1-2)

[5] Exceptions to this convention include unit vectors denoted by $\mathbf{e}$, such as $\mathbf{e}_i$ of Eq. (L26), for which the caret is omitted. To be on the safe side, it is good practice to always define unit vectors explicitly.



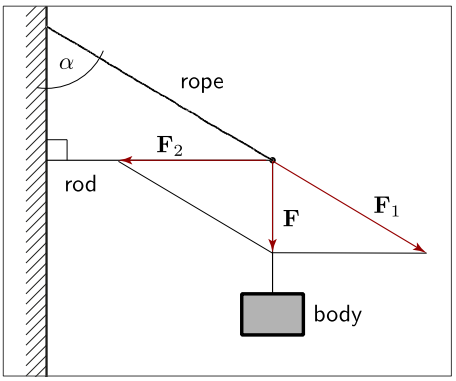
For later reference, let us apply the above relations to derive a useful formula for the **area of a parallelogram**, $A(\mathbf{v},\mathbf{w})$, spanned by two vectors $\mathbf{v},\mathbf{w} \in \mathbb{R}^n$. From elementary geometry we know that $A(\mathbf{v},\mathbf{w}) = \|\mathbf{v}_\perp\|\|\mathbf{w}\|$: the area equals the length of one edge of the parallelogram, say $\|\mathbf{w}\|$, multiplied by its height relative to this edge, $\|\mathbf{v}_\perp\|$ (see figure). An alternative representation for the area reads as

$$A(\mathbf{v},\mathbf{w}) \overset{(L39)}{=} \|\mathbf{v} - \hat{\mathbf{w}}\langle\hat{\mathbf{w}},\mathbf{v}\rangle\|\|\mathbf{w}\| = \left[\|\mathbf{v}\|^2\|\mathbf{w}\|^2 - \langle\mathbf{w},\mathbf{v}\rangle^2\right]^{1/2} \tag{L40}$$

$$\overset{(L35)}{=} \|\mathbf{v}\|\|\mathbf{w}\|\left[1-\cos^2\big(\angle(\mathbf{v},\mathbf{w})\big)\right]^{1/2} = \|\mathbf{v}\|\|\mathbf{w}\|\sin\big(\angle(\mathbf{v},\mathbf{w})\big)\,. \tag{L41}$$

The decomposition of vectors into perpendicular and parallel components has many applications. More generally, scalar products can be used to decompose vectors into contributions pointing in arbitrary directions.

EXAMPLE Let us illustrate the utility of vector decompositions with an example from statics. A mass is suspended by rigid rod and a rope (see figure). To assess the stability of the construction we need to know the magnitude of the forces acting on rope and rod, respectively. To this end we decompose the gravitational force, $\mathbf{F}$, exerted by the body as



$$\mathbf{F} = \mathbf{F}_1 + \mathbf{F}_2\,, \tag{L42}$$

into contributions $\mathbf{F}_1$ and $\mathbf{F}_2$ acting in the directions parallel to the rope and rod, respectively. Expressing each force as unit vector times norm, $\mathbf{F} = \hat{\mathbf{F}}F$, $\mathbf{F}_1 = \hat{\mathbf{F}}_1F^1$, and $\mathbf{F}_2 = \hat{\mathbf{F}}_2F^2$, the goal is to find the two unknowns F^1 and F^2 in terms of the known force, F, and the given angle α. To this end, we write Eq. (L42) as $\hat{\mathbf{F}}F = \hat{\mathbf{F}}_1F^1 + \hat{\mathbf{F}}_2F^2$ and take scalar products with $\hat{\mathbf{F}}$ and $\hat{\mathbf{F}}_2$ to obtain

$$\langle\hat{\mathbf{F}},\hat{\mathbf{F}}\rangle F = \langle\hat{\mathbf{F}},\hat{\mathbf{F}}_1\rangle F^1 + \langle\hat{\mathbf{F}},\hat{\mathbf{F}}_2\rangle F^2,$$
$$\langle\hat{\mathbf{F}}_2,\hat{\mathbf{F}}\rangle F = \langle\hat{\mathbf{F}}_2,\hat{\mathbf{F}}_1\rangle F^1 + \langle\hat{\mathbf{F}}_2,\hat{\mathbf{F}}_2\rangle F^2.$$

We know that $\langle\hat{\mathbf{F}},\hat{\mathbf{F}}\rangle = \langle\hat{\mathbf{F}}_2,\hat{\mathbf{F}}_2\rangle = 1$ and deduce by elementary geometry that $\langle\hat{\mathbf{F}},\hat{\mathbf{F}}_1\rangle = \cos(\alpha)$, $\langle\hat{\mathbf{F}},\hat{\mathbf{F}}_2\rangle = 0$, and $\langle\hat{\mathbf{F}}_2,\hat{\mathbf{F}}_1\rangle = \cos(\frac{\pi}{2}+\alpha) = -\sin(\alpha)$. This leads to the solutions

$$F^1 = \frac{F}{\cos\alpha}, \qquad F^2 = F\tan\alpha.$$

Can you explain intuitively why F^1 grows indefinitely in the limit $\alpha \to \frac{\pi}{2}$?

L3.3 Inner product spaces

REMARK In this and many later sections the caret symbol ($\hat{}$) is used to discriminate vectors, $\hat{\mathbf{v}} \in V$, of generic vector spaces from their component representations, $\mathbf{v} \in \mathbb{R}^n$, with respect to some basis. Scalar products in V are denoted by $\langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle_V$ and the corresponding scalar product of $\mathbb{R}^n$ by $\langle \mathbf{v}, \mathbf{w} \rangle_{\mathbb{R}^n}$. This definition of $\hat{\mathbf{v}}$ is totally unrelated to the unit-vector notation of the previous section.

Although our discussion so far focused on the standard scalar product of $\mathbb{R}^n$, the algebraic form of the formula Eq. (L30) was not essential in any way. Indeed, all results were derived solely on the basis of its three fundamental features (i-iii) listed above. In this section we invert the logic of the argument and *define* scalar products for general vector spaces as vector-pairing operations that obey the criteria (i)-(iii). Equation (L30) then has the status of just one of many possible realizations of scalar products on $\mathbb{R}^n$. Generalized scalar products can be rather abstract and need not have straightforward geometric interpretations. However, they always endow a vector space with powerful computational structures which often facilitate the solution of problems. For example, the vector spaces relevant to quantum theory all have scalar products and operations based on these are of profound physical importance, although these scalar products do not lend themselves to a direct geometric interpretation.

Scalar product: general definition

A **scalar product**[6] of an $\mathbb{R}$-vector space V is a map

$$\langle\ ,\ \rangle : V \times V \to \mathbb{R}, \qquad (\hat{\mathbf{v}}, \hat{\mathbf{w}}) \mapsto \langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle\ , \tag{L43}$$

with the following properties $(\hat{\mathbf{u}}, \hat{\mathbf{v}}, \hat{\mathbf{w}} \in V, a \in \mathbb{R})$:

(i) **symmetry**: $\langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle = \langle \hat{\mathbf{w}}, \hat{\mathbf{v}} \rangle$,

(ii) **linearity**: $\langle a\hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle = a\langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle$,
$\langle \hat{\mathbf{u}} + \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle = \langle \hat{\mathbf{u}}, \hat{\mathbf{w}} \rangle + \langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle$,

(iii) **positive definiteness**: $\hat{\mathbf{v}} \neq \mathbf{0} : \langle \hat{\mathbf{v}}, \hat{\mathbf{v}} \rangle > 0$. (L44)

A vector space, V equipped with a scalar product, $(V, \langle\ ,\ \rangle)$, is called a **normed vector space**, **inner product space** or **Euclidean vector space**.

INFO In the literature, the term **Euclidean space** is used in three different ways:

- ▷ A general vector space V equipped with a scalar product, $(V, \langle\ ,\ \rangle)$.
- ▷ The standard space $\mathbb{R}^n$ with its standard scalar product Eq. (L30).

[6] The general scalar product is sometimes called **inner product** and a vector space equipped with it an **inner product space**.

▷ The affine space $\mathbb{E}^n$ discussed on p. 24.

Although the usage of one term for seemingly different objects may seem confusing, the discussion of this section will show that there is no contradiction and that the three definitions are equivalent to each other.

EXAMPLE

▷ In **Euclidean space**, $\mathbb{E}^d$, with $d = 2$ or 3, lengths and angles between vectors may be determined geometrically (by using a ruler). One may then *define* the scalar product of two vectors $\mathbf{v}$ and $\mathbf{w}$ through Eq. (L35), i.e. the product of their length and the enclosed angle. It is straightforward to check that this geometrically constructed scalar product obeys all criteria required by the general definition.

▷ In the **function space** $L^2(I)$ (see 26), consider two functions $f, g : I \to \mathbb{R}$ and define the map $\langle\,,\,\rangle : I \times I \to \mathbb{R}$ in terms of the integral

$$\langle f, g\rangle = \int_I \mathrm{d}x\, f(x)g(x), \tag{L45}$$

where we used the shorthand $\int_I \equiv \int_a^b$ for $I = [a, b]$, and $a < b \in \mathbb{R}$. This operation defines a scalar product. (→ L3.3.1)

▷ For an example of an unconventional scalar product defined on $\mathbb{R}^2$, see problem L3.3.2.

EXERCISE Identities derived from scalar products often have an intuitive or even trivial interpretation. As an example, consider the **triangle inequality**

$$\|\hat{\mathbf{v}}\| + \|\hat{\mathbf{w}}\| \geq \|\hat{\mathbf{v}} - \hat{\mathbf{w}}\|. \tag{L46}$$

In the Euclidean space $\mathbb{E}^3$ this identity states that the sum of the lengths of two sides of a triangle exceeds the length of the third side.

However, one should also learn to think about such relations in more general terms which are not tied to an obvious geometric picture. Practice this understanding by proving the triangle identity from the general definition of the scalar product. Hint: Use the Cauchy-Schwarz inequality to show that $(\|\hat{\mathbf{v}}\| + \|\hat{\mathbf{w}}\|)^2 \geq \|\hat{\mathbf{v}} - \hat{\mathbf{w}}\|^2$, which implies (L46). Discuss the interpretation of the triangle inequality in the case of the function space scalar product (L45).

INFO The condition of positive definiteness is sometimes abandoned, which then leads to the definition of **positive semidefinite** ($\langle\hat{\mathbf{v}}, \hat{\mathbf{v}}\rangle = 0$ for $\hat{\mathbf{v}} \neq \mathbf{0}$ is allowed) or **positive indefinite** ($\langle\hat{\mathbf{v}}, \hat{\mathbf{v}}\rangle < 0$ is allowed) scalar products. An indefinite scalar product of great physical significance, known as the **Minkovski metric**, is defined in $\mathbb{R}^4$. In applications involving the Minkovski metric it is customary to label the standard basis vectors of $\mathbb{R}^4$ as $\hat{\mathbf{e}}_0, \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3$. The scalar product is defined by the

relations[7] $\langle \hat{\mathbf{e}}_0, \hat{\mathbf{e}}_0 \rangle = 1$, $\langle \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_i \rangle = -1$, $i = 1, 2, 3$, and $\langle \hat{\mathbf{e}}_\mu, \hat{\mathbf{e}}_\nu \rangle = 0, \mu \neq \nu$.[8] In physics, $\mathbb{R}^4$ equipped with a Minkovski metric is understood as **space-time**, where $\mathbf{e}_0$ represents a 'time-like' direction, and $\mathbf{e}_i$ are 'space-like' directions. A point with coordinates (ct, x^1, x^2, x^3) then labels a space time-event taking place at time t, and having spatial coordinates x^i. Here the *speed of light*, $c \simeq 3 \times 10^8 \mathrm{m/s}$, is included in the definition of $x^0 = ct$ to give $x^\mu, \mu = 0, \ldots, 3$ all the same dimension of physical length.

Some physical contexts require a scalar product which is not positive definite but satisfies the weaker condition of non-degeneracy: a **non-degenerate inner product** has the property that $\langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle = 0$, $\forall \hat{\mathbf{w}} \in V$ implies $\hat{\mathbf{v}} = 0$. For example, the Minkovski metric is indefinite and admits vectors of vanishing norm ($\hat{\mathbf{e}}_0 + \hat{\mathbf{e}}_1$ is an example). However, it is non-degenerate. Indeed, if $\hat{\mathbf{v}} = \hat{\mathbf{e}}_\mu v^\mu$ has vanishing scalar product with all other vectors, then $\langle \hat{\mathbf{v}}, \hat{\mathbf{e}}_\nu \rangle = 0$ certainly holds for the basis vectors $\hat{\mathbf{e}}_\nu$, implying $v^0 = \langle \hat{\mathbf{v}}, \hat{\mathbf{e}}_0 \rangle = 0$ and $v^i = -\langle \hat{\mathbf{v}}, \hat{\mathbf{e}}_i \rangle$. Hence all the expansion coefficients of the vector $\hat{\mathbf{v}}$ vanish, thus it was the null vector to begin with.

Metric tensor

Consider a basis $\{\hat{\mathbf{v}}_i\}$ of a space $(V, \langle\ ,\ \rangle_V)$, where the subscript on the scalar $\langle\ ,\ \rangle_V$ emphasizes that it belongs to V. Evaluating the scalar product for all possible pairs of basis vectors yields the so-called **metric (tensor)**, $g \equiv \{g_{ij}\}$,

$$\boxed{g_{ij} \equiv \langle \hat{\mathbf{v}}_i, \hat{\mathbf{v}}_j \rangle_V\,,} \tag{L47}$$

where the symmetry of the scalar product implies the relation $g_{ij} = g_{ji}$. Now consider two generic vectors $\hat{\mathbf{x}} = \hat{\mathbf{v}}_i x^i$ and $\hat{\mathbf{y}} = \hat{\mathbf{v}}_j y^j$ in V. Their scalar product can be expressed as

$$\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_V = \left\langle \hat{\mathbf{v}}_i x^i, \hat{\mathbf{v}}_j y^j \right\rangle_V = x^i \langle \hat{\mathbf{v}}_i, \hat{\mathbf{v}}_j \rangle_V\, y^i = x^i\, g_{ij}\, y^j. \tag{L48}$$

This formula suggests introducing a **generalized scalar product of $\mathbb{R}^n$** by defining

$$\boxed{\langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{R}^n} \equiv x^i g_{ij} y^j,} \tag{L49}$$

where $\mathbf{x} = (x^1, \ldots, x^n)^T$ and $\mathbf{y} = (y^1, \ldots, y^n)^T$ are component vectors in $\mathbb{R}^n$. With this definition we obtain

$$\boxed{\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_V = \langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{R}^n} = x^i g_{ij} y^j.} \tag{L50}$$

The advantage of this definition is that the scalar product of two vectors in V is equal to the scalar product of their component representations in $\mathbb{R}_n$.

[7] Some texts use the opposite sign convention for the Minkovski metric, defining $\langle \hat{\mathbf{e}}_0, \hat{\mathbf{e}}_0 \rangle = -1$, and $\langle \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_i \rangle = 1$, $i = 1, 2, 3$.

[8] It is customary to index the full set of four basis vectors of a Minkovski space by Greek indices, $\mu = 0, 1, 2, 3$. However, the restricted set of indices excluding zero, $i = 1, 2, 3$, is labeled by latin letters.

INFO Given two vector spaces, $(V, \langle\ ,\ \rangle_V)$ and $(W, \langle\ ,\ \rangle_W)$, we call a map $F : V \to W$ an **isometry**, if $\forall \hat{\mathbf{x}}, \hat{\mathbf{y}} \in V$, $\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_V = \langle F(\hat{\mathbf{x}}), F(\hat{\mathbf{y}}) \rangle_W$, i.e. if the V-scalar product of its arguments is equal to the W-scalar product of its images. The definition of the scalar product (L49) is such that the component representation $\phi_{\mathbf{v}} : V \to \mathbb{R}^n, \hat{\mathbf{x}} \to \mathbf{x}$ becomes an isometry of the vector spaces $(V, \langle\ ,\ \rangle_V)$ and $(\mathbb{R}^n, \langle\ ,\ \rangle_{\mathbb{R}^n})$. Whenever possible one should aim to work with isometries to benefit from the fact that they leave the scalar product, and hence also lengths, angles, etc. invariant.

It is customary to abbreviate the notation by introducing components with covariant indices as[9]

$$x_j \equiv x^i g_{ij}. \tag{L51}$$

This **index-lowering convention** may be applied to represent the scalar product (L50) between two vectors compactly as

$$\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_V = \langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{R}^n} = x_j y^j. \tag{L52}$$

Be aware, however, that the positioning of indices (upstairs vs. downstairs) has now become crucially important: $x_i \neq x^i$, unless $g_{ij} = \delta_{ij}$.

For later reference, we note that it is often convenient to introduce an 'inverse' metric tensor $\{g^{ij}\}$ through the relation

$$g_{kj} g^{ji} = \delta_k{}^i, \tag{L53}$$

where i and k are arbitrary and the repeated index j is summed over. For example, if

$$g_{11} = g_{22} = 1, \qquad g_{12} = g_{21} = \tfrac{1}{\sqrt{2}}, \tag{L54}$$

it is straightforward to verify that $g^{11} = g^{22} = 2$ and $g^{12} = g^{21} = -\sqrt{2}$.[10]

The inverse metric can be used to define an **index-raising** relation analogous to Eq. (L51):

$$x^i = x_j g^{ji}. \tag{L55}$$

The index-lowering and -raising relations (L51) are (L55) consistent with each other in the sense that $x^i = x_j g^{ji} = (x^k g_{kj}) g^{ji} = x^k \delta_k{}^i = x^i$. In operations involving numerous index summations this is a useful and important consistency check!

To **summarize**, a generic scalar product, $\langle\ ,\ \rangle_V$, of a vector space, V, motivates the definition of the metric tensor, Eq. (L47). Its components g_{ij} define a non-standard scalar product (L49) of $\mathbb{R}^n$. The correspondence $(V, \langle\ ,\ \rangle_V) \cong (\mathbb{R}^n, \langle\ ,\ \rangle_{\mathbb{R}^n})$ then becomes an isometry for which the scalar product between vectors and their component representation is given by (L50).

[9] Since the metric tensor is symmetric, $g_{ij} = g_{ji}$, Eq. (L51) can equivalently be written as $x_j \equiv g_{ji} x^i$.

[10] In many applications, 'off-diagonal' elements of the metric tensor vanish, $g_{ij} = 0$ for $i \neq j$. The elements of the inverse metric tensor then also have this property, $g^{ij} = 0$ for $i \neq j$, and the diagonal elements are obtained as $g^{ii} = (g_{ii})^{-1}$. Methods for finding the inverse metric in situations with non-diagonal metric tensors are discussed in section L5.4.

EXERCISE Define a generalized scalar product of $\mathbb{R}^n$ through Eq. (L49) with a priori unspecified coefficients g_{ij}. What conditions have to be imposed on the coefficients g_{ij} to satisfy the criteria (L44) defining an scalar product? Show that these conditions hold if $g_{ij} = \langle \hat{\mathbf{v}}_i, \hat{\mathbf{v}}_j \rangle_V$ is defined through a scalar product of a vector space, V.

Given a basis $\{\hat{\mathbf{v}}_i\}$, it can in general be difficult to determine the expansion of a general vector, $\hat{\mathbf{x}} = \hat{\mathbf{v}}_i x^i$, i.e. to **compute the expansion coefficients** x^i. However, the problem becomes a lot easier if a scalar product is available and the metric tensor, g_{ij}, and its inverse, g^{ij}, are known. To see this, we define a set of **contravariant basis vectors** with *raised* indices, $\{\hat{\mathbf{v}}^i\}$, using an index-raising relation analogous to Eq. (L55):

$$\hat{\mathbf{v}}^i \equiv g^{ij} \hat{\mathbf{v}}_j. \tag{L56}$$

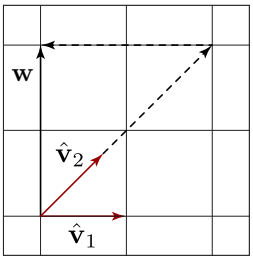
Then we compute $\langle \hat{\mathbf{v}}^i, \hat{\mathbf{v}}_k \rangle_V = \langle g^{ij} \hat{\mathbf{v}}_j, \hat{\mathbf{v}}_k \rangle_V = g^{ij} \langle \hat{\mathbf{v}}_j, \hat{\mathbf{v}}_k \rangle_V = g^{ij} g_{jk} = \delta^i{}_k$. Thus, the two sets of vectors $\{\hat{\mathbf{v}}^i\}$ and $\{\hat{\mathbf{v}}_k\}$ satisfy the **orthonormality relation**

$$\langle \hat{\mathbf{v}}^i, \hat{\mathbf{v}}_k \rangle_V = \delta^i{}_k. \tag{L57}$$

The expansion coefficients of $\hat{\mathbf{x}}$ can now be obtained by taking its scalar product with a contravariant basis vector: $\langle \hat{\mathbf{v}}^i, \hat{\mathbf{x}} \rangle_V = \langle \hat{\mathbf{v}}^i, \hat{\mathbf{v}}_k x^k \rangle_V = \langle \hat{\mathbf{v}}^i, \hat{\mathbf{v}}_k \rangle_V x^k = \delta^i{}_k x^k = x^i$. This leads to the result

$$\boxed{\hat{\mathbf{x}} = \hat{\mathbf{v}}_i \langle \hat{\mathbf{v}}^i, \hat{\mathbf{x}} \rangle_V.} \tag{L58}$$

The statement made by this formula is that the expansion coefficients of a generic vector $\hat{\mathbf{x}}$ can be found using a four step-program: (1) Compute the metric tensor, g_{ij}, and (2) its inverse, g^{ij}. Then, (3) build the linear combinations $\hat{\mathbf{v}}^i = g^{ij} \hat{\mathbf{v}}_j$ of basis vectors, and (4) compute the components of $\hat{\mathbf{x}}$ using the scalar product $x^i = \langle \hat{\mathbf{v}}^j, \hat{\mathbf{x}} \rangle_V$. Although this may look complicated, the steps of this program are often easy to perform, and generally are an efficient method for of obtaining expansion coefficients. (→ L3.3.5-6).



EXAMPLE Consider the vector space $V = \mathbb{E}^2$ equipped with its geometrically defined scalar product (L35). As basis we use the vectors $\{\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2\}$ indicated in the figure. In coordinates corresponding to the grid they have a component representation $\hat{\mathbf{v}}_1 = (1,0)^T$ and $\hat{\mathbf{v}}_2 = \frac{1}{\sqrt{2}}(1,1)^T$, respectively. It is straightforward to verify (do it!) that the metric tensor defined by this basis is given by Eq. (L54). What is the component representation of the vector $\mathbf{w}$ in the given basis? Compute its norm from the component representation and check that the result agrees with the geometrically computed length.

Orthonormal bases of inner product spaces

Given an inner product space $(V, \langle\ ,\ \rangle_V)$ it is natural to work with bases for which the metric tensor $\{g_{ij}\}$ assumes a simple form. This eases all operations involving the metric, such

as finding its inverse, taking scalar products and computing vector decompositions. A basis, $\{\hat{\mathbf{e}}_i\}$, yields maximal metric simplicity if its vectors have unit norm, $||\hat{\mathbf{e}}_i|| = \sqrt{\langle \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_i \rangle_V} = 1$, and are mutually orthogonal, $\langle \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j \rangle_V = 0, i \neq j$. These two criteria specify the form of the metric tensor as

$$\langle \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j \rangle_V = g_{ij} = \delta_{ij}. \tag{L59}$$

Here, the Kronecker-δ is defined as usual, $\delta_{ij} = 1$ for $i = j$ and 0 otherwise. A basis obeying these properties is called an **orthonormal basis**.

Before demonstrating that for any scalar product orthogonal bases can indeed by found, let us discuss some of their properties. For an orthonormal basis, the component scalar product representation assumes a particularly simple form, too: given two arbitrary vectors $\hat{\mathbf{x}} = \hat{\mathbf{e}}_i x^i$ and $\hat{\mathbf{y}} = \hat{\mathbf{e}}_j y^j$ in V we obtain (cf. Eq. (L50))

$$\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_V = \left\langle \hat{\mathbf{e}}_i x^i, \hat{\mathbf{e}}_j y^j \right\rangle_V = x^i \langle \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j \rangle_V y^j = x^i \delta_{ij} y^j = \langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{R}^n}, \tag{L60}$$

where in the last equality we encounter the *standard scalar product* (L30) of the component representation in $\mathbb{R}^n$, $x^i \delta_{ij} y^j = x^j y^j$. This leads to the conclusion that

> The scalar product of vectors represented in an orthonormal basis equals the standard $\mathbb{R}^n$-scalar product of their components.

The construction above entails a re-interpretation of the standard scalar product formula (L30). The latter does not conform to the conventions of covariant notation (cf. 32), in that it contains a pairwise summation over two contravariant (raised) indices. Our present discussion suggests to rewrite (L30) as $x^j y^i = x^j \delta_{ij} y^j$. While at first sight the inclusion of the Kronecker-δ may look artificial, we now understand that it represents a particularly simple metric, $g_{ij} = \delta_{ij}$. In other words, the misalignment of indices in Eq. (L30) tells us that the the placeholder of a metric tensor is 'missing' there.

Having identified this missing element, we can bring Eq. (L30) into a form consistent with the general scalar product of Eq. (L52), by writing $\langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{R}^n} = x^j y^j = x^i \delta_{ij} y^j = x_j y^j$. Here we used the fact that for an orthonormal basis contra- and covariant components are equal,[11] $x^j = x^i \delta_{ij} = x_j$.

Working with orthonormal bases has many advantages. For example, the evaluation of the expansion formula (L58) becomes particularly easy because $\hat{\mathbf{e}}^i = \delta^{ij} \hat{\mathbf{e}}_j = \hat{\mathbf{e}}_i$, so that the **expansion of a vector in an orthonormal basis** assumes the simple form

$$\hat{\mathbf{x}} = \hat{\mathbf{e}}_i \left\langle \hat{\mathbf{e}}^i, \hat{\mathbf{x}} \right\rangle_V = \mathbf{e}_i x^i, \tag{L61}$$

where $x^i = \langle \hat{\mathbf{e}}^i, \hat{\mathbf{x}} \rangle_V = \langle \hat{\mathbf{e}}_i, \hat{\mathbf{x}} \rangle_V$ is straightforwardly obtained by taking the scalar product of $\hat{\mathbf{x}}$ with the corresponding basis vector. (→ L3.3.3-4).

To summarize, for a generic scalar product, $\langle\ ,\ \rangle_V$, there are two options:

[11] This is the reason why many introductory textbooks refrain from distinguishing co- and contravariant notation in the first place. However, one should be aware of the fact that the corresponding material is then strictly limited to the case of *orthonormal* bases.

- ▷ If one works with a generic basis $\{\hat{\mathbf{v}}_i\}$ in V, a metric tensor, g_{ij}, needs to be introduced, and the scalar product appropriate to the description of the component representation of vectors becomes a non-standard scalar product in $\mathbb{R}^n$.
- ▷ If instead one works with an orthonormal basis $\{\hat{\mathbf{e}}_i\}$ in V, the metric tensor is trivial, $g_{ij} = \delta_{ij}$, co- and contravariant components are equal, $x_i = x^i$ and $\hat{\mathbf{e}}^i = \hat{\mathbf{e}}_i$, and the corresponding scalar product of components is the standard scalar product of $\mathbb{R}^n$.

Obviously, the second approach is simpler and one will usually aim to work with orthonormal bases of scalar products. However, sometimes there are compelling reasons to single out a non-orthonormal basis. The covariant representation of the metric introduced above then is the best way to describe the situation.

EXAMPLE As an example for constructions using an orthonormal basis, let us represent the geometric area, $A(\mathbf{v},\mathbf{w})$, spanned by two vectors $\mathbf{v},\mathbf{w} \in \mathbb{R}^n$ in terms of their components in the standard basis, $\{\mathbf{e}_i\}$. To this end, we insert the expansions $\mathbf{v} = \mathbf{e}_i v^i$, $\mathbf{w} = \mathbf{e}_j w^j$ into Eq. (L40), and obtain:

$$\begin{aligned} A^2(\mathbf{v},\mathbf{w}) &= \|\mathbf{v}\|^2\|\mathbf{w}\|^2 - \langle\mathbf{v},\mathbf{w}\rangle^2 = \sum_{ij}\left[(v^i)^2(w^j)^2 - (v^i w^i)(v^j w^j)\right] \\ &= \sum_{i<j}\left[(v^i)^2(w^j)^2 + (v^j)^2(w^i)^2 - 2(v^i w^i)(v^j w^j)\right] = \sum_{i<j}\left[v^i w^j - v^j w^i\right]^2 . \end{aligned} \tag{L62}$$

In the sum of the first line terms with $i = j$ cancel. We split the remaining contribution into sums $\sum_{i<j}$ and $\sum_{j<i}$, and in the latter sum relabel indices as $i \leftrightarrow j$ to arrive at the second line.

For two-dimensional vectors, $n = 2$, this reduces to

$$A(\mathbf{v},\mathbf{w}) = |v^1 w^2 - v^2 w^1| . \tag{L63}$$

We will need this result when discussing area integrals with curvilinear coordinates in chapter C4.2. It is left as an exercise to verify that for three-dimensional vectors, $n = 3$, Eq. (L62) reproduces the cross product formula (L86), $A(\mathbf{v},\mathbf{w}) = \|\mathbf{v}\times\mathbf{w}\|$, to be derived in section L4.2 below.

Orthonormalization

Given that orthonormal bases are very convenient to work with, two obvious questions present themselves: for an arbitrary inner product space, $(V, \langle\ ,\ \rangle_V)$, do orthonormal bases always exist? And if so, are there methods for obtaining them? Fortunately, the answer to both is affirmative. By a procedure known as **Gram-Schmidt orthonormalization** any basis $\{\hat{\mathbf{v}}_i\}$ can be constructively transformed into an orthonormal basis.

The algorithm starts by picking one of the basis vectors, say $\hat{\mathbf{v}}_1$. By normalizing it we obtain the first vector of the new basis, $\hat{\mathbf{e}}_1 \equiv \hat{\mathbf{v}}_1/\|\hat{\mathbf{v}}_1\|$. We next define $\hat{\mathbf{v}}_{2,\perp} \equiv \hat{\mathbf{v}}_2 - \hat{\mathbf{e}}_1\langle\hat{\mathbf{e}}^1,\hat{\mathbf{v}}_2\rangle$ as the orthogonal complement of $\hat{\mathbf{v}}_2$ with respect to $\hat{\mathbf{e}}_1$, obtained by subtracting the component of $\hat{\mathbf{v}}_2$ parallel to $\hat{\mathbf{e}}_1$ (cf. Eq. (L39)). Here $\hat{\mathbf{e}}^1 \equiv \hat{\mathbf{e}}_1$, as appropriate for an orthonormal basis with

metric tensor δ_{ij} and $\hat{\mathbf{e}}_i = \delta_{ij}\hat{\mathbf{e}}^j$. The vector $\hat{\mathbf{v}}_{2,\perp}$ is non-vanishing. (Why? Remember linear independence.) Moreover, it is perpendicular to $\hat{\mathbf{e}}^1$ by construction,

$$\big\langle \hat{\mathbf{e}}^1, \hat{\mathbf{v}}_{2,\perp} \big\rangle = \big\langle \hat{\mathbf{e}}^1, \hat{\mathbf{v}}_2 - \hat{\mathbf{e}}_1 \langle \hat{\mathbf{e}}^1, \hat{\mathbf{v}}_2 \rangle \big\rangle = \langle \hat{\mathbf{e}}^1, \hat{\mathbf{v}}_2 \rangle - \langle \hat{\mathbf{e}}^1, \hat{\mathbf{v}}_2 \rangle = 0,$$

where we wrote $\langle\ ,\ \rangle_V \equiv \langle\ ,\ \rangle$ for brevity. Normalization of $\hat{\mathbf{v}}_{2,\perp}$ yields $\hat{\mathbf{e}}_2 \equiv \hat{\mathbf{v}}_{2,\perp}/|\hat{\mathbf{v}}_{2,\perp}|$. We continue in this manner to define $\hat{\mathbf{v}}_{3,\perp} \equiv \hat{\mathbf{v}}_3 - \hat{\mathbf{e}}_1\langle \hat{\mathbf{e}}^1, \hat{\mathbf{v}}_3\rangle - \hat{\mathbf{e}}_2\langle \hat{\mathbf{e}}^2, \hat{\mathbf{v}}_3\rangle$, then normalize it, and so on, until we arrive at $\hat{\mathbf{e}}_n$:

$$\begin{array}{lcllcl}
\hat{\mathbf{v}}_{1,} & & & \hat{\mathbf{e}}_1 & \equiv & \hat{\mathbf{v}}_{1,\perp}/\|\hat{\mathbf{v}}_{1,\perp}\| \\
\hat{\mathbf{v}}_{2,\perp} & \equiv & \hat{\mathbf{v}}_2 - \hat{\mathbf{e}}_1\langle \hat{\mathbf{e}}^1, \hat{\mathbf{v}}_2\rangle, & \hat{\mathbf{e}}_2 & \equiv & \hat{\mathbf{v}}_{2,\perp}/\|\hat{\mathbf{v}}_{2,\perp}\| \\
\vdots & & \vdots & \vdots & & \vdots \\
\hat{\mathbf{v}}_{i,\perp} & \equiv & \hat{\mathbf{v}}_i - \sum_{j=1}^{i-1} \hat{\mathbf{e}}_j\langle \hat{\mathbf{e}}^j, \hat{\mathbf{v}}_i\rangle, & \hat{\mathbf{e}}_i & \equiv & \hat{\mathbf{v}}_{i,\perp}/\|\hat{\mathbf{v}}_{i,\perp}\|, \\
\vdots & & \vdots & \vdots & & \vdots \\
\hat{\mathbf{v}}_{n,\perp} & \equiv & \hat{\mathbf{v}}_n - \sum_{j=1}^{n-1} \hat{\mathbf{e}}_j\langle \hat{\mathbf{e}}^j, \hat{\mathbf{v}}_n\rangle, & \hat{\mathbf{e}}_n & \equiv & \hat{\mathbf{v}}_{n,\perp}/\|\hat{\mathbf{v}}_{n,\perp}\|.
\end{array} \tag{L64}$$

We note that the basis resulting from a Gram-Schmidt procedure is non-canonical in that it depends on the order in which the vectors are orthonormalized (see the example below). It is also worth noting that the algorithm may be applied to arbitrary sets $U = \{\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_m\}$ of vectors, even if $m > n$ exceeds the dimensionality of V and the set is linearly dependent. In this case, the algorithm will produce the vector $\mathbf{0}$ at some of its steps (why?). Vectors whose orthonormalization vanishes will be discarded. If U contained k linearly independent vectors, the result of the operation will be an orthonormal basis of the k-dimensional subspace $\mathrm{span}(U)$. For $k = n$, we obtain a basis of V.

EXERCISE Convince yourself that all vectors $\{\hat{\mathbf{v}}_{i,\perp}, i = 1, \ldots n\}$ are indeed mutually orthogonal! This is best proven by **induction**. We know the validity of the statement for the first two vectors, i.e. prove that $\hat{\mathbf{e}}_{2,\perp} \perp \hat{\mathbf{e}}_{1,\perp}$. It remains to show that if the statement holds for the first $1, 2, \ldots, j$ objects, then it will also be true for the $(j+1)$th one. This proves the orthogonality statement for the remaining vectors $\hat{\mathbf{e}}_{3,\ldots,n}$.

EXERCISE Apply the **Gram-Schmidt orthonormalization** algorithm to the $\mathbb{R}^3$-basis

$$\mathbf{v}_1 = \begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} 2 \\ 2 \\ 3 \end{pmatrix}, \quad \mathbf{v}_3 = \begin{pmatrix} -4 \\ 0 \\ 4 \end{pmatrix}. \tag{L65}$$

Before doing the calculation think a little and try to anticipate the geometric orientation of the orthonormal basis. Show how different bases are produced depending on whether you start the procedure with $\mathbf{v}_1, \mathbf{v}_2$, or $\mathbf{v}_3$. (→ L3.3.7-8).

INFO The Gram-Schmidt algorithm relies on the positive definiteness of a scalar product. For **semi- and indefinite scalar products**, vectors of ill-defined norm can arise (the square root of a

vector with $\langle \mathbf{v}, \mathbf{v} \rangle < 0$ does not yield a real number). This would invalidate essential steps of the normalization procedure. However, it may be adapted to obtain a basis $\{\mathbf{e}_i\}$ in which the scalar product is represented by a metric tensor $g_{ij} \equiv \eta_{ij}$, with diagonal elements $\eta_{ii} = 1$ for $i = 1, \ldots, r$ and $\eta_{ii} = -1, i = r+1, \ldots, n$, with vanishing off-diagonal elements, $\eta_{i \neq j} = 0$. Here η is the standard symbol for the representation of the metric in this form. n is the vector space dimension, and the number r is an invariant called the **signature of the metric**. A positive definite metric has signature $r = n$. The Minkovski metric defined on p. 45 is an example of a metric of signature 1.

L3.4 Complex scalar product

REMARK This section can be skipped at first reading. It is a prerequisite for chapters L8 and C6.

So far our focus has been on $\mathbb{R}$-vectors spaces, and in particular on the standard vector space $\mathbb{R}^n$. We here discuss how the concept of inner products can be generalized to complex vector spaces. A **complex inner product** of a $\mathbb{C}$-vector space, V, is a map

$$\langle\ ,\ \rangle : V \times V \to \mathbb{C}, \qquad (\hat{\mathbf{v}}, \hat{\mathbf{w}}) \mapsto \langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle\ , \tag{L66}$$

with the following properties:

(i) **symmetry**: $\langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle = \overline{\langle \hat{\mathbf{v}}, \hat{\mathbf{u}} \rangle}$,

(ii) **complex linearity**: $\langle a\hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle = \bar{a} \langle \mathbf{v}, \mathbf{w} \rangle$,
$\langle \hat{\mathbf{v}}, a\hat{\mathbf{w}} \rangle = a \langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle$,
$\langle \hat{\mathbf{u}} + \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle = \langle \hat{\mathbf{u}}, \hat{\mathbf{w}} \rangle + \langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle$,

(iii) **positive definiteness**: $\hat{\mathbf{v}} \neq \mathbf{0} : \langle \hat{\mathbf{v}}, \hat{\mathbf{v}} \rangle > 0$. (L67)

These properties are analogous to those of Eq. (L44) for a scalar product on a $\mathbb{R}$-vector space. Notice, however, that complex conjugation is involved in the symmetry relation, and when 'pulling out' a scalar factor multiplying the first (but not the second!) vector. A complex vector space, V, equipped with such an inner product, $(V, \langle\ ,\ \rangle)$, is called a **unitary vector space**.

Now consider the **standard complex vector space**, $\mathbb{C}^n = \{\mathbf{z} = (z^1, \ldots, z^n)^T | z^i \in \mathbb{C}\}$. As for $\mathbb{R}^n$ (cf. Eq. (L49)), a generic scalar product for $\mathbb{C}^n$ is described by a metric tensor $g = \{g_{ij}\}$ as

$$\boxed{\langle \mathbf{u}, \mathbf{w} \rangle_{\mathbb{C}^n} = \overline{u^i} g_{ij} w^j,} \tag{L68}$$

where the complex conjugation of the *left* vector components is required to satisfy the complex linearity property (ii) of Eq. (L67). The symmetry relation of the same equation further implies the condition

$$g_{ij} = \overline{g_{ji}}. \tag{L69}$$

Eq. (L68) can also be written as

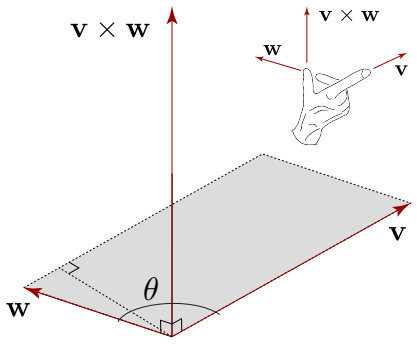
$$\langle \mathbf{u}, \mathbf{w} \rangle_{\mathbb{C}^n} \equiv \overline{u_j} w^j. \tag{L70}$$

where $u_j = u^i g_{ij}$ hides the metric via index-lowering. If the metric is trivial, $g_{ij} = \delta_{ij}$, so that $u_j = u^j$, we arrive at the **(standard) complex scalar product**,

$$\langle \mathbf{u}, \mathbf{w} \rangle \equiv \overline{u^j} w^j. \tag{L71}$$

Unlike in the real case of Eq. (L30), this scalar product is not usually denoted by a dot notation ($\mathbf{v} \cdot \mathbf{w}$). Note that the complex conjugation in Eq. (**??**) ensures positivity: $\langle \mathbf{v}, \mathbf{v} \rangle = \overline{v_i} v^i = \sum_i^n |v^i|^2 \geq 0$.

L4 Vector product



In this chapter we focus on the Euclidean space $\mathbb{E}^3 \simeq \mathbb{R}^3$. This space is special not only because it is the space of our daily experience but also because it admits the definition of a product operation between vectors that is very different from the scalar product discussed above. This so-called vector product assigns to two vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^3$ another 'vector' which is usually denoted $\mathbf{v} \times \mathbf{w}$. (The quotation marks hint at the fact that $\mathbf{v} \times \mathbf{w}$ actually is not a real vector, a point to be discussed below.) In the following, we introduce the vector product from two different perspectives; the first is geometric and the second emphasizes the algebraic features of the vector product.

L4.1 Geometric formulation

The **vector product** or **cross product** is a map, $\times : \mathbb{E}^3 \times \mathbb{E}^3 \to V$, $(\mathbf{v}, \mathbf{w}) \mapsto \mathbf{v} \times \mathbf{w}$, that assigns to two $\mathbb{E}^3$-vectors $\mathbf{v}$ and $\mathbf{w}$ an element $\mathbf{v} \times \mathbf{w}$ of another three-dimensional vector space, V. The mathematical identity of V is discussed in precise terms in chapter L11. For the moment we note that being three-dimensional, $V \cong \mathbb{E}^3$ is isomorphic (in one-to-one correspondence) to $\mathbb{E}^3$ and each of its elements can be described as a three-component object. For this reason, the physics literature often does not distinguish between V and $\mathbb{E}^3$ and considers the cross product to be a map

$$\times : \mathbb{E}^3 \times \mathbb{E}^3 \to \mathbb{E}^3, \qquad (\mathbf{v}, \mathbf{w}) \mapsto \mathbf{v} \times \mathbf{w}, \tag{L72}$$

that assigns to two vectors $\mathbf{v}$ and $\mathbf{w}$ another $\mathbb{E}^3$-vector, $\mathbf{v} \times \mathbf{w}$. The image, $\mathbf{v} \times \mathbf{w}$, of the cross-product is defined implicitly by the following geometric properties:

1. **Perpendicularity:** By definition, $\mathbf{v} \times \mathbf{w}$ points in a direction perpendicular to the two-dimensional plane[1] spanned by $\mathbf{v}$ and $\mathbf{w}$ (unless $\mathbf{v} \parallel \mathbf{w}$, in which case $\mathbf{v} \times \mathbf{w} \equiv \mathbf{0}$). In other words, $\mathbf{v} \times \mathbf{w}$ is **perpendicular to both $\mathbf{v}$ and $\mathbf{w}$**.

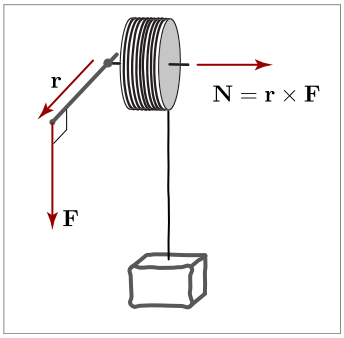
[1] Here we use the fact that we are operating in $\mathbb{E}^3$. In $\mathbb{E}^2$ a direction perpendicular to a two-dimensional plane does not exist and in and in $\mathbb{E}^{n>3}$ a plane does not uniquely identify a perpendicular direction.

2. **Orientation:** Perpendicularity to a plane still leaves two possible directions, 'upwards' or 'downwards'. The orientation of $\mathbf{v} \times \mathbf{w}$ is defined according to the **right-hand rule**: if index and middle finger of a right hand point in the direction of $\mathbf{v}$ and $\mathbf{w}$, respectively, then its thumb indicates the direction of $\mathbf{v} \times \mathbf{w}$ (see the figure above).

3. **Norm**: By definition, $\|\mathbf{v} \times \mathbf{w}\|$ is equal to the geometric area of the parallelogram spanned by $\mathbf{v}$ and $\mathbf{w}$. According to Eq. (L41), this area is given by

$$\|\mathbf{v} \times \mathbf{w}\| = \|\mathbf{v}\| \|\mathbf{w}\| \sin\theta, \tag{L73}$$

where $\theta = \angle(\mathbf{v}, \mathbf{w}) \in [0, \pi]$ is the angle between $\mathbf{v}$ and $\mathbf{w}$, as defined in Eq. (L35).



INFO The vector product plays an important role in **physics**. Generally speaking, vector products appear whenever the two physical concepts 'vector' and 'rotation' meet.

Let us illustrate this point with an example from mechanics. Consider a weight lifted by a lever (see figure). The influence of the lever on the weight depends on three factors: (i) the point at which the lifting force $\mathbf{F}$ is applied to the lever, described by the vector $\mathbf{r}$ connecting the axis of rotation to that point; (ii) the magnitude of the force; and (iii) its direction. The applied force will be maximally efficient if it acts in a direction perpendicular to $\mathbf{r}$ (as drawn in the figure). All these factors are combined in the definition of **torque**,

$$\mathbf{N} = \mathbf{r} \times \mathbf{F}. \tag{L74}$$

The torque is defined to be perpendicular to both $\mathbf{r}$ and $\mathbf{F}$ and this defines an imaginary axis around which it tries to induce rotational motion. (A torque acts *efficiently* if it is aligned with an axis around which mechanical motion is actually possible, such as the cylindrical axis of the structure shown in the figure.) Taking the norm, $\|\mathbf{N}\| = \|\mathbf{r}\| \|\mathbf{F}\| |\sin\angle(\mathbf{r}, \mathbf{F})|$, we see that the torque is largest if $\mathbf{r} \perp \mathbf{F}$. The norm also expresses the 'law of levers' (Hebelgesetz), according to which the effect of the force depends on the product of its magnitude, $\|\mathbf{F}\|$, and the distance of application relative to the rotation axis, $\|\mathbf{r}\|$.

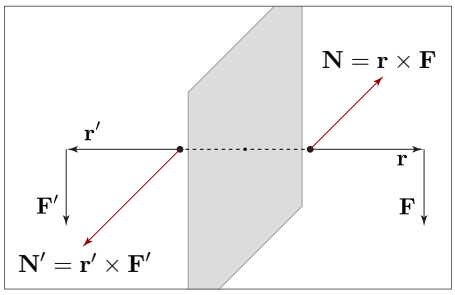
From its geometric construction it follows that the vector product is

antisymmetric: $\mathbf{v} \times \mathbf{w} = -\mathbf{w} \times \mathbf{v}$, (L75a)

distributive: $\mathbf{u} \times (\mathbf{v} + \mathbf{w}) = \mathbf{u} \times \mathbf{v} + \mathbf{u} \times \mathbf{w}$, (L75b)

in general not associative: $\mathbf{u} \times (\mathbf{v} \times \mathbf{w}) \neq (\mathbf{u} \times \mathbf{v}) \times \mathbf{w}$. (L75c)

The lack of associativity can be shown by constructing counter examples (consider, for example, the vector product of three orthonormal basis vectors). The verification of distributivity on the basis of the geometric definition of the product is tricky – take it as a challenging exercise – and will not be discussed here. However, distributivity will follow as a trivial consequence of the alternative definition of the vector product to be discussed in the next section.

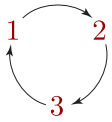


INFO We mentioned above that **the vector product, $\mathbf{v} \times \mathbf{w}$, is not an element of the space $\mathbb{E}^3$ in which $\mathbf{v}$ and $\mathbf{w}$ are defined**. Though $\mathbf{v} \times \mathbf{w}$ does live in a three-dimensional vector space, called V above, this space is different from the $\mathbb{E}^3$ of the argument vectors, and this difference shows up in various ways. As a physically motivated example, let us consider the torque, $\mathbf{N} = \mathbf{r} \times \mathbf{F}$, of two vectors assumed to be perpendicular for simplicity, $\mathbf{r} \perp \mathbf{F}$, and study its properties under reflection[2] with respect to a plane. Let us denote the image of a vector $\mathbf{v}$ under this reflection by $\mathbf{v}'$. For reflections with respect to the shaded plane in the figure we thus have $\mathbf{r}' = -\mathbf{r}$ and $\mathbf{F}' = \mathbf{F}$. The torque $\mathbf{N} = \mathbf{r} \times \mathbf{F}$ is parallel to the plane. If it were an element of $\mathbb{E}^3$, its reflection would thus be equal to $\mathbf{N}$. However, the torque is actually an element of V, and as such its reflection is *defined* to be the torque computed from the reflected argument vectors, $\mathbf{N}' \equiv \mathbf{r}' \times \mathbf{F}' = -\mathbf{r} \times \mathbf{F}$. This points in the direction *opposite* to $\mathbf{N}$, showing that under planar reflections *the cross product transforms differently from an $\mathbb{E}^3$-vector*. In view of this oddity, the vector product of two vectors is sometimes called a **pseudo-vector** or **axial vector**. However, the mathematically clean view, presented in section L11.8, is that the cross-product lives in the three-dimensional vector space of 'covariant tensors of second degree'. In three dimensions, these objects can be described in terms of three components, thus resembling vectors, hence it is standard practice in physics to represent them using the same notation as used for vectors. However, the above construction shows that both physically and mathematically, they are *different* from vectors, and confusion can be avoided by keeping this point in mind.

L4.2 Algebraic formulation

REMARK The non-vectorial nature of the vector product not only shows in its geometric features (cf. preceding info block) but also algebraically: relations involving the vector product typically involve index positions that violate the conventions of covariant notation (cf. p. 32). This happens because the proper algebraic formulation of the vector product, discussed in section L11.8, requires keeping track of the metric tensor. However, one looses sight of it when employing an orthonormal basis with $g_{ij} = \delta_{ij}$, such as the Cartesian basis used throughout this chapter. On the other hand, when using an orthonormal basis inconsistencies in index position can simply be ignored, since index position does not matter: $v_i = g_{ij} v^j = \delta_{ij} v^j = v^i$. For the sake of notational consistency, we will nevertheless adhere to the convention introduced in chapter L2: we write the expansion of a vector w.r.t. an orthonormal basis as $\mathbf{v} = \mathbf{e}_i v^i$, with lower and upper indices on basis vectors or components, respectively.

[2] Formally, a **reflection with respect to a plane** is a map $\mathbb{E}^3 \to \mathbb{E}^3, \mathbf{v} \equiv \mathbf{v}_\parallel + \mathbf{v}_\perp \mapsto \mathbf{v}' \equiv \mathbf{v}_\parallel - \mathbf{v}_\perp$ where $\mathbf{v} = \mathbf{v}_\parallel + \mathbf{v}_\perp$ is a decomposition of the argument into components parallel and perpendicular to the plane, respectively. The reflection inverts the sign of the perpendicular component.



The geometric definition of the vector product presented in Sec. L4.1 is intuitive but cumbersome to work with. To introduce a more efficient computational approach we consider an orthonormal basis, $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. The vector product makes reference to the right-hand orientation, and so it will be natural to label the basis vectors such that $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ point in the direction of the index finger, middle finger, and thumb, respectively. A basis obeying this criterion is called **positively oriented**. Any orthonormal basis can be converted into a positively oriented basis by a relabeling of basis vectors.[3]

The positive orientation of a basis defines a cyclic ordering of basis vectors as shown in the figure. Computing the geometrically defined vector product of any two consecutive vectors in this sequence we obtain the third, e.g. $\mathbf{e}_2 \times \mathbf{e}_3 = \mathbf{e}_1$. Computing a product in 'reverse order', we obtain the third vector with a minus sign, e.g. $\mathbf{e}_2 \times \mathbf{e}_1 = -\mathbf{e}_3$. It is convenient to introduce notation representing these relations in compact form: we call a triple of three unequal indices (i, j, k) **cyclically ordered** if they are ordered in the sequence 123, 231 or 312, as indicated in the figure, and anti-cyclically ordered if the sequence of ordering is reversed, 213, 321 or 132. Geometric reasoning similar to the above shows that the three basis vectors of a right-handed orthonormal basis satisfy $\mathbf{e}_i \times \mathbf{e}_j = \pm\mathbf{e}_k$, where the upper or lower sign applies if the indices ijk are ordered cyclicly or anti-cyclicly, respectively.

We will now show that these relations can be summarized in compact form using the three-index version of the **Levi-Civita symbol** introduced on p. 11:

$$\epsilon_{123} = 1, \quad \epsilon_{ijk} = -\epsilon_{jik} = -\epsilon_{ikj} = -\epsilon_{kji} \qquad (i, j, k \in \{1, 2, 3\}). \tag{L76}$$

By definition, it is **antisymmetric** under the exchange of any two of its indices. It therefore vanishes if two indices cooincide, $\epsilon_{112} = 0$, etc. As is apparent from the two right-most equalities in Eq. (L76), the Levi-Civita symbol is also **invariant** under cyclic permutations of its indices. The reason is that cyclic permutations of three indices always involve two index exchanges, e.g. $\epsilon_{123} \mapsto \epsilon_{213} \mapsto \epsilon_{231}$, implying a sign of $(-1)^2 = 1$. The values of ϵ_{ijk} can thus be summarized as

$$\epsilon_{ijk} = \begin{cases} 1, & (i, j, k) \text{ cyclic}, \\ -1, & (i, j, k) \text{ anti-cyclic}, \\ 0, & \text{else (two or three indices coincide)}. \end{cases} \tag{L77}$$

Remarkably, these values perfectly match those arising in the above-mentiond relation $\mathbf{e}_i \times \mathbf{e}_j = \pm\mathbf{e}_k$. The Levi-Civita symbol can thus be used to summarize all vector products of vectors of a right-handed basis (including the case $\mathbf{e}_i \times \mathbf{e}_i = \mathbf{0}$) in a single compact equation:

$$\boxed{\mathbf{e}_i \times \mathbf{e}_j = \epsilon_{ijk}\, \mathbf{e}_k.} \tag{L78}$$

Another useful result is obtained by projecting Eq. (L78) onto $\mathbf{e}_k$:

$$(\mathbf{e}_i \times \mathbf{e}_j) \cdot \mathbf{e}_k = \epsilon_{ijk}. \tag{L79}$$

[3] For example, if $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ is positively oriented, then $\{\mathbf{e}_2, \mathbf{e}_1, \mathbf{e}_3\}$ is negatively oriented.

Although the Levi-Civita formulation of the cross product Eq. (L78) may not look very intuitive, it is a potent aid in performing fault-proof computations. In the following, we apply it to describe the vector product between generic vectors $\mathbf{v} = \mathbf{e}_i v^i$ and $\mathbf{w} = \mathbf{e}_j w^j$ as

$$\mathbf{v} \times \mathbf{w} = (\mathbf{e}_i v^i) \times (\mathbf{e}_j w^j) = v^i w^j (\mathbf{e}_i \times \mathbf{e}_j) \overset{(L79)}{=} v^i w^j \epsilon_{ijk}\, \mathbf{e}_k. \tag{L80}$$

This relation shows that the kth component of $\mathbf{v} \times \mathbf{w}$ is given by:[4]

$$\boxed{(\mathbf{v} \times \mathbf{w})^k = v^i w^j \epsilon_{ijk}.} \tag{L81}$$

Formulated in column-vector notation, this reads

$$\begin{pmatrix} v^1 \\ v^2 \\ v^3 \end{pmatrix} \times \begin{pmatrix} w^1 \\ w^2 \\ w^3 \end{pmatrix} = \begin{pmatrix} v^2 w^3 - v^3 w^2 \\ v^3 w^1 - v^1 w^3 \\ v^1 w^2 - v^2 w^1 \end{pmatrix} . \tag{L82}$$

This relation is useful for computing a vector product explicitly. (→ L4.2.1-2) However, it leads to very tedious expressions in calculations involving more than one vector product. In such cases, great simplifications can be achieved by employing the Levi-Civita symbol. The reason is that this symbol obeys the **contraction identity** (→ L4.2.3-4)

$$\boxed{\epsilon_{ijk}\epsilon_{mnk} = \delta_{im}\delta_{jn} - \delta_{in}\delta_{jm},} \tag{L83}$$

where, as usual with pairs of indices, k is summed over. (Verify this identity, ideally without using the hint given in the footnote.[5]) In practice, this identity converts two-fold cross products (encoded via $\epsilon\epsilon$) into combinations of scalar products (encoded via $\delta\delta - \delta\delta$). This is illustrated in the following example, and in problems L4.3.1-2.

EXAMPLE Let us illustrate the usage of the Levi-Civita tensor by checking that Eq. (L81) conforms with the geometric definition of the vector product. The orthogonality $\mathbf{v} \perp (\mathbf{v} \times \mathbf{w})$ is verified by taking the scalar product:

$$\mathbf{v} \cdot (\mathbf{v} \times \mathbf{w}) \overset{(L81)}{=} v^k\, v^i w^j \epsilon_{ijk} \overset{(L76)}{=} -v^k\, v^i w^j \epsilon_{kji} = -v^i\, v^k w^j \epsilon_{ijk}\ . \tag{L84}$$

In the second equality we used the antisymmetry of the Levi-Civita symbol and in the third relabeled the summation indices $i \leftrightarrow k$ (the dummy index in a summation can always be relabeled without

[4] Eq. (L81) is an example of how relations involving the vector product do not conform to consistent covariant notation: the index k sits upstairs on the left but downstairs on the right. As mentioned on p. 56, the reason is that we are working in an orthonormal basis with metric tensor $g_{ij} = \delta_{ij}$ and have chosen to not keep track of its role. If one does keep track of it, Eq. (L81) takes the form $(\mathbf{v} \times \mathbf{w})^k = \sqrt{\det(g)}\, v^i w^j\, \epsilon_{ijl}\, g^{lk}$, where $\det(g)$ denotes the 'determinant' of g_{ij}, a construction introduced in chapter L6.1. This expression does conform to consistent covariant notation, but its justification requires an extended discussion of several more advanced concepts, which we reserve for section V6.5.

[5] Without loss of generality, assume $(i, j) = (1, 2)$. The sum over k in Eq. (L83) then yields nonzero only for $k = 3$. For this value of k, $\epsilon_{mnk} = 1$ if $(m, n) = (1, 2) = (i, j)$ while $\epsilon_{mnk} = -1$ if $(m, n) = (2, 1) = (j, i)$. This agrees with the value produced by the combination of Kronecker δ's on the r.h.s. of Eq. (L83).

changing the result). Comparing the 2nd and 4th terms in (L84), we see that $\mathbf{v}\cdot(\mathbf{v}\times\mathbf{w})$ equals its negative, and therefore must vanish. Similarly one shows that $\mathbf{w}\perp(\mathbf{v}\times\mathbf{w})$. We thus confirm that the vector product computed by (L81) is perpendicular to the plane spanned by $\mathbf{v}$ and $\mathbf{w}$. Its orientation (upward or downward) relative to this plane follows the right-hand rule as described by (L78). A little more work is needed to verify Eq. (L73), according to which the norm of $\mathbf{v}\times\mathbf{w}$ is equal to the area of the parallelogram spanned by $\mathbf{v}$ and $\mathbf{w}$. Using the contraction identify, we find:

$$\begin{aligned}\|\mathbf{v}\times\mathbf{w}\|^2 &\overset{(L32)}{=} (\mathbf{v}\times\mathbf{w})\cdot(\mathbf{v}\times\mathbf{w}) \overset{(L81)}{=} (v^i w^j \epsilon_{ijk})(v^m w^n \epsilon_{mnk}) \overset{(L83)}{=} v^i w^j v^m w^n (\delta_{im}\delta_{jn}-\delta_{in}\delta_{jm})\\ &= v^i w^j v^i w^j - v^i w^j v^j w^i = (\mathbf{v}\cdot\mathbf{v})\,(\mathbf{w}\cdot\mathbf{w}) - (\mathbf{v}\cdot\mathbf{w})^2. \qquad \text{(L85)}\end{aligned}$$

Taking the square root, we indeed obtain the area $A(\mathbf{v},\mathbf{w})$ of the stated parallelogram:

$$\|\mathbf{v}\times\mathbf{w}\| = [(\mathbf{v}\cdot\mathbf{v})\,(\mathbf{w}\cdot\mathbf{w}) - (\mathbf{v}\cdot\mathbf{w})^2]^{1/2} \overset{(L41)}{=} \|\mathbf{v}\|\|\mathbf{w}\|\sin(\angle(\mathbf{v},\mathbf{w}) = A(\mathbf{v},\mathbf{w}). \qquad \text{(L86)}$$

L4.3 Further properties of the vector product

The algebraic definition of the vector product leads to a number of secondary relations:

Grassmann identity: $$\mathbf{u}\times(\mathbf{v}\times\mathbf{w}) = \mathbf{v}(\mathbf{u}\cdot\mathbf{w}) - \mathbf{w}(\mathbf{u}\cdot\mathbf{v}), \qquad \text{(L87a)}$$

Jacobi identity: $$\mathbf{u}\times(\mathbf{v}\times\mathbf{w}) + \mathbf{v}\times(\mathbf{w}\times\mathbf{u}) + \mathbf{w}\times(\mathbf{u}\times\mathbf{v}) = \mathbf{0}, \qquad \text{(L87b)}$$

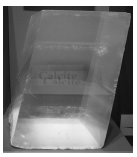
Lagrange identity: $$(\mathbf{v}\times\mathbf{w})\cdot(\mathbf{t}\times\mathbf{u}) = (\mathbf{v}\cdot\mathbf{t})(\mathbf{w}\cdot\mathbf{u}) - (\mathbf{v}\cdot\mathbf{u})(\mathbf{w}\cdot\mathbf{t}), \qquad \text{(L87c)}$$

$$(\mathbf{v}\times\mathbf{w})^2 = \|\mathbf{v}\|^2\|\mathbf{w}\|^2 - (\mathbf{v}\cdot\mathbf{w})^2. \qquad \text{(L87d)}$$

All of these have geometric interpretations which, however, are not entirely obvious (try to find them as an exercise). Their algebraic proofs, utilizing the contraction identity (L83), are more straightforward and likewise left as an exercise (→ L4.3.1-2).

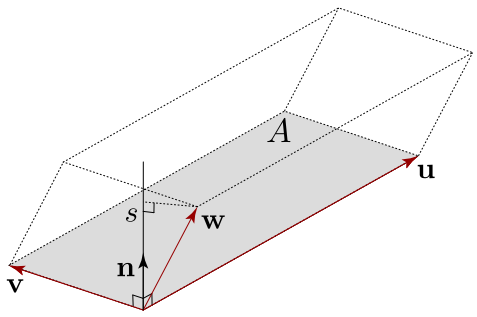
Given the scalar- and the vector product, we can introduce a combined product operation, the so-called **scalar triple product**, as

$$(\mathbf{u},\mathbf{v},\mathbf{w}) \mapsto (\mathbf{u}\times\mathbf{v})\cdot\mathbf{w} \overset{(L78)}{=} u^i v^j w^k\,\epsilon_{ijk}\ . \qquad \text{(L88)}$$



The German denotation '*Spat*produkt' refers to a class of materials known as 'Spate' which mineralize into parallelepipedal[6] geometries (the figure shows an example).

[6] A **parallelepiped** is the three-dimensional generalization of a parallelogram.



The scalar triple product specifies the geometric volume of the parallelepiped[6] spanned by its three argument vectors:

$$\mathrm{Vol}(\mathbf{u},\mathbf{v},\mathbf{w}) = |(\mathbf{u}\times\mathbf{v})\cdot\mathbf{w}|. \qquad \text{(L89)}$$

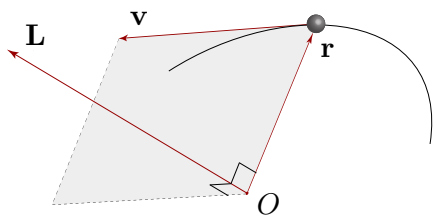
To see this, notice that the volume of a parallelepiped is given by the area of one of its faces times its height in the direction perpendicular to that face. (This statement generalizes the area formula for parallelograms, area = (base line) × (height), to three dimensions.) For example, the volume of the parallelepiped shown in the figure can be computed as the product of the shaded area, A, spanned by $\mathbf{u}$ and $\mathbf{v}$, and the length, s, of the projection of $\mathbf{w}$ onto a line perpendicular to that area. This volume, As, can conveniently be produced by a combination of scalar- and vector products: $\mathbf{u}\times\mathbf{v} = A\mathbf{n}$, where $\mathbf{n}$ is a unit vector perpendicular to the base area, and $\mathbf{n}\cdot\mathbf{w} = s$. Thus $|(\mathbf{u}\times\mathbf{v})\cdot\mathbf{w}| = As$, as stated.[7] Finally, the volume does not depend on which of the three different faces is chosen at the outset. This freedom is reflected in the **cyclic invariance** of the scalar triple product,

$$(\mathbf{u}\times\mathbf{v})\cdot\mathbf{w} = (\mathbf{v}\times\mathbf{w})\cdot\mathbf{u} = (\mathbf{w}\times\mathbf{u})\cdot\mathbf{v}, \qquad \text{(L90)}$$

which follows from the cyclic invariance of the Levi-Civita symbol in Eq. (L88).

The triple product can be used to diagnose whether three vectors are linearly independent or not. If they are linearly independent, they span a parallelepiped with nonzero volume, hence $(\mathbf{u}\times\mathbf{v})\cdot\mathbf{w} \neq 0$. In contrast, if they are linearly dependent, all three lie in the same plane. They thus span a 'flat parallelepiped' with zero volume, hence their triple product vanishes. (→ L4.3.3-4) This method for diagonizing linear independence can be generalized to an arbitrary number of vectors using the notion of **determinants**, to be discussed in chapter L6.1.

INFO We know from daily experience that rotating bodies resist changes of their axis of rotation. For example it takes a strong force to change the rotation of a wheel in motion and this is what keeps bicycles from falling. The same principle maintains the rotational axis of the planets of the solar system in their motion around sun.



The quantity that is 'conserved' in free rotational motion is called **angular momentum**. For any body of mass m and velocity $\mathbf{v}$ its angular momentum relative to a point, O is defined as (see the figure below)

$$\mathbf{L} \equiv m\mathbf{r}\times\mathbf{v}, \qquad \text{(L91)}$$

where $\mathbf{r}$ is the vector connecting O and the body. The angular momentum vector $\mathbf{L}$ is perpendicular to the plane spanned by $\mathbf{r}$ and the direction of instantaneous motion specified by $\mathbf{v}$. In the particular case of a body travelling along a planar orbit, e.g.

[7] The absolute value is needed due to the antisymmetry of the vector product, $(\mathbf{u}\times\mathbf{v})\cdot\mathbf{w} = -(\mathbf{v}\times\mathbf{u})\cdot\mathbf{w}$. The scalar triple product can thus be either positive or negative, depending on whether its argument vectors satisfy a right-hand rule or not. However, in both cases $|(\mathbf{u}\times\mathbf{v})\cdot\mathbf{w}|$ gives the volume of the parallelepiped.

the earth orbiting around the sun, the angular momentum relative to a point in the orbital plane stands perpendicular to that plane.

The **conservation law** expressing the 'stability' of rotational motion reads,

$$\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t} = \mathbf{N}, \tag{L92}$$

where $\mathbf{N} = \mathbf{r} \times \mathbf{F}$ is the torque acting on the body relative to the point of definition of angular momentum. In the absence of torque, angular momentum is conserved. Notice that the absence of torque does not necessitate the absence of forces. For example, the earth experiences a gravitational force, $\mathbf{F}$, from the sun. However, that force is radial, $\mathbf{F} \parallel \mathbf{r}$, i.e. directed along the line connecting the centers of earth and sun. This means that it does not create a torque, and so the rotational motion of our planet is (approximately) conserved. For an extended discussion of angular momentum, consult a lecture course in classical mechanics.

L5 Matrices I: general theory

REMARK Much of the following discussion applies to both real and complex vector spaces. To avoid excessive notation we will focus on the complex case throughout. At all stages the imaginary part of complex numbers may be set to zero (i.e. replacing $a \in \mathbb{C}$ by $a \in \mathbb{R}$) to obtain the corresponding theory of real matrices. In the few cases where the real and the complex theory differ both variants will be discussed in turn.

L5.1 Linear maps

We now understand the structure of vector spaces. However, beyond this descriptive level not much has really been 'done' with them. This will now change when we consider *maps* between vector spaces. Of particular interest are maps that are compatible with the 'linear structure' of the theory: a map $F : V \to W$ between two vector spaces (this includes the case $V = W$ of maps acting within one vector space) is called a **linear map** if $F(a\mathbf{v} + b\mathbf{w}) = aF(\mathbf{v}) + bF(\mathbf{w})$ for $a, b \in \mathbb{R}$ and $\mathbf{v}, \mathbf{w} \in V$.[1]

This definition states that the same result is obtained if we first add the vectors in V and then apply F, or first apply F and then add the resulting vectors in V'. We have already encountered an important class of such maps, viz. the isomorphisms $\phi_{\mathbf{v}} : V \to \mathbb{R}^n$ of section L2.5, which map V-vectors onto corresponding $\mathbb{R}^n$-representations for a given V-basis.

It is customary to denote linear maps by capitalized early latin letters, i.e. $A, B, \ldots$ instead of $F, G, \ldots$. The brackets enclosing the argument vector are usually dropped, i.e. one writes $A\mathbf{v}$ instead of $A(\mathbf{v})$.

EXAMPLE A **photo** is a map of 3-dimensional objects onto a 2-dimensional image. This defines an (approximately) linear map $\mathbb{E}^3 \to \mathbb{E}^2$: Doubling the object size leads to an image twice as large, and displacing the object (formally, adding a fixed vector to the vectors defining it) leads to a proportionally displaced image. Notice, however, that it is not in general possible to reconstruct the original object from its image: the photographic 'map' is not invertible. In contrast, photos taken of two-dimensional objects do allow for reconstruction. This anticipates a point to be discussed in more detail below: invertible linear maps, i.e. vector space *isomorphisms*, can exist only between vector spaces of equal dimensionality.

[1] As an example of a *non*linear map consider $F : V \to V$, $\mathbf{v} \mapsto \mathbf{v}\|\mathbf{v}\|$. Why is this map not linear?

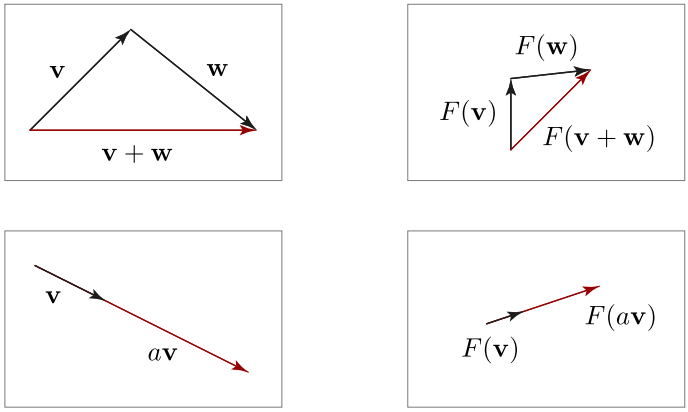


Figure L12: On the definition of linear maps, F, between vector spaces, illustrated for a map that rotates all vectors by 45deg and shrinks them by a factor of 2. Top panels: it does not matter whether vectors are first added and then mapped by F, or first mapped and then added. Bottom panels: in the same sense, the map is compatible with scalar multiplication.

Before discussing the mathematics of linear maps it is worthwhile to outline the **importance of the concept to physics**. First, many operations of physical significance are described by linear maps. Examples include rotation, dilatation, the reflection of space and time, and others more. Second, we will see that even very complicated general maps between vector spaces can be 'locally' approximated by linear maps. The heuristics behind this statement is that arbitrary smooth structures (think of a curve winding through three-dimensional space) look 'linear' (the curve approximately becomes a straight line) if one zooms in sufficiently closely. The description of 'linear structures' and of maps between them may therefore serve as a local (close-up) approximation to the more complicated 'global' picture. Third, the mathematics of quantum mechanics is essentially one of linear maps between vector spaces known as Hilbert spaces (see chapter L10). This list is not exhaustive but illustrates that linear maps have many important applications in physics.

INFO The importance of linear maps is also reflected in the physics curriculum where linear algebra is routinely taught in the first or second terms. It was not always like this. When the 'modern' theory of quantum mechanics was formulated in the third decade of the last century, linear maps and their description in terms of so-called matrices were unfamiliar to a majority of physicists. They were certainly unknown to Werner Heisenberg when he formulated the foundations of the operator approach to **quantum mechanics**. It was Max Born, together with his collaborator Pascual Jordan, who realized that Heisenberg's theory could be formulated in the language of linear maps, and this observation was published in the joint paper M. Born, W. Heisenberg, P. Jordan, *Zur Quantenmechanik II*. Zeitschrift für Physik **35**, 557 (1926). This first formulation of quantum mechanics in terms of linear maps marked the beginning of quantum theory as it is taught to date. Since then linear algebra has become an indispensable tool in modern physics.

L5.2 Matrices

REMARK We begin by discussing linear maps between standard vector spaces, $V = \mathbb{C}^n$, $W = \mathbb{C}^m$. In section L5.5 we will see how this discussion includes most of the mathematics required to describe the theory of linear maps between general spaces.

Consider the simplest of all complex vector spaces, $\mathbb{C}^1 \cong \mathbb{C}$. A general linear map acts on 'vectors'[2] $x \in \mathbb{C}$ by $x \mapsto Ax$, multiplying them by a fixed complex number, $A \in \mathbb{C}$. Indeed, it is straightforward to verify (try it) that multiplication by a number meets the linearity criterion formulated above. The distinguishing feature of the map is that Ax does not contain additive constants, or higher powers of x ($Ax + B$ or $Ax^{\alpha \neq 1}$ are not allowed) . Now let us generalize this construction to maps $A : \mathbb{C}^2 \to \mathbb{C}$. Here, $\mathbf{x} = (x^1, x^2)^T$ has two components and $A\mathbf{x} \in \mathbb{C}$ is a number that depends on these. Again, it is not difficult to verify that the most general linear map reads $A\mathbf{x} = A_1 x^1 + A_2 x^2$, linear in both x^1 and x^2, with complex coefficients, $A_1, A_2 \in \mathbb{C}$. For a map $A : \mathbb{C}^2 \to \mathbb{C}^2$ the image $A\mathbf{x}$ has two components which must both be linear functions of x^1 and x^2. Thus, the most general image vector can be parameterized as

$$A \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} = \begin{pmatrix} A^1{}_1 x^1 + A^1{}_2 x^2 \\ A^2{}_1 x^1 + A^2{}_2 x^2 \end{pmatrix}, \tag{L93}$$

in terms of four complex numbers $\{A^i{}_j\}$.
Everything we have said so far also applies to linear maps between real instead of complex vector vector spaces. In this case, of course, real instead of complex coefficients are involved.

EXERCISE Consider the map $A : \mathbb{R}^2 \to \mathbb{R}^2$ between real vector spaces described by

$$A = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \tag{L94}$$

and let it act on some simple vectors such as $\mathbf{x} = (1, 0)^T$, or $\mathbf{x} = (1, 1)^T$. Convince yourself that A describes the **rotation** of vectors by an angle θ. Argue entirely in geometric terms (not using formulas) why rotations of space are linear maps.

The generalization to maps between two vector spaces, each of arbitrary dimension, should now be obvious. The most general linear map $A : \mathbb{C}^n \mapsto \mathbb{C}^m$ is specified by

$$\mathbf{x} = \begin{pmatrix} x^1 \\ x^2 \\ \vdots \\ x^m \end{pmatrix} \longmapsto A\mathbf{x} = \begin{pmatrix} A^1{}_1 x^1 + A^1{}_2 x^2 + \cdots + A^1{}_n x^n \\ A^2{}_1 x^1 + A^2{}_2 x^2 + \cdots + A^2{}_n x^n \\ \vdots \\ A^m{}_1 x^1 + A^m{}_2 x^2 + \cdots + A^m{}_n x^n \end{pmatrix} = \begin{pmatrix} A^1{}_j\, x^j \\ A^2{}_j\, x^j \\ \vdots \\ A^m{}_j\, x^j \end{pmatrix}, \tag{L95}$$

[2] For one-component vectors, we avoid the boldface convention, i.e. we write $x = \mathbf{x} = (x)$ for simplicity.

i.e. the ith component of the vector $A\mathbf{x}$ is given by

$$\boxed{(A\mathbf{x})^i = A^i{}_1 x^1 + A^i{}_2 x^2 + \cdots + A^i{}_n x^n = A^i{}_j x^j \,,} \tag{L96}$$

with $i = 1, \ldots, m$ and $j = 1, \ldots, n$. The coefficients $\{A^i{}_j\}$ are all complex numbers, hence

> A linear map $A : \mathbb{C}^n \to \mathbb{C}^m$ is fully specified by $m \times n$ complex numbers $\{A^i{}_j\}$.

This means that linear maps are comparatively 'simple'. To appreciate this statement, consider the case $n = m = 1$. Then just a single number is needed to specify a linear function, whereas describing a generic function $F : \mathbb{C} \to \mathbb{C}$, $x \mapsto F(x)$ requires specifying infinitely many function values. Similarly, $m \times n$ numbers contain much less information than required to specify an arbitrary higher-dimensional function $F : \mathbb{C}^n \to \mathbb{C}^m$.

In the following, arrays of sums as in Eq. (L95) will appear so often that it pays to switch to a more **efficient notation**: we define the rectangular array

$$A = \begin{pmatrix} A^1{}_1 & \ldots & A^1{}_j & \ldots & A^1{}_n \\ \vdots & & \vdots & & \vdots \\ A^i{}_1 & \ldots & A^i{}_j & \ldots & A^i{}_n \\ \vdots & & \vdots & & \vdots \\ A^m{}_1 & \ldots & A^m{}_j & \ldots & A^m{}_n \end{pmatrix}, \tag{L97}$$

called the **matrix** 'representing' the linear map A, or its **matrix representation**. The matrix fully specifies the linear map and is customarily denoted by the same symbol, A. Occasionally we want to draw a more marked distinction between a map, $\hat{A}$, and its matrix, A, in which case the former will carry a caret. The entries, $A^i{}_j$, of a matrix A are called its **components** or **matrix elements**. The full matrix is often denoted as $A = \{A^i{}_j\}$, where the index range is left implicit. By convention, the left index i labels rows, the right index j columns (also when noncovariant notation, A_{ij}, is used for the matrix elements).

The action of this matrix on a vector $\mathbf{x}$ — which is more commonly called the **multiplication of a vector by a matrix** — is now *defined* through the relation:

$$\boxed{\begin{pmatrix} A^1{}_j x^j \\ \vdots \\ A^i{}_j x^j \\ \vdots \\ A^m{}_j x^j \end{pmatrix} \equiv \begin{pmatrix} A^1{}_1 & \ldots & A^1{}_j & \ldots & A^1{}_n \\ \vdots & & \vdots & & \vdots \\ A^i{}_1 & \ldots & A^i{}_j & \ldots & A^i{}_n \\ \vdots & & \vdots & & \vdots \\ A^m{}_1 & \ldots & A^m{}_j & \ldots & A^m{}_n \end{pmatrix} \begin{pmatrix} x^1 \\ \vdots \\ x^j \\ \vdots \\ x^n \end{pmatrix}.} \tag{L98}$$

One may visualize how the ith component of $A\mathbf{x}$ is computed by moving stepwise from left to right along the ith row of the matrix A, and at the same time from top to bottom along the single column of the vector representing $\mathbf{x}$. At each step the corresponding matrix element

$A^i{}_j$ and vector element x^j are multiplied and the results added up, $A^i{}_1 x^1 + \cdots + A^i{}_n x^n$, to obtain $(A\mathbf{x})^i = A^i{}_j x^j$, as given in Eq. (L96).

EXAMPLE Let us illustrate the operation of multiplying a vector by a matrix with a number of basic examples:

$$\begin{pmatrix} 1 & 4 \\ 5 & 3 \end{pmatrix} \cdot \begin{pmatrix} 2 \\ 1 \end{pmatrix} = \begin{pmatrix} 1\cdot 2 + 4 \cdot 1 \\ 5 \cdot 2 + 3 \cdot 1 \end{pmatrix} = \begin{pmatrix} 6 \\ 13 \end{pmatrix},$$

$$\begin{pmatrix} 2 & 5 \\ 3 & 3 \\ 6 & 1 \end{pmatrix} \cdot \begin{pmatrix} 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 2\cdot 3 + 5 \cdot 2 \\ 3 \cdot 3 + 3 \cdot 2 \\ 6 \cdot 3 + 1 \cdot 2 \end{pmatrix} = \begin{pmatrix} 16 \\ 15 \\ 20 \end{pmatrix}$$

$$2 \cdot 2 = 4. \tag{L99}$$

For an $m \times n$ matrix $A = \{A^i{}_j\}$, the jth **column** defines a vector,

$$\mathbf{A}_j = (A^1{}_j, \ldots, A^m{}_j)^T = \begin{pmatrix} A^1{}_j \\ \vdots \\ A^m{}_j \end{pmatrix}, \tag{L100}$$

with components $(\mathbf{A}_j)^i = A^i{}_j$. For example, the 1st column of the 2×2-matrix $A = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ defines $\mathbf{A}_1 = \left(\begin{smallmatrix} a \\ c \end{smallmatrix}\right)$. A general matrix can be written as an n-tuple

$$A = (\mathbf{A}_1, \ldots, \mathbf{A}_n), \tag{L101}$$

formed by its n column vectors. Likewise, the ith **row** can be identified with the transpose of a vector, $\mathbf{A}^{iT} = (A^i{}_1, \ldots, A^i{}_n)$. For example, the second row of the 2×2 matrix corresponds to $\mathbf{A}^{2T} = (c, d)$. We can think of a general matrix in terms of a stack

$$A = \begin{pmatrix} \mathbf{A}^{1T} \\ \vdots \\ \mathbf{A}^{nT} \end{pmatrix} \tag{L102}$$

of n of these objects. Using this notation, Eq. (L96) can be expressed as $(A\mathbf{x})^i = \mathbf{A}^{iT} \cdot \mathbf{x}$, thus the ith element of $A\mathbf{x}$ equals the scalar product of the ith row of the matrix with $\mathbf{x}$.

The **action of A on the jth standard basis vector**, $\mathbf{e}_j = (0, \ldots, 1, \ldots, 0)^T$ (the 1 at the jth position, of course), is given by

$$A\mathbf{e}_j = \begin{pmatrix} A^1{}_1 & \ldots & A^1{}_j & \ldots & \ldots & A^1{}_n \\ \vdots & & \vdots & & & \vdots \\ \vdots & & \vdots & & & \vdots \\ A^i{}_1 & \ldots & A^i{}_j & \ldots & \ldots & A^i{}_n \\ \vdots & & \vdots & & & \vdots \\ A^m{}_1 & \ldots & A^m{}_j & \ldots & \ldots & A^m{}_n \end{pmatrix} \cdot \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} A^1{}_j \\ \vdots \\ \vdots \\ A^i{}_j \\ \vdots \\ A^m{}_j \end{pmatrix}, \tag{L103}$$

i.e. by the jth column of the matrix A. In the column vector notation introduced above this can be written as

$$A\mathbf{e}_j = \mathbf{A}_j. \tag{L104}$$

Linear maps are often *defined* by their action on the standard basis vectors, i.e. by an assignment $\mathbf{e}_j \mapsto \mathbf{v}_j$, where $\mathbf{v}_j$ are the known image vectors of the standard basis vectors. Eq. (L104) implies that the matrix representing the map can then be represented as $A = (\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n)$, i.e. as an array containing the n image vectors $\mathbf{v}_j = \mathbf{A}_j$ as column vectors.

EXAMPLE If $A : \mathbb{C}^2 \to \mathbb{C}^3$ is a linear map whose action on the standard basis of $\mathbb{C}^2$ is defined by the first two expressions in Eq. (L105), then its matrix representation A is given by the third:

$$\begin{pmatrix}1\\0\end{pmatrix} \overset{A}{\mapsto} \begin{pmatrix}3\\2\\1\end{pmatrix}, \qquad \begin{pmatrix}0\\1\end{pmatrix} \overset{A}{\mapsto} \begin{pmatrix}-1\\0\\1\end{pmatrix}, \qquad A = \begin{pmatrix}3 & -1\\2 & 0\\1 & 1\end{pmatrix}. \tag{L105}$$

EXERCISE The set of all matrices containing m rows and n columns of real numbers is sometimes called $\mathrm{mat}(\mathbb{C}, m, n)$. Two matrices $A, B \in \mathrm{mat}(\mathbb{C}, m, n)$ may be added by adding their components, i.e. we define $A + B \in \mathrm{mat}(\mathbb{C}, m, n)$ through $(A + B)^i{}_j \equiv A^i{}_j + B^i{}_j$. Similarly, we may multiply A by a scalar, $a \in \mathbb{C}$, to obtain a matrix aA with matrix elements $(aA)^i{}_j \equiv aA^i{}_j$. Show that with these definitions, $\mathrm{mat}(\mathbb{C}, m, n)$ is an $\mathbb{C}$-vector space. Show that the dimension of this space is given by $m \cdot n$.

The transpose and the adjoint of a matrix

We conclude our introduction of matrices by defining two operations that will become increasingly important in our discussion below. Given an $m \times n$ matrix A we may define a corresponding $n \times m$ matrix A^T (spoken A-transpose) by exchanging rows and columns. This is illustrated in the following examples:

$$\begin{aligned} A = \begin{pmatrix}2 & 3 & 1\\2 & 4 & 7\end{pmatrix} &\longrightarrow A^T = \begin{pmatrix}2 & 2\\3 & 4\\1 & 7\end{pmatrix},\\ A = \begin{pmatrix}4 & 2\\1 & 5\end{pmatrix} &\longrightarrow A^T = \begin{pmatrix}4 & 1\\2 & 5\end{pmatrix},\\ A = \begin{pmatrix}1\\3\\0\end{pmatrix} &\longrightarrow A^T = (1\ 3\ 0). \end{aligned} \tag{L106}$$

The third example shows how the extreme case of a $1 \times n$ matrix, i.e. a vector, transposes to a $n \times 1$ matrix. We have used this notation before as shorthand for column vectors, e.g.

$(0,1)^T = \binom{0}{1}$. For a matrix with elements $A^i{}_j$, the elements of the **transpose matrix** are given by

$$(A^T)_j{}^i = A^i{}_j, \tag{L107}$$

where on both sides of the equation the left index labels rows, the right index columns. For example, $(A^T)_2{}^1 = 3$ in the first example given above. Transposing a matrix by interchanging rows and columns can thus be memorized as an operation which slides both indices to the respective 'other side', $(A^T)_j{}^i = A^{\rightarrow i}_{j\leftarrow}$. The prescription works in either direction, i.e. for a matrix with elements $B_j{}^i$ we define $(B^T)^i{}_j = B_j{}^i$. Notice that when using covariant notation, as we do here, upper indices stay up and lower ones down during transposition. (The rationale behind this convention will be discussed later in section L11.4.) If instead one chooses to use non-covariant notation, with all indices downstairs, transposition amounts to interchanging them, $(A^T)_{ij} = A_{ji}$.

For a **complex vector space**, we define the **adjoint matrix** $A^\dagger$ (spoken 'A-adjoint' or 'A-dagger') through transposition followed by complex conjugation

$$A^\dagger = \overline{A^T}, \qquad (A^\dagger)_j{}^i = \overline{A^i{}_j}. \tag{L108}$$

For example

$$A = \begin{pmatrix} 1+2i & 5 \\ 4-i & 3i \end{pmatrix} \longrightarrow A^\dagger = \begin{pmatrix} 1-2i & 4+i \\ 5 & -3i \end{pmatrix}. \tag{L109}$$

L5.3 Matrix multiplication

The power of matrix calculus becomes apparent when we consider the *composition* of linear maps. For example, a graphics designer might might rotate, stretch and rotate a figure in three consecutive steps on a computer. All three operations are linear maps and the joint operation amounts to their composition.

The composition, $C \equiv B \circ A : \mathbb{C}^n \to \mathbb{C}^l$, of two linear maps, $A : \mathbb{C}^n \to \mathbb{C}^m$ and $B : \mathbb{C}^m \to \mathbb{C}^l$ is again linear and hence described by a matrix. The $l \times n$ matrix $\{C^k{}_j\}$ representing map C can be found from the $l \times m$ and $m \times n$ matrices $\{B^k{}_i\}$ and $\{A^i{}_j\}$ of B and A, respectively. To this end, observe that A maps a $\mathbb{C}^n$-vector with components x^j onto a $\mathbb{C}^m$-vector with components $A^i{}_j x^j$. This image vector, in turn, is mapped by B onto a $\mathbb{C}^l$-vector with components $B^k{}_i \left(A^i{}_j x^j\right) = \left(B^k{}_i A^i{}_j\right) x^j$. The matrix of the composite map, $C = B \circ A$, thus has matrix elements

$$\boxed{C^k{}_j = B^k{}_i A^i{}_j.} \tag{L110}$$

There exists an efficient scheme to compute these matrix elements directly from the rectangular arrays of the individual matrices:

$$\begin{pmatrix} C^1{}_1 & \dots & C^1{}_j & \dots & C^1{}_n \\ \vdots & & \vdots & & \vdots \\ C^k{}_1 & \dots & C^k{}_j & \dots & C^k{}_n \\ \vdots & & \vdots & & \vdots \\ C^l{}_1 & \dots & C^l{}_j & \dots & C^l{}_n \end{pmatrix} \equiv \begin{pmatrix} B^1{}_i A^i{}_1 & \dots & B^1{}_i A^i{}_j & \dots & B^1{}_i A^i{}_n \\ \vdots & & \vdots & & \vdots \\ B^k{}_i A^i{}_1 & \dots & B^k{}_i A^i{}_j & \dots & B^k{}_i A^i{}_n \\ \vdots & & \vdots & & \vdots \\ B^l{}_i A^i{}_1 & \dots & B^l{}_i A^i{}_j & \dots & B^l{}_i A^i{}_n \end{pmatrix}$$

$$\equiv \begin{pmatrix} B^1{}_1 & \dots & B^1{}_i & \dots & B^1{}_m \\ \vdots & & \vdots & & \vdots \\ B^k{}_1 & \dots & B^k{}_i & \dots & B^k{}_m \\ \vdots & & \vdots & & \vdots \\ B^l{}_1 & \dots & B^l{}_i & \dots & B^l{}_m \end{pmatrix} . \begin{pmatrix} A^1{}_1 & \dots & A^1{}_j & \dots & A^1{}_n \\ \vdots & & \vdots & & \vdots \\ A^i{}_1 & \dots & A^i{}_j & \dots & A^i{}_n \\ \vdots & & \vdots & & \vdots \\ A^m{}_1 & \dots & A^m{}_j & \dots & A^m{}_n \end{pmatrix} . \qquad \text{(L111)}$$

To compute element $C^k{}_j$ of the matrix $C = BA$ (sometimes also denoted $B \cdot A$) , proceed from left to right along row k of B and from top to bottom along column j of A. Multiply the respective elements of the matrices B and A and add up, $C^k{}_j = B^k{}_1 A^1{}_j + \cdots + B^k{}_m A^m{}_j = B^k{}_i A^i{}_j$, in agreement with Eq. (L110). This amounts to taking the scalar product of row k of B and row j of A, in other words $C^k{}_j = \mathbf{B}^{kT} \cdot \mathbf{A}_j$.

EXAMPLE Let us illustrate the operation of matrix multiplication on a number of examples:

$$\begin{pmatrix} 1 & 4 \\ 5 & 3 \end{pmatrix} \cdot \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} = \begin{pmatrix} 1\cdot 2 + 4 \cdot 1 & 1 \cdot 1 + 4 \cdot 3 \\ 5 \cdot 2 + 3 \cdot 1 & 5 \cdot 1 + 3 \cdot 3 \end{pmatrix} = \begin{pmatrix} 6 & 13 \\ 13 & 14 \end{pmatrix},$$

$$\begin{pmatrix} 1 & 2 \\ 3 & 3 \\ 2 & 4 \end{pmatrix} \cdot \begin{pmatrix} 3 & 1 \\ 2 & 1 \end{pmatrix} = \begin{pmatrix} 1\cdot 3 + 2 \cdot 2 & 1 \cdot 1 + 2 \cdot 1 \\ 3 \cdot 3 + 3 \cdot 2 & 3 \cdot 1 + 3 \cdot 1 \\ 2 \cdot 3 + 4 \cdot 2 & 2 \cdot 1 + 4 \cdot 1 \end{pmatrix} = \begin{pmatrix} 7 & 3 \\ 15 & 6 \\ 14 & 6 \end{pmatrix},$$

$$(2) \cdot (2) = (4).$$

The take-home message of our discussion so far is:

> The composition of linear maps is described by the product of the matrices representing them, where the product operation is defined by Eq. (L111).

Of course, we can consider compositions of more than two maps. For example, if three maps are applied in succession, say first A, then B, then C, one obtains the composite map

$C\circ(B\circ A)=(C\circ B)\circ A=C\circ B\circ A$ where the associativity of the composition means that we do not need to put brackets. In the language of matrices this means $C\cdot B\cdot A=C\cdot(B\cdot A)=(C\cdot B)\cdot A$ where all '$\cdot$' operations are matrix products. When working with products containing more than two matrices it sometimes pays to think about the 'most economic' way to compute the product; matrix multiplication is time consuming and some orders of taking products are more efficient than others. In general, the proliferation of terms to be added/multiplied makes higher-order multiplications cumbersome. Sometimes, however, matrix multiplication leads to simple results, as is illustrated by the following example.

EXERCISE Verify that the product of the matrices A, B and A' given below has the 'diagonal' form indicated on the right:

$$A=\frac{1}{\sqrt{2}}\begin{pmatrix}1&1\\-1&1\end{pmatrix},\qquad B=\begin{pmatrix}0&1\\1&0\end{pmatrix},\qquad A'=\frac{1}{\sqrt{2}}\begin{pmatrix}1&-1\\1&1\end{pmatrix},\qquad ABA'=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

In Sec. L7 we will discuss why the product ABA' assumes a simple form.

We finally note that it is sometimes useful to think of **vectors as matrices**. Indeed, you may identify a vector

$$\mathbf{v}=\begin{pmatrix}v^1\\\vdots\\v^n\end{pmatrix} \tag{L112}$$

with a matrix containing n rows and 1 column. Likewise, the vector $\mathbf{w}^T=(w^1,\ldots,w^n)$ is a matrix containing 1 row and n columns. If $\mathbf{v},\mathbf{w}\in\mathbb{R}^n$ are real, then their scalar product

$$\langle\mathbf{w},\mathbf{v}\rangle=\mathbf{w}^T\mathbf{v}, \tag{L113}$$

may be identified with the matrix product between an $1\times n$ and an $n\times 1$ matrix, which yields an 1×1 matrix, i.e. a number.

Properties of matrix multiplication

Matrix multiplication is one of the most important operations of linear algebra. The matrix product is ($a,a'\in\mathbb{C}$)

- ▷ **associative**: $C\cdot(B\cdot A)=(C\cdot B)\cdot A=C\cdot B\cdot A,$ (L114)
- ▷ **compatible with scalar multiplication**: $(aB)\cdot A=B\cdot(aA)=aB\cdot A,$ (L115)
- ▷ **distributive**: $C\cdot(aB+a'B')=aC\cdot B+a'C\cdot B'.$ (L116)
- ▷ **not commutative** (except in special cases): $A\cdot B\neq B\cdot A.$ (L117)
- ▷ The **transpose** of a matrix product equals the reverse product of transposed matrices:

$$(A\cdot B)^T=B^T\cdot A^T, \tag{L118}$$

By iteration, this formula generalizes to: $(A{\cdot}B{\cdot}C{\cdot}sE)^T = E^T{\cdot}sC^T{\cdot}B^T{\cdot}A^T$.

The **associativity** of matrix multiplication reflects the associativity of the composition of the corresponding linear maps. It also follows directly from the definition (L111) of matrix multiplication: $C^l{}_k(B^k{}_iA^i{}_j) = (C^l{}_kB^k{}_i)A^i{}_j$, implying Eq. (L114). The **distributivity** of the matrix product and its **compatibility with scalar multiplication** are trivial consequences of the definition. The **lack of commutativity** means that linear maps carried out in different orders generally lead to different results. This point is illustrated in the example below. Finally, Eq. (L118) for transposing a matrix product follows from $((A{\cdot}B)^T)_j{}^i = (A{\cdot}B)^i{}_j = A^i{}_kB^k{}_j = (A^T)_k{}^i(B^T)_j{}^k = (B^T)_j{}^k(A^T)_k{}^i = (B^T{\cdot}A^T)_j{}^i$. For the next-to-last equality we used the fact that *individual* matrix elements commute, since they are just numbers, not matrices. (Make sure you understand the difference between this statement and $A \cdot B \neq B \cdot A$ for matrices.)

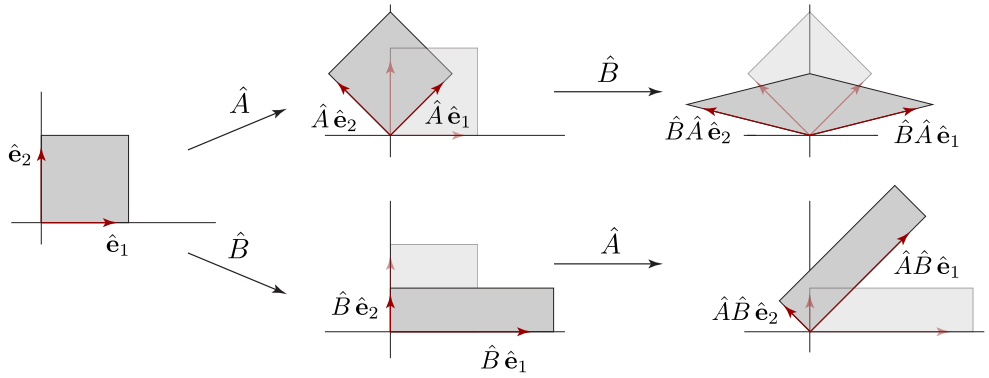


Figure L13: Illustration of the action of the maps $\hat{A}$ and $\hat{B}$ defined in Eq. (L119), and of their compositions $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$ in $\mathbb{E}^2$.

INFO A (real) **algebra** is an $\mathbb{R}$-vector space W with a product operation

$$W \times W \to W, \qquad (u, v) \mapsto u \cdot v,$$

subject to the following conditions ($u, v, w \in W,\ c \in \mathbb{R}$):

- $(u + v) \cdot w = u \cdot w + v \cdot w$,
- $u \cdot (v + w) = u \cdot v + u \cdot w$,
- $c(v \cdot w) = (cv) \cdot w + v \cdot (cw)$.

Our discussion above shows that the space of $n \times n$ matrices $(\mathrm{mat}(\mathbb{R}, n, n), \cdot)$ forms an algebra. Its elements are matrices, $A, B, \ldots$ and its product operation is the matrix multiplication $A \cdot B = C$. Due to the associativity of this operation, the matrix algebra is called an associative algebra.

EXERCISE Consider two maps in $\mathbb{R}^2$ A and B, with matrix representation

$$A = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 2 & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \tag{L119}$$

Compute the action of these matrices act on the standard vectors $(1,0)^T$ and $(0,1)^T$. Convince yourself that A describes a rotation by an angle $\pi/4$ in the counter-clockwise direction, while B describes stretching and shrinking by a factor two in the 1- and 2-directions, respectively (cf. Fig. L13). Now compute the matrix products

$$BA = \begin{pmatrix} 2 & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 2 & -2 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix},$$

$$AB = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 2 & 0 \\ 0 & \frac{1}{2} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 2 & -\frac{1}{2} \\ 2 & \frac{1}{2} \end{pmatrix},$$

that describe rotating then stretching, or stretching then rotating, respectively. Let these composites act on the standard basis vectors to explore how they are changed.

L5.4 The inverse of a matrix

General remarks on invertible linear maps

In section L1.1 we learned that if a map is bijective then an inverse map exists. Specifically, for an invertible linear map $A : \mathbb{C}^n \to \mathbb{C}^m$ there is an inverse map $A^{-1} : \mathbb{C}^m \to \mathbb{C}^n$ such that $A^{-1}A$ is the identity map on $\mathbb{C}^n$ (and AA^{-1} the identity on $\mathbb{C}^m$). These statements raise a number of questions: do invertible maps exist between spaces of arbitrary dimension n and m (try to find an answer in advance)? How can we know if a map possesses an inverse? If it does, how can we obtain it?

First, it turns out that

> Invertible maps $A : \mathbb{C}^n \to \mathbb{C}^m$ can exist only between vector spaces of equal dimension $n = m$.

This statement is intuitively understandable. If $A : \mathbb{C}^n \to \mathbb{C}^m$, and $m > n$, then the target space is 'too big' to be surjectively covered. Conversely, if $m < n$ then it is 'too small' for an injective assignment. Consider, then, maps between spaces of equal dimension, $n = m$. According to our discussion of section L1.1 the bijectivity of maps depends on whether they are both injective and surjective. Whereas for general maps these two features are independent of each other, the situation with linear maps turns out to be simpler:

> For linear maps $A : \mathbb{C}^n \to \mathbb{C}^n$ between vector spaces of equal dimension, the conditions of injectivity and surjectivity are equivalent.

To check the invertibility of a linear map it is therefore sufficient to test either one of the two criteria. In practice, however, the following two turn out to be the most **useful test criteria** for the invertibility of a map $A : \mathbb{C}^n \to \mathbb{C}^n$:

- ▷ Consider a basis, for example the standard basis $\{\mathbf{e}_i\}$, and verify whether the set of image vectors, $\{A\mathbf{e}_i\}$, is also a basis.
- ▷ Equivalently, you may verify that no non-zero vector gets mapped to zero: $\forall \mathbf{v} \neq \mathbf{0} : \ A\mathbf{v} \neq \mathbf{0}$.

If either one of these conditions is met, then A is invertible. (For a proof, see the next subsection.)

We finally remark that for a general matrix, $A : \mathbb{C}^n \to \mathbb{C}^m$, the **kernel** is defined as the set of vectors, $\mathrm{Ker}A \equiv \{\mathbf{v} \in \mathbb{C}^n | A\mathbf{v} = \mathbf{0}\} \subset A$, which get annihilated by A. The kernel of A is a subspace of $\mathbb{C}^n$ (why?). Likewise, the image of A, $\mathrm{Im}(A) = A(\mathbb{C}^n)$, is a subspace of $\mathbb{C}^m$ (why?). The dimension of the image space, $\dim(\mathrm{Im}(A))$, is called the **rank** of the matrix. The invertibility criteria above require that for a matrix $A : \mathbb{C}^n \to \mathbb{C}^n$ the image must span the full space $\mathbb{C}^n$, i.e. its dimension equals the maximal possible value, n:

An invertible matrix $A : \mathbb{C}^n \to \mathbb{C}^n$ has maximal rank n.

The dimension formula

REMARK In this subsection we verify the various statements made in the previous subsection. It can be skipped on first reading

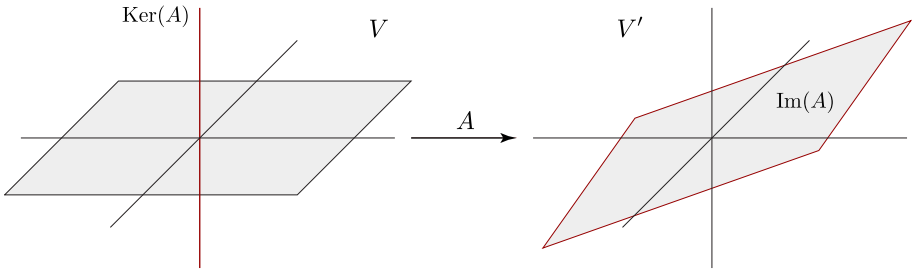


Figure L14: Schematic of the one-dimensional kernel and the two-dimensional image of a linear map $A : V \to V'$ between two three-dimensional vector spaces. For a discussion, see info section below.

Above, we introduced the kernel, $\mathrm{Ker}(A)$, and the image, $\mathrm{Im}(A)$, of a matrix $A : \mathbb{C}^n \to \mathbb{C}^m$ as subspaces of $\mathbb{C}^n$ and $\mathbb{C}^m$, respectively. All that we seem to know *a priori* about the dimensions of these spaces, is that they are smaller or equal to n and m, respectively. However, it turns out that they are related to each other by a stronger relation, known as the **dimension formula**. A simple construction (see info section) shows that

$$\boxed{\dim \mathrm{Ker}(A) + \dim \mathrm{Im}(A) = n.} \tag{L120}$$

For a graphical illustration in the case $n = 3$, $\dim \mathrm{Ker}(A) = 1, \dim \mathrm{Im}(A) = 2$, see Fig. L14. In this case, the dimension of the kernel and the image obviously add to three, i.e. the dimension

of the space where the map is defined. Notice that the formula does not make reference to the dimension, m, of the target space.

INFO

The **proof of Eq.** (L120) is straightforward. Let $k \equiv \dim \mathrm{Ker}(A) \leq n \equiv \dim(\mathbb{C}^n)$. Now construct a basis, $\{\mathbf{v}_i\}$ of $\mathbb{C}^n$ such that $\{\mathbf{v}_1, \ldots, \mathbf{v}_k\}$ span $\mathrm{Ker}(A)$. (For a degenerate kernel, $\mathrm{Ker}(A) = \{\mathbf{0}\}$, containing just the null-vector, we have $k = 0$ and the kernel basis is empty.) The image of A is then spanned by the $n - k$ vectors $\mathbf{w}_1 \equiv A\mathbf{v}_{k+1}, \ldots, \mathbf{w}_{n-k} \equiv A\mathbf{v}_n$, i.e. $\mathrm{span}\{\mathbf{w}_1, \ldots, \mathbf{w}_{n-k}\} = \mathrm{Im}(A)$. It remains to be shown that these vectors are linearly independent. For in this case, $\mathrm{span}\{\mathbf{w}_1, \ldots, \mathbf{w}_{n-k}\} = \mathrm{Im}(A)$ is an $n - k$ dimensional subspace of $\mathbb{C}^m$, which in turn implies $\dim \mathrm{Im}(A) + \dim \mathrm{Ker}(A) = (n - k) + k = n$. To show that the vectors $\mathbf{w}_j$ are linearly independent, assume the opposite, i.e. the existence of a nontrivial linear combination, $\mathbf{0} = a^i \mathbf{w}_i = a^i A\mathbf{v}_{k+i} = A(a^i \mathbf{v}_{k+i})$. This, however, is a contradiction, because the linear combination $a^i \mathbf{v}_{k+i}$ does not lie in $\ker(A)$ and hence it cannot map to the null vector.

Eq. (L120) has a number of important consequences. For example, it implies that invertible maps can exist only between spaces of equal dimension, $n = m$. This follows from Eq. (L120) because an invertible map must be surjective and injective and this requires $\dim \mathrm{Im}(A) = m$ and $\dim \mathrm{Ker}(A) = 0$, respectively. Our relation thus assumes the form $n = m$. Moreover, the formula also implies that if $n = m$, then injectivity and surjectivity are equivalent. To understand this, assume surjectivity, i.e. $\dim \mathrm{Im}(A) = n$. Eq. (L120) then states $\dim \mathrm{Ker}(A) = 0$, which means injectivity. The reverse conclusion, that injectivity implies surjectivity, is shown in the same way.

Finally, notice that the above arguments did not rely on properties distinguishing $\mathbb{C}^n$ from **generic n-dimensional vector spaces**. For maps $A : V \to V'$ between generic spaces, the dimension formula assumes the form

$$\dim \mathrm{Ker}(A) + \dim \mathrm{Im}(A) = \dim V. \tag{L121}$$

All statements regarding injectivity, surjectivity, and bijectivity carry over to the general case.

Matrix inversion

A matrix A representing a map $A : \mathbb{C}^n \to \mathbb{C}^n$ has as many rows as columns and is therefore called a **square matrix**. Assume that A is invertible, i.e. that an inverse map A^{-1} exists. The latter will be represented by an **inverse matrix**, denoted by A^{-1} as well. Its defining property, $A^{-1}A = AA^{-1} = \mathbb{1}$, corresponds to a matrix equation in which $\mathbb{1}$ is the so-called **unit matrix**,

$$\mathbb{1} = \begin{pmatrix} 1 & 0 & \ldots & \\ 0 & 1 & & \\ \vdots & & \ddots & 0 \\ & & 0 & 1 \end{pmatrix}, \tag{L122}$$

or $\mathbb{1}^i{}_j = \delta^i{}_j$, i.e. a matrix whose action on any vector $\mathbb{1}\mathbf{v} = \mathbf{v}$ leaves the vector invariant.

INFO Recall the concept of groups introduced in section L1.2. The set of invertible maps acting on an n-dimensional vector space forms a group: the composition of two invertible maps is again invertible, invertible maps have inverse maps, and we have a neutral element, i.e. the identity map. In the present context, the composition of maps is represented by matrix multiplication. The ensuing group is called the **general linear group** and denoted $\mathrm{GL}(n,\mathbb{F})$, where $\mathbb{F}=\mathbb{R}$ or $\mathbb{C}$, depending on whether V is a real or complex vector space.

In explicit matrix multiplication notation, the equation defining the inverse matrix assumes the form

$$A^{-1}\cdot A=\begin{pmatrix}(A^{-1})^1{}_1 & (A^{-1})^1{}_2 & \cdots & \\ (A^{-1})^2{}_1 & (A^{-1})^2{}_2 & & \\ \vdots & & \ddots & \\ & & & (A^{-1})^n{}_n\end{pmatrix}\cdot\begin{pmatrix}A^1{}_1 & A^1{}_2 & \cdots & \\ A^2{}_1 & A^2{}_2 & & \\ \vdots & & \ddots & \\ & & & A^n{}_n\end{pmatrix}=\begin{pmatrix}1 & 0 & \cdots & \\ 0 & 1 & & \\ \vdots & & \ddots & \\ & & & 1\end{pmatrix}, \tag{L123}$$

where $A^{-1}\equiv\{(A^{-1})^i{}_k\}$. This equation may be equivalently expressed as

$$\boxed{i,j=1,\ldots,n:\qquad (A^{-1})^i{}_kA^k{}_j=\delta^i{}_j.} \tag{L124}$$

EXAMPLE For $n=2$, a straightforward check shows that the matrix inverse is obtained as

$$A=\begin{pmatrix}a & b\\ c & d\end{pmatrix}\Rightarrow A^{-1}=\frac{1}{ad-bc}\begin{pmatrix}d & -b\\ -c & a\end{pmatrix}. \tag{L125}$$

Notice that no inverse exists if $ad=bc$. The reason is that the matrix A then fails the test criteria formulated in the foregoing section. For example, $\mathrm{Ker}(A)$ is not empty, since the vector $\binom{d}{-c}$ is annihilated by A. Equivalently, the image vectors $A\mathbf{e}_1$ and $A\mathbf{e}_2$ are not linearly independent.

Unfortunately, there is no quick and painless way of **computing matrix inverses** for general n. For $n\gtrsim 4$ matrix inversion is often done on a computer. In fact, the optimization of matrix inversion algorithms is a field of active research in computer science which underpins the applied relevance of the problem.

In low dimensions such as $n=2,3,4,\ldots$, a matrix may be constructively inverted as follows: start from the column vector representation (cf. Eq. (L101)) $A^{-1}=(\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_n)$. Substituting this into the matrix equation $AA^{-1}=\mathbb{1}$ we observe that the jth column vector, $\mathbf{a}_j$, is determined by the equation

$$A\mathbf{a}_j=\mathbf{e}_j. \tag{L126}$$

Each vector equation defines a **system of n linear equations** $(A\mathbf{a}_j)^i=A^i{}_k(\mathbf{a}_j)^k=\delta^i{}_j$, which need to be solved for each j. Altogether we thus need to solve $n\times n$ scalar linear equations, or n vector equations. Once we are done with this task the n vectors $\mathbf{a}_j$ define the

desired A^{-1}. An efficient scheme for solving linear systems of equations is discussed in the info section below.

INFO In linear algebra we often need to solve problems such as

$$A\mathbf{x} = \mathbf{b}, \tag{L127}$$

where A is an $m \times n$ matrix, $\mathbf{b} \in \mathbb{C}^m$ a known vector, and $\mathbf{x} \in \mathbb{C}^n$ is sought. Written in components, this assumes the form of a **system of linear equations**,

$$A^i{}_j x^j = b^i, \qquad i = 1, \ldots, m. \tag{L128}$$

For $\mathbf{b} = \mathbf{0}$ the system is called **homogenous**, otherwise it is called **inhomogeneous**. A homogeneous system determines $\mathbf{x}$ only up to a multiplicative constant: if $\mathbf{x}$ satisfies $A\mathbf{x} = \mathbf{0}$ then any $(c\mathbf{x})$, $c \in \mathbb{C}$ does too.

There are different ways to approach problems of this type. The most straightforward one is to proceed by iteration: pick any of the equations $A^i{}_j x^j = b^i$ and solve for x^1 in terms of the unknowns x^2 to x^n as $x^1 = -\frac{1}{A^i{}_1}\left(b^i - \sum_{j=2}^n A^i{}_j x^j\right)$. (Of course, the choice of x^1 is arbitrary. It might be more convenient to start with another component, ideally one for which the r.h.s. contains the smallest number of variables x^j.) Substitute this result into the remaining equations and the problem has been reduced to one of $m-1$ equations for the $n-1$ variables $x^2 \ldots x^n$. This procedure must now be repeated until one of the following situations occur, depending on the values of m and n:

- If there are **as many equations as variables** $m = n$, the system may or may not have a solution. It does not if one of the equations states a contradiction (such as $0 \cdot x^n = b^m$, where b^m is non-vanishing). If no contradiction is encountered and if the system is homogeneous, $\mathbf{b} = \mathbf{0}$, the final equation specifies x^n only up to a multiplicative constant, see remarks above and the example below. If the system is inhomogeneous its **solution is unique**, i.e. the final equation uniquely specifies $x^n = x^n(A, b)$ in terms of the given coefficients $A^i{}_j$, and b^i. One may now iterate backwards by expressing x^{n-1} in terms of x^n, then x^{n-2} in terms of x^{n-1} and x^n, until all $x^j(A, b)$ are specified.

- If there are **fewer equations than variables**, $m < n$, the procedure ends at a point where all m equations have been processed but $n - m$ variables, $x^{m+1,\ldots,n}$, are still unspecified. These variables then have the status of free parameters, i.e. for each choice of $\{x^{m+1}, \ldots, x^n\}$ one can find a solution for all the equations, so that the system has infinitely many solutions. Such systems of equations are called **under-determined**, i.e. the number of equations does not suffice to fix all variables. For an under-determined system one may apply the procedure outlined above to express m variables as $x^j(A, b, x^{m+1,\ldots,n})$ for $j = 1, \ldots m$, i.e. as functions of the given coefficients and the free parameters.

- If there are **more equations than variables**, $m > n$, we run out of variables to eliminate before the last $m-n$ equations have been processed. Such systems are **over-determined** and in general have no solutions.[3]

[3] If the values of all variables are held fixed, the remaining $m-n$ equations assume a purely numerical form, like $3 = 4$ or $3 = 3$. The former, a contradiction, would signify an over-determined system. The latter, a redundancy, would imply that these remaining equations were actually not 'independent' of the first n ones.

For an example of an underdetermined system, consider the homogeneous system $A\mathbf{x} = \mathbf{0}$ defined by the matrix

$$A = \begin{pmatrix} 6 & -1 & 5 \\ 2 & 0 & 2 \\ -8 & 1 & -7 \end{pmatrix}. \tag{L129}$$

Expanded into a system of three equations, this reads

$$\begin{aligned} 6x^1 - x^2 + 5x^3 &= 0, \\ 2x^1 + 2x^3 &= 0, \\ -8x^1 + x^2 - 7x^3 &= 0. \end{aligned} \tag{L130}$$

Start with the second equation to obtain $x_3 = -x_1$. Inserting this result into the first and third equations, they simplify to

$$\begin{aligned} x^1 - x^2 &= 0, \\ -x^1 + x^2 &= 0. \end{aligned}$$

The first of these equations now implies $x^1 = x^2$. The fact that this is compatible with the second equation signals that the system is solvable. Defining $x^3 = c$, we obtain $x^1 = x^2 = -c$ and hence the set of solutions

$$\mathbf{x} = c \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix},$$

parameterized by a free running variable, c. It is good practice to always substitute the result $\mathbf{x}$ back into the defining equations to check that no mistakes have been made. Then, confirm by matrix-vector multiplication that our solution indeed satisfies $A\mathbf{x} = 0$.

EXAMPLE Let us illustrate the algorithm for computing matrix inverses with the example

$$A = \begin{pmatrix} 1 & 1 & -1 \\ 1 & 0 & -\frac{1}{2} \\ -1 & -1 & \frac{3}{2} \end{pmatrix}. \tag{L131}$$

Following the general algorithm, we need to solve three systems of equations, $A\mathbf{a}_j = \mathbf{e}_j$, for $j = 1, 2, 3$. Each of these is processed according to the solution scheme discussed in the info section above. In this way we find,

$$\mathbf{a}_1 = \begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix}, \qquad \mathbf{a}_2 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \qquad \mathbf{a}_3 = \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix},$$

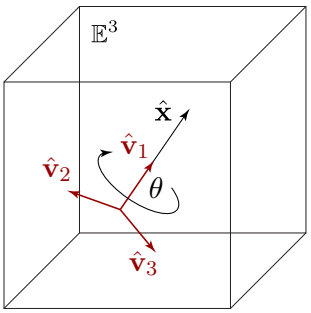
and this is then combined into the matrix

$$A^{-1} = \begin{pmatrix} 1 & 1 & 1 \\ 2 & -1 & 1 \\ 2 & 0 & 2 \end{pmatrix}. \tag{L132}$$

Check by matrix multiplication that $AA^{-1} = \mathbb{1}$ indeed holds.

L5.5 General linear maps and matrices

REMARK Throughout this section, vectors $\hat{\mathbf{v}} \in V$ of general vector spaces will carry a caret to distinguish them from their column vector representations $\mathbf{v} \in \mathbb{C}^n$. General linear maps $\hat{A} : V \to W$ will distinguished by the same symbol from their matrix representations $A : \mathbb{C}^n \to \mathbb{C}^m$.



While our discussion so far was restricted to the standard vector spaces $\mathbb{C}^n$, we now consider linear maps between generic spaces, V. To motivate this generalization, consider the example of Euclidean space $\mathbb{E}^3$. Pick a vector $\mathbf{x}$ and consider rotating space around the direction of $\mathbf{x}$ by an angle θ. In this way a map, A, obeying the linearity criteria is defined (why?). This raises questions like how the action of A can be described in terms of formulas or how this linear map can be included as a building block in more complicated operations. For example, we might want to describe a succession of two rotations around different rotation axes $\mathbf{x}$ and $\mathbf{x}'$. Such operations are no longer easily visualized and we need an efficient formalism for their description.

To this end, let $\hat{A} : V \to W$ be an arbitrary linear map between vector spaces. In both, V and W, we pick (not necessarily orthonormal) bases, $\{\hat{\mathbf{v}}_j\}$ and $\{\hat{\mathbf{w}}_i\}$, respectively. The discussion includes the case $V = W$ of linear maps operating within one vector space (such as the rotation above), $V = W$, in which case identical bases may be chosen, $\hat{\mathbf{w}}_j = \hat{\mathbf{v}}_j$. We may now apply the map $\hat{A}$ to the basis vectors $\hat{\mathbf{v}}_j$ and expand their image vectors, $\hat{\mathbf{u}}_j \equiv A\hat{\mathbf{v}}_j \in W$, in the $\{\hat{\mathbf{w}}_i\}$ basis as

$$j = 1, \ldots, n : \qquad \hat{\mathbf{u}}_j \equiv \hat{A}\hat{\mathbf{v}}_j = \hat{\mathbf{w}}_i A^i{}_j, \tag{L133}$$

where the coefficients $A^i{}_j$ specify the action of the map. Note that for the purposes of the present discussion it is convenient to write the coefficients describing the map *behind* the vectors. This ordering is naturally suggested by the covariant notation, i.e. $\hat{\mathbf{w}}_i A^i{}_j$ puts the summation indices i next to each other and looks more natural than the (identical) expression $A^i{}_j \hat{\mathbf{w}}_i$.

EXAMPLE In our rotation example above, it would be convenient to choose a basis containing a unit vector $\hat{\mathbf{v}}_1$ pointing in the direction of the rotation axis. This vector can be complemented by two mutually orthogonal $\hat{\mathbf{v}}_2 \perp \hat{\mathbf{v}}_3$ unit vectors in the plane perpendicular to $\hat{\mathbf{v}}_1$ to yield a basis $\{\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2, \hat{\mathbf{v}}_3\}$. Only one basis is needed, because our rotation map acts within one vector space. It is then not difficult to see that the rotation acts as

$$\begin{aligned}
\hat{A}\hat{\mathbf{v}}_1 &= \hat{\mathbf{v}}_1, \\
\hat{A}\hat{\mathbf{v}}_2 &= \hat{\mathbf{v}}_2 \cos\theta - \hat{\mathbf{v}}_3 \sin\theta, \\
\hat{A}\hat{\mathbf{v}}_3 &= \hat{\mathbf{v}}_2 \sin\theta - \hat{\mathbf{v}}_3 \cos\theta.
\end{aligned}$$

Given the basis, any V-vector, $\hat{\mathbf{x}}$, may be represented by a column vector $\mathbf{x} \equiv \phi_{\hat{\mathbf{v}}}(\hat{\mathbf{x}})$ in $\mathbb{C}^n$ (see section L2.5). Specifically, the basis vectors $\hat{\mathbf{v}}_j$ get mapped onto the standard basis vectors $\phi_{\hat{\mathbf{v}}}(\hat{\mathbf{v}}_j) = \mathbf{e}_j = (0, \ldots, 1, \ldots, 0)^T$. Likewise, vectors $\hat{\mathbf{y}} \in W$ get represented by column vectors $\mathbf{y} \equiv \phi_{\hat{\mathbf{w}}}(\hat{\mathbf{y}}) \in \mathbb{C}^m$, and basis vectors $\hat{\mathbf{w}}_i$ by standard basis vectors $\mathbf{f}_i = (0, \ldots, 1, \ldots, 0)^T \in \mathbb{C}^m$. Eq. (L133) then states that under $\hat{A}$ a basis vector with component representation $\mathbf{e}_j$ gets mapped onto one with component representation $\mathbf{u}_j \equiv \mathbf{f}_i A^i{}_j = (A^1{}_j, A^2{}_j, \ldots, A^m{}_j)^T$. We thus conclude that the map $\hat{A}$ defines a unique assignment of $\mathbb{C}^n$-standard basis vectors to $\mathbb{C}^m$-component vectors. As discussed in section L5.2, this defines an $m \times n$ matrix $A = (\mathbf{u}_1, \ldots, \mathbf{u}_n)$ containing the image component vectors as columns, and the numbers $A^i{}_j$ (cf. Eq. (L97)) as entries. This map is defined by the equation $A\mathbf{e}_j = \mathbf{u}_j$, i.e. much like $\mathbf{e}_j$ represents the vector $\hat{\mathbf{v}}_j$, the matrix $A : \mathbf{e}_j \mapsto \mathbf{u}_j$ represents the map $\hat{A} : \hat{\mathbf{v}}_j \mapsto \hat{\mathbf{u}}_j$. The situation is summarized in the diagram below. However, always remember that the matrix representation, A, is specific to a choice of basis.

$$
\begin{array}{ccc}
V & \xrightarrow{\hat{A}} & W \\
\hat{\mathbf{v}}_j & \longmapsto & \hat{\mathbf{u}}_j = \hat{A}\mathbf{v}_j \\
{\scriptstyle \phi_{\hat{\mathbf{v}}}}\downarrow & & \downarrow{\scriptstyle \phi_{\hat{\mathbf{w}}}} \\
\mathbf{e}_j & \longmapsto & \mathbf{u}_j = A\mathbf{e}_j \\
\mathbb{C}^n & \xrightarrow{A} & \mathbb{C}^m
\end{array}
$$

EXERCISE Compute the matrix representing the rotation map discussed above.

The discussion above shows how a generic linear map, $\hat{A}$, may be described by a matrix, A. Since these matrix representations are a powerful aid in computations, the typical **workflow for working with linear maps** is as follows:

- ▷ The first step often is the choice of a basis adjusted to the action of the linear map. For example, in the case of rotations, axes of rotation present themselves as directions of basis vectors. For a reflection with respect to a plane one might choose vectors within that plane and complement them by vectors perpendicular to the plane to a basis, etc.
- ▷ Next, one constructs the matrix representating the map, as discussed above.
- ▷ Concrete calculations are then usually performed using matrices. For example, the composition of two linear maps (represented in the same basis, of course) would be described in terms of their matrix product, etc.
- ▷ At the end of a matrix-based computation, the map $\mathbf{x} \mapsto \hat{\mathbf{x}}$ may be applied to switch back to V-vectors.

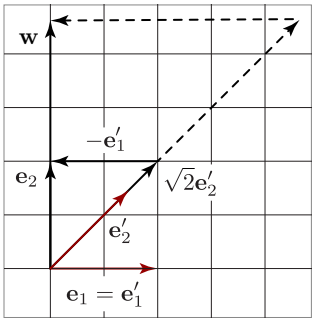
EXERCISE Consider the space (cf. discussion on p. 27) P_4 of all **real-valued polynomials**, $p(x) = ex^4 + dx^3 + cx^2 + bx + a$ of degree equal to or less than 4. Within this space consider differentiation,

$\mathrm{d}_x : P_4 \to P_4$, as a linear map acting on a polynomial as $\mathrm{d}_x p(x) = 4ex^3 + 3dx^2 + 2cx + b$. (Make sure you understand why the differentiation of polynomials of finite degree, n, is a linear map acting in the subspace of polynomials, P_n.) Identify the matrix representing this map in the basis defined by the polynomials $\{x^4, x^3, x^2, x, 1\}$.

L5.6 Matrices describing coordinate changes

REMARK Throughout this section, vectors living in general spaces will be denoted $\hat{\mathbf{x}}$ (i.e. they carry a caret). Their $\mathbb{C}^n$-component representation relative to a basis $\{\hat{\mathbf{v}}_j\}$ will be denoted $\mathbf{x}$, and the representation relative to a basis $\{\hat{\mathbf{v}}'_j\}$ by $\mathbf{x}'$. The formulas discussed in this section are easiest to read if expansion coefficients are written to the right of vectors, i.e. we write $\hat{\mathbf{x}} = \hat{\mathbf{v}}_j x^j$ instead of $x^j \hat{\mathbf{v}}_j$. However, this notation convention is not imperative.

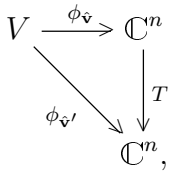
In section L2.5 we discussed how a choice of basis $\{\hat{\mathbf{v}}_j\}$ of a vector space V defines an isomorphism, $\phi_{\hat{\mathbf{v}}} : V \to \mathbb{C}^n$, assigning to each vector $\hat{\mathbf{x}} = \hat{\mathbf{v}}_j x^j \in V$ a component vector $\mathbf{x} = (x^1, \ldots, x^n)^T$. Likewise, we saw that a choice of basis assigns to any linear map, $\hat{A} : V \to V$, a corresponding matrix representation A. If we now choose a different basis, $\{\hat{\mathbf{v}}'_j\}$, the component representation of vectors changes, $\mathbf{x} \mapsto \mathbf{x}'$, and so does the matrix representation, $A \mapsto A'$, but the vectors, $\hat{\mathbf{x}}$, and linear maps, $\hat{\mathbf{A}}$, themselves remain invariant, of course. In a sense, a basis change means a change of 'language' by which the invariant objects $\hat{\mathbf{x}}$ and $\hat{A}$ are described in $\mathbb{C}^n$. Such changes are important operations and in this section we will learn how to describe them efficiently.



EXAMPLE Let us revisit the kitchen example of p. 19 to exemplify how the change of coefficients accompanying a change of bases can be computed in elementary terms. For example, on p. 19 we asked how the components of a vector with representation $\mathbf{w} = (0, 90)^T$ change if we switch from coordinates measured along the walls to ones in which one of the coordinate directions is rotated by 45 deg (see figure, where the vector $\mathbf{w}$ has been shortened for better visibility). Such questions can be conveniently addressed in terms of basis changes. The phrase 'coordinates along the walls' actually means that vectors are represented in terms of two unit length basis vectors, $\mathbf{e}_1$ and $\mathbf{e}_2$, parallel to the walls. Vectors may then be written as, e.g., $\hat{\mathbf{w}} = \hat{\mathbf{e}}_1 0 + \hat{\mathbf{e}}_2 90$, to identify their expansion coefficients in that basis. Suppose now we keep 1 as one coordinate direction but choose the other coordinate direction at a 45 deg angle to the first (see figure). This defines an alternative basis, with $\hat{\mathbf{e}}'_1 = \hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ replaced by $\hat{\mathbf{e}}'_2 = \frac{1}{\sqrt{2}}(\hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_2)$ (make sure you understand this point). To find the coefficients $w^{i\prime}$ of a vector $\hat{\mathbf{w}} = \hat{\mathbf{e}}'_1 w^{1\prime} + \hat{\mathbf{e}}'_2 w^{2\prime}$ expanded in the new basis, we first represent the old basis vectors as linear combinations of the new ones: $\hat{\mathbf{e}}_1 = \hat{\mathbf{e}}'_1$ and $\hat{\mathbf{e}}_2 = -\hat{\mathbf{e}}'_1 + \sqrt{2}\hat{\mathbf{e}}'_2$

(see the figure above). Now substitute this result into the old basis vector expansion to obtain $\hat{\mathbf{w}} = \hat{\mathbf{e}}_1 0 + \hat{\mathbf{e}}_2 90 = \hat{\mathbf{e}}'_1 0 + (-\hat{\mathbf{e}}'_1 + \sqrt{2}\hat{\mathbf{e}}'_2)90 = -\hat{\mathbf{e}}'_1 90 + \hat{\mathbf{e}}'_2\sqrt{2}\,90$. We thus obtain $\hat{\mathbf{w}}' = 90(-1, \sqrt{2})^T$ for the component representation in the new basis. The geometric interpretation of this expansion is shown in the figure above.

The discussion above shows that basis changes are not really complicated operations. All we need to do is solve linear equations, i.e. equations containing the unknowns (such as the expansion coefficients of the old basis vectors in terms of the new ones) to linear order[4] and rearrange terms. At the same time, it should also be evident that calculations of this sort can become cumbersome in higher dimensions where lots of coefficients are involved. In the next subsection, we will discuss how the required operations can be streamlined to maximal efficiency. But before doing so, it is worth understanding the **change of representation** induced by a change of basis on a conceptual level. The situation is summarized in the diagram below, where the maps $\phi_{\hat{\mathbf{v}}}$ and $\phi_{\hat{\mathbf{v}}'}$ assign to vectors $\hat{\mathbf{x}}$ the component representations $\mathbf{x}$ and $\mathbf{x}'$, respectively.



These maps are vector space isomorphisms (i.e. invertible linear maps), which means that the composite map,

$$T = \phi_{\hat{\mathbf{v}}'} \circ \phi_{\hat{\mathbf{v}}}^{-1} : \mathbb{C}^n \to \mathbb{C}^n, \qquad \mathbf{x} \mapsto \phi_{\hat{\mathbf{v}}'}(\phi_{\hat{\mathbf{v}}}^{-1}(\mathbf{x})) = \mathbf{x}', \tag{L134}$$

is an isomorphism, too. The linear map $T : \mathbb{C}^n \to \mathbb{C}^n$, $\mathbf{x} \mapsto T\mathbf{x} = \mathbf{x}'$, describes how the coordinates of the vector $\hat{\mathbf{x}}$ change upon a change of basis. Being a linear map $\mathbb{C}^n \to \mathbb{C}^n$, we can think of T as a matrix. Next we learn how to identify this **transformation matrix** in practical terms.

Transformation matrix

REMARK In this subsection, we sometimes use primed indices like $x'^{j'}$, where $\mathbf{x}'$ defines the component representation of a vector in a new basis, $\{\hat{\mathbf{v}}'_{j'}\}$. While this notation does not look nice, it serves as a reminder indicating whether a index refers to components of the new basis (j') or not (j). However, this notational twist is purely cosmetic (and certainly not standard), the naming of summation indices remains completely arbitrary. It will be abandoned in later sections after some familiarity with basis transformations has been gained.

In the old and the new basis representation, respectively, the expansion of a V-vector $\hat{\mathbf{x}}$ assumes

[4] A quantity x appears to 'linear order' if only its first power appears, i.e. if no terms such as x^α, with $\alpha \neq 1$, are present. For example, $x + 1 = 0$ is a linear equation, but $x^{2/3} + 1 = 0$ or $\sin(x) + 1 = 0$ are not.

the form

$$\hat{\mathbf{x}} = \hat{\mathbf{v}}_j x^j,$$
$$\hat{\mathbf{x}} = \hat{\mathbf{v}}'_{j'} x'^{j'}, \tag{L135}$$

which defines the representation vectors $\mathbf{x} = (x^1, \ldots, x^n)^T$ and $\mathbf{x}' = (x'^1, \ldots, x'^n)^T$. Assume that the expansion of the old basis vectors in terms of the new ones is given by

$$\hat{\mathbf{v}}_j = \hat{\mathbf{v}}'_{j'} T^{j'}{}_j. \tag{L136}$$

Substituting this expansion into the first of the equations above, $\hat{\mathbf{x}} = \mathbf{v}'_{j'} T^{j'}{}_j x^j$, and comparing with the second equation, we obtain the identification

$$x'^{j'} = T^{j'}{}_j x^j. \tag{L137}$$

Eq. L98 then tells us that the basis change is represented by the **transformation matrix**

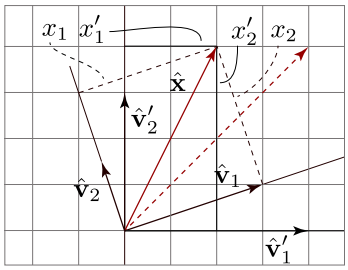
$$T = \begin{pmatrix} T^1{}_1 & \ldots & T^1{}_j & \ldots & T^1{}_n \\ \vdots & & \vdots & & \vdots \\ T^{j'}{}_1 & \ldots & T^{j'}{}_j & \ldots & T^{j'}{}_n \\ \vdots & & \vdots & & \vdots \\ T^n{}_1 & \ldots & T^n{}_j & \ldots & T^n{}_n \end{pmatrix}, \tag{L138}$$

as $\mathbf{x}' = T\mathbf{x}$. Our discussion shows that the contents of the matrix T can be interpreted and used in several different ways:

- ▷ The jth column of this matrix, $\mathbf{T}_j$, with components $T^{j'}{}_j$, contains the expansion coefficients of the jth old basis vector $\hat{\mathbf{v}}_j$ in terms of the new basis vectors $\{\hat{\mathbf{v}}'_{j'}\}$ (Eq. (L136)).
- ▷ The basis vector $\hat{\mathbf{v}}_j$, that used to have the representation $\mathbf{e}_j$ in the old basis, is now represented by the column vector $\mathbf{T}_j = T\mathbf{e}_j$.
- ▷ The vectors $\mathbf{x}'$ and $\mathbf{x}$ in $\mathbb{C}^n$ that represent a general vector $\hat{\mathbf{x}} \in V$ in the new and old bases, respectively, are related by matrix multiplication, $\mathbf{x}' = T\mathbf{x}$ (see Eq. (L137)).

The transformation matrix T tells us how the form of a $\mathbb{C}^n$-vector changes as we pass from the old to the new representation. However, it also specifies the **inverse transformation**, i.e. the question of how a vector assuming a known form in the new representation looked in the old one. To understand how, notice that a change from the old basis to the new one, and then back to the old one amounts to the identity operation. We just discussed how old–to–new is described by a matrix T. The change new–to–old must undo the effect of this transformation, which means that it is described by the **inverse of the transformation matrix**, T^{-1}. A transformation from the old to the new representation and then back is then correctly described as $T^{-1} \cdot T = \mathbb{1}$, i.e. an identity operation.

EXAMPLE Consider the $\mathbb{E}_2$-bases $\{\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2\}$ and $\{\hat{\mathbf{v}}'_1, \hat{\mathbf{v}}'_2\}$ shown in the figure. The old basis vectors are expressed in terms of the new ones as



$$\begin{aligned} \hat{\mathbf{v}}_1 &= \tfrac{3}{4}\hat{\mathbf{v}}'_1 + \tfrac{1}{3}\hat{\mathbf{v}}'_2, \\ \hat{\mathbf{v}}_2 &= -\tfrac{1}{8}\hat{\mathbf{v}}'_1 + \tfrac{1}{2}\hat{\mathbf{v}}'_2, \end{aligned} \tag{L139}$$

and this gives us

$$T = \begin{pmatrix} \frac{3}{4} & -\frac{1}{8} \\ \frac{1}{3} & \frac{1}{2} \end{pmatrix}. \tag{L140}$$

For example, we read off the matrix element $T^1{}_2 = -\frac{1}{8}$ from the first term in the expression $\hat{\mathbf{v}}_2 = \hat{\mathbf{v}}'_1 T^1{}_2 + \hat{\mathbf{v}}'_2 T^2{}_2$. Now consider a vector $\hat{\mathbf{x}} = \hat{\mathbf{v}}_j x^j$ with components $\mathbf{x} = \binom{1}{2}$ with respect to the old basis. According to our discussion above, the representation of $\hat{\mathbf{x}}$ in the new basis, $\hat{\mathbf{x}} = \hat{\mathbf{v}}'_{j'} x'^{j'}$ is obtained as

$$\mathbf{x} \mapsto \mathbf{x}' = T\mathbf{x} = \begin{pmatrix} \frac{3}{4} & -\frac{1}{8} \\ \frac{1}{3} & \frac{1}{2} \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{4}{3} \end{pmatrix}.$$

We conclude that $\hat{\mathbf{x}} = 1\hat{\mathbf{v}}_1 + 2\hat{\mathbf{v}}_2 = \frac{1}{2}\hat{\mathbf{v}}'_1 + \frac{4}{3}\hat{\mathbf{v}}'_2$. This can be confirmed by inspection of the figure. Let us also consider the inverse transformation

$$T^{-1} = \frac{12}{5}\begin{pmatrix} \frac{1}{2} & \frac{1}{8} \\ -\frac{1}{3} & \frac{3}{4} \end{pmatrix}. \tag{L141}$$

(Verify by matrix multiplication that $T^{-1}T = \mathbb{1}$.) We may use it, for example, to check how the representation $(\frac{3}{4}, \frac{1}{3})^T$ of the vector $\hat{\mathbf{v}}_1$ in the *new* basis transforms under a change to the old basis:

$$T^{-1}\begin{pmatrix} \frac{3}{4} \\ \frac{1}{3} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

This confirms that in the old basis $\hat{\mathbf{v}}_1$ was represented by a standard basis vector.

Change of matrix representation

We now understand how basis changes are described by invertible transformation matrices, T, and how they cause a change of component vectors as $\mathbf{x}' = T\mathbf{x}$. Next we address the related question of how matrix representations of linear maps $\hat{\mathbf{y}} = \hat{A}\hat{\mathbf{x}}$ transform under a change of basis.

The defining property of the matrices A and A' which represent the map $\hat{A}$ in the old and the new basis, respectively, is that $\mathbf{y} = A\mathbf{x}$ and $\mathbf{y}' = A'\mathbf{x}'$. Substitution of $\mathbf{y}' = T\mathbf{y}$ and $\mathbf{x}' = T\mathbf{x}$ into the second relation yields $T\mathbf{y} = A'T\mathbf{x}$. We multiply this vector relation by T^{-1}

to obtain $\mathbf{y} = T^{-1}A'T\mathbf{x} \stackrel{!}{=} A\mathbf{x}$. Since this equality holds for arbitrary $\mathbf{x}$, we arrive at the identification

$$\boxed{A = T^{-1}A'T.} \tag{L142}$$

This important formula affords a straightforward interpretation. The application of the map to some vector in the *old* representation (A) is equivalent to the following set of steps:

1. First, pass from the vector's old representation to the new one by applying the matrix T.
2. Then apply the map in the new representation by using the new form of the matrix, A'.
3. Finally, transform the resulting image vector back to the old representation by applying T^{-1}.

Note that Eq. (L142) may be multiplied from the left and right by T and T^{-1}, respectively, to obtain $TAT^{-1} = T(T^{-1}A'T)T^{-1} = A'$, or

$$A' = TAT^{-1}. \tag{L143}$$

Read: the matrix representation in the new basis is obtained from the old representation by applying the inverse transformation matrices. The transformations (L142) and (L143) are sometimes called **similarity transformations**. The name indicates that matrices related by a similarity transformation describe the same linear map, albeit in a different representation.

EXAMPLE Let us illustrate this transformation procedure with the example of the vectors defined in Eq. (L139). Assume that we have a linear map which stretches all vectors in the horizontal direction by a factor of 2. For example, the vector $\hat{\mathbf{x}}$ would map to the dashed vector indicated in the figure. In the language of the ('new') $\hat{\mathbf{v}}'$-basis, this transformation assumes a simple form: $\hat{\mathbf{v}}'_1 \mapsto 2\hat{\mathbf{v}}'_1$ and $\hat{\mathbf{v}}'_2 \mapsto \hat{\mathbf{v}}'_2$, which means that this map has the matrix representation

$$A' = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}. \tag{L144}$$

The application of the transformation matrix (L140) and its inverse (L141) yields the representation of the map in the ('old') $\hat{\mathbf{v}}$-basis:

$$A = T^{-1}A'T = \frac{12}{5}\begin{pmatrix} \frac{1}{2} & \frac{1}{8} \\ -\frac{1}{3} & \frac{3}{4} \end{pmatrix}\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \frac{3}{4} & -\frac{1}{8} \\ \frac{1}{3} & \frac{1}{2} \end{pmatrix} = \frac{1}{10}\begin{pmatrix} 19 & -\frac{3}{2} \\ -6 & 11 \end{pmatrix}. \tag{L145}$$

Let us check that this – awkward looking – result makes sense. Application of the matrix on the right to the 'old–basis–representation' of $\hat{\mathbf{v}}_1$, i.e. $(1,0)^T$, produces the image vector $(19/10, -6/10)^T$, i.e. almost $(2, -0.6)^T$. This tells us that $\hat{\mathbf{v}}_1$ is approximately mapped to $2\hat{\mathbf{v}}_1 - 0.6\,\hat{\mathbf{v}}_2$. Inspect the figure to verify that this statement is consistent with the graphical representation of the transformation.

Matrix trace

The discussion above shows how the matrices representing a linear map transform under changes of basis. However, a linear map also possesses some characteristic properties that are independent of the choice of basis. The simplest of these (others will be discussed below) is the **trace of a matrix** A defined as the sum of all matrix elements on the diagonal:

$$\boxed{\mathrm{tr}(A) \equiv \sum_i A^i{}_i.} \tag{L146}$$

The most important algebraic property of the trace is its so-called **cyclic invariance**. Given two matrices A, B we have

$$\boxed{\mathrm{tr}(AB) = \mathrm{tr}(BA).} \tag{L147}$$

This identity is trivially verified as $\mathrm{tr}(AB) = (AB)^i{}_i = A^i{}_j B^j{}_i = B^j{}_i A^i{}_j = (BA)^j{}_j = \mathrm{tr}(BA)$. The denotation 'cyclic invariance' is motivated by the obvious generalization of the exchange identity to n matrices $A_1, \ldots, A_n$:

$$\mathrm{tr}(A_1 A_2 \ldots A_{n-1} A_n) = \mathrm{tr}(A_n A_1 A_2 \ldots A_{n-1}), \tag{L148}$$

i.e. we may 'cyclically' exchange matrices under the trace.

The cyclic invariance immediately implies that the trace is invariant under a change of basis. We have seen above that under a basis change mediated by a transformation matrix T the matrix representation of a linear transformation A changes as $A \mapsto A' = T^{-1}AT$. However, the trace remains invariant,

$$\mathrm{tr}(A') = \mathrm{tr}(T^{-1}AT) = \mathrm{tr}(TT^{-1}A) = \mathrm{tr}(A). \tag{L149}$$

For example, the matrix A' of Eq. (L144) has the trace $\mathrm{tr}(A') = 2 + 1 = 3$, which equals the trace of its transform, $\mathrm{tr}(A) = \frac{19}{10} + \frac{11}{10} = 3$.

We finally notice that the **matrix trace** is invariant under transposition,

$$\mathrm{tr}(A) = \mathrm{tr}(A^T), \tag{L150}$$

where $\mathrm{tr}(A^T) \equiv \sum_i (A^T)_i{}^i$. This follows trivially from $A^i{}_i = (A^T)_i{}^i$.

Summary

The above discussion conveys an important message: depending on the chosen basis, the matrix representations of linear maps may be nice or ugly (cf. Eq. (L144) vs. Eq. (L145)). We favor to work with nice representations and in the following sections will discuss how such forms can be found. As a reminder, table L5.1 provides a summary of the essential facts about matrix endomorphisms discussed above.

general linear map, $\hat{A} : V \to W$	$\hat{A}(\hat{\mathbf{v}}_j) = \hat{\mathbf{w}}_i A^i{}_j$
~~representation matrix~~ matrix representation, A	$A = \{A^i{}_j\}$
image of standard basis vector $\mathbf{e}_j$ under A	jth column vector of A, $\mathbf{A}_j$
matrix representation of $\hat{A} : \hat{\mathbf{x}} \mapsto \hat{\mathbf{y}}$	$\mathbf{y} = A\mathbf{x}$
basis transformation within V	$\hat{\mathbf{v}}_j = \hat{\mathbf{v}}'_{j'} T^{j'}{}_j$
~~representation matrix~~ matrix representation, T	$T = \{T^{j'}{}_j\}$
jth old standard basis vector in new representation	jth column vector of T, $\mathbf{T}_j$
relation between old and new representations of $\hat{\mathbf{x}}$	$\mathbf{x}' = T\mathbf{x}$
inverse transformation	$\hat{\mathbf{v}}'_{j'} = \hat{\mathbf{v}}_j (T^{-1})^j{}_{j'}$
j'th new standard basis vector in old representation	j'th column vector of T^{-1}, $\mathbf{T}^{-1}_{j'}$
matrix representation of $\hat{A}$ in new basis	$A' = TAT^{-1}$

Table L5.1: Formulas describing matrix representations of linear maps and their changes under basis transformations. In the table, $\{\hat{\mathbf{v}}_j\}$ and $\{\hat{\mathbf{v}}'_{j'}\}$ are distinct bases of the same vector space V.

L6 Matrices II: determinants

At the end of the previous chapter we have introduced the trace of a matrix A as a number — the sum of its diagonal elements — which does not change under changes of basis. There exists one more basis-invariant scalar quantity, the so-called determinant, $\det(A) \in \mathbb{C}$. The very important role played by the determinant is somewhat difficult to describe before it has been defined and applied. However, let us mention in advance that the determinant provides a powerful test for the invertibility of a matrix (it is invertible if and only if the determinant is non-vanishing), and plays a key role in obtaining the simplest possible matrix representation of a linear map. In this chapter we will define the determinant, and discuss its characteristic properties. In later chapters will then be applied in a number of different contexts.

L6.1 Determinant

The **determinant** is a function

$$\det : \mathrm{mat}(\mathbb{C}, n, n) \to \mathbb{C}, \qquad A \mapsto \det(A), \tag{L151}$$

producing numbers from square matrices. The determinant of a matrix is sometimes denoted by $\det(A) \equiv |A|$, or $\det \left(\begin{smallmatrix} 1 & 2 \\ 0 & 3 \end{smallmatrix}\right) \equiv \left|\begin{smallmatrix} 1 & 2 \\ 0 & 3 \end{smallmatrix}\right|$.

Permutations

Gottfried Wilhelm Leibniz (1646-1716)

A German mathematician and philosopher. Leibniz developed infinitesimal calculus independently of Newton. Being fascinated with automated computation, he invented various types of mechanical calculators, and refined the binary number system. In the humanities Leibniz is known for his 'philosophical optimism', e.g. the view that our universe is the best a god could possibly have created.

Before explaining how the determinant is computed, we need to discuss some mathematical aspects of **permutations** (of n objects). A permutation is a reordering of these objects. There are different notations for permutations. For example, labeling the objects as $1, 2, 3, 4$, the symbol $[3, 2, 4, 1]$ denotes the permutation $1 \to 3$, $2 \to 2$, $3 \to 4$, and $4 \to 1$. Alternatively, we may label a permutation by P, where $P(j) \in \{0, 1, \ldots, n\}$ is the number to which j is permuted. Sometimes, the shorthand notation $Pj \equiv P(j)$ is used instead. In this language, $[3, 2, 4, 1]$ is represented as $P1 = 3$, $P2 = 2$, $P3 = 4$, $P4 = 1$.

The set of all permutations of n objects (or numbers) is denoted S_n. For example,

$$S_3 = \{[1, 2, 3], [2, 1, 3], [3, 2, 1], [2, 3, 1], [3, 1, 2], [1, 3, 2]\}. \tag{L152}$$

Exercise: convince yourself that the number of permutations contained in S_n equals $n! \equiv n \cdot (n-1) \cdot \ldots 2 \cdot 1$. For example, S_3 contains $3! = 6$ elements.

INFO Although permutations are easy to define, the underlying mathematics is complex. The set S_n forms a group, the so-called **permutation group**, or **symmetric group**. Composition in this group is the iteration of permutations. For example, if we are given three balls, labeled $1, 2, 3$, we may first exchange the first and the second ball, to obtain $[2, 1, 3]$ and then the second and the third to arrive at the 'product' $[2, 3, 1]$. A permutation can be undone (the inverse) and there is the neutral or identical permutation, $P = \mathrm{id}$, which permutes nothing. Beyond these simple statements, the mathematics of permutations quickly becomes complicated. (The richness of the underlying structures is illustrated, for example, by Rubik's cube whose solution can be understood in terms of the permutation of 54 differently colored squares covering the six faces of the cube.)

Each permutation can be reduced to a sequence of *pair* permutations, i.e. permutations which exchange just two objects at a time. This statement is easy to understand: any re-ordering of n objects can be achieved manually (with one's own two hands) by sequentially swapping pairs of objects. Now, for a given permutation $P \in S_n$ we have two options:[1] the number of pair permutations needed to arrive at P may be even or odd (determine the even/odd attribute for the six permutations of S_3). In the former/latter case, we call P an **even/odd permutation** and define

$$\mathrm{sgn}(P) = \begin{cases} +1, & P \text{ even}, \\ -1, & P \text{ odd}. \end{cases} \tag{L153}$$

[1] Notice that the even/odd attribute is not entirely innocent: there are different ways of realizing a given P by a sequence of pair permutations. However, the 'parity', i.e. the even- or oddness of the number of pair permutations, is an invariant. This makes the function sgn well defined.

as the **signum of a permutation**.

Determinant definition and calculation

We are now in a position to define the **determinant** of an $n \times n$ matrix $A = \{A^i{}_j\}$ as

$$\boxed{\det(A) = \sum_{P \in S_n} \operatorname{sgn}(P) A^1{}_{P1} A^2{}_{P2} \dots A^n{}_{Pn}.} \tag{L154}$$

Let us write down the determinant for the three simplest cases, $n = 1, 2, 3$:

$$\begin{aligned} n = 1: \quad & \det(A) = A^1{}_1, \\ n = 2: \quad & \det(A) = A^1{}_1 A^2{}_2 - A^1{}_2 A^2{}_1, \qquad \text{(L155)} \\ n = 3: \quad & \det(A) = A^1{}_1 A^2{}_2 A^3{}_3 - A^1{}_2 A^2{}_1 A^3{}_3 - A^1{}_3 A^2{}_2 A^3{}_1 \\ & \quad - A^1{}_1 A^2{}_3 A^3{}_2 + A^1{}_2 A^2{}_3 A^3{}_1 + A^1{}_3 A^2{}_1 A^3{}_2 \qquad \text{(L156)} \end{aligned}$$

For example,

$$\begin{aligned} \det \begin{pmatrix} 1 & 3 \\ 2 & 5 \end{pmatrix} &= 1 \cdot 5 - 2 \cdot 3 = -1, \\ \det \begin{pmatrix} 2 & 3 & 1 \\ -1 & 4 & 3 \\ 0 & 2 & 2 \end{pmatrix} &= 2 \cdot 4 \cdot 2 - 3 \cdot (-1) \cdot 2 - 1 \cdot 4 \cdot 0 \\ &\quad - 2 \cdot 3 \cdot 2 + 3 \cdot 3 \cdot 0 + 1 \cdot (-1) \cdot 2 = 8. \end{aligned} \tag{L157}$$

For $n = 4$ the number of terms grows to 24, which illustrates that manually computing determinants of dimension larger than three is cumbersome.

INFO The determinants of real matrices afford a concrete **geometric interpretation**: the absolute value of the determinant of an $n \times n$ matrix A, $|\det A|$, equals the *volume* of the n-dimensional parallelepiped spanned by the column vectors of A. The general proof of this identity requires integration theory and will not be discussed here. However, for two- and three-dimensional matrices the statement can be checked by straightforward computation: for a two-dimensional matrix $A = (\mathbf{A}_1, \mathbf{A}_2)$ with column vectors $\mathbf{A}_1$ and $\mathbf{A}_2$, Eq. (L155) gives

$$n = 2: \quad |\det(A)| = |A^1{}_1 A^2{}_2 - A^1{}_2 A^2{}_1| \overset{\text{(L63)}}{=} A(\mathbf{A}_1, \mathbf{A}_2), \tag{L158}$$

where $A(\mathbf{v}, \mathbf{w})$ is the area of the parallelogram spanned by two vectors, $\mathbf{v}, \mathbf{w}$ (cf. Eq. (L63)). Similarly, for a three-dimensional matrix $A = (\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3)$, Eq. (L156) gives

$$n = 3: \quad |\det(A)| = |\epsilon_{ijk} A^i{}_1 A^j{}_2 A^k{}_3| \overset{\text{(L88)}}{=} |(\mathbf{A}_1 \times \mathbf{A}_2) \cdot \mathbf{A}_3| \overset{\text{(L89)}}{=} V(\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3), \tag{L159}$$

where $V(\mathbf{u}, \mathbf{v}, \mathbf{w})$ is the volume of the parallelepiped spanned by three vectors, $\mathbf{u}, \mathbf{v}, \mathbf{w}$, and the Levi-Civita tensor generates the sign factors occurring in Eq. (L156).

INFO Eq. (L154) is known as the **Leibniz rule**. It defines one of several ways of computing determinants. For completeness we mention an alternative formula, the **Laplace rule**. This rule is useful in computing determinants of matrices containing rows or columns containing a large number of zeros, so-called **sparse matrices**. Laplace's algorithm proceeds in three steps:

1. Choose an arbitrary matrix row, i, (or column, j) of a matrix A. Ideally, choose a row (column) containing a maximum number of zeros.

2. If column no. j has been chosen and ${A^i}_j \neq 0$ compute the so-called **minors** $M^{ij} \in \mathbb{C}$. It is defined as the determinant of the $(n-1) \times (n-1)$ matrix obtained by crossing out column j and row i of A. For example, with column $j = 1$ and A the 3×3 matrix in (L157),

$$M^{11} = \det \begin{pmatrix} 4 & 3 \\ 2 & 2 \end{pmatrix} = 2, \quad M^{21} = \det \begin{pmatrix} 3 & 1 \\ 2 & 2 \end{pmatrix} = 4, \quad M^{31} = \det \begin{pmatrix} 3 & 1 \\ 4 & 3 \end{pmatrix} = 5.$$

   If the rule is applied with reference to a fixed *row* i, the minors M^{ij} need to be computed for varying j.

3. Finally compute the sum

$$\det(A) = \sum_i {A^i}_j (-)^{i+j} M^{ij}, \tag{L160}$$

   where j is fixed and $(-)^{i+j} \equiv (-1)^{i+j}$. One can show that the result thus obtained does not depend on j. For completeness we mention that the product $(-)^{i+j} M^{ij}$ is called the **cofactor** of the matrix element ${A^i}_j$. The formula shows why only minors corresponding to non-vanishing matrix elements enter the scheme. For our 3×3 matrix from Eq. (L157), the evaluation of the sum for $j = 1$ yields

$$\det(A) = 2M^{11} - (-1)M^{21} + 0M^{31} = 2 \cdot 2 + 4 = 8.$$

Laplace's rule reduces the computation of an $n \times n$ determinant to that of the computation of $\leq n$ determinants of lower order $(n-1) \times (n-1)$. Exercises: Apply the rule to the third row of the matrix A.

We will not show the equivalence of Laplace's and Leibniz' rules for computing determinants. However, it is an instructive exercise to rearrange terms in the 3×3 Leibniz expression (L156) such that the determinant assumes the form of Laplace's sum (L160). The general proof is left as a challenging exercise in combinatorics.

INFO There are few **types of matrices for which the calculation of determinants can be simplified**. Consider, for example, the case of **triangular matrices** for which ${A^i}_j = 0$ for either all $i > j$ (upper triangular matrix), or all $i < j$ (lower triangular matrix). These matrices are called 'triangular' because all matrix element to the lower left of the diagonal, or upper right of the diagonal, respectively, vanish by the above condition. The **determinant of a triangular matrix** is simply given by $\det(A) = \prod_i {A^i}_i$. Show how this is a straightforward consequence of Leibniz' rule. (Hint: think which permutations obey the condition $Pi \geq i$ for all i.)

A **matrix block structure** is defined as

$$X = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \tag{L161}$$

where $A \in \mathrm{mat}(r, r, \mathbb{C})$, $D \in \mathrm{mat}(s, s, \mathbb{C})$, and $r+s = n$. The complementary blocks are rectangular matrices $B \in \mathrm{mat}(r, s, \mathbb{C})$ and $A \in \mathrm{mat}(s, r, \mathbb{C})$ of non-quadratic form if $r \neq s$. Any matrix of dimension $n > 1$ carries a block structure with blocks of arbitrary dimension r and $s = n - r$, respectively. Although this is a formal statement, the distinction of blocks really makes sense if the sub-blocks carry distinct meaning. For example, consider an atom containing r electrons and s nucleons (the protons and neutrons forming its nucleus). Let $X^i{}_j$ be the strength of the magnetic interaction between these particles. The interaction strength between the electrons $X^i{}_j$, $i, j \leq r$, or the matrix block A will be qualitatively different from that between the nucleons (block D), or the electron-nucleon interaction B, C. The magnetic interaction matrix therefore naturally carries a block structure.

It can be shown that

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A - BD^{-1}C) \det(D), \tag{L162}$$

i.e. the determinant of the block matrix can be represented as the product of determinants of the $s \times s$ matrix D and the $r \times r$ matrix $A - BD^{-1}C$. Whether or not this representation simplifies the calculation of the determinant depends on the structure of the blocks A, B, C, D. A dramatic simplification arises, e.g., if either $B = 0$ or $C = 0$. In this case the formula collapses to

$$\det \begin{pmatrix} A & 0 \\ C & D \end{pmatrix} = \det \begin{pmatrix} A & B \\ 0 & D \end{pmatrix} = \det(A) \det(D). \tag{L163}$$

INFO Determinants appear frequently in various mathematical contexts and it is important to be able to recognize them as such even if they are not represented exactly as in (**??**). In fact, there exist various popular **alternative determinant representations building on the Leibniz rule** some of which we review here for later reference.

All these re-formulations rely on the option to rearrange permutations in different orders. For example, the matrix elements in (**??**) may be reordered as $\sum_{P \in S_n} \mathrm{sgn}(P) A^{P^{-1}1}{}_1 \dots A^{P^{-1}n}{}_n$, where $P^{-1}j$ is the inverse permutation acting on j. In this form, the covariant (downstairs) indices are arranged in ascending order. (For example, $A^1{}_2 A^2{}_1 A^3{}_3$ may be rearranged as $A^2{}_1 A^1{}_2 A^3{}_3$ where the permutation appearing in the second representation downstairs is the inverse of the permutation appearing in the first representation upstairs.) Now, $\mathrm{sgn}(P) = \mathrm{sgn}(P^{-1})$ (why?) and $\sum_P F(P^{-1}) = \sum_P F(P)$, i.e. the for arbitrary functions, F, the summation over all inverse group elements equals the summation over all group elements. This allows us to rewrite the determinant as

$$\det(A) = \sum_{P \in S_n} \mathrm{sgn}(P) A^{P1}{}_1 A^{P2}{}_2 \dots A^{Pn}{}_n, \tag{L164}$$

with ascending contravariant indices. Also note that the index configuration $(1, 2, \dots, n)$ appearing in these expressions is not 'speicial'. It is just one (viz. the identity) permutation, and can be replaced

by any other $Q(1,2,\ldots,n) \equiv (i_1,\ldots,i_n)$ with no consequence if $\mathrm{sgn}(Q) = 1$ or a sign change if $\mathrm{sgn}(Q)$ is odd. The formal way to see this is by writing

$$\sum_{P\in S_n} \mathrm{sgn}(P) A^{P1}{}_{Q1}\ldots A^{Pn}{}_{Qn} = \sum_{P\in S_n} \mathrm{sgn}(P) A^{Q^{-1}P1}{}_{1}\ldots A^{Q^{-1}Pn}{}_{n} =$$
$$= \sum_{P\in S_n} \mathrm{sgn}(QQ^{-1}P) A^{Q^{-1}P1}{}_{1}\ldots A^{Q^{-1}Pn}{}_{n} = \mathrm{sgn}(Q)\sum_{P\in S_n} \mathrm{sgn}(Q^{-1}P) A^{Q^{-1}P1}{}_{1}\ldots A^{Q^{-1}Pn}{}_{n} =$$
$$= \mathrm{sgn}(Q)\sum_{P\in S_n} \mathrm{sgn}(P) A^{P1}{}_{1}\ldots A^{Pn}{}_{n}.$$

The final sum equals $\det(A)$, and so we have obtained another Leibniz rule clone,

$$\det(A)\,\mathrm{sgn}(Q) = \sum_{P\in S_n} \mathrm{sgn}(P) A^{P1}{}_{Q1} A^{P2}{}_{Q2}\ldots A^{Pn}{}_{Qn} \tag{L165}$$

We finally note that the formula can be written in a more compact form by introducing the fully antisymmetric tensor

$$\epsilon_{j_1,j_2,\ldots,j_n} \equiv \epsilon^{j_1,j_2,\ldots,j_n} \equiv \begin{cases} \mathrm{sgn}[j_1,\ldots,j_n], & (j_1,\ldots,j_n) \text{ a permutation of } (1,\ldots,n) \\ 0, & \text{else.} \end{cases} \tag{L166}$$

This is the generalization of the Levi-Civita symbol (L77) to index arguments of higher order. Using this symbol, the determinant formula assumes the compact form

$$\det A = \epsilon^{j_1,j_2,\ldots,j_n} A^1{}_{j_1} A^2{}_{j_2}\ldots A^n{}_{j_n} = \epsilon_{j_1,j_2,\ldots,j_n} A^{j_1}{}_1 A^{j_2}{}_2\ldots A^{j_n}{}_n. \tag{L167}$$

With $\mathrm{sqn}([i_1,\ldots,i_n]) = \epsilon_{i_1,\ldots,i_n}$ the generalization Eq. (L165) assumes the compact form

$$\boxed{\det A\,\epsilon_{i_1,\ldots,i_n} = \epsilon_{j_1,j_2,\ldots,j_n} A^{j_1}{}_{i_1} A^{j_2}{}_{i_2}\ldots A^{j_n}{}_{i_n}.} \tag{L168}$$

Determinant properties

Much like the trace, the determinant is a 'fingerprint' of a linear map in that it does not change under changes of basis. Besides, it has many other useful properties summarized below. All of these are straightforward consequences of the definition, although in some cases the proof may not be entirely obvious. (In such cases we refer to lecture courses in linear algebra or mathematics textbooks for detailed discussions.) In subsequent chapters the usefulness of the **properties of the determinant function** discussed below will show in concrete applications.

1. For a **diagonal matrix**, $D = \mathrm{diag}(\lambda_1,\ldots,\lambda_n)$ Leibniz' formula implies that the determinant is given by the product of the diagonal elements,[2]

$$\det(D) = \prod_{i=1}^{n} \lambda_i. \tag{L169}$$

The determinant of a diagonal matrix containing zeroes on the diagonal vanishes.

[2] The symbol $\prod$ is the product analog of the sum, $\sum$, i.e. $\prod_{i=1}^n x_i = x_1\cdot x_2\cdot\cdots\cdot x_n$.

2. The determinant is **invariant under transposition**,

$$\boxed{\det(A^T) = \det A.} \tag{L170}$$

(This can be proven by exchanging matrix indices in the Leibniz formula and using that for any set of objects $\{X_{ij}\}$, $\sum_P \prod_i X_{i\,Pi} = \sum_P \prod_i X_{Pii}$ (why?).)

We also note that under complex conjugation it behaves as

$$\overline{\det(A)} = \det(\overline{A}), \tag{L171}$$

where $\overline{A} = \{\overline{A^i{}_j}\}$ is the complex conjugate of the matrix. Combining this with Eq. (L170), we obtain

$$\det(A^\dagger) = \overline{\det A}, \tag{L172}$$

where the adjoint is defined in Eq. (L108).

3. The determinant is **antisymmetric** under the pairwise **exchange** of two rows **columns** or of two **rows**,

$$\det(\dots, \mathbf{A}_i, \dots, \mathbf{A}_j, \dots) = -\det(\dots, \mathbf{A}_j, \dots, \mathbf{A}_i, \dots), \tag{L173}$$

$$\det \begin{pmatrix} \vdots \\ \mathbf{A}^{iT} \\ \vdots \\ \mathbf{A}^{jT} \\ \vdots \end{pmatrix} = -\det \begin{pmatrix} \vdots \\ \mathbf{A}^{jT} \\ \vdots \\ \mathbf{A}^{iT} \\ \vdots \end{pmatrix}. \tag{L174}$$

Here, the ellipses represent rows or columns that remain unchanged. The sign change implies that for matrices containing identical rows or columns the determinant equals its own negative, i.e. it vanishes.

4. **Multilinearity**: The determinant is **linear in each column**. With $r, r' \in \mathbb{C}$,

$$\det(\dots, r\mathbf{A}_j + r'\mathbf{A}'_j, \dots) = r\det(\dots, \mathbf{A}_j, \dots) + r'\det(\dots, \mathbf{A}'_j, \dots). \tag{L175}$$

Similarly, the determinant is **linear each row**,

$$\det \begin{pmatrix} \vdots \\ r\mathbf{A}^{iT} + r'\mathbf{A}^{i'T} \\ \vdots \end{pmatrix} = r\det \begin{pmatrix} \vdots \\ \mathbf{A}^{iT} \\ \vdots \end{pmatrix} + r'\det \begin{pmatrix} \vdots \\ \mathbf{A}^{i'T} \\ \vdots \end{pmatrix}. \tag{L176}$$

Notice the similar behavior of the determinant with respect to operations affecting rows or columns, respectively. Convince yourself that this is a consequence of the invariance of the determinant under transposition, Eq. (L170).

5. For $r \in \mathbb{C}$, the determinant obeys the relation

$$\det(rA) = r^n \det(A), \tag{L177}$$

where $(rA)_{ij} \equiv rA_{ij}$. This formula can be proven by repeated application of Eq. (L175) for $r' = 0$.

6. The determinant of a matrix vanishes if it contains **linearly dependent rows or columns**. For example, if $\mathbf{A}_1 = \sum_{i=2}^n c^i \mathbf{A}_i$ Eq. (L175) may be applied to reduce $\det(A)$ to a sum of determinants of the form $\det(\mathbf{A}_i, \dots, \mathbf{A}_i, \dots)$. The antisymmetry relation (L173) implies that each determinant in the sum vanishes individually. Notice that the above relation implies the vanishing of $A(\mathbf{e}_1 - \sum_{i=2}^n c^i \mathbf{e}_i) = \mathbf{A}_i - \sum_{i=2} c^i \mathbf{A}_i$, i.e. the existence of a non-vanishing vector that is annihilated by A. Conversely, if we have a vector $\mathbf{v} = c^i \mathbf{e}_i$ with this property, $\mathbf{0} = A(c^i \mathbf{e}_i) = c^i \mathbf{A}_i$, then the column vectors of A are linearly independent and the determinant vanishes. This leads us to the important conclusion,

7. The **determinant vanishes if and only if a matrix is non-invertible**, i.e. if it annihilates a non-vanishing vector. This criterion provides a rather **powerful test for the invertibility of a matrix**: compute its determinant and if a non-vanishing result is obtained, invertibility is guaranteed.

8. Crucially, the **determinant of a product of matrices** equals the product of determinants,

$$\boxed{\det(AB) = \det(A)\det(B),} \tag{L178}$$

for $A, B \in \mathrm{mat}(\mathbb{C}, n, n)$. The proof is based on direct algebraic manipulations of the Leibniz formula and can be found in mathematics textbooks.

9. Eq. (L178) implies an important formula for the **inverse of determinants**. From Eq. (L169) we know that the unit matrix has unit determinant, $\det(\mathbb{1}) = 1$. Now use that $1 = \det(\mathbb{1}) = \det(AA^{-1}) = \det(A)\det(A^{-1})$ to obtain

$$\boxed{\det(A^{-1}) = \frac{1}{\det(A)}.} \tag{L179}$$

10. An important consequence of Eqs. (L178) and (L179) is that

the determinant of a matrix is invariant under a change of basis.

If the new representation of a matrix A after a basis change is $A' = TAT^{-1}$, then we have

$$\det(A') = \det(TAT^{-1}) \overset{(L178)}{=} \det(T)\det(A)\det(T^{-1}) \overset{(L179)}{=} \det(A). \tag{L180}$$

Above, we have seen that all invertible matrices, i.e. all elements of the matrix group $\mathrm{GL}(n,\mathbb{C})$ have a non-vanishing determinant. The subset, $\mathrm{SL}(n,\mathbb{C}) \subset \mathrm{GL}(n,\mathbb{C})$, defined by the condition that the determinant equals unity,

$$\mathrm{SL}(n,\mathbb{C}) = \{A \in \mathrm{GL}(n,\mathbb{C}) | \det(A) = 1\}, \tag{L181}$$

is called the **special linear group**. It is a group (with matrix multiplication as composition), rather than just a subset, because the group axioms are satisfied: it contains the unit matrix, $\mathbb{1} \in \mathrm{SL}(n,\mathbb{C})$, which acts as the group's unit element; if $\det(A) = \det(B) = 1$, then $\det(AB) = \det(A)\det(B) = 1$, i.e. matrix multiplication is compatible with the group definition; and if $\det(A) = 1$, then $\det(A^{-1}) = (\det(A))^{-1} = 1$, hence the inverse of A also lies in the group. The special linear group, both in its complex and real version $\mathrm{SL}(n,\mathbb{C})$ and $\mathrm{SL}(n,\mathbb{R})$, respectively, is one of several subgroups of $\mathrm{GL}(n,\mathbb{C})$ which are used to describe certain linear physical transformations. However, the full meaning of these objects becomes apparent only in the middle of the curriculum when disciplines such as relativity or particle physics are discussed.

EXAMPLE It is instructive to verify the **properties of the determinant** for the simple case of a 2×2 matrix

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{L182}$$

with determinant

$$\det(A) = ad - bc. \tag{L183}$$

1. For a diagonal matrix, $b = c = 0$, Eq. (L183) indeed reduces to $\det A = ad$, the product of diagonal elements.
2. Invariance under transposition follows from the invariance of (L183) under exchange $c \leftrightarrow b$.
3. Column antisymmetry is illustrated by $\det \left(\begin{smallmatrix} b & a \\ d & c \end{smallmatrix}\right) = bc - ad = -\det(A)$.
4. Column-linearity (L175) is illustrated by $\det \left(\begin{smallmatrix} (a+a') & b \\ (c+c') & d \end{smallmatrix}\right) = (a+a')d - b(c+c') = (ad-bc) + (a'd - bc') = \det \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) + \det \left(\begin{smallmatrix} a' & b \\ c' & d \end{smallmatrix}\right)$, row linearity is shown in the same way.
5. To verify Eq. (L177) consider $\det(rA) = \det \left(\begin{smallmatrix} ra & rb \\ rc & rd \end{smallmatrix}\right) = (ra)(rd) - (rb)(rc) = r^2(ad-bc) = r^2 \det(A)$.
6. If the determinant vanishes, this fixes one parameter of the matrix, for example $a = bc/d$. Verify that the same condition is required to obtain a non-trivial solution, $\mathbf{v}$, of $A\mathbf{v} = 0$.
7. Eq. (L178) is verified by defining two 2×2 matrices, A and B, computing the product AB, and comparing its determinant with the product of the determinants of the individual matrices.
8. The inverse of the matrix (L182) is given by Eq. (L125). Taking its determinant we indeed obtain $\det A^{-1} = \frac{1}{(ad-bc)^2}(da - bc) = \frac{1}{ad-bc} = 1/\det(A)$.

INFO For the purpose of illustration, let us discuss the proof of the exchange identity (L174). The proofs of other identities are of comparable complexity and use similar arguments. Most **proofs of determinant properties** use the Leibniz rule (L154) and the group property of permutations. To illustrate this, let $P_{[1,2]}$ denote the pair permutation exchanging the first and the second elements of a set of n numbers, e.g. $P_{[1,2]}\{3,4,2,1\} = \{4,3,2,1\}$. For an arbitrary permutation, P, the composition $P' = P \circ P_{[1,2]}$ is again a permutation — the group property. The composite permutation P' acts as $P'2 = P1$, $P'1 = P2$, and $P'l = Pl$ for $l > 2$. We also know that $\mathrm{sgn}(P') = -\mathrm{sgn}(P)$, because P and P' differ by one pair permutation (if P is even P' is odd, and vice versa). Now, consider two matrices A and A' differing by an exchange of the first and the second row:

$$A = \begin{pmatrix} \mathbf{A}^{1T} \\ \mathbf{A}^{2T} \\ \mathbf{A}^{3T} \\ \vdots \\ \mathbf{A}^{nT} \end{pmatrix}, \qquad A' = \begin{pmatrix} \mathbf{A}^{2T} \\ \mathbf{A}^{1T} \\ \mathbf{A}^{3T} \\ \vdots \\ \mathbf{A}^{nT} \end{pmatrix}. \tag{L184}$$

We thus know that ${A'^1}_i = {A^2}_i$ and ${A'^2}_i = {A^1}_i$, while all components taken from rows other than 1 and 2 are equal. Now let us apply the Leibniz rule to the computation of the respective determinants:

$$\begin{aligned}
\det(A') &= \sum_{P\in S_n} \mathrm{sgn}(P) {A'^1}_{P1} {A'^2}_{P2} {A'^3}_{P3} \dots {A'^n}_{Pn} \\
&= \sum_{P\in S_n} \mathrm{sgn}(P) {A^2}_{P1} {A^1}_{P2} {A^3}_{P3} \dots {A^n}_{Pn} \\
&= -\sum_{P\in S_n} \mathrm{sgn}(P') {A^2}_{P'2} {A^1}_{P'1} {A^3}_{P'3} \dots {A^n}_{P'n} \\
&= -\sum_{P'\in S_n} \mathrm{sgn}(P') {A^1}_{P'1} {A^2}_{P'2} {A^3}_{P'3} \dots {A^n}_{P'n} = -\det(A).
\end{aligned}$$

In the second equality we used the exchange relation (L184) between A' and A; in the third the relation between P' and P; and in the fourth, that if P runs over all permutations in S_n so does P', i.e. $\sum_{P\in S_n} = \sum_{P'\in S_n}$. The final equality is just the definition of the determinant where the summation 'variable' P' replaces P.

L7 Matrices III: diagonalizing matrices

L7.1 Diagonal matrices

Next to the unit matrix, the so-called **diagonal matrices** are the simplest of matrices. As is indicated by the name a diagonal matrix, D, has its only non-vanishing matrix elements on the 'matrix diagonal', ${D^i}_j = {\delta^i}_j \lambda_j$, or

$$D = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix}.$$

In writing such matrices it is customary to leave areas with vanishing matrix elements blank, i.e. zeros are omitted unless they occur on the diagonal itself. An even more compact notation reads

$$D = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n). \tag{L185}$$

The problem with diagonal matrices is that they are fragile objects: under a transformation of bases represented by a transformation matrix T, D transforms as

$$D \overset{\text{(L143)}}{\longmapsto} A = TDT^{-1},$$

which will *not* in general be diagonal.
These observations motivate a number of questions:

- ▷ Given a general matrix, A, how can we know if it is a diagonal matrix 'in disguise'? I.e. does there exist a transformation such that $A = TDT^{-1}$? This would mean that the matrix T describes the transformation to a new basis in which A assumes the particularly simple form of a diagonal matrix.
- ▷ Can every matrix A be transformed into a diagonal matrix?
- ▷ Does there exist an algorithm to compute the matrices T which transform a given matrix into a diagonal representation?

INFO At first sight these may seem like abstract questions. However, the problem of finding simple (diagonal) representations of matrices is of great **practical importance** not just in physics but also in engineering, computer science, biology, and other contexts. The reason is that many phenomena in nature, or in statistical sciences can be approximately described in terms of matrices representing linear maps. The generic representation especially of large matrices generally does not tell much about their action. However, its action becomes much more transparent if we know a diagonal representation.

The importance of the problem shows in that physicists, mathematicians and computer scientists alike are investing a lot of effort into improving algorithms for the constructive 'diagonalization' of complex linear maps.

L7.2 Eigenvectors and eigenvalues

A diagonal matrix acts on the ith standard basis vector, $\mathbf{e}_i$, by scalar multiplication:

$$D\mathbf{e}_i = \lambda_i \, \mathbf{e}_i \tag{L186}$$

Generally a vector, $\mathbf{v}$, that remains invariant up to scalar multiplication under the application of a matrix, A, $A\mathbf{v} = \lambda\mathbf{v}$ is called an **eigenvector**[1] of that matrix, and $\lambda \in \mathbb{C}$ is called its **eigenvalue**. Eq. (L186) states that the standard basis vectors $\mathbf{e}_i$ are eigenvectors of D and that the corresponding eigenvalues λ_i are given by the diagonal elements. Eigenvectors and eigenvalues are a concept of key relevance to the diagonalization of matrices.

To understand why, assume now that we had switched to a different basis. The previously diagonal matrix would now assume the form $A = TDT^{-1}$, which will be non-diagonal in general. However, a key feature of the new representation is that it still possesses n linearly independent eigenvectors $\mathbf{e}'_i \equiv T\mathbf{e}_i$. This is checked by computing $A\mathbf{e}'_i = (TDT^{-1})(T\mathbf{e}_i) = TD\mathbf{e}_i = T\lambda_i\mathbf{e}_i = \lambda_i T\mathbf{e}_i = \lambda_i\mathbf{e}'_i$. While the eigenvectors change their form under the transformation (from standard basis vectors $\mathbf{e}_i$ to $T\mathbf{e}_i$),

the set of eigenvalues $\{\lambda_i\}$ of a matrix is not affected by a transformation of bases.

The key to matrix diagonalization, i.e. the constructive transformation of a given matrix to diagonal form, lies in reversing the above construction: assume we were given an arbitrary matrix A and had succeeded in finding n linearly independent eigenvectors, $\mathbf{v}_i$, with eigenvalues λ_i. As we will discuss in the rest of the chapter, A can then be transformed to a diagonal representation and $T = (\mathbf{v}_1, \ldots, \mathbf{v}_n)$ is the matrix describing this transformation.

L7.3 Characteristic polynomial

The key to the diagonalization of a matrix, A, lies in its eigenvectors and eigenvalues. How can these be found? An eigenvector, $\mathbf{v}$, obeys the equation $A\mathbf{v} = \lambda\mathbf{v}$ or $(A - \lambda\mathbb{1})\mathbf{v} = 0$, where

[1] The word 'eigen', loaned from German, translates to 'own'.

λ is its as yet unknown eigenvalue. If this equation is to have a non-vanishing solution, then the matrix $A - \lambda\mathbb{1}$ must have a vanishing determinant, $Z(\lambda) \equiv \det(A - \lambda\mathbb{1}) = 0$ (because it annihilates a non-vanishing vector, $\mathbf{v}$). This condition should be read as a necessary and sufficient criterion for λ to be an eigenvalue:

Every eigenvalue λ of a matrix A satisfies the condition $\det(A - \lambda\mathbb{1}) = 0$.

We may evaluate the determinant using the Leibniz formula (L154),

$$Z(\lambda) = \sum_{P\in S_n} \operatorname{sgn}(P)(A - \lambda\mathbb{1})^1{}_{P1}(A - \lambda\mathbb{1})^2{}_{P2}\dots(A - \lambda\mathbb{1})^n{}_{Pn}. \tag{L187}$$

to notice that $Z(\lambda)$ is a *polynomial* of degree n in λ. The polynomial nature of $Z(\lambda)$ follows from the observation that the highest power of λ present in the product of n factors $(A-\lambda\mathbb{1})^i{}_{Pi}$ is given by λ^n.[2] In general, the sum will contain arbitrary lower powers of λ as well, so it may be represented as

$$Z(\lambda) = \sum_{i=0}^{n} c_n\lambda^n, \tag{L188}$$

with coefficients $c_i \in \mathbb{C}$ depending on the matrix elements A_{ij}.

The polynomial $Z(\lambda)$ is called the **characteristic polynomial** of A. It is a 'characteristic' feature of the matrix, A, in that it does not change under transformations of basis. This follows from the fact that for $A' = T^{-1}AT$, $\det(A' - \lambda\mathbb{1}) = \det(T^{-1}AT - \lambda T^{-1}\mathbb{1}T) = \det(T^{-1}(A - \lambda\mathbb{1})T) = \det(A - \lambda\mathbb{1})$, where we used that $T^{-1}\mathbb{1}T = \mathbb{1}$ and the invariance of the determinant Eq. (L182). The invariance of the characteristic polynomial is, of course, an expected feature of a function determining the invariant eigenvalues.

INFO There is not much that can be said in general about the **coefficients of the characteristic polynomial**. For $\lambda = 0$ we obtain $Z(0) = \det(A)$ by definition of the characteristic polynomial and $Z(0) = c_0$ according to Eq. (L188). This yields the identification $c_0 = \det(A)$. The two highest possible powers, λ^n and λ^{n-1}, are obtained from the contribution $\prod_i(A^i{}_i - \lambda) = (-\lambda)^n + (-\lambda)^{n-1}\sum_{i=1}^n A^i{}_i + \dots$ of the unit permutation $Pi = i$ to the sum. Here, the ellipses denote terms of order λ^{n-2} and less. We thus conclude $c_n = (-)^n$ and $c_{n-1} = -\sum_{i=1}^n A^i{}_i = -\mathrm{tr}(A)$. All other coefficients, $c_1, \dots, c_{n-2}$, have a more complicated structure.

Once a value λ has been found for which the characteristic polynomial vanishes, $Z(\lambda) = 0$, the corresponding eigenvector, $\mathbf{v}$, is obtained by solving the system of linear equations $(A-\lambda\mathbb{1})^i{}_j v^j$ for the coefficients v^j. This can be done by the methods discussed on p.76. Before discussing how the program can be iterated to achieve a systematic diagonalization of matrices, let us illustrate it on the simple example of a 2×2-matrix.

[2] To see this, consider the contribution of the unit perturbation $Pi = i$ to the sum and evaluate $(A - \lambda\mathbb{1})^1{}_1(A - \lambda\mathbb{1})^2{}_2\dots(A - \lambda\mathbb{1})^n{}_n = (-\lambda)^n + \dots$, where the ellipses represent powers in λ of lower order.

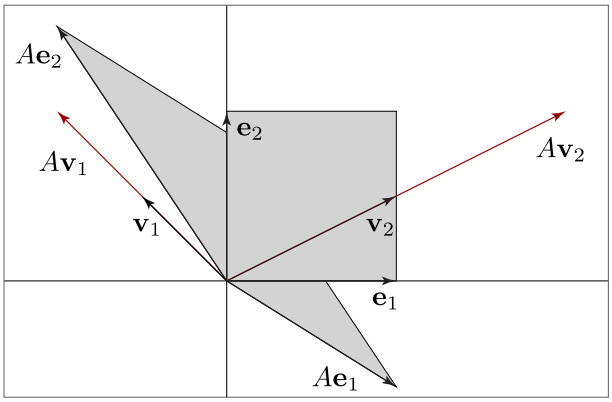


Figure L15: Action of the matrix (L189) in the two dimensional plane. Discussion, see text.

EXAMPLE Consider the 2×2 matrix

$$A = \begin{pmatrix} 1 & -1 \\ -\frac{1}{2} & \frac{3}{2} \end{pmatrix}. \tag{L189}$$

This matrix acts on the unit vectors $\mathbf{e}_{1,2}$ as shown in Fig. L15. It simultaneously stretches and rotates the vectors, which leads to a distortion of the plane, as indicated in the figure. Now let us identify the eigenvectors, $\mathbf{v}_{1,2}$, of the matrix. Following the above procedure the first step is to set up the characteristic polynomial

$$Z(\lambda) = \det(A - \lambda \mathbb{1}) = \det \begin{pmatrix} 1-\lambda & -1 \\ -\frac{1}{2} & \frac{3}{2}-\lambda \end{pmatrix} = (1-\lambda)(\tfrac{3}{2}-\lambda) - \tfrac{1}{2} = \lambda^2 - \tfrac{5}{2}\lambda + 1.$$

The ensuing equation $Z(\lambda) = 0$ is quadratic and its two solutions are given by $\lambda_1 = 2$ and $\lambda_2 = \frac{1}{2}$. We may now find the corresponding eigenvectors by solution of

$$(A - \lambda_1 \mathbb{1})\mathbf{v}_1 = \begin{pmatrix} -1 & -1 \\ -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} {v^1}_1 \\ {v^2}_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow \mathbf{v}_1 = c_1 \begin{pmatrix} 1 \\ -1 \end{pmatrix},$$
$$(A - \lambda_2 \mathbb{1})\mathbf{v}_2 = \begin{pmatrix} \frac{1}{2} & -1 \\ -\frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} {v^1}_2 \\ {v^2}_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Rightarrow \mathbf{v}_2 = c_2 \begin{pmatrix} 2 \\ 1 \end{pmatrix},$$

where $c_{1,2}$ are arbitrary constants which may be set, e.g., to unity, $c_{1,2} = 1$. We may now verify the eigenvector property by checking $A\mathbf{v}_{1,2} = \lambda_{1,2}\mathbf{v}_{1,2}$ (try it yourself). It is easy to make mistakes when computing eigenvectors, so a check should be a routine element of the program. Along the direction specified by $\mathbf{v}_{1,2}$ the matrix A acts by stretching by the factors $2, 1/2$. The two vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ are linearly independent, and the matrix transforming A into a diagonal representation is given by (cf. the general discussion of section L7.2)

$$T = (\mathbf{v}_1, \mathbf{v}_2) = \begin{pmatrix} 1 & 2 \\ -1 & 1 \end{pmatrix}, \qquad T^{-1} = \frac{1}{3}\begin{pmatrix} 1 & -2 \\ 1 & 1 \end{pmatrix}.$$

It is straightforward to verify that $T^{-1}AT = \mathrm{diag}(2, \frac{1}{2})$ assumes a diagonal form.

EXERCISE Consider the matrices shown in the example of p.70 and discuss in which sense they can be understood as part of a diagonalization program.

EXERCISE Consider the matrix A from Eq. (L129). Show that its characteristic polynomial is given by

$$Z(\lambda) = -\lambda^3 - \lambda^2 + 2\lambda = -\lambda(\lambda - 1)(\lambda + 2), \tag{L190}$$

with zeros $\lambda_0 = 0$, $\lambda_1 = 1$, $\lambda_2 = -2$.

L7.4 Matrix diagonalization

General structures

We are now in a good position to discuss the diagonalizability of matrices from a general perspective. The previous section has shown that the zeros of the characteristic polynomial, $Z(\lambda)$, play a key role in the process. A first question to ask then is whether every characteristic polynomial need to have zeros. The answer depends on whether we are operating in real or complex vector spaces. For example the characteristic polynomial of the real matrix

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{L191}$$

is given by $Z(\lambda) = \lambda^2 + 1$ and does not have *real* zeros. This means that no real eigenvalues can be found and that the matrix is not diagonalizable in terms of real matrices.

The situation in the complex vector space $\mathbb{C}^n$ is different. According to the **fundamental theorem of algebra** (whose proof is a subject of 'algebra', not 'linear algebra'), every polynomial of degree n has an equal number of complex zeros $\lambda_i \in \mathbb{C}$ and can hence be factorized as

$$Z(\lambda) = \prod_{i=1}^{n} (\lambda - \lambda_i), \qquad \lambda_i \in \mathbb{C}. \tag{L192}$$

For example, the characteristic polynomial of the matrix A in Eq. (L191) can be factored as $Z(\lambda) = \lambda^2 + 1 = (\lambda - i)(\lambda + i)$ with complex zeros $\lambda_1 = i$ and $\lambda_2 = -i$. Considered as an element of $\mathrm{mat}(2, 2, \mathbb{C})$ the matrix A therefore *is* diagonalizable. A simple and important corollary of Eq. (L192) is that

The determinant of a matrix $\det(A) = \prod_i \lambda_i$ equals the product of its eigenvalues.

This follows from the observation that on the one hand $Z(0) = \det(A)$ while on the other hand Eq. (L192) states that $Z(0) = \prod_i \lambda_i$.

EXERCISE Show that the eigenvectors of the matrix A of Eq. (L191) are given by $\mathbf{v}_1 = \frac{1}{\sqrt{2}}(-\mathrm{i}, 1)^T$ and $\mathbf{v}_2 = \frac{1}{\sqrt{2}}(\mathrm{i}, 1)^T$, where the normalization factors $1/\sqrt{2}$ fix the complex norm of the eigenvectors as $\|\mathbf{v}_i\| \equiv |v^1{}_i|^2 + |v^2{}_i|^2 = 1$. Verify that

$$T = (\mathbf{v}_1, \mathbf{v}_2) = \frac{1}{\sqrt{2}} \begin{pmatrix} -\mathrm{i} & \mathrm{i} \\ 1 & 1 \end{pmatrix} \Rightarrow T^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathrm{i} & 1 \\ -\mathrm{i} & 1 \end{pmatrix},$$

transforms the matrix to the diagonal form $T^{-1}AT = \mathrm{diag}(i, -i)$.

We conclude that

> If a real matrix cannot be diagonalized within the matrix space $\mathrm{mat}(n, n, \mathbb{R})$, it may still be diagonalizable by complex matrices in $\mathrm{mat}(n, n, \mathbb{C})$.

The existence of n eigenvalues is a necessary but not sufficient condition for the diagonalizability of a matrix. Complications may arise if eigenvectors coincide, $\lambda_i = \lambda_j$. Such eigenvalues are called 'degenerate' (entartet) and the number, r, of eigenvalues λ_i of a given value is called their degree of **degeneracy**. (For example, the unit matrix has n degenerate eigenvalues, each equal to unity.)

Let us first discuss the simpler situation in which **no degeneracies** are present. In this case, the **eigenvectors, $\mathbf{v}_i$, of the n different eigenvalues are linearly independent** and hence form a basis, $\{\mathbf{v}_i\}$, a so-called **eigenbasis** of the matrix A. The transformation matrix $T = (\mathbf{v}_1, \ldots, \mathbf{v}_n)$ then achieves the diagonalization as $D = T^{-1}AT$.

INFO The **linear independence of eigenvectors with different eigenvalues** is best shown by induction. First take two eigenvectors, $\mathbf{v}_{1,2}$ and assume that a nontrivial linear combination $\mathbf{0} = c_1\mathbf{v}_1 + c_2\mathbf{v}_2$ exists, with $c_{1,2} \neq 0$. Now subtract the two equations

$$\begin{aligned} \mathbf{0} = A\mathbf{0} = A(c_1\mathbf{v}_1 + c_2\mathbf{v}_2) &= c_1\lambda_1\mathbf{v}_1 + c_2\lambda_2\mathbf{v}_2, \\ \mathbf{0} = \lambda_2\mathbf{0} &= c_1\lambda_2\mathbf{v}_1 + c_2\lambda_2\mathbf{v}_2, \end{aligned}$$

from each other to obtain $c_1(\lambda_1 - \lambda_2)\mathbf{v}_1 = \mathbf{0}$. This is a contradiction, because all three, $c_1, \lambda_1 - \lambda_2$, and $\mathbf{v}_1$ are non-vanishing. The two vectors $\mathbf{v}_1, \mathbf{v}_2$ therefore cannot be linearly dependent. Now assume that the first j eigenvectors are linearly independent, $j = 1, \ldots, n-1$, and assume that a linear combination exists for which $\mathbf{0} = \sum_{i=1}^{j+1} c_i\mathbf{v}_i$. Arguing as before, we then find that

$$\begin{aligned} \mathbf{0} = A\mathbf{0} = A\left(\sum_i c_i\mathbf{v}_i\right) &= \sum_{i=1}^{j+1} c_i\lambda_i\mathbf{v}_i, \\ \mathbf{0} = \lambda_{j+1}\mathbf{0} &= \sum_{i=1}^{j+1} c_i\lambda_{j+1}\mathbf{v}_i. \end{aligned}$$

Subtraction yields $0 = \sum_{i=1}^{j} c_i(\lambda_i - \lambda_{j+1})\mathbf{v}_i$, which contradicts the starting assumption. We are therefore led to the conclusion that the eigenvectors bv_i are all linearly independent.

The situation gets a little more involved if degenerate eigenvalues occur. We first notice that the set of eigenvectors corresponding to a given eigenvalue, λ, form a subspace of $\mathbb{C}^n$ called the **eigenspace** of that eigenvalue. This is because for any two eigenvectors, $\mathbf{v}, \mathbf{w}$ with $A\mathbf{v} = \lambda\mathbf{v}$ and $A\mathbf{w} = \lambda\mathbf{w}$, the linear combination $c\mathbf{v} + d\mathbf{w}$, $c, d \in \mathbb{C}$, is again an eigenvector with the same eigenvalue. For non-degenerate eigenvalues, λ_i, the eigenspaces are all one-dimensional and are spanned by the corresponding eigenvectors, $\mathbf{v}_i$. Eigenvalues of degeneracy r can have eigenspaces of higher dimensionality up to r (For an extreme example, consider the unit matrix with its $r = n$ degenerate eigenvalues unity where the standard unit vectors $\mathbf{e}_i$ span the n-dimensional eigenspace $\mathbb{C}^n$). If the eigenspaces of all r-fold degenerate eigenvalues have maximal dimension, r, then we have as many linearly independent eigenvectors as eigenvalues. Since there are n eigenvalues in total (some of which may be degenerate) the corresponding n eigenvectors span the full vector space and the matrix is diagonalizable. By contrast, it is **not diagonalizable** if r-fold degenerate eigenvectors with eigenspaces of lower dimensionality $< r$ occur.

To illustrate the phenomenon with a simple example, consider the matrix $A = \left(\begin{smallmatrix} 1 & a \\ 0 & 1 \end{smallmatrix}\right)$. Its characteristic polynomial is given by (check!) $Z(\lambda) = (\lambda - 1)^2$ with the two-fold degenerate zero $\lambda = 1$. However, for $a \neq 0$ the corresponding eigenvector equation $(A - 1 \cdot \mathbb{1})\mathbf{v} = \left(\begin{smallmatrix} 0 & a \\ 0 & 0 \end{smallmatrix}\right)\mathbf{v}$ has only the solution, $\mathbf{v} = (0, c)^T$, where c is a normalization constant. The eigenspace for $\lambda = 1$ is one-dimensional and the matrix cannot be diagonalized.

INFO In physical applications, non-diagonalizable matrices with degenerate eigenvalues do not occur very often. Still it is good to know how the simplest possible representation of a matrix with degenerate eigenvalues looks like. The answer is shown in the schematic below,

$$\begin{pmatrix} \ddots & & & & & & \\ & \lambda & 1 & & & & \\ & 0 & \lambda & & & & \\ & & & \mu & 1 & 0 & \\ & & & 0 & \mu & 1 & \\ & & & 0 & 0 & \mu & \\ & & & & & & \ddots \end{pmatrix}, \tag{L193}$$

where λ and μ are two- and three-fold degenerate eigenvalues with only one-dimensional eigenspaces. The statement is that for each eigenvalue of degeneracy r the matrix can be reduced to one containing r copies of the eigenvalues on the diagonal and $r - 1$ copies of unity on the next diagonal as shown in the figure. Such matrices are said to be in **Jordan form** and the constituent blocks are known as **Jordan blocks**.

For the general discussion of algorithms of transforming matrices into a Jordan form we refer to specialized textbooks on linear algebra. However, the general idea may be illustrated using a simple example. Consider the matrix

$$A = \begin{pmatrix} 0 & 1 \\ -1 & -2 \end{pmatrix}. \tag{L194}$$

Its characteristic polynomial is obtained via $Q(\lambda) = (\lambda + 1)^2$ with two degenerate zeros $\lambda = -1$. The corresponding eigenvector equation,

$$\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

yields (always up to normalization) only one solution, $\mathbf{v}_1 = (1, -1)^T$. We aim to transform A into its Jordan representation $A' = \left(\begin{smallmatrix} 1 & a \\ 0 & 1 \end{smallmatrix}\right)$, where a is a parameter to be determined. To this end we consider the ansatz for the transforming matrix $T^{-1} = (\mathbf{v}_1, \mathbf{w})$, where $\mathbf{v}_1$ is A's eigenvector and and $\mathbf{w}$ a complementing vector of the new basis which also remains to be determined. The equation fixing $\mathbf{w}$ and a then is given by $TAT^{-1} = A'$. It is a straightforward exercise to compute T^{-1} and to write out the matrix equation above in terms of four equations for the coefficients of TAT^{-1}. A solution of these equations is given by $a = 1$, $w_1 = 1$ and $w_2 = 0$. Substituting this into the defining equation, we obtain

$$\begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & -2 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ 0 & -1 \end{pmatrix},$$

as can be checked by direct matrix multiplication. The matrix on the r.h.s. is the Jordan representation of A. The computation of general Jordan representations generalizes the above program to the solution of systems of linear equations of higher order.

Matrix diagonalization recipe

We are now in a position to discuss the algorithm for diagonalizing a matrix $A \in \mathrm{mat}(n, n, \mathbb{C})$ in concrete terms. To diagonalize,

1. Compute the characteristic polynomial $Z(\lambda)$, then
2. Find its zeros, λ_i. If the eigenvalues are all different then the matrix is diagonalizable. In this case, find the eigenvectors by solving the linear systems $(A - \lambda_i \mathbb{1})\mathbf{v}_i = 0$.
3. The matrix $T = (\mathbf{v}_1, \ldots, \mathbf{v}_n)$ then describes the transformation into a diagonal form $T^{-1}AT = D \equiv \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$.
4. Check that no mistakes have been made by explicit verification of the matrix equation of the previous step.

EXAMPLE Consider the 3×3 **matrix** A given in Eq. (L129). The zeros of its characteristic polynomial (L190) are given by $z_0 = 0$, $z_1 = 1$, and $z_2 = -2$, i.e.

$$D = \mathrm{diag}(0, 1, -2).$$

Solving the equations $(A - z_i \mathbb{1})\mathbf{v}_i$, we find (check!)

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}, \qquad \mathbf{v}_2 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \qquad \mathbf{v}_3 = \begin{pmatrix} -1 \\ -\frac{1}{2} \\ \frac{3}{2} \end{pmatrix},$$

and hence

$$T = \begin{pmatrix} 1 & 1 & -1 \\ 1 & 0 & -\frac{1}{2} \\ -1 & -1 & \frac{3}{2} \end{pmatrix}.$$

The inverse of this matrix has been computed in the example on p. 77 (where it was called A), with the result

$$T^{-1} = \begin{pmatrix} 1 & 1 & 1 \\ 2 & -1 & 1 \\ 2 & 0 & 2 \end{pmatrix}.$$

It may be checked by direct matrix multiplication that $TDT^{-1} = A$.

In the case of **eigenvalues with degeneracy** r, the first step is to find as many eigenvectors as possible. If r linearly independent eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_r$ can be found, we include them as part of our transformation matrix T^{-1} and A remains diagonalizable. In the exceptional case where only $s < r$ eigenvectors can be found A is not diagonalizable. It then contains a Jordan block of size $r - s + 1$ which must be computed by procedures similar to those exemplified on p.L7.4.

The characteristic polynomials of **real matrices** often have fewer real zeros than their rank. In such cases they are not diagonalizable in terms of real transformation matrices but may still be complex-diagonalizable as discussed in the exercise of section L7.4.

One final remark: our discussion above has covered all possible scenarios and this may somewhat over-emphasize the role played by non-diagonalizable matrices. In fact, most matrices met in **physical applications** *are* diagonalizable and this includes the real diagonalizability of real matrices. The point is that the matrices met in disciplines such as mechanics, electrodynamics, or quantum mechanics usually obey conditions which grant diagonalizability from the outset. For example, real matrices which equal their own transpose, $A = A^T$, or which obey the condition $A^T = A^{-1}$ are categorically diagonalizable. The characteristic polynomials of such matrices factorize and even degenerate eigenvalues are not harmful to diagonalizability. Similar statements apply to complex matrices obeying the conditions $A = A^\dagger$ or $A^\dagger = A^{-1}$. In the next chapter we will discuss the mathematics and some of the applications of matrices satisfying conditions of this type.

L7.5 Functions of matrices

REMARK This section can be skipped on first reading. It requires familiarity with Taylor series, chapter C5.

Given a square matrix, $A \in \mathrm{mat}(\mathbb{C}, n)$, the product $AA \in \mathrm{mat}(\mathbb{C}, n)$ is a again a square matrix. This observation may be interpreted by saying that the complex function $f : \mathbb{C} \to$

$\mathbb{C}, z \mapsto z^2 = zz$ has a natural generalization, which involves generalizing the domain of definition from the complex numbers to the n-dimensional square matrices, $f : \mathrm{mat}(\mathbb{C}, n) \to \mathrm{mat}(\mathbb{C}, n), A \mapsto AA$. We denote this function by the same symbol f to keep the notation slim.

This idea can be extended to arbitrary functions $f : \mathbb{C} \to \mathbb{C}, z \mapsto z^2$ possessing a Taylor expansion around $z = 0$. Given the Taylor series representation,

$$f(z) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} z^n,$$

we define a function $f : \mathrm{mat}(\mathbb{C}, n) \to \mathrm{mat}(\mathbb{C}, n), A \mapsto f(A)$ by

$$\boxed{f(A) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} A^n,} \tag{L195}$$

where $A \in \mathrm{mat}(\mathbb{C}, c)$, and

$$A^n \equiv \underbrace{AA \ldots A}_{n \text{ times}}, \qquad \text{and} \quad A^0 \equiv \mathbb{1}.$$

For example, the **exponential function of a matrix** is now defined as $\exp(A) = \sum_n \frac{A^n}{n!}$, etc. In many ways, one may work with functions of matrices as with ordinary functions. However, care must be exercised not to apply function relations which rely on the commutativity of numbers. For example, the relation $\exp(z+z') = \exp(z)\exp(z')$ does not extend to matrices, $\exp(A+B) \neq \exp(A)+\exp(B)$ in general. The origin of the inequality can be understood by separate Taylor expansion of the two sides of the (in)equality in A and B up to second order. For the l.h.s. we have $1+(A+B)+\frac{1}{2}(A+B)^2+\cdots = 1+(A+B)+\frac{1}{2}(A^2+AB+BA+B^2)+\ldots$, while the r.h.s. yields $(1+A+\frac{1}{2}A^2+\ldots)(1+B+\frac{1}{2}B^2+\ldots) = 1+(A+B)+\frac{1}{2}(A^2+2AB+B^2)$. The two expressions are different, unless the matrices A and B commute, $AB = BA$. The rule of thumb is that functions of a single matrix, $f(A)$, behave like ordinary functions ($\exp(A+A) = \exp(A)\exp(A)$), etc., because the commutativity issue does not arise. However, when functions of *different* matrices appear, one has to be careful.

The function of a matrix becomes rather easy to evaluate if we know the matrix in diagonal form, $A = TDT^{-1}$. In this case, $A^n = (TDT^{-1})(TDT^{-1})\ldots(TDT^{-1}) = TD^nT^{-1}$, where D^n is a diagonal matrix containing the nth power, λ_i^n, of A's eigenvalues on its diagonal. The matrix function can now be evaluated as

$$f(A) = T^{-1}\left(\sum_{n=0}^{\infty} f^{(n)}(0) D^n\right) T = T^{-1} f(D) T, \tag{L196}$$

where $f(D) = \mathrm{diag}(f(\lambda_1), \ldots, f(\lambda_n))$ is a diagonal matrix containing on its diagonal the complex function $f(z)$ evaluated on the eigenvalues λ_i.

L8 Orthogonality and unitarity

REMARK In this chapter minor differences between real and complex vector spaces need to be addressed. To avoid repetition, we discuss both cases in parallel.

In both physics and mathematics we often encounter linear maps preserving the scalar product between vectors. Simple examples of such transformations include the rotation or reflection of vectors. In quantum mechanics, linear maps of functions (cf. chapter L10) which do not alter a scalar product defined on the space of functions, Eq. (L218) play a distinguished role, etc. This chapter will introduce the mathematical features of scalar product preserving maps. Specifically, we will see that these maps are much easier to work with than generic linear maps.

L8.1 Orthogonal and unitary maps

The defining feature of a scalar product preserving map is that

$$\boxed{\forall \hat{\mathbf{v}}, \hat{\mathbf{w}} \in V, \qquad \langle \hat{A}\hat{\mathbf{v}}, \hat{A}\hat{\mathbf{w}} \rangle = \langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle.} \tag{L197}$$

Depending on whether V is complex or real, maps obeying this criterion are called **unitary** or **orthogonal maps**, respectively.

Unitary (orthogonal) maps have a trivial kernel. The reason is that for every non-vanishing vector $\hat{\mathbf{v}}$ we have $\|\hat{A}\hat{\mathbf{v}}\|^2 = \langle \hat{A}\hat{\mathbf{v}}, \hat{A}\hat{\mathbf{v}} \rangle = \langle \hat{\mathbf{v}}, \hat{\mathbf{v}} \rangle = \|\hat{\mathbf{v}}\|^2 \neq 0$, i.e. the image $\hat{A}\hat{\mathbf{v}}$ cannot be the null-vector. From our discussion above we conclude that **unitary (orthogonal) maps are invertible**.

Given two unitary or maps, $\hat{A}, \hat{B}$, the product $\hat{A}\hat{B}$ is again unitary (orthogonal), since

$$\langle \hat{A}\hat{B}\hat{\mathbf{v}}, \hat{A}\hat{B}\hat{\mathbf{w}} \rangle = \langle \hat{A}(\hat{B}\hat{\mathbf{v}}), \hat{A}(\hat{B}\hat{\mathbf{w}}) \rangle = \langle \hat{B}\hat{\mathbf{v}}, \hat{B}\hat{\mathbf{w}} \rangle = \langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle.$$

Similarly, the inverse of an unitary (orthogonal) map $\hat{A}$ is also unitary (orthogonal);

$$\langle \hat{A}^{-1}\hat{\mathbf{v}}, \hat{A}^{-1}\hat{\mathbf{w}} \rangle = \langle \hat{A}(\hat{A}^{-1}\hat{\mathbf{v}}), \hat{A}(\hat{A}^{-1}\hat{\mathbf{w}}) \rangle = \langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle,$$

where the unitarity (orthogonality) of $\hat{A}$ was used. Finally, the unit map is trivially orthogonal (unitary). We conclude the set of unitary (orthogonal) maps define a group embedded in the

larger group of invertible maps. These groups are denoted the **unitary group**, $\mathrm{U}(n)$, and the **orthogonal group**, $\mathrm{O}(n)$, respectively.

We finally note that linear maps which are element of the unitary group are frequently denoted by Latin letters starting with the $\hat{U}, \hat{V}, ... \in \mathrm{U}(n)$ and elements of the orthogonal group as $\hat{O}, \hat{P}, \hat{Q}, ... \in \mathrm{O}(n)$.

L8.2 Orthogonal and unitary matrices

Definition

Let us now explore what unitarity (orthogonality) of $\hat{U}$ ($\hat{O}$) implies for the associated matrices U (O). Given that we work in an inner product space, it is natural to work with an **orthonormal basis**, $\langle \hat{\mathbf{e}}_i, \hat{\mathbf{e}}_j \rangle = \delta_{ij}$ (the generalization to a non-orthonormal basis is addressed in the info block on p.111 below). The scalar product of two vectors is then given by (cf. Eq. (L60)) $\langle \hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle = \overline{v^i} \delta_{ij} w^j$. Representing the coefficients of $\hat{U}\hat{\mathbf{v}}$ as $(U\mathbf{v})^l = U^l{}_i v^i$[1] and using $\overline{U^l{}_i v^i} = \overline{U^l{}_i}\,\overline{v^i}$ the unitarity condition (L197) becomes

$$\overline{U^l{}_i}\,\overline{v^i}\,\delta_{lm}\,U^m{}_j w^j = \overline{v^i}\delta_{ij}w^j. \tag{L198}$$

This condition must hold for arbitrary $\mathbf{v}$ and $\mathbf{w}$ which implies the matrix condition $\overline{U^l{}_i}\,\delta_{lm}\,U^m{}_j = \delta_{ij}$. Recalling the definition (L108) of the **adjoint matrix**, $(U^\dagger)_i{}^l = \overline{U^l{}_i}$ we may write it as

$$(U^\dagger)_i{}^l\,\delta_{lm}U^m{}_j = \delta_{ij}. \tag{L199}$$

To **simplify the notation**, we define

$$\boxed{(U^\dagger)^i{}_j \equiv \delta^{ik}(U^\dagger)_k{}^l\delta_{lj}.}$$

Conceptually, this definition changes covariant indices to contravariant ones (and vice versa). This is done by application of the index raising operation Eq. (L55) with standard metric $g_{ij} = \delta_{ij}$. Note that the index-raising operation does not affect the concrete values of matrix elements, $(U^\dagger)^i{}_j = (U^\dagger)_i{}^j$, element-wise. For example, for

$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad U^\dagger = \overline{U}^T = \begin{pmatrix} \overline{a} & \overline{c} \\ \overline{b} & \overline{d} \end{pmatrix}$$

with $(U^\dagger)^1{}_2 = (U^\dagger)_1{}^2 = \overline{c}$, etc. (In the info section on p. 111 we will extend the definition of unitarity to the case of non-standard scalar products, $g_{ij} \neq \delta_{ij}$. For such scalar products, the index-positioning becomes essential, and $(U^\dagger)^i{}_j \neq (U^\dagger)_i{}^j$.)

[1] Recall that $\mathbf{v}$ and A refer to the $\mathbb{C}^n$-component representation and the matrix representation of the vector $\mathbf{v}$ and the linear map $\hat{A}$ in a given basis.

The unitarity condition now assumes the form

$$\boxed{(U^\dagger)^i{}_k U^k{}_j = \delta^i{}_j.} \tag{L200}$$

Matrices obeying this condition are called **unitary matrices**. In a similar manner the orthogonality condition of a real map, $\hat{O}$, implies the matrix relation $(O^T)_l{}^i\,\delta_{ij}O^j{}_m = \delta_{lm}$ (i.e. the same as above, only that the complex conjugation is absent). In an analogous manner, we raise/lower indices as $(O^T)^i{}_j = \delta^{ik}(O^T)_k{}^l\delta_{lj}$ to obtain the condition as

$$\boxed{(O^T)^i{}_k\, O^k{}_j = \delta^i{}_j.} \tag{L201}$$

Matrices obeying this condition are called **orthogonal matrices**. The essential statement made by Eqs. (L200) and (L201) is that

> The adjoint, $U^\dagger$, and the transpose, O^T, of a unitary matrix U and an orthogonal matrix, O, respectively, equal their inverse. Conversely, a matrix whose inverse is given by its adjoint (transpose) is unitary (orthogonal).

In other words, the inverse of a unitary (orthogonal) matrix is obtained without any elaborate calculation. Consider, for example, the matrix $U = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} 1 & \mathrm{i} \\ \mathrm{i} & 1 \end{smallmatrix}\right)$. It is straightforward to verify that it is unitary: $U^\dagger = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} 1 & -\mathrm{i} \\ -\mathrm{i} & 1 \end{smallmatrix}\right)$ obeys the condition (L200) and the matrices are inverse to each other, $U^\dagger U = \mathbb{1}$.

In an index-free notation the equations defining unitarity and orthogonality, respectively, read

$$\boxed{\begin{array}{ll} \hat{O} \text{ orthogonal} & \Leftrightarrow O^T O = \mathbb{1}, \\ \hat{U} \text{ unitary} & \Leftrightarrow U^\dagger U = \mathbb{1}. \end{array}} \tag{L202}$$

These equations imply an economic way to **test for the unitarity (orthogonality) of a matrix**: build the adjoint (transpose), $U^\dagger$ (O^T), and check whether $UU^\dagger = \mathbb{1}$ ($OO^T = \mathbb{1}$). While unitarity (orthogonality) cannot usually be 'seen' with the naked eye (is $U = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} \mathrm{i} & 1 \\ 1 & \mathrm{i} \end{smallmatrix}\right)$ unitary?) this operation can be performed with relatively little effort.

We finally mention that the **non-covariant index representation** of the unitarity/orthogonality conditions reads as

$$U^\dagger_{il}U_{li} = \delta_{ij}, \qquad O^T_{il}O_{lj} = \delta_{ij}, \tag{L203}$$

where $U^\dagger_{ij} = \overline{U_{ji}}$ and $O^T_{ij} = O_{ji}$.

The group of unitary and orthogonal matrices

We have seen that the abstract unitary and orthogonal maps form subgroups $\mathrm{U}(n)$ and $\mathrm{O}(n)$ of the group of invertible linear maps. Likewise, the sets of unitary and orthogonal

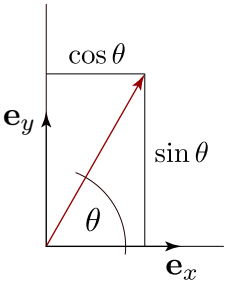
matrices define subgroups of the group of invertible matrices, $\mathrm{GL}(n,\mathbb{C})$ and $\mathrm{GL}(n,\mathbb{R})$. These groups are denoted by $\mathrm{U}(n)$ and $\mathrm{O}(n)$, respectively, i.e. by the same symbol as their abstract siblings.[2] They are called the **group of unitary and orthogonal matrices**, respectively, and defined as

$$\begin{aligned}\mathrm{U}(n) &= \{U \in \mathrm{GL}(n,\mathbb{C}) | U^\dagger = U^{-1}\},\\ \mathrm{O}(n) &= \{O \in \mathrm{GL}(n,\mathbb{R}) | O^T = O^{-1}\}.\end{aligned} \tag{L204}$$

Their group property follows from the fact that they are matrix representations of of the groups $\mathrm{U}(n)$ and $\mathrm{O}(n)$ introduced in the previous section (think about this point). However, it is a good exercise to check the group criteria explicitly, i.e. that the product of two unitary (orthogonal) matrices is again unitary (orthogonal), that the same holds for the inverse, and that the unit matrix lies in each group.

INFO As mentioned in the beginning of the chapter, orthogonal and unitary maps play an important **role in physics**. The reason being that there are many linear transformation which preserve the norm of vectors. Important examples include rotations of vectors, reflections of vectors at a point or at a plane and others.

Consider, for example, the case of a two-dimensional real vector space, $n = 2$. The matrix



$$R(\theta) = \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix} \tag{L205}$$

describes a rotation of vectors by the angle θ. This can be seen by applying $R(\theta)$ to the vector $(1,0)^T$ representing the unit basis vector in x-direction. The inverse of this matrix is given by $R^{-1}(\theta) = R(-\theta)$ since it must rotate by the same angle in opposite direction. Using $\cos(-\theta) = \cos\theta$ and $\sin(-\theta) = -\sin\theta$ we find that

$$R^{-1}(\theta) = \begin{pmatrix}\cos\theta & \sin\theta\\ -\sin\theta & \cos\theta\end{pmatrix} = R^T(\theta). \tag{L206}$$

(Check by matrix multiplication that $RR^{-1} = \mathbb{1}$.) The reflection of vectors at the origin, $\mathbf{x} \mapsto -\mathbf{x}$, another orthogonal map, is represented by the negative of the unit matrix, $-\mathbb{1}$. For example, a 90deg rotation ($\theta = \pi/2$) followed by a reflection and another 90deg rotation is not expected to have any effect. Show this by verifying that $R(\pi/2)(-\mathbb{1})R(\pi/2) = \mathbb{1}$.

The most important applications of **unitary maps** in physics are found in **quantum mechanics**. A brief teaser introduction to the description of quantum phenomena in terms of unitary maps will be given on pp L9.2 after a some more material has been introduced.

[2] Do not be confused by the double-usage of the symbol $\mathrm{U}(n)$. In the abstract context, it denotes the set of linear maps of an n-dimensional complex vector space obeying the criterion (L197). In the matrix-context it denotes a set of matrices acting in the standard space $\mathbb{C}^n$ and obeying the condition (L202). Once a basis has been chosen, each element of the abstract $U(n)$ has a corresponding element of the matrix $U(n)$, and this assignment is compatible with the rules of group composition. The groups are therefore 'almost identical', and it is justified to denote them by the same symbol.

INFO In applications, we sometimes need to work with **non-orthonormal bases** $\{\hat{\mathbf{v}}_i\}$ for which the scalar product $\langle \hat{\mathbf{v}}_i, \hat{\mathbf{v}}_j \rangle = g_{ij}$ defines the elements of a metric tensor. In section L3.3 we saw that in this case we should work with a non-standard $\mathbb{C}^n$-scalar product $\langle \mathbf{v}, \mathbf{w} \rangle = \overline{v^i} g_{ij} w^j$.

Representing the coefficients of $\hat{U}\hat{\mathbf{v}}$ as $(U\mathbf{v})^l = U^l{}_i v^i$,[3], the unitarity condition (L197) becomes $\overline{U^l{}_i}\,\overline{v^i}\, g_{lm}\, U^m{}_j w^j = \overline{v^i} g_{ij} w^j$. Comparison with Eq. (L198) shows that the presence of a metric tensor amounts to a replacement $\delta_{ij} \to g_{ij}$. Accordingly, the condition (L199) for the adjoint of the transformation now reads

$$(U^\dagger)_l{}^i\, g_{ij} U^j{}_m = g_{lm}. \tag{L207}$$

The difference to the orthonormal relation (L199) is the generalization $\delta_{ij} \to g_{ij}$. Again we observe that the appearance of spurious Kronecker-δs in the covariant notation signifies a formula which generalizes as before if a metric enters the stage. This should be considered a strength of the notation. For example, the non-covariant formulation of unitarity, Eq. (L203) does not contain any 'hints' as to how its generalization to a non-orthonormal basis looks like.

INFO The simplest representative of a signature-r **indefinite metric** is the diagonal tensor $\eta = \mathrm{diag}(1, \ldots, 1, -1, \ldots, -1)$, containing r elements 1 and $n-r$ elements -1 on its diagonal. Complex matrices preserving this scalar product obey the relation $(U^\dagger)_l{}^i\, \eta_{ij} U^j{}_m = \eta_{lm}$. This is the defining relation of the **specical unitary group**, $\mathrm{U}(r, n-r)$. The analogous relation for the real case, $(O^T)_l{}^i\, \eta_{ij} O^j{}_m = \eta_{lm}$, defines the **special orthogonal group** $\mathrm{O}(r, n-r)$. As an example, consider $n = 2$ and $r = 1$. The condition

$$\Lambda^T \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \Lambda = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \tag{L208}$$

is satisfied by matrices of the form $\Lambda = \left(\begin{smallmatrix} \cosh\alpha & \sinh\alpha \\ \sinh\alpha & \cosh\alpha \end{smallmatrix}\right)$. A group of great physical significance is the **Lorentz group**, $\mathrm{O}(1,3)$. This is the group of real matrices satisfying $\Lambda^T \eta \Lambda = \eta$ for the Minkovski metric introduced on p. 45, for which $r = 1$, $n = 4$. Elements, $\Lambda \in \mathrm{O}(1,3)$, of the Lorentz group are called **Lorentz transformations** and play an important role in the theory of **special relativity**.

Eigenvalues

Unitary matrices are invertible and therefore possess non-vanishing eigenvalues. However there is an even stronger statement constraining the eigenvalues of unitary matrices: assume $U\mathbf{v} = \lambda\mathbf{v}$ and use that $\langle \mathbf{v}, \mathbf{v} \rangle = \langle U\mathbf{v}, U\mathbf{v} \rangle = \langle \lambda\mathbf{v}, \lambda\mathbf{v} \rangle = |\lambda|^2 \langle \mathbf{v}, \mathbf{v} \rangle$, which requires $|\lambda|^2 = 1$:

> The n eigenvalues, λ_n, of a unitary matrix are complex unit-modular numbers, $\lambda_n = \mathrm{e}^{\mathrm{i}\phi_n}$, with real $\phi_n \in [0, 2\pi]$.

The same argument applied to an orthogonal matrix, O, shows that its eigenvalues must have unit modulus, too, $|\lambda| = 1$. However, these eigenvalues need not be real, i.e. there is

[3] Recall that $\mathbf{v}$ and A refer to the $\mathbb{C}^n$-component representation and the matrix representation of the vector $\hat{\mathbf{v}}$ and the linear map $\hat{A}$ in a given basis.

no guarantee that the characteristic polynomial of an orthogonal matrix has real zeros. For example, the orthogonal matrix $\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$ has the two imaginary unit-modular eigenvalues $\pm\mathrm{i}$. If an orthogonal matrix has real eigenvalues, they must equal ± 1, the only two real numbers with modulus one.

L8.3 Special unitary and special orthogonal matrices

The determinant of a matrix equals the product of its eigenvalues. Above we have seen that for unitary (orthogonal) matrices the latter are unit-modular numbers. Since the product of unit-modular numbers is again unit-modular (why?), we know that[4]

> The **determinant of a unitary matrix** is a complex number of *unit modulus*, $\det(U) = \mathrm{e}^{\mathrm{i}\phi}$, where $\phi \in [0, 2\pi]$ is real. Likewise, the **determinant of an orthogonal matrix** is a real number of unit modulus, i.e. $\det(O) = \pm 1$.

It is instructive to prove this statement without reference to the eigenvalues. To this end, take a unitary matrix, U, define $z = \det(U)$, and compute $|z|^2 = \det(U)\overline{\det(U)} = \det(U)\det(U^\dagger) = \det(UU^\dagger) = \det(\mathbb{1}) = 1$ where Eq. (L172) has been used. The same construction applied to an orthogonal matrix shows $\det(O) = \pm 1$.

Unitary (orthogonal) matrices possessing the special value $\det(U) = 1$ ($\det O = 1$) are called **special unitary (orthogonal) matrices**. The unit-determinant property is preserved under matrix multiplication, $\det(UV) = 1$ for $\det(U) = \det(V) = 1$, the building of the inverse, $\det(U^{-1}) = 1$, for $\det(U) = 1$, and the unit-matrix of course has determinant one. This means that the set of special unitary (orthogonal) matrices forms a sub*group* of the set of unitary (orthogonal) matrices known as the **special unitary (orthogonal) group**, $\mathrm{SU}(n)$ ($\mathrm{O}(n)$),

$$\begin{aligned}\mathrm{SU}(n) &\equiv \{A \in \mathrm{U}(n) | A^\dagger = A, \det A = 1\},\\ \mathrm{SO}(n) &\equiv \{A \in \mathrm{O}(n) | A^T = A, \det A = 1\}.\end{aligned} \tag{L209}$$

We note that the special unitary group can also be understood as a subgroup of $\mathrm{SL}(n, \mathbb{C})$, i.e. the group of unit-determinant (but not necessarily unitary) complex matrices. Similarly, the special orthogonal group can be understood as a subgroup of $\mathrm{SL}(n, \mathbb{R})$, containing real matrices of unit determinant, which are not necessarily orthogonal.

INFO Special unitary matrices play an important **role in physics**, notably in quantum mechanics and particle physics. For example, the quantum mechanics of spin (which is the quantum generalization of classical angular momentum) is mathematically described in terms of $\mathrm{SU}(2)$. () The groups $\mathrm{SU}(2)$ and $\mathrm{SU}(3)$ played a decisive role in the sixties of the past century when their mathematical structure

[4] Notice that even if an orthogonal matrix has no real eigenvalues its determinant is real by construction. At the same time, the determinant is the product of n (possibly complex) unit modular eigenvalues. Combining these two facts we conclude that the product must be real and unit-modular, i.e. it must equal ± 1.

was linked to the properties of known elementary particles and the so-called **standard model** of matter emerged.

The groups $\mathrm{SO}(2)$ and $\mathrm{SO}(3)$ feature in **classical mechanics** where they describe the mathematics of rotations in two- and three-dimensional space, respectively. We have argued above that rotations are mathematically represented by orthogonal matrices. In fact, they are *special* orthogonal matrices. This follows from the fact that any rotation specfied in terms of a set of rotation angles can be continuously 'deformed' to a unit operation by reducing the angles to zero. Consider, for example, the rotation matrix $R(\theta)$ defined in Eq. (L205). It can be deformed to the unit matrix by a continuous reduction of θ to zero. The unit matrix has unit determinant, and so must have any *continuous* deformation of it. A sudden 'jump' to a determinant -1 would be in conflict with continuity. The above rotation matrix has unit determinant, , $R(\theta) \in \mathrm{SO}(2)$, and so does any other. By contrast, matrices describing reflections, for example, $R = \left(\begin{smallmatrix} 1 & \\ & -1 \end{smallmatrix}\right)$ describing a reflection at the x-axis (why?) can have determinant -1.

Summarizing, the set of complex (real) matrix groups encountered so far contains $\mathrm{mat}(n,n,\mathbb{C}) \supset \mathrm{GL}(n,\mathbb{C}) \supset \mathrm{U}(n), \mathrm{SL}(n,\mathbb{C}) \supset \mathrm{SU}(n)$ (and analogously for the real case). There are a few more groups of relevance to the physics curriculum, however, the ones above are arguably the most important ones. The hierarchical relation between them is illustrated in Fig. L16.

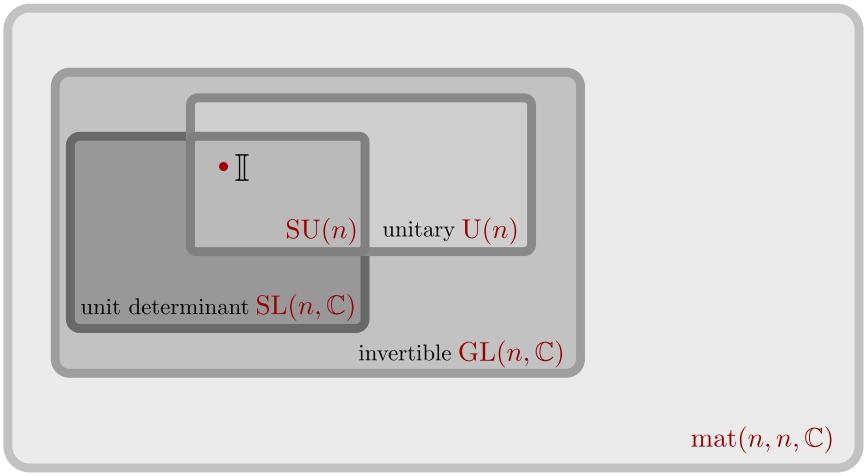


Figure L16: The most imortant matrix subgroups of $\mathrm{mat}(n,n,\mathbb{C})$. The 'smallest' group $\mathrm{SU}(n) = \mathrm{SL}(n,\mathbb{C}) \cap \mathrm{U}(n)$ is the intersection of the groups of unit determinant, $\mathrm{SL}(n,\mathbb{C})$, and the unitary group, $\mathrm{U}(n)$, respectively. For the real case, replace $\mathbb{C} \to \mathbb{R}$ and $\mathrm{U} \to \mathrm{O}$.

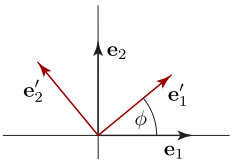
INFO For any unitary matrix U with determinant $\det(U) = \mathrm{e}^{\mathrm{i}\phi}$, a matrix of unit determinant may be defined as $U' = \mathrm{e}^{-\mathrm{i}\phi/n}\,U$. This follows from $\det U' = \det(\mathrm{e}^{-\mathrm{i}\phi/n}U) = (\mathrm{e}^{-\mathrm{i}\phi/n})^n \det(U) = \mathrm{e}^{-\mathrm{i}\phi}\mathrm{e}^{\mathrm{i}\phi} = 1$, where Eq.(L177) has been used. For example, the unitary matrix $U = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} \mathrm{i} & 1 \\ 1 & \mathrm{i} \end{smallmatrix}\right)$ has determinant $\mathrm{e}^{\mathrm{i}\pi} = -1$. Multiply it by $\mathrm{e}^{-\mathrm{i}\pi/2} = -\mathrm{i}$ to obtain the special unitary matrix $U' = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} 1 & -\mathrm{i} \\ -\mathrm{i} & 1 \end{smallmatrix}\right)$. Since matrices differing by a multiplicative factor are 'almost equivalent', the manipulation above is often used to pass from a unitary matrix to its slightly simpler unit-determinant version.

For orthogonal matrices, this prescription does not work since $\det(O)^{-1/n} = (-1)^{-1/n}$ is not a real number so multiplication by it takes us outside the set of real matrices.

L8.4 Orthogonal and unitary basis changes

In section L5.6 we considered a basis transformation, $\hat{T}$, from a basis $\{\mathbf{v}_i\}$ to a new basis $\{\mathbf{v}'_i\}$, and found that finding the ~~representing~~ matrix of the inverse transformation, $\hat{T}^{-1}$, generally requires inverting the matrix T. Much less work is required if we work with orthonormal bases, i.e. if both the old, $\{\mathbf{e}_i\}$, and the new basis $\{\mathbf{e}'_i\}$ are orthonormal. In this case, the transformation matrix $\mathbf{e}_i = \mathbf{e}'_j T^j{}_i$ preserves the scalar product, $\langle \mathbf{e}_i, \mathbf{e}_j \rangle = \langle \mathbf{e}'_i, \mathbf{e}'_j \rangle = \delta_{ij}$. This means that **the transformation matrix is unitary (orthogonal)** and that its inverse is obtained 'for free' just by building $T^\dagger$ (T^T).

EXERCISE Apply elementary trigonometry to compute the matrix describing the transformation between the basis vectors shown in the figure. Verify its orthogonality by building the transpose and checking that Eq. (L201) holds.



To make these statements more concrete, let us write $T \equiv U$ to emphasize the unitarity of the transform and consider the inverse relation $\mathbf{e}'_i = \mathbf{e}_j (U^{-1})^j{}_i$. Multiplication of Eq. (L200) from the right by U^{-1} yields $(U^{-1})^i{}_j = (U^\dagger)^i{}_j$, and this gives us the transformation relations

$$\mathbf{e}_j = \mathbf{e}'_k \, U^k{}_j, \qquad \mathbf{e}'_j = \mathbf{e}_k \, (U^\dagger)^k{}_j. \tag{L210}$$

For the orthonormality preserving transformations $T \equiv O$ of a **real vector space**, these relations are to be replaced by

$$\mathbf{e}_j = \mathbf{e}'_k \, O^k{}_j, \qquad \mathbf{e}'_j = \mathbf{e}_k \, (O^T)^k{}_j. \tag{L211}$$

L9 Hermiticity and symmetry

Besides the unitary (orthogonal) maps there exists a second family of linear maps defined in relation to the scalar product. These so-called Hermitian (symmetric) maps are of great importance to physics, notably to quantum mechanics (see the info section on p.118 for a brief discussion). Following the same strategy as in the previous chapter we first define the hermiticity (symmetry) of linear maps to then discuss the structure of their associated matrices.

L9.1 Hermitian and symmetric maps

We call a linear map $\hat{A} : V \to V$ of a complex (real) inner product space a **Hermitian (symmetric)** linear map, if

$$\boxed{\forall \hat{\mathbf{v}}, \hat{\mathbf{w}} \in V, \qquad \langle \hat{A}\hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle = \langle \hat{\mathbf{v}}, \hat{A}\hat{\mathbf{w}} \rangle.} \tag{L212}$$

Unlike with unitary (orthogonal) maps the relation above does *not* define a group property: if $\hat{A}, \hat{B}$ are Hermitian (symmetric) then we know that $\langle \hat{A}\hat{B}\hat{\mathbf{v}}, \hat{\mathbf{w}} \rangle = \langle \hat{B}\hat{\mathbf{v}}, \hat{A}\hat{\mathbf{w}} \rangle = \langle \hat{\mathbf{v}}, \hat{B}\hat{A}\hat{\mathbf{w}} \rangle$. However, this does not equal $\langle \hat{\mathbf{v}}, \hat{A}\hat{B}\hat{\mathbf{w}} \rangle$, unless $\hat{A}\hat{B} = \hat{B}\hat{A}$. So, in general, the composition of two Hermitian (symmetric) maps, $\hat{A}\hat{B}$, is not Hermitian (symmetric). However, the absence of a group structure notwithstanding, the matrices representing Hermitian (symmetric) maps possess strong mathematical structure to be discussed in the next section:

L9.2 Hermitian and symmetric matrices

Definition

The availability of a scalar product suggests to representing Hermitian (symmetric) linear maps in an orthonormal basis $\{\hat{\mathbf{e}}_i\}$. With $(A\mathbf{v})^i = A^i{}_j v^j$ the condition $\langle A\mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{v}, A\mathbf{w} \rangle$ then takes the form

$$\overline{A^i{}_j}\, \overline{v^j} \delta_{ik} w^k = \overline{v^j} \delta_{jl} A^l{}_k w^k.$$

This must hold for arbitrary $\mathbf{v}, \mathbf{w}$ which requires $\overline{A^i{}_j}\delta_{ik} = \delta_{jl}A^l{}_k$. Recalling the definition of the adjoint matrix (L108), and multiplying with δ^{mj} we obtain

$$\delta^{mj}(A^\dagger)_j{}^i\delta_{ik} \equiv (A^\dagger)^m{}_k = A^m{}_k. \tag{L213}$$

The same construction carried out for a symmetric matrix acting on a real vector space shows that $(A^T)^m{}_k = A^m{}_k$. We have thus found that

> The matrices, A, representing Hermitian (symmetric) linear maps in an orthonormal basis are equal their adjoint (transpose), $A^i{}_j = (A^\dagger)^i{}_j$ ($A^i{}_j = (A^T)^i{}_j$).

EXAMPLE The matrices

$$A \equiv \begin{pmatrix} -1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}, \qquad B \equiv \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \tag{L214}$$

are examples of a Hermitian and a symmetric matrix, respectively.

Eigenvalues and determinant

All n eigenvalues, λ, of a Hermitian (symmetric) matrix are real. To see this, let $\mathbf{v}$ be the corresponding eigenvector and compute $\lambda\langle\mathbf{v},\mathbf{v}\rangle = \langle\mathbf{v},\lambda\mathbf{v}\rangle = \langle\mathbf{v},A\mathbf{v}\rangle = \langle A\mathbf{v},\mathbf{v}\rangle = \langle\lambda\mathbf{v},\mathbf{v}\rangle = \overline{\lambda}\langle\mathbf{v},\mathbf{v}\rangle$. Since $\langle\mathbf{v},\mathbf{v}\rangle \neq 0$, the first and the last entry in this chain of equalities require $\lambda = \overline{\lambda}$. The result also implies that unlike a generic real matrix a symmetric matrix has n real eigenvalues. We know that its characteristic polynomial has n zeros λ_n (which for a generic matrix may be complex). However, the argument above shows that these solutions must be real. To summarize,

> A Hermitian (symmetric) matrix of an n-dimensional complex (real) vector space has n real eigenvalues.

As a corollary we observe that

> The determinant of a Hermitian matrix is real.

This is because it is the product of its n real eigenvalues. (Of course, if a symmetric matrix is real, then its determinant is too.)

EXERCISE Show that the eigenvalues of the symmetric matrix A of Eq. (L214) are given by $(1,-2,-2)$ and those of the Hermitian matrix B by $(1,-1)$.

Diagonalization

Hermitian (symmetric) matrices have the important property that they can always be diagonalized. The transformation matrices effecting the diagonalization are unitary (orthogonal). These statements are proven in the info section below.

However, not only can these be diagonalized as a matter of principle, it also turns out that the practical diagonalization procedure is much simpler than that for generic matrices. The key simplification lies in the fact that

> Eigenvectors $\mathbf{v}_1$ and $\mathbf{v}_2$ corresponding to different eigenvalues $\lambda_1 \neq \lambda_2$ of a Hermitian (symmetric) matrix are perpendicular to each other $\langle \mathbf{v}_1, \mathbf{v}_2 \rangle = 0$.

To show this, consider two different eigenvalues λ_1, λ_2. Then compute $\lambda_1 \langle \mathbf{v}_2, \mathbf{v}_1 \rangle = \langle \mathbf{v}_2, \lambda_1 \mathbf{v}_1 \rangle = \langle \mathbf{v}_2, A\mathbf{v}_1 \rangle = \langle A\mathbf{v}_2, \mathbf{v}_1 \rangle = \lambda_2 \langle \mathbf{v}_2, \mathbf{v}_1 \rangle$, or $0 = (\lambda_1 - \lambda_2)\langle \mathbf{v}_2, \mathbf{v}_1 \rangle$. Since $\lambda_1 - \lambda_2 \neq 0$, this equality requires $\langle \mathbf{v}_2, \mathbf{v}_1 \rangle = 0$. This observation suggests starting the diagonalization by computing as many eigenvectors $\hat{\mathbf{v}}_i$ of different eigenvalues λ_i. Choosing these vectors to be normalized, we know that they form an orthonormal set, $\langle \hat{\mathbf{v}}_i, \hat{\mathbf{v}}_j \rangle = \delta_{ij}$. If all eigenvalues are different they form a basis and the matrix $T = (\mathbf{v}_1, \ldots, \mathbf{v}_n)$ transforms A into diagonal form, $D = T^{-1}AT$. The procedure becomes a little more complicated if degenerate eigenvalues λ of multiplicity $l > 1$ are present. The proven diagonalizability of A means that l linearly independent eigenvectors $\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_l$ with eigenvalue λ exist, i.e. that we do not run into the same complications that characterize the Jordan matrices discussed on p. 103. In situations with degenerate eigenvalues we therefore need to find l linearly independent solutions of the equation $(A - \lambda \mathbb{1})\mathbf{v} = 0$ and then construct an orthonormal basis in the l-dimensional subspace of those solutions.

INFO A proof of principle **showing the diagonalizability of Hermitian (symmetric) matrices** goes as follows. Let A be a Hermitian matrix and pick one of its eigenvalues, λ_1. Denote the corresponding (normalized) eigenvector $\hat{\mathbf{v}}_1$. Next define $V_1 \subset V$ to be the subspace of V containing all vectors perpendicular to $\hat{\mathbf{v}}_1$, i.e. $\forall \mathbf{w} \in \mathbf{V}_1$, $\langle \mathbf{w}, \hat{\mathbf{v}}_1 \rangle = 0$. The key observation now is that A acts *within* V_1, i.e. for $\mathbf{w} \in V_1$, $A\mathbf{w} \in V_1$ is perpendicular to $\hat{\mathbf{v}}_1$ too. To see this, compute $\langle \hat{\mathbf{v}}_1, A\mathbf{w} \rangle = \langle A\hat{\mathbf{v}}_1, \mathbf{w} \rangle = \langle \lambda_1 \hat{\mathbf{v}}_1, \mathbf{w} \rangle = \lambda_1 \langle \hat{\mathbf{v}}_1, \mathbf{w} \rangle = 0$, where in the last step the assumed orthogonality of $\mathbf{w}$ and $\mathbf{v}_1$ was used.

We may now iterate the procedure by picking a second eigenvector λ_2 and computing a normalized eigenvector $\hat{\mathbf{v}}_2 \in V_1$. Then determine the subspace of $V_2 \subset V_1$ of all vectors in V_1 perpendicular to $\hat{\mathbf{v}}_2$ (and automatically perpendicular to $\hat{\mathbf{v}}_1$ because we are working in V_1). In each step, the dimension of the spaces $V_1, V_2, \ldots$ reduces by one. Continue the procedure until the one-dimensional vector space $V_{n-1} \subset V_{n-1} \subset \cdots \subset V_1 \subset V$ with its unique normalized basis vector $\mathbf{v}_n$ and eigenvalue λ_n have been determined.

As a result of this procedure, a basis of orthonormal eigenvectors, $\langle \hat{\mathbf{v}}_i, \mathbf{v}_j \rangle = \delta_{ij}$ is obtained. This means that the corresponding transformation matrix $T \equiv (\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2, \ldots, \hat{\mathbf{v}}_n)$ is unitary (orthogonal), cf. section L8.4. However, while this procedure is straightforward in principle it requires us to determine subspaces of vectors perpendicular to a set of chosen vectors. This can be cumbersome in practice and for this reason Hermitian (symmetric) are usually diagonalized differently, as discussed in the main text.

EXERCISE Apply the procedure above to show that the matrices given in Eq. (L214) are diagonalized by

$$A = TDT^T, \qquad D = \mathrm{diag}(1,-2,-2), \qquad T = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & -\frac{2}{\sqrt{6}} & 0 \end{pmatrix}$$

and

$$B = TDT^\dagger, \qquad D = \mathrm{diag}(1,-1), \qquad T = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ \mathrm{i} & -\mathrm{i} \end{pmatrix}. \tag{L215}$$

We conclude this section by **summarizing** the most essential properties of Hermitian (symmetric) matrices:

- ▷ Every Hermitian (symmetric) matrix is diagonalizable.
- ▷ Its eigenvalues, $\{\lambda_i\}$, are real, and
- ▷ an orthonormal basis of eigenvectors can always be found.
- ▷ The transformation matrices, T, to an orthonormal basis of eigenvectors are unitary, $T^{-1} = T^\dagger$ (symmetric, $T^{-1} = T^T$), which means that
- ▷ Hermitian (symmetric) matrices can be represented as $A = TDT^\dagger$, $D = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$.

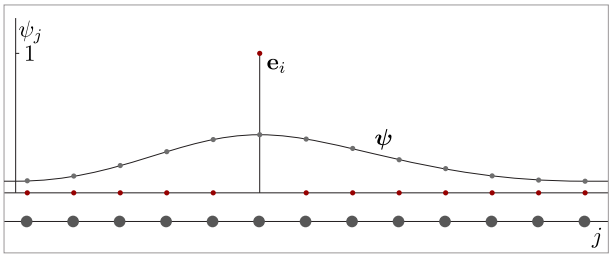


Figure L17: Cartoon of a one-dimensional crystal. Individual atoms are labeled by n. The components ψ_i of a quantum mechanical state are a measure of the probability amplitude to find the state at site n, and $|\psi_i|^2$ is the corresponding probability.

INFO Although this is not the place for an in-depth discussion let us motivate the formal structures introduced above by a brief outlook to the application of **linear algebra in quantum mechanics**. We begin by formulating a few key *axioms* of quantum mechanics. These are all statements that cannot be proven (much like Newton's laws of classical mechanics cannot be 'proven') from more fundamental principles. They have been formulated in axiomatic terms on the basis that they successfully explain experimental observation.

▷ The physical state of a system is described in terms of a unit normalized vector $\psi \in V$, $\langle\psi,\psi\rangle = 1$ defined in a complex vector space (cf. section L3.4). The dimension of that space, N, may be infinite, in which case a number of extra conditions need to be imposed. Vector spaces equipped with these properties are called **Hilbert spaces** (see chapter L10 for more information). For all practical purposes we may think of a Hilbert space as a complex inner product space. Following standard conventions we denote Hilbert space state vectors, ψ, in a non-boldface ($\boldsymbol{\psi}$) notation. Their components, ψ_j, are generally written as subscripts, i.e. in non-covariant notation.

Consider, for example, a 'one-dimensional crystal' consisting of N equally spaced atoms, as shown schematically in the bottom of Fig. L17. We assume the crystal to be closed into a ring, i.e. atom no N is adjacent to atoms number $N-1$ and 1. The Hilbert space representing this system then is $\mathbb{C}^N$. Our 'system' in this context is an **electron**, i.e. a quantum particle which may move in the crystal by hopping from one atom to the next.

▷ The components ψ_j are a measure for the so-called **probability amplitude** that the particle is located at atom no. j, and the real number $|\psi_j|^2$ gives us the actual probability to find it at j in a measurement. In this context the jth standard basis vector $(0,\ldots,1,\ldots,0)^T$ describes a state in which the electron is found with certainty (probability one) at site no. j. A general state describes a 'superposition' in which the probability to find the electron is delocalized over different sites with probability $|\psi_j|^2$. The unit normalization $1 = \langle\psi,\psi\rangle = \sum_j |\psi_j|^2$ means that these probabilities add to unity, i.e. the particle will be found *somewhere* in the crystal.

▷ **Physical observables**, A, i.e. quantities which can be measured (position, momentum, angular momentum, etc.) are described by Hermitian linear maps, $\hat{A}$, acting in V. In the present context these maps are called **(Hilbert space) operators**, and their eigenvectors, ψ_n are called **eigenstates** (Eigenzustand). An axiom of quantum mechanics states states that a **measurement of the observable** must yield an eigenvalue, λ_n, of $\hat{A}$ as a result.

For example, the **position operator**, $\hat{X}$, describing the position of a quantum particle in the lattice is described by a diagonal matrix

$$X = \begin{pmatrix} 1 & & & & & \\ & 2 & & & & \\ & & 3 & & & \\ & & & \ddots & & \\ & & & & N-1 & \\ & & & & & N \end{pmatrix}.$$

When we make a position measurement we find the electron at one of the N possible sites, i.e. we measure one of the eigenvalues $j = 1,\ldots,N$ of the position operator.

However, *before* the measurement it cannot be known with certainty where the electron will be found – the probabilistic nature of quantum mechanics. The best we can achieve is statements about the *expected* result, denoted $\langle A\rangle$, of the measurement of A. For example, an electron with probability amplitude $\psi_1 = \psi_2 = \frac{1}{\sqrt{2}}$, $\psi_{j>2} = 0$ will be at site 1 and 2 with equal probability $|\psi_{1,2}|^2 = 1/2$. In this case, we expect a position measurement to yield the result 1 or 2 with equal probability, and the *expected* value of the measurement, which by definition equals the average

over many repeated measurements, will be $1 \times \frac{1}{2} + 2 \times \frac{1}{2} = 1.5$. Notice that the expected value may take fractional values even if each measurement yields an integer result.

An axiom of quantum mechanics condenses all this into the mathematical statement that the **expectation value, $\langle A \rangle$, of the measurement of an observable**, A, on a system in a state ψ is given by the scalar product,

$$\langle A \rangle = \langle \psi, \hat{A}\psi \rangle.$$

The hermiticity of $\hat{A}$ guarantees that this yields a real value, $\overline{\langle \psi, \hat{A}\psi \rangle} = \langle \hat{A}\psi, \psi \rangle = \langle \psi, \hat{A}\psi \rangle$, as we require of a probability. The meaning of the formula is easiest to interpret in a basis in which $\hat{A}$ assumes a diagonal form. For example, the position operator acts on a state as $(\hat{X}\psi)_j = j\psi_j$, i.e. by multiplication of ψ by the diagonal matrix given above. We then obtain the expectation value as

$$\langle \hat{X} \rangle = \langle \psi, \hat{X}\psi \rangle = \sum_j \overline{\psi_j} (\hat{X}\psi)_j = \sum_j j|\psi_j|^2.$$

This formula expresses the fact that the result j is found with probability $|\psi_j|^2$ and that the expected value is the sum over all these contributions. For the state mentioned above, application of this formula indeed yields $\langle \hat{X} \rangle = 1\frac{1}{\sqrt{2}^2} + 2\frac{1}{\sqrt{2}^2} = 1.5$.

▷ Another axiom of quantum mechanics states that a measurement of an observable A on a state ψ will affect that state. Assume that a the measurement yielded a particular eigenvalue λ_n. Quantum mechanics then says that right after the measurement the system will be in the corresponding eigenstate ψ_n. Unlike with classical physics, where measurements can be made purely observatory and non-invasive, **a quantum measurement on a state ψ causes a state change $\psi \to \psi_n$.** For example, the measurement of an electron at position j means that after the measurement the system is in the state described by the jth standard vector $(0, \ldots, 1, \ldots, 0)$. This reflects that after the measurement we know with probability one that the electron is at j.

▷ In classical physics the instantaneous position, $\mathbf{x}$, of a particle does not contain the full information about its motion. We also need to know its velocity, $\mathbf{v}$, or momentum, $\mathbf{p} = m\mathbf{v}$, where m is the particle mass. The pair $(\mathbf{x}, \mathbf{p})$, fully specifies the state of the particle in the sense that knowledge of $(\mathbf{x}, \mathbf{p})(0)$ at an initial time $t = 0$ is sufficient information to solve Newton's equations and to predict the future motion $(\mathbf{x}, \mathbf{p})(t)$.

To discuss how these structures carry over to the quantum world we turn back to our lattice example. Without explanation we state that the Hermitian (check!) matrix representing the Hermitian operator $\hat{P}$ of the observable 'momentum' acts on quantum states as $(P\psi)_j = \frac{1}{2i}(\psi_{j+1} - \psi_{j-1})$. The corresponding matrix reads

$$P = \frac{1}{2\mathrm{i}} \begin{pmatrix} 0 & 1 & & & & -1 \\ -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & & \ddots & & \\ & & & -1 & 0 & 1 \\ 1 & & & & -1 & 0 \end{pmatrix},$$

where all empty positions are filled with zeros.[1]

We may now ask what values possible values a **quantum measurement of momentum** might yield. According to the measurement axiom formulated above these must be eigenvalues of the matrix P, i.e. to answer the question we need to diagonalize the latter. Let us denote the eigenstates of the momentum operator by ψ_l, $l = 1, \ldots, N$ i.e. $\hat{P}\psi_l = \lambda_l \psi_l$, where λ_l is the eigenvalue. To find these states, let us start from an eigenvector ansatz, $\psi = c\exp(zl)$, where c, z are complex parameters. If we substitute this into the matrix equation, we find that for site-indices inside the system, $j \neq 1, N$, the eigenvector condition is satisfied,

$$(\hat{P}\psi)_j = \frac{1}{2i}(\psi_{j+1} - \psi_{j-1}) = \frac{c}{2i}\left(e^{z(j+1)} - e^{z(j-1)}\right) = \frac{1}{2i}\left(e^{z} - e^{-z}\right)\psi_j, \qquad 1 < j < N,$$

with eigenvalue $\lambda = (e^z - e^{-z})/2i$. A constraint for the parameter z follows from the condition that the equation hold at the boundaries, too:

$$(\hat{P}\psi)_N = \frac{1}{2i}(\psi_1 - \psi_{N-1}) = \frac{c}{2i}\left(e^{z} - e^{z(N-1)}\right) = \frac{c}{2i}\left(e^{z}e^{-zN} - e^{-z}\right)\psi_N.$$

The eigenvalue equation is satisfied, provided $\exp(-zN) = 1$. This condition is resolved by the N different choices $z = 2\pi i l/N$, where $l = 1, \ldots, N$. These values lead to N different eigenvectors and eigenvalues

$$\psi_{l,j} = \frac{1}{\sqrt{N}} e^{\mathrm{i}\frac{2\pi l}{N}j}, \qquad \lambda_l = \sin(2\pi l/N),$$

where we have chosen the second free parameter, $c = 1/\sqrt{N}$ to obtain normalization, $\sum_l |\psi_{l,j}|^2 = 1$, and $(e^z - e^{-z})/2i = \sin(2\pi l/N)$ was used. These N different states form a basis, the **eigenbasis of the momentum operator**.

Physically, the axioms of quantum mechanics imply that a measurement of the momentum on a lattice can yield only the *discrete* values $\lambda_l = \sin(2\pi l/N)$, $l = 1, \ldots, N$. Unlike in classical physics, the momentum of a quantum particle moving on a ring does not assume arbitrary values but is **quantized**. The full set of real eigenvalues of an hermitean operator is called its **spectrum**.[2] Specifically, neighboring eigenvalues in the discrete spectrum of the momentum operator differ by $|\sin(2\pi(l+1)/N) - \sin(2\pi l/N)| \simeq |\cos(2\pi l/N)|2\pi/N = \mathcal{O}(N^{-1})$ where a first order Taylor expansion was applied and we used that the cosine is of order unity. This shows how the quantization becomes more pronounced for 'small systems'.

The above diagonalization procedure also shows that the eigenstates of the momentum operator extend over the whole lattice, with components of uniform magnitude $|\psi_{k,l}|^2 = N^{-1}$. Now suppose we had measured the position of the quantum particle and got j_0 as an answer (i.e. an eigenvalue of the position operator $\hat{X}$). According to the collapse postulate, the state of the particle immediately after the measurement will be described by the state vector $\psi_j = \delta_{j,j_0}$, a

[1] The corner elements 1 and -1 appearing in the momentum matrix describe the action of $\hat{P}$ on boundary states: $(\hat{P}\psi)_N = \frac{1}{2i}(\psi_1 - \psi_{N-1})$, i.e. the operator takes the difference of neighboring sites as in the 'inner' parts of the ring. (The neighboring sites of the terminal site N are $N-1$ and 1.)

[2] The denotation 'spectrum' is physically motivated and reflects that the eigenvalues of operators carrying physical significance are often determined by spectroscopic methods.

state concentrated at the lattice site j_0. But this is very different from any of the delocalized momentum eigenstates! Conversely, suppose we had measured the momentum and obtained any of the eigenvalues $\sin(2\pi l/N)$. After the measurement the particle will then be in the states ψ_l which is completely smeared over the lattice. This is very different from any position eigenstate. These observations show that the observables **position and momentum cannot be simultaneously determined with certainty**. The more accurately one is determined, the more undetermined gets the other. The degree to which the maximizing the precision of one measurement increases the uncertainty of the other is made precise by **Heisenbergs uncertainty relation** which we do not discuss here. In lecture courses of quantum mechanics it is shown how the 'incompatibility' of simultaneous measurements of observables is at the root of most quantum phenomena.

The discussion above is meant to hint at the connections between the abstract operations discussed earlier in the text (basis change, matrix diagonalization, etc.) and the phenomena of quantum mechanics. For an in-depth development of the the axiomatic of quantum mechanics and its formulation in terms of linear algebra we refer to advanced lecture courses on quantum theory.

L9.3 Relation between Hermitian and unitary matrices

REMARK This section discusses connections between Hermitian and unitary matrices and can be skipped at first reading.

Both Hermitian and unitary matrices were introduced with reference to a scalar product. One may wonder if this means that they have more in common than our so far discussion revealed. To understand the actual connection between these two sets of matrices, let A be an Hermitian matrix and consider its exponential

$$U \equiv \exp(\mathrm{i}A), \tag{L216}$$

where the exponential function is defined in Eq. (L195). We claim that U is unitary. To see this, compute the Hermitian adjoint,

$$U^\dagger = \left(\sum_n \frac{(\mathrm{i}A)^n}{n!}\right)^\dagger = \sum_n \frac{((\mathrm{i}A)^n)^\dagger}{n!} = \sum_n \frac{(-\mathrm{i}A)^n)}{n!} = \exp(-\mathrm{i}A) = U^{-1}.$$

Here, we used $(X^n)^\dagger = (X^\dagger)^n$, and $(\mathrm{i}A)^\dagger = -\mathrm{i}A$. In the last equality we noted that $\exp(-\mathrm{i}A)\exp(\mathrm{i}A) = \mathbb{1}$, i.e. $U^{-1} = \exp(-\mathrm{i}A)$. We have thus found that

The exponential of $\mathrm{i}\times$(a Hermitian matrix) is unitary.

EXAMPLE Consider the Hermitian matrix $A = \theta \left(\begin{smallmatrix} & -\mathrm{i} \\ \mathrm{i} & \end{smallmatrix}\right)$, where θ is a real parameter. Multiplication by i yields $\mathrm{i}A = \theta J$, where the matrix $J = \left(\begin{smallmatrix} & 1 \\ -1 & \end{smallmatrix}\right)$. We observe that $J^2 = -\mathbb{1}$, and $J^{2n} = (-)^n \mathbb{1}$, $J^{2n+1} = (-)^n J$. From these identities we obtain

$$\exp(\mathrm{i}A) = \sum_n \left(\frac{1}{(2n+1)!}(\mathrm{i}A)^{2n+1} + \frac{1}{2n!}(\mathrm{i}A)^{2n} \right) = \sum_n \left(\frac{(-)^n \theta^{2n+1}}{(2n+1)!} J + \frac{(-)^n \theta^{2n}}{2n!} \mathbb{1} \right) =$$

$$= \quad \sin(\theta) J + \cos(\theta) \mathbb{1} = \left(\begin{smallmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{smallmatrix}\right).$$

It is straightforward to verify that the resulting matrix is unitary.

In fact, an even stronger statement can be made. A Hermitian matrix, A, of dimension n is fixed by n^2 real parameters. To understand this counting, note that the relation $A^\dagger = A$, or $\overline{A^i{}_j} = A^j{}_i$ requires all n diagonal elements, $A^i{}_i$ to be real. The $n(n-1)/2$ elements $A^i{}_j$, $i > j$, defining the upper right triangle of the matrix can be chosen as arbitrary complex numbers. The elements of the lower left triangle are then fixed through the above hermiticity condition. Noting that a complex number contains two real parameters, we conclude that $n + 2\frac{n(n-1)}{2} = n^2$ free real parameters need to be specified to define a Hermitian matrix. For example, a general two-dimensional Hermitian matrix is of the form $A = \left(\begin{smallmatrix} a & b+\mathrm{i}c \\ b-\mathrm{i}c & d \end{smallmatrix}\right)$, and thus described by $4 = 2^2$ real parameters a, b, c, d.

The unitary matrices of dimension n, too, are parameterized by n^2 real parameters. This follows from the fact that the relation $U^\dagger U = \mathbb{1}$, or $(U^\dagger)^i{}_k U^k{}_i = \delta^i{}_j$ can be understood as a set of n^2 *real* equations[3] constraining the n^2 complex or $2n^2$ real parameters describing an arbitrary complex matrix. Each equation effectively fixes one free parameter, so that the set of unitary matrices is parameterizable in terms of $2n^2 - n^2 = n^2$ real parameters. For example, a two dimensional unitary matrix, $U = \left(\begin{smallmatrix} r & s \\ t & u \end{smallmatrix}\right)$ is constraint by the condition $U^\dagger U = \left(\begin{smallmatrix} \bar{r} & \bar{t} \\ \bar{s} & \bar{u} \end{smallmatrix}\right)\left(\begin{smallmatrix} r & s \\ t & u \end{smallmatrix}\right) = \left(\begin{smallmatrix} 1 & \\ & 1 \end{smallmatrix}\right)$. Building the matrix product, we see that this implies the two real equations $|r|^2 + |t|^2 = |s|^2 + |u| = 1$ and a complex one, $\bar{r}s + \bar{t}u = 0$. (The fourth component relation is the complex conjugate of the third relation and does not introduce further constraints). Since a complex relation implies two separate real equations for real and imaginary part, we have a total of four real equations for the eight real parameters entering the complex numbers r, t, s, u. This leaves $4 = 2^2$ free real parameters determining a two-dimensional unitary matrix.

The key observation is that unitary and hermitian matrices of the same dimension contain equally many free real parameters. We have also seen that for a Hermitian A, $U = \exp(\mathrm{i}A)$ is unitary. This suggests that *every* unitary matrix can be expressed as the exponential of i times a Hermitian matrix. It is non-trivial to show that this is indeed the case and that (L216) represents a proper **exponential parameterization of the group of unitary matrices**. This representation plays a rather important role in physics. For example, in quantum mechanics (see info section above), physical observables are represented by Hermitian matrices,

[3] The counting follows from the observation that for $i > j$, $(U^\dagger)^i{}_k U^k{}_j = 0$ is an equation fixing the *complex* number $(U^\dagger)^i{}_k U^k{}_j$. This gives a totality of twice as many, $2n(n-1)/2 = n(n-1)$, real equations. The equations for $i < j$ are obtained by complex conjugation of those for $i > j$ (why?) and must not be counted separately. For $i = j$, $(U^\dagger)^i{}_k U^k{}_i = \sum_k |U^i{}_k|^2 = 1$ are n real conditions, so that we have a totality of $n + 2n(n-1)/2 = n^2$ real equations.

the evolution of observables in time is described by unitary matrices, and the exponential representation establishes the correspondence between these two descriptions. Another important consequence of the exponential representation is that a unitary matrix can be factorized as

$$U = e^{iA} = e^{iA/N} e^{iA/N} \dots e^{iA/N}, \tag{L217}$$

i.e. as a product of N factors $\exp(iA/N)$. (Explain on the basis of the results of section L7.5 why this relation holds.) If $N \gg 1$ is very large, the matrices A/N (containing the matrix elements of A divided by N) are close to zero and an expansion $\exp(iA/N) \simeq \mathbb{1} + iA/N$ is permissible. The decomposition above represents a possibly complicated unitary matrix as a product of a large number of relatively simple (close to the unit matrix) factors described by 'small' anti-hermitian matrices iA/N.[4] For example, if $U = \left(\begin{smallmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{smallmatrix}\right)$ is a rotation as in the example above, and N is chosen asymptotically large, the decomposition is in terms of N factors $\left(\begin{smallmatrix} 1 & \theta/N \\ -\theta/N & 1 \end{smallmatrix}\right)$. Convince yourself that the application of this matrix to a two-dimensional vector, $\mathbf{v}$, generates an 'infinitesimal rotation' of $\mathbf{v}$ by an angle θ/N. Specifically, check that the norm of the transformed vector equals that of $\mathbf{v}$ up to corrections of $\mathcal{O}(N^{-2})$ neglected in the first order expansion in iA/N. The above decomposition thus describes a finite angle rotation as a product of an infinitely large number of 'infinitesimal' rotations. Representations of this type play an important role in many physical applications.

A similar relation holds between the set of *anti*symmetric real matrices, $A^T = -A$, and the orthogonal matrices $O^T = O^{-1}$. It is a good exercise (try it!) to show that $\exp(A) = O$ is orthogonal and that the sets of antisymmetric matrices and orthogonal matrices contain the same number of parameters, namely $n(n-1)/2$. However, in this case, $\exp(A)$ does not cover the full group of orthogonal matrices. (Only the subgroup $\mathrm{SO}(n) \subset \mathrm{O}(n)$ of unit determinant orthogonal matrices is obtained.) This correspondence and its applications in physics are discussed in advanced lecture courses.

[4] A matrix X is called **anti-hermitian** if $X^\dagger = -X$. The matrices iA are anti-hermitian because $(iA)^\dagger = -iA^\dagger = -iA$.

L10 Linear algebra in function spaces

REMARK This chapter looks at the mathematics of functions (i.e. mathematics commonly subsumed under the roof of 'calculus') from a linear algebraic perspective. It should be read at a relatively late stage and requires familiarity with major parts of chapter C. Specifically, we will make reference to section C6.1 on the δ-function and section C6.2 on Fourier series. Some familiarity with linear differential equations is also required. Throughout this chapter we will often use a column vector notation such as $f \leftrightarrow \mathbf{v}$ where on the l.h.s we have an object belonging to a function space, and on the r.h.s. the analogous object of a finite dimensional vector space. Occasionally we will consider spaces with non-trivial metrics and familiarity with section L3.3 and covariant notation is required to understand these parts of the chapter.

Earlier in part L (cf. section L2.3) we had introduced function spaces as an example of vector spaces. However, so far we have not discussed any of the central concepts of linear algebra – changes of basis, linear maps, etc. – in this context. This extension will be the subject of the present chapter. It provides important foundations for the mathematical understanding of various physical disciplines and notably of quantum mechanics. The mathematical framework of quantum mechanics is essentially a synthesis of analysis and linear algebra, and the most efficient way to penetrate it is to regard functions as vectors to which all operations of linear algebra may be applied. In the rest of this chapter, we will discuss how this works in practice.

There are two aspects in which function spaces differ from the conventional vector spaces discussed so far. The first is different notation. For example, the 'components' specifying a function f are denoted $f(x)$ and not v^i like those of a vector $\mathbf{v}$. As with any change of notation it may take some time to get used to this, but after a while the linear-algebraic way of handling functions will begin to feel natural. The second point is more serious: function spaces are infinite dimensional. For example, we need infinitely many 'components' $f(x)$ to fully describe a function f, indices labeling function-bases run over infinite index-sets, etc. Infinite dimensionality may also lead to existence problems. For example, linear maps of function spaces can be thought of as infinitely large matrices. Determinants and traces of such matrices then assume the form of infinite products and sums whose convergence must be checked. All this indicates that the mathematically rigorous treatment of infinite dimensional vector spaces requires substantial extensions of the framework of finite dimensional linear algebra, and this is the subject of **functional analysis**. While a mathematically rigorous introduction to functional analysis is beyond the scope of this text, we will point out convergence issues where they occur and suggest pragmatic ways of handling them. This approach should be

sufficient for the majority of situations encountered in physics.

Throughout, we will consider function spaces $X \equiv \{f : I \to \mathbb{C}\}$ containing functions mapping a *bounded*[1] domain of definition $I \subset \mathbb{R}^n$ into the complex numbers. Our focus on complex valued functions is largely motivated by applications. The choice of a compact domain of definition eases the discussion of some of the convergence issues mentioned above. Some of the modifications required for the treatment of unbounded domains of definition will be listed at the end of the chapter.

David Hilbert (1862–1943)
One of the most influential and versatile mathematicians of his time. Hilbert is considered one of the last 'universal' mathematicians, capable of overseeing the field as a whole. He made important contributions not only to many areas of mathematics but also to physics, notably to the development of general relativity and to the mathematical foundations of quantum mechanics.

Throughout this chapter we will also assume square integrability $f \in L^2(I)$ which means that X is an inner product space with the standard scalar product

$$\langle f, f' \rangle = \int_I \mathrm{d}x\, \overline{f(x)} f'(x). \qquad \text{(L218)}$$

For $n > 1$ the integral on the right hand side becomes a higher dimensional integral. Although this generalization is straightforward, we will mostly use $n = 1$ notation for simplicity. In a number of applications Eq. (L218) is replaced by the non-standard scalar product

$$\langle f, f' \rangle \equiv \int_I \mathrm{d}x\, \overline{f(x)} g(x) f'(x) \qquad \longleftrightarrow \qquad \langle \mathbf{v}, \mathbf{v}' \rangle = \sum_{ij} \overline{v^i} g_{ij} v^j \equiv \sum_i \overline{v^i} v_i, \qquad \text{(L219)}$$

where g is some positive function.[2] Function spaces equipped with such scalar products define an important an important class of so-called **Hilbert spaces**.[3]

L10.1 The standard basis of a function space

In section L2.3 we established a correspondence between functions f and vectors $\mathbf{v}$ as

$$f \qquad \longleftrightarrow \qquad \mathbf{v},$$

[1] A set $I \subset \mathbb{R}^n$ is bounded if for any $\mathbf{x} \in I$ and all $i = 1, \ldots, n$ the components x^i lie between an upper and a lower bound $a^i < |x^i| < b^i$, where $a^i < b^i$ are positive real numbers.

[2] One might consider even more general scalar products, viz. $\langle f, f' \rangle \equiv \int_I \mathrm{d}x\, \mathrm{d}y \overline{f(x)} g(x,y) f'(y)$ where the weight function $g(y,x) = \overline{g(x,y)}$ assumes the role of the metric $g_{ij} = \overline{g_{ji}}$ (check that this defines a scalar product if g has suitable positivity properties). However such generalizations do not often occur in practice and we will not discuss them.

[3] Hilbert spaces are generalizations of the Euclidean spaces discussed earlier in this chapter. They are inner product spaces equipped with an extra condition ensuring that the norm of a vector (L32) exists. Denoting the components of a vector f by f_k, this amounts to existence conditions on sums such as $\langle f, f \rangle = \sum_k f_k^2 < \infty$. In the case of finite dimensional Euclidean spaces this condition is trivially fulfilled. The detailed discussion of the Hilbert condition for infinite dimensional spaces is beyond the scope of the present text. However, we note that the requirement of finite $\langle f, f \rangle = \int_I dx f(x)^2 < \infty$ is a condition of this sort if we understand the integral as a generalized 'sum' over squared 'components' $f(x)^2$.

$$\begin{aligned} f(x) \quad &\longleftrightarrow \quad v^i, \\ x \quad &\longleftrightarrow \quad i, \end{aligned} \tag{L220}$$

i.e. if $f \in L^2(I)$ is thought of as a vector, then $x \in I$ would play the role of the index $i = \{1, \ldots, n\}$, and the $f(x)$ values would be its components.

However, when we speak of components we implicitly refer to a basis, and the function f must be expandable as

$$f = \int \mathrm{d}x \, \delta_x \, f(x) \qquad \longleftrightarrow \qquad \mathbf{v} = \sum_i \mathbf{e}_i \, v^i, \tag{L221}$$

where now $\delta_y \leftrightarrow \mathbf{e}_i$ assumes the role of a **basis function** and $\int \mathrm{d}y \leftrightarrow \sum_i$ is a 'sum' over the infinitely large number of these functions. The distinguishing property of the finite dimensional standard basis $\{\mathbf{e}_i\}$ in (L221) is its orthonormality $\langle \mathbf{e}_i, \mathbf{e}_j \rangle \equiv g_{ij} = \delta_{ij}$, i.e. it is a basis in which the metric assumes the form of a unit matrix. The component representation of these basis vectors is as simple as possible, $(\mathbf{e}_i)^j = \delta^j{}_i$ has zeros everywhere except for a one at position i. What would a basis function δ_x with analogous properties look like? A preliminary answer to this question was given early in the text, on p. 33, where we argued that the basis function which is to be multiplied by the coefficient $f(x)$ in the linear expansion must be focused on the point x with infinite precision. This is the defining property of the δ-function introduced in section C6.1. The function has δ_x has the required properties that $\delta_x(y)$ vanishes for $y \neq x$ in such a way that its 'infinitely narrow' support is compensated by the infinite amplitude $\delta_x(x) = \infty$, i.e.

$$\delta_y(x) = \delta(x - y) \leftrightarrow (\mathbf{e}_i)^j = \delta^j{}_i, \tag{L222}$$

assumes the role of the Kronecker-δ valued components of a standard basis vector. The components $f(y)$ of a function expanded in the standard basis can then be expressed as

$$f(y) = \int \mathrm{d}x \, \underbrace{\delta_x(y)}_{\delta(x-y)} \, f(x) \qquad \longleftrightarrow \qquad v^j = \sum_j \underbrace{(\mathbf{e}_i)^j}_{\delta^j{}_i} \, v^i. \tag{L223}$$

Much like the standard basis of $\mathbb{R}^n$ is orthonormal, $\langle \mathbf{e}_i, \mathbf{e}_{i'} \rangle = \delta_{ii'}$, the δ-function basis $\{\delta_x\}$ satisfies and **orthonormality relation**, too: $\langle \delta_x, \delta_y \rangle = \int_I \mathrm{d}z \, \delta_x(z)\delta_y(z) = \int_I \mathrm{d}z \, \delta(x-z)\delta(z-y) = \delta(x-y)$, so we have the correspondence

$$\langle \delta_x, \delta_y \rangle = \delta(x - y) \qquad \longleftrightarrow \qquad \langle \mathbf{e}_i, \mathbf{e}_j \rangle = \delta_{ij}. \tag{L224}$$

The components of a vector can be obtained by taking the scalar product with a basis vector $v^i = \langle \mathbf{e}^i, \mathbf{v} \rangle = \sum_j \langle \mathbf{e}^i, \mathbf{e}_j \rangle \, v^j = \sum_j \delta^i{}_j v^j$, where the conventions of Eq. (L56) where used. Likewise, the 'components' $f(x)$ can be obtained as $\langle \delta_x, f \rangle = \int \mathrm{d}y \, \delta_x(y) f(y)$, i.e.

$$f(x) = \langle \delta_x, f \rangle \qquad \longleftrightarrow \qquad v^i = \left\langle \mathbf{e}^i, \mathbf{v} \right\rangle. \tag{L225}$$

We note that for function spaces, there is no such thing as covariant notation of indices. If a metric enters the stage, it needs to be written in explicit form and cannot be 'hidden' in raised or lowered indices.

	vector space		function space	
	invariant	components	invariant	components
elements	$\mathbf{v}$	$v^j=\langle\mathbf{e}^j,\mathbf{v}\rangle$	f	$f(x)=\langle\delta_x,f\rangle$
scalar product	$\langle\mathbf{u},\mathbf{v}\rangle$	$\overline{u^i}g_{ij}v^j\equiv\overline{u^i}v_i$	$\langle f,g\rangle$	$\int\mathrm{d}x\,\overline{f(x)}g(x)$
standard basis	$\mathbf{e}_i$	$e^i{}_j=\delta^i{}_j$	δ_y	$\delta_y(x)=\delta(y-x)$
alternative basis	$\mathbf{w}_\alpha$	$(\mathbf{w}_\alpha)^j=\langle\mathbf{e}^j,\mathbf{w}_\alpha\rangle$	ψ_k	$\psi_k(x)=\langle\delta_x,\psi_k\rangle=\frac{1}{\sqrt{L}}\mathrm{e}^{\mathrm{i}kx}$
orthonormality	$\langle\mathbf{w}_\alpha,\mathbf{w}_\beta\rangle\equiv g_{\alpha\beta}=\delta_{\alpha\beta}$	$\overline{(\mathbf{w}_\alpha)^i}(\mathbf{w}_\beta)_i=\delta_{\alpha\beta}$	$\langle\psi_k,\psi_p\rangle=\delta_{kp}$	$\frac{1}{L}\int\mathrm{d}x\,\mathrm{e}^{\mathrm{i}(p-k)x}=\delta_{kp}$
expansion	$\mathbf{v}=\mathbf{w}_\alpha v^\alpha$	$v^j=(\mathbf{w}_\alpha)^j v^\alpha$	$f=\psi_k\tilde{f}_k$	$f(x)=\frac{1}{\sqrt{L}}\sum_k\mathrm{e}^{\mathrm{i}kx}\tilde{f}_k$
coefficients	$v^\alpha=\langle\mathbf{w}^\alpha,\mathbf{v}\rangle$	$v^\alpha=\overline{(\mathbf{w}^\alpha)_i}v^i$	$\tilde{f}_k=\langle\psi_k,f\rangle$	$\tilde{f}_k=\frac{1}{\sqrt{L}}\int\mathrm{d}x\,\mathrm{e}^{-\mathrm{i}kx}f(x)$
completeness	$\langle\mathbf{e}_j,\mathbf{e}_i\rangle=\langle\mathbf{e}_j,\mathbf{w}^\alpha\rangle\langle\mathbf{w}_\alpha,\mathbf{e}_i\rangle$	$\delta_{ji}=(\mathbf{w}^\alpha)_j\overline{(\mathbf{w}_\alpha)_i}$	$\delta(x-y)=\langle\delta_x,\psi_k\rangle\langle\psi_k,\delta_y\rangle$	$\delta(x-y)=\frac{1}{L}\sum_k\mathrm{e}^{\mathrm{i}k(x-y)}$

Table L10.1: Summarizing the linear algebraic interpretation of basis changes in function space. Einstein summation over the repeated indices α or k is used. For completeness, the table makes reference to a general metric $g=\{g_{ij}\}$, and an index lowering convention $v_i\equiv g_{ij}v^j$ is used (cf. Eq. (L51)). Similarly, $w_\alpha=g_{\alpha\beta}w^\beta$. Our discussion in the main text assumes orthonormal bases, $g_{ij}=\delta_{ij}$ and $g_{\alpha\beta}=\delta_{\alpha\beta}$ where $v_i=v^i$ and $w_\alpha=w^\alpha$. If you are not yet familiar with these index conventions you may regard all indices as subscripts.

Non-standard bases of function space

The relations above would be of little more than pedagogical value if there were not interesting function bases different from the standard δ-basis. We have already met one important example of non-standard bases, viz. the basis of Fourier functions discussed in section C6.2. To understand how Fourier series representations of functions can be seen as a change of basis, we consider the case $I=[0,L]$ and the function space $X=\{f\in L^2(I)|f(0)=f(L)\}$, i.e. the space of complex valued square integrable functions on the interval I with 'periodic boundary conditions' $f(0)=f(L)$. Now consider the set of functions $\{\psi_k\in X|k\in(2\pi/L)\mathbb{Z}\}$ where

$$\psi_k(x)\equiv\frac{1}{\sqrt{L}}\exp(\mathrm{i}kx). \tag{L226}$$

Apart from the normalization factor $L^{-1/2}$, these functions coincide with the Fourier modes $\exp(\mathrm{i}kx)$ introduced in Sec. C6.2. As we are going to show next the set $\{\psi_k\}$ defines an **orthonormal basis** of $L^2(I)$ different from the standard basis $\{\delta_x\}$. To explore these connections we again refer to the analogous situation in a finite dimensional vector space: let $\{\mathbf{w}_\alpha|\alpha=1,\ldots,N\}$ be an orthonormal system of basis vectors different from the standard basis $\{\mathbf{e}_i|i=1,\ldots,N\}$.[4]

The function values

$$\psi_k(x)\qquad\longleftrightarrow\qquad(\mathbf{w}_\alpha)^j \tag{L227}$$

are the components of the new basis vectors written in terms of the old basis. In the language of section **??** they define the entries of an 'infinite dimensional' transformation matrix $(T^{-1})_{x,k}$.

[4] We use different basis indices i and α, respectively, to foster comparison to the functions $\{\delta_y\}$ and $\{\psi_k\}$ which, likewise, are labeled by different indices x and k.

Thanks to the orthonormalization of the standard basis $\{\delta_y\} \leftrightarrow \{\mathbf{e}_i\}$, we may understand the function *values*, $\psi_k(x)$ (i.e. the analog of vector components) as scalar products taken between the Fourier functions, ψ_k, (the analog of vectors) and the basis functions, δ_x of the standard basis (cf. Eq. (L225))

$$\psi_k(x) = \langle \delta_x, \psi_k \rangle \qquad \longleftrightarrow \qquad (\mathbf{w}_\alpha)^j = \langle \mathbf{e}^j, \mathbf{w}_\alpha \rangle. \tag{L228}$$

It is straightforward to check the **orthonormalization of the Fourier basis**:

$$\begin{aligned} \langle \psi_k, \psi_p \rangle &= \int_I \mathrm{d}x\, \overline{\psi_k(x)} \psi_p(x) = \frac{1}{L} \int_0^L \mathrm{d}x\, \mathrm{e}^{\mathrm{i}(p-k)x} = \delta_{kp} \\ &\longleftrightarrow \\ \langle \mathbf{w}_\alpha, \mathbf{w}_\beta \rangle &= \sum_j \overline{(\mathbf{w}_\alpha)_j} (\mathbf{w}_\beta)^j = \delta_{\alpha\beta}. \end{aligned} \tag{L229}$$

The second line of Eq. (L229) states the orthonormality of the $\{\mathbf{w}_\alpha\}$ basis; the first line shows that the Fourier modes $\{\psi_k\}$ satisfy an analogous orthogonality relation.

Completeness relations

Eq. (L229) shows that the functions $\{\psi_k\}$ are orthonormal and hence linearly independent. However, we do not yet know whether they represent a *complete* set. Unlike an n-dimensional vector space where n mutually orthogonal vectors will automatically form a basis, $L^2(I)$ is infinite dimensional. But ∞ is not a well defined number and we cannot determine by counting whether the *infinitely many* functions $\{\psi_k\}$ suffice to span it. (Maybe twice as many functions $2 \times \infty = \infty$ would be needed for that task?) Unlike with finite dimensional vector spaces, completeness needs to be established in different ways.

It will turn out that for function bases of practical interest, completeness follows from general principles and need not be checked 'manually'. Occasionally, however, this needs to be done and we here show how. A set of functions $\{\psi_k\}$ is complete, if every function can be expanded as $f = \sum_k \psi_k c_k$, where c_k are expansion coefficients. Taking the scalar product $\langle \psi_k, f \rangle$ and using the orthonormality relation (L229) we obtain the identification $c_k = \langle \psi_k, f \rangle$, so completeness requires the existence of expansions

$$f = \sum_k \psi_k \langle \psi_k, f \rangle \qquad \longleftrightarrow \qquad \mathbf{v} = \sum_\alpha \mathbf{w}_\alpha \langle \mathbf{w}^\alpha, \mathbf{v} \rangle. \tag{L230}$$

An equivalent condition is that every element of a function basis, for example those of the standard basis $\{\delta_x\}$, is expandable

$$\forall x \in I: \quad \delta_x = \sum_k \psi_k \langle \psi_k, \delta_x \rangle \qquad \longleftrightarrow \qquad \forall i = 1, \ldots, N: \quad \mathbf{e}_i = \sum_\alpha \mathbf{w}_\alpha \langle \mathbf{w}^\alpha, \mathbf{e}_i \rangle\ . \tag{L231}$$

Since a generic function can be expanded in the standard basis, Eq. (L231) suffices to guarantee expandability in elements of the $\{\psi_k\}$ basis. Taking scalar products $\langle \delta_y, \ \rangle$ of this relation with generic standard basis vectors we obtain the equivalent set of relations

$$\delta(y-x) \overset{(L224)}{=} \langle \delta_y, \delta_x \rangle \overset{(L231)}{=} \sum_k \langle \delta_y, \psi_k \rangle \langle \psi_k, \delta_x \rangle \overset{(L228)}{=} \sum_k \psi_k(y)\overline{\psi_k(x)}$$

$$\longleftrightarrow$$

$$\delta_{ji} \overset{(L224)}{=} \langle \mathbf{e}_j, \mathbf{e}_i \rangle \overset{(L231)}{=} \sum_\alpha \langle \mathbf{e}_j, \mathbf{w}_\alpha \rangle \langle \mathbf{w}^\alpha, \mathbf{e}_i \rangle \overset{(L228)}{=} \sum_\alpha (\mathbf{w}_\alpha)_j \overline{(\mathbf{w}^\alpha)_i} \ . \tag{L232}$$

These relations are easy to conceptualize: in the finite dimensional case (cf. Eq. (L228)) $(T^{-1})^j{}_\alpha = (T^\dagger)^j{}_\alpha = \langle \mathbf{e}^j, \mathbf{w}_\alpha \rangle = (\mathbf{w}_\alpha)^j$ are elements of the *unitary* transformation matrix T^{-1} describing the basis change and $T^\alpha{}_i = \langle \mathbf{w}^\alpha, \mathbf{e}_i \rangle = \overline{(\mathbf{w}^\alpha)_i}$. Eq. (L231) simply is a rewriting of the unitarity relation $(T^\dagger)^j{}_\alpha T^\alpha{}_i = \delta^j{}_i$ with matrix elements expressed as scalar products.[5] In an analogous manner, the first of the relations identifies $\{\psi_k(x)\}$ as the elements of an infinite dimensional unitary 'matrix' describing the change from the standard basis to the basis $\{\psi_k\}$. Equations like

$$\boxed{\delta(y-x) = \sum_k \psi_k(y)\, \overline{\psi_k(x)},} \tag{L233}$$

are called **completeness relations**. For the specific case of the Fourier functions (L226) the completeness has been checked by explicit construction, cf. Eq. (**??**). The orthonormality relation (L229) and the completeness relation prove that

Fourier series expansion amounts to a change of basis in function space.

Below, we will introduce a few more examples of function bases and demonstrate how their completeness follows in different ways from general criteria. However, before that we need to adapt another key concept of linear algebra to function spaces:

L10.2 Linear operators

Linear maps $\hat{A} : X \to X, f \mapsto \hat{A}f$ which send functions $f \in X$ to new functions $\hat{A}f$ are generally called **linear operators**. The general linearity conditions discussed in section L5.1 require that for a sum of two functions $f, g \in X$ the map act as $\hat{A}(f+g) = \hat{A}f + \hat{A}g$, and that it be linearly compatible with scalar multiplication $\hat{A}(cf) = c\hat{A}f$ for $x \in \mathbb{R}$.

EXAMPLE Consider the space $X \subset L^2([0,1])$ of complex valued functions on the unit interval subject to the periodicity condition $f(0) = f(1)$. Linear operators $\hat{A} : X \to X$ respecting the

[5] To make the equivalence perfect, one may raise the index j in Eq. (L232) (by multiplication with a trivial $\delta^k{}_j$ and summation over j) to obtain $\delta^k{}_i = \langle \mathbf{e}^k, \mathbf{e}_i \rangle = (\mathbf{w}_\alpha)^k \overline{(\mathbf{w}^\alpha)_i}$.

periodicity condition are easily constructed. For example, consider the function $h \in X$ with $h(x) = \cos(2\pi x)$. Multiplication by h defines the linear operator $\hat{A}_h : X \to X, f \mapsto hf$, where $(hf)(x) = h(x)f(x)$. Like h and f the function $\hat{A}_h f = hf$ is periodic, i.e. $\hat{A}_h$ acts *within* the space X. Multiplication by h satisfies the linearity criteria $\hat{A}_h(f+g) = \hat{A}_h f + \hat{A}_h g$ and $\hat{A}_h(cf) = c\, A_h f$ for $f, g \in X$ and $c \in \mathbb{R}$ and hence $\hat{A}_h$ is a linear operator on the space X.

The linear operators playing the most important role in applications involve derivative operations and are called **differential operators**. As an example consider the operator $-\mathrm{i}\,\mathrm{d}_x$ acting on functions by differentiation, e.g. $-\mathrm{i}\,\mathrm{d}_x \cos(2\pi x) = 2\pi\,\mathrm{i}\,\sin(2\pi x)$, where the factor of $-\mathrm{i}$ has been introduced for later convenience. This map, too, satisfies the periodicity condition (why?) and linearity and so defines a linear operator in X.

Later in the chapter, we will see that this operator plays an important role in the description of periodic functions and we will use it as a case study to illustrate various generic features of differential operators. Sums and products of linear operators are again linear operators. For example $(-\mathrm{i}\,\mathrm{d}x)^2 = -\mathrm{d}_x^2$ and $-\mathrm{d}_x^2 + \cos(2\pi x)$, too, act linearly in X.

L10.3 Eigenfunctions

In previous sections we have seen that the essential information on a linear map $\hat{A} : V \to V$ of a finite dimensional vector space is contained in its eigenvectors $\mathbf{v}_i$, i.e. vectors on which $\hat{A}$ acts as $\hat{A}\mathbf{v}_i = \lambda_i \mathbf{v}_i$ where λ_i is the corresponding eigenvalue. In cases where a *basis* of eigenvectors could be found, the linear map $\hat{A}$ assumed the simple form of a diagonal matrix in that basis. Generic vectors could then be expanded in the basis of eigenvectors and the action of the $\hat{A}$ was essentially under control.

Very similar things can be said about linear operators of function spaces. For an operator $\hat{A} : X \to X$ a function f_n satisfying the relation

$$\hat{A} f_k = \lambda_k\, f_k \tag{L234}$$

is called an **eigenfunction** with eigenvalue λ_k. We attach a subscript k to f_k because in cases where eigenfunctions play a role we will want to number them and k plays the role of a counting index. Unlike with finite dimensional spaces, linear operators on function spaces generally possess infinitely many eigenfunctions so the counting index will generally run over an infinite set. Typical examples include $k \in \mathbb{Z}$, or double-indices such as $(k_1, k_2) \in \mathbb{Z} \times \mathbb{Z}$. If I is unbounded, dense sets of eigenvalue indices may occur, see section L10.5 the end of this chapter.

If an eigenfunction $\tilde{f}_k$ has been found it will often be convenient to normalize it. As with vectors this is done by computing the square of its norm $\mathcal{N} \equiv \langle \tilde{f}_k, \tilde{f}_k \rangle = \int_I \mathrm{d}x\, |\tilde{f}_k|^2$. We may then define the unit-normalized eigenfunction $f_k \equiv \frac{1}{\sqrt{\mathcal{N}}} \tilde{f}_k$. We note that the seemingly innocent normalization operation may become tricky if I is non-compact and again refer to section L10.5 for a discussion of this case.

EXAMPLE As an example consider the space of periodic functions on the unit interval discussed

in the previous section L10.2. The eigenfunction equation for the linear operator $(-\mathrm{i})\mathrm{d}_x$ reads

$$(-\mathrm{i})\mathrm{d}_x f(x) = \lambda f(x), \tag{L235}$$

where we temporarily omitted the counting index k. We verify by substitution that this equation is solved by the function $a\mathrm{e}^{\mathrm{i}\lambda x}$ where $a, \lambda \in \mathbb{C}$ and λ features as the eigenvalue. Given this result, we need to ask two follow-up questions: the first is whether there are other eigenfunctions with the same eigenvalue. The answer to this question requires some background in the theory of differential equations. Eq. (L235) is an ordinary first order linear differential equation. In section C7.8 we will show that up to normalization such equations possess a unique solution. The freedom of different choices of normalization is represented by the pre-factor a in our family of eigenfunctions, so we have found the full set of solutions.[6] The second question is whether the eigenfunctions actually belong to the function space X. They do if the periodicity condition $f(0) = f(1)$, or $a = ae^{\lambda}$ is obeyed. This is satisfied *iff* $\lambda = 2\pi\mathrm{i}k$, $k \in \mathbb{Z}$. What this tells us is that the proper eigenvalues of our operator in X are given by $\lambda = \lambda_k \equiv 2\pi\mathrm{i}k$ and that $a\exp(2\pi\mathrm{i}kx)$ are the corresponding eigenfunctions. Finally, we verify that the norm of these functions is given by $|a|$ and that for $a = 1$ or other unit-modular constants we have unit normalization.

To summarize our results, we have found that the linear operator $(-\mathrm{i})\mathrm{d}_x$ possesses the set of eigenfunctions

$$f_k(x) \equiv \mathrm{e}^{2\pi\mathrm{i}kx}, \qquad k \in \mathbb{Z}. \tag{L236}$$

These functions are just the **Fourier modes** on the unit-interval. We now understand that the Fourier basis is just the basis of eigenfunctions of the linear operator $-\mathrm{i}\,\mathrm{d}_x : X \to X$.

The discussion of the example above contains a few general **guiding principles for the identification of eigenfunctions**:

- ▷ Technically, the 'eigenequations' $\hat{A}f = \lambda f$ associated with a linear differential operator are linear differential equations. Start by identifying a complete set of linearly independent solutions. The cardinality of that set depends on both the order of the highest derivative operator contained in $\hat{A}$ and on the dimensionality of I. If $\dim(I) = 1$ as in the example above the order of $\hat{A}$ determines the number of linearly independent solutions. For higher dimensional I the situation can become more complicated (think of the Fourier expansion of higher dimensional functions discussed in section **??** for example).
- ▷ Next check that the general solutions actually lie in the function space X, i.e. that they satisfy the defining properties of elements of X. It may happen that some solutions have to be disposed of (such as those with $\lambda \notin 2\pi\mathrm{i}\,\mathbb{Z}$ discussed above). The appropriately restricted set then defines your set of eigenfunctions.
- ▷ Finally, it may be expedient to normalize the functions as discussed above.

[6] The situation would be different had we considered the operator $-\mathrm{d}_x^2 = ((-\mathrm{i})\mathrm{d}_x)^2$. Its eigenequation $-\mathrm{d}_x^2 f = \lambda f$ is a second order differential equation with an eigenspace spanned by *two* linearly independent solution functions $e^{\pm\lambda x}$. The general solution is then given by all linear combinations $c_+e^{+\lambda x} + c_-e^{-\lambda x}$ with constants $c_\pm$. More generally an nth order differential operator has n linearly independent solutions and an n-dimensional eigenspace.

L10.4 Self adjoint linear operators

In section **??** we discussed the specific properties of Hermitian linear maps. We learned that a Hermitian matrix can always be diagonalized. The diagonalizability property means that the set of eigenvectors of a Hermitian matrix is complete. In fact, the set eigenvectors could be conveniently chosen so as to form an orthonormal basis. All these niceties carry over to the case of linear operators.

Definition

Assume our function space X is equipped with a scalar product (L219). For concreteness, we may consider the space X of periodic functions on the interval $[0, L]$ with complex standard scalar product $\langle f, g\rangle = \int_0^L \mathrm{d}x\, \overline{f(x)} g(x)$. An operator $\hat{A} : X \to X$ is called **self adjoint** if

$$\forall f, g \in X : \quad \left\langle \hat{A} f, g \right\rangle = \left\langle f, \hat{A} g \right\rangle \qquad \longleftrightarrow \qquad \forall \mathbf{v}, \mathbf{w} \in V : \quad \left\langle \hat{A}\mathbf{v}, \mathbf{w} \right\rangle = \left\langle \mathbf{v}, \hat{A}\mathbf{w} \right\rangle . \tag{L237}$$

We observe that a self adjoint linear operator is the analog of an Hermitian matrix. In fact, it is common practice (in physics) to use the terminology of 'Hermitian operators', and we will do so in the following.

For example, the operator $(-\mathrm{i})\mathrm{d}_x$ considered above enjoys the hermiticity property:

$$\begin{aligned}\langle (-\mathrm{i})\mathrm{d}_x f, g\rangle &= \int_0^L \mathrm{d}x\, \overline{(-\mathrm{i})\mathrm{d}_x f(x)} g(x) = \mathrm{i}\int_0^L \mathrm{d}x\, \mathrm{d}_x \overline{f(x)} g(x) = \int_0^L \mathrm{d}x\, \overline{f(x)}\, (-\mathrm{i})\mathrm{d}_x g(x) = \\ &= \langle f, (-\mathrm{i})\mathrm{d}_x g\rangle ,\end{aligned}$$

where we integrated by parts, noting that no boundary terms arise due to the assumed periodicity of the integrand. [7]

EXERCISE Recapitulate the arguments of section **??** to verify that they carry over to the case of function spaces.

As in the case of finite dimensional vector spaces, the hermiticity of a linear operator makes strong statements about its eigenvalues and eigenfunctions: all eigenvalues λ_k are real, eigenfunctions ψ_k with different eigenvalues are mutually orthogonal $\langle \psi_k, \psi_{k'}\rangle = 0$ if $\lambda_k \neq \lambda_{k'}$, and the full system of eigenfunctions is complete. The Fourier eigenfunctions of $(-\mathrm{i})d_x$ are a nice example of this.

Importantly, the knowledge that an operator is Hermitian and that we have found all of its eigenfunctions is sufficient to establish the completeness of that set of functions. In applications, it is usually the theory of differential equations that tells us that we have found a complete set of solutions of an operator eigenequation (L234). Once we know that all

[7] At this point it becomes evident why we included a factor $(-\mathrm{i})$ in the definition of the differential operator: it serves to make the latter Hermitian.

solutions are under control, completeness is granted by the hermiticity of the operator, and no explicit verification of completeness relations is necessary. This is why we said above that explicit verifications of completeness are often not needed.

INFO Hermitian differential operators play an important role both in mathematics and physics. For example, the **axioms of quantum mechanics** state that to each physical 'observable' (position, momentum, angular momentum, etc.) there corresponds one Hermitian operator $\hat{A}$. The expected state[8] of that observable is given by the 'matrix element' $\langle\psi, \hat{A}\psi\rangle$ of $\hat{A}$ in a state vector ψ describing the physical state of the system. Depending on the context, $\hat{A}$ and ψ may belong to a finite-dimensional vector space or to a function space, in which case ψ is called a wave function. We can clearly learn a great deal about a physical observable from the eigenfunctions of its corresponding operator. Moreover, if a given operator plays an especially important role in a problem, then its eigenfunctions will typically be a natural basis to work with. In the case of infinite-dimensional operators, the eigenequations are determined by differential equations. For example, the two differential operators discussed in the examples below are relevant to the quantum mechanical description of the hydrogen atom.

Example: Legendre polynomials

Consider the function space $X \equiv \{f : [-1, 1] \to \mathbb{R}\}$, i.e. the real valued functions on the interval $[-1, 1]$ (no boundary conditions specified), with standard scalar product $\langle f, g\rangle = \int_{-1}^{1} \mathrm{d}x\, f(x)g(x)$. On this space, we define the second order differential operator

$$\hat{A} = \frac{\mathrm{d}}{\mathrm{d}x}(1 - x^2)\frac{\mathrm{d}}{\mathrm{d}x}. \tag{L238}$$

It is straightforward to check, that this operator is *symmetric* relative to the standard scalar product, $\langle \hat{A}f, g\rangle = \langle f, \hat{A}g\rangle$.

EXERCISE Verify the symmetry of the differential operator (L238). Do this using integration by parts and show why no boundary terms arise.

The eigenequation of $\hat{A}$, $\hat{A}P_l = \lambda_l P_l$ is called **Legendre differential equation** and the eigenfunctions P_l are known as **Legendre polynomials**. (We will see shortly why they are polynomials in x.) Finding a complete set of solutions of the Legendre equation is a non-trivial task, often discussed in lecture courses on ordinary differential equations, theoretical electrodynamics, or quantum mechanics. Referring to the info section below for a quick sketch of the solution strategy, here we just state the result: non-singular solutions of the Legendre differential equation are found for eigenvalues $\lambda_l = -l(l + 1)$, where $l = 0, 1, 2, \ldots$ is a positive integer. The corresponding Legendre polynomials can be represented in different

[8] In quantum mechanics observables generally cannot be determined with mathematical precision, there remains 'quantum uncertainty'.

ways, among them the so-called **Rodrigues formula**

$$P_l(x) = \frac{1}{2^l l!}\frac{\mathrm{d}^l}{\mathrm{d}x^l}(x^2-1)^l. \tag{L239}$$

A list of the first four polynomials reads,

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{1}{2}(3x^2-1), \quad P_3(x) = \frac{1}{2}(5x^3-3x),$$
$$P_4(x) = \frac{1}{8}(35x^4-30x^2+3). \tag{L240}$$

It is customary to normalize the Legendre polynomials as $P_l(1) = 1$, i.e. by fixing their value at $x = 1$. For a visual representation of a few Legendre polynomials, see Fig. L18.

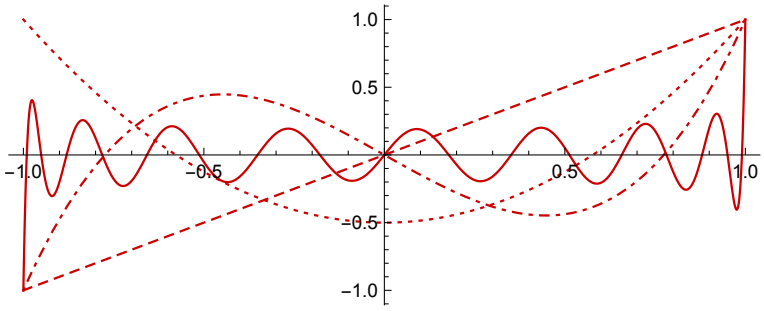


Figure L18: The Legendre polynomials P_1, dashed; P_2 dotted; P_3 dash-dotted, P_{17}, solid.

INFO Let us sketch the derivation of the result (L239).[9] The fact that the differential operator $\hat{A}$ contains a polynomial $(1-x^2)$ suggests that polynomial solutions to the eigenequation might exist. (This is a really weak argument, but better than none.) Indeed, we may check by direct substitution that $P_0 \equiv 1$ is a solution with eigenvalue $\lambda_0 = 0$ and $P_1 \equiv x$ one with eigenvalue $\lambda_1 = 2$. Encouraged by these findings, we may speculate that more complex solutions $P(x)$ of the equation $\hat{A}P(x) = \lambda P(x)$ also assume the form of a series

$$P(x) = \sum_{j=0}^{\infty} a_j x^{\alpha+j},$$

Here, the parameter $0 \leq \alpha < 1$ has been introduced to include the option of fractional, yet positive powers of x. If we act on this ansatz with the Legendre differential operator (try it!) we obtain a function

$$\hat{A}P(x) = \sum_{j=0}^{\infty}\left(a_j(\alpha+j)(\alpha+j+1)x^{\alpha+j} - a_j(\alpha+j)(\alpha+j-1)x^{\alpha+j-2}\right).$$

[9] As a word of caution we note that a comprehensive discussion would need to cover various aspects of convergence whose discussion is beyond the scope of this text. You may try to spot possible convergence issues or consult the literature if you are interested in knowing how a watertight derivation proceeds.

It will be convenient to combine the two contributions to this series into one. This can be done by rearranging terms as follows:

$$\sum_{j=0}^{\infty} a_j(\alpha+j)(\alpha+j-1)x^{\alpha+j-2} =$$
$$= \sum_{j=2}^{\infty} a_j(\alpha+j)(\alpha+j-1)x^{\alpha+j-2} + X(x) = \sum_{j=0}^{\infty} a_{l+2}(\alpha+j+2)(\alpha+j+1)x^{\alpha+j} + X(x),$$

where the term $X(x) \equiv a_0\alpha(\alpha-1)x^{\alpha-2}+a_1(\alpha+1)\alpha x^{\alpha-1}$, contains the first two summands $j=0,1$ of the series and in the second line we renamed the summation index as $j \to j-2$. Combining terms we have

$$\hat{A}P(x) = \sum_{j=0}^{\infty} \left(a_j(\alpha+j)(\alpha+j+1) - a_{j+2}(\alpha+j+2)(\alpha+j+1)\right) x^{\alpha+j} - X(x).$$

This series must be equal to the series $\lambda P(x)$. Representing these conditions in the form of a series, we get

$$0 \stackrel{!}{=} \hat{A}P(x) - \lambda P(x) = \sum_{j=0}^{\infty} \left(a_j((\alpha+j)(\alpha+j+1)-\lambda) - a_{j+2}(\alpha+j+2)(\alpha+j+1)\right) x^{\alpha+j} - X(x). \tag{L241}$$

The fact that the l.h.s vanishes everywhere demands that the coefficients of each power $x^{\alpha+k}$ are individually zero (why?). We first notice that terms of $\mathcal{O}(x^{\alpha-2}, x^{\alpha-1})$ are contained only in the contribution $X(x)$. These two must be individually zero which leads to the condition $\alpha = 0$ if either a_0 or a_1 are different from zero. The vanishing of higher powers $x^{\alpha+j}$ demands that

$$a_j((\alpha+j)(\alpha+j+1)-\lambda) - a_{j+2}(\alpha+j+2)(\alpha+j+1) = 0 \Leftrightarrow$$
$$a_{j+2} = \frac{(\alpha+j)(\alpha+j+1)-\lambda)}{(\alpha+j+2)(\alpha+j+1)} a_j.$$

The second equation can be seen as a relation recursively fixing coefficients as $a_0 \to a_2 \to a_4 \to \ldots$ and $a_1 \to a_3 \to a_5 \to \ldots$. To avoid the solution vanishing everywhere, at least one of its 'anchors' a_0 or a_1 must be non-vanishing, which in turn requires that the fractional power $\alpha = 0$ vanishes. Turning to the termination of the series, we are after solutions of *polynomial* form, i.e. we require that $a_j = 0$ after a finite number of terms. Inspection of the recursion relation shows that this condition requires the eigenvalue to assume the form $\lambda \equiv l(l+1)$ where $l \in \mathbb{N}_+$ is a positive integer. Assume that l is an even/odd integer. We then observe that the series of even/odd coefficients vanishes, while the odd/even series remains infinite. (These are the two linearly independent solutions of the Legendre differential equation at given l, there won't be other solutions.) Closer inspection shows that the unbounded solution has convergence issues and that we should discard it. It is an easy matter to compute the first few good solutions by hand and as a result one obtains the list (L241). A less easy exercise (try it!) is to verify that the recurrence relations defining the Legendre polynomials are generated by the Rodrigues formula (L239).

EXERCISE Prove the **orthogonality of the Legendre polynomials**

$$\int_{-1}^{1} \mathrm{d}x\, P_l(x) P_{l'}(x) \propto \delta_{ll'}, \tag{L242}$$

for $l = 2$ and $l' = 3$. The general proof is not easy, unless we use our linear algebraic background knowledge: use that $\hat{A}P_l = l(l+1)P_l$ and the symmetry of $\hat{A}$, $\int (\hat{A}P_l)P_{l'} = \int P_l(\hat{A}P_{l'})$ to show that the integral vanishes unless $l = l'$.

In the next section we will see where the Legendre differential operator appears in a larger framework of applications.

Exampe: spherical harmonics

REMARK Requires sections V2.4 and **??**

In physics and mathematics we are often working with problems defined on a sphere, i.e. a surface of points at fixed distance from a common origin. A convenient way to parameterize such surfaces is in terms of spherical coordinates (θ, ϕ). We saw that the natural 'surface element' assigning a spherical surface element to a change $(\mathrm{d}\theta, \mathrm{d}\phi)$ of coordinates is given by $\mathrm{d}S \equiv \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi$ and this suggests that we should consider the scalar product

$$\langle f, g\rangle = \int_0^{\pi} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, \sin\theta \overline{f(\theta,\phi)} g(\theta,\phi), \tag{L243}$$

defined on the space $X \equiv L^2(S^2)$ of square-integrable functions on the sphere, where the latter is identified with $S^2 = \{(\theta,\phi) | \theta \in (0,\pi), \phi \in (0, 2\pi)\}$[10]. This coordinate parameterization of the sphere implies that for all $f \in X$ we have the periodicity condition $f(\theta, 0) = f(\theta, 2\pi)$.

A differential operator important for the description of problems in electrodynamics and quantum mechanics is the **Laplacian on the sphere** $\Delta : X \to X$. This operator is obtained from the cartesian three-dimensional Laplace operator (**??**), $\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2$ by passing to spherical coordinates $(x, y, z) \mapsto (r, \theta, \phi)$. The result of this transformation is the complicated looking differential operator Eq. (V99) containing second derivatives w.r.t. the three coordinates, r, θ, ϕ. Its restriction to functions $f(\theta, \phi)$, i.e. functions depending on angles but not on radial coordinates, is given by

$$\Delta = \frac{1}{\sin\theta} \partial_\theta \sin\theta\, \partial_\theta + \frac{1}{\sin^2\theta} \partial_\phi^2. \tag{L244}$$

This operator is Hermitian w.r.t. the scalar product defined above as can be verified by an instructive little calculation (try it!). Conceptually, its hermiticity is inherited from that of

[10] As discussed in section V2.4 these coordinates parameterize the sphere up to a single line connecting the north and the south pole. However, as long as the focus is on integration theory, the omission of a line out of a two dimensional surface is not a problem.

the Laplacian $\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2$ of functions in *three*-dimensional space $L^2(\mathbb{R}^3)$ relative to the standard three dimensional scalar product $\langle f, g\rangle = \int \mathrm{d}x\mathrm{d}y\mathrm{d}z\, \overline{f(x,y,z)}\, g(x,y,z)$. The hermiticity of the cartesian Laplace follows straightforwardly upon partial integration w.r.t. the coordinates x, y, z. Since the 'parent' three dimensional Laplacian is Hermitian, its restriction to the subset of spherical functions must be so too.

Let us now proceed to identify the **eigenfunctions, f_λ, of the Laplace operator**, i.e. solutions of the second order partial (!) differential equation $\Delta f_\lambda(\theta,\phi) = \lambda f_\lambda(\theta,\phi)$. The solution of this problem would be tough if there were not a little trick by which the complicated looking equation can be transformed into two simpler ones: let us start by multiplying the equation with $\sin^2\theta$ and rearranging terms,

$$\left[\left(\sin\theta\partial_\theta \sin\theta\, \partial_\theta - \lambda\sin^2\theta\right) + \partial_\phi^2\right] f(\theta,\phi) = 0,$$

where we temporarily omitted the subscript λ for notational clarity. The important point now is that the differential operator appearing in this equation is the sum of two terms each depending only on θ or on ϕ. Multivariate operators separating into additive single-variate contributions are called **separable**. They have the nice property that the corresponding solutions can be obtained as *products* of single variate solution functions. In the present context this can be seen as follows: we make an ansatz $f(\theta,\phi) = g(\theta)h(\phi)$. Substituting this into the equation and multiplying from the left by $g^{-1}(\theta)h^{-1}(\phi)$, we obtain

$$g^{-1}(\theta)\left(\sin\theta\partial_\theta \sin\theta\, \partial_\theta - \lambda\sin^2\theta\right) g(\theta) = -h^{-1}(\phi)\partial_\phi^2 h(\phi).$$

The right side of this equation does not depend on θ, which means that the right side must be a constant independent of θ too. Conversely, the left side must be a constant independent of ϕ. Since these constants are equal to each other the left and the right side individually must be equal to the same constant, independent of both θ and ϕ. Let us call this constant m^2. Equating both the left and the right side of the equation to this constant, we obtain two separate *ordinary* equations,

$$\begin{aligned}\left(\sin\theta\mathrm{d}_\theta \sin\theta\, \mathrm{d}_\theta - \lambda\sin^2\theta\right) g(\theta) &= m^2 g(\theta),\\ \mathrm{d}_\phi^2 h(\phi) &= -m^2 h(\phi).\end{aligned}$$

The second of these equations is solved by the Fourier modes $h = h_m$ where $h_m(\phi) \equiv \exp(i\phi m)$ and the periodicity condition $h_m(0) = h_m(2\pi)$ requires $m \in \mathbb{Z}$ to be an integer. In the first equation, we apply a variable substitution $x \equiv \cos(\theta) \in [-1,1]$. Defining $g(\theta(x)) \equiv P(x)$ and using that $(\sin\theta)^{-1}\mathrm{d}_\theta = \mathrm{d}_x$ and $\sin^2(\theta) = 1 - x^2$ a little calculation shows that the equation assumes the form

$$\left(\mathrm{d}_x(1-x^2)\mathrm{d}_x - \lambda - m^2(1-x^2)^{-1}\right) P(x) = 0.$$

For $m = 0$ this is just the Legendre differential equation discussed in the previous section. In this case, we have the solutions $P(x) = P_l(x)$ with corresponding eigenvalues $\lambda = -l(l+1)$. The generalization of the solutions to arbitrary m are known as **Legendre functions** P_l^m.

These functions exist for values of $m \in \{-l, \ldots, l\}$ and the corresponding eigenvalues are given by $-l(l+1)$, independent of m. For positive m they are defined by

$$P_l^m = (-1)^m (1-x^2)^{m/2} \frac{\mathrm{d}^m}{\mathrm{d}x^m} P_l(x), \tag{L245}$$

while the solutions for negative m are $P_l^{m<0} = \frac{(l-m)!}{(l+m)!} P_l^{-m}$. Summarizing, we have found that the eigenfunctions of the spherical Laplace operator are given by the so-called **spherical harmonics**

$$\boxed{Y_l^m(\theta,\phi) \equiv \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\, \mathrm{e}^{im\phi} P_l^m(\cos(\theta)),} \tag{L246}$$

where the prefactor ensures unit-normalization $\left\langle Y_l^m, Y_j^n \right\rangle = \delta_{lj}\delta^{mn}$. (The proof of this is not straightforward.)

EXERCISE Convince yourself of the generality of the above argument, i.e. of the fact that every differential equation $\hat{A}f = 0$ defined by a separable differential operator of n variables and their derivatives $\hat{A}(x_1, \partial_1, \ldots, x_n, \partial_n) = \sum_i \hat{A}_i(x_i, \partial_i)$ can be diagonalized in terms of a product ansatz $f(x_1, \ldots, x_n) = \prod_i f_i(x_i)$, where all f_i are solutions of the ordinary equation $\hat{A}_i f_i = c f_i$ with a common constant c.

It is instructive to write down a few of these functions explicitly

$$\begin{aligned}
l = 0 : Y_0^0(\theta,\phi) &= \frac{1}{\sqrt{4\pi}}, \\
l = 1 : Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\cos\theta, \\
Y_1^{\pm 1}(\theta,\phi) &= \sqrt{\frac{3}{8\pi}}\sin\theta\, \mathrm{e}^{\pm i\phi}, \\
l = 2 : Y_2^0(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1), \\
Y_2^{\pm 1}(\theta,\phi) &= \mp\sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta\, \mathrm{e}^{\pm i\phi}, \\
Y_2^{\pm 2}(\theta,\phi) &= \mp\sqrt{\frac{15}{32\pi}}\sin^2\theta\, \mathrm{e}^{\pm 2i\phi}.
\end{aligned} \tag{L247}$$

We notice a trend of increasingly complex dependence on the angular arguments at higher (l, m). Fig. L19 shows a visual representation of the first few spherical harmonics. If these images faintly remind you of your chemistry classes this is no accident. The spherical harmonics are a key element of the description of atomic and molecular orbitals which is a consequence of their central role in the solution of the Schrödinger equations of atoms. These applications are generally discussed in lecture courses on quantum mechanics.

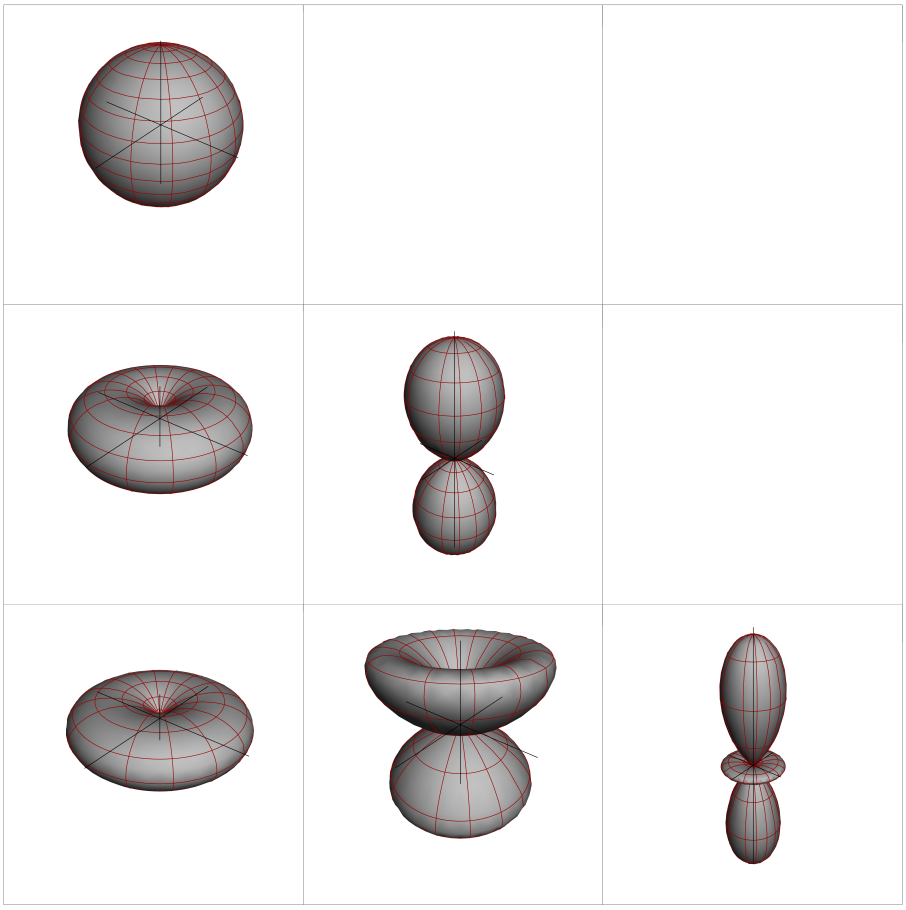


Figure L19: Plot of the first few spherical harmonics, Y_0^0 (first row), $Y_1^{-1,0,1}$ (second row), $Y_2^{-2,-1,0,1,2}$ (third row). The surfaces shown are generated by plotting the spherical-coordinate points $(r, \theta, \phi) = (|Y_l^m|^2(\theta, \phi), \theta, \phi)$ as a function of the angles (θ, ϕ).

The spherical harmonics are the complete set of eigenfunctions of an hermitean differential operator acting on functions $f \in L^2(S^2)$ on the sphere. From linear algebra we know that these functions define a **function basis on the sphere**, i.e. that every f can be expanded in the basis functions Y_l^m as

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_l^m \, Y_l^m(\theta, \phi),$$

$$a_l^m = \langle Y_l^m, f \rangle = \int_0^{\pi} \sin\theta \, \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi \, \overline{Y_l^m(\theta, \phi)} \, f(\theta, \phi), \tag{L248}$$

where the orthonormality of the spherical harmonics, $\left\langle Y_l^m, Y_j^n \right\rangle = \delta_{lj} \delta^{mn}$, implies that the expansion coefficients are obtained by the straightforward computation of scalar products as indicated in the second line.

Functions of one variable can often be approximated in terms of only a few Fourier harmonics. Similarly, low order spherical harmonics expansions are generally sufficient to obtain good descriptions of functions on the sphere (provided the latter do not exhibit wild variations). For an illustration of this point, consider the randomly generated function $f(\theta, \phi)$ shown in the first panel of Fig. L20. The remaining panels show the expansion of this function in terms of spherical harmonics from $l = 0$ (second panel) up to $l = 4$ (last panel). The $l = 4$ approximation already does a rather good job at describing our function in terms of the 24 expansion coefficients needed for an $l = 4$ expansion. What our example shows is that the spherical harmonics are the 'Fourier modes of the sphere' and play an equally useful role in the description of functions with angular variation.

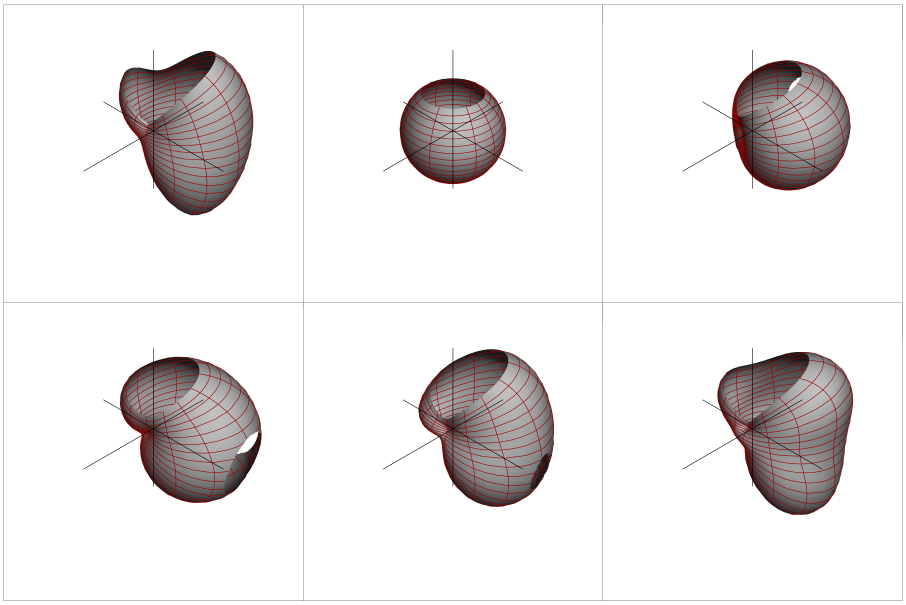


Figure L20: First panel: a randomly generated positive function f on the sphere plotted in the polar representation $f(\theta, \phi), \theta, \phi)$. Remaining panels: expansion of this function in terms of spherical harmonics up to level $l = 4$. For visual clarity the plots of all functions are limited to an angular window $\theta \in [0.6, \pi - 0.6]$.

L10.5 Function spaces with unbounded support

We conclude this chapter with a few qualitative remarks on function spaces with unbounded support, for example the space $X = L^2(\mathbb{R})$ of square integrable functions on the real axis. With few modifications, most of the concepts developed in previous sections carry over to this case. For example, we have seen in section C6.3 how Fourier series become Fourier *transforms* when functions defined on the entire real axis are considered. In practical terms this means that sums become integrals, however, the general structure of the concept remains unchanged. The importance one attributes to the differences between the bounded and the unbounded

case depend a lot one one's individual perspective:
Rigorous perspective: when we pass to spaces of functions with unbounded support, a lot of things happen. For example, the eigenfunctions $\psi_k(x) \equiv \exp(\mathrm{i}kx)$ of the differential operator $(-\mathrm{i})\mathrm{d}_x$ lie *outside* X, which follows from the fact that $|\psi_k|^2 = 1$ cannot be integrated over the whole real line.

This lack of integrability means that scalar products between the eigenfunctions cannot be taken, unless properly 'regularized' (see below). Relatedly, the Fourier 'index' k now becomes a continuous variable, and we need to ask how the discrete sums over eigenfunctions turn into integrals of sorts. There are several other elements of finite dimensional linear algebra — traces, determinants, etc. — whose mathematically rigorous generalization to the case of function spaces with unbounded support is far from trivial. However, being physicists we may ask how severe these complications are from the point of view of a
Pragmatic perspective: in section C6.3 we saw that the non-integrability of the Fourier modes ψ_k could be dealt with by introducing convergence generating factors. Alternatively it is often legitimate, and in fact convenient, to consider functions on a large but finite domain of definition $[-L, L]$, and send $L \to \infty$ in the end. (In practice this means to make L bigger than any other length scale of the physics problem at hand.) As long as L remains finite, the concepts discussed in previous sections may safely be applied. Provided nothing dangerous happens as the limit $L \to \infty$ is eventually taken, the case of an unbounded integration domain then effectively is under control. Pragmatic strategies of this sort usually work in physics. However, it should not go unmentioned that there are important exceptions to the rule. For example, so-called Dirac (differential) operators play a very important role in particle physics and more recently also in condensed matter physics. Such operators are distinguished for exceptionally poor convergence behavior and their 'regularization' is a delicate subject. These issues are discussed in lecture courses on quantum field theory at a late stage of the physics curriculum.

L11 Multilinear algebra

REMARK In this chapter, vectors, $\mathbf{v}$, matrices, A, and other objects of linear algebra will be understood from a unified perspective. It therefore becomes pointless distinguish vectors by a boldface notation and we will denote them as $v \in V$ throughout. Unless mentioned otherwise we will work with real vector spaces throughout.

Linear algebra is the mathematical discipline of objects that satisfying certain linearity criteria. So far, we have seen two representatives of these, vectors and matrices. However, there are other classes of 'linear objects' and the cumulative term for all of them – including vectors and matrices – is *tensors*. Much like vectors can be generalized to vector *fields*, one may define tensor fields. Tensors and tensor fields play an important role in various fields of physics including in general relativity, in hydrodynamics, quantum information and others.

In this chapter, we introduce the algebraic foundations of tensor algebra and in this way a new and unifying approach to linear algebra. The extension to tensor fields, along with an introductory discussion of physical applications, is the subject of the later chapters V4 to V6.

L11.1 Direct sum and direct product of vector spaces

Starting from an n-dimensional vector space, V, multilinear algebra builds more structured – and as we will see useful – vector spaces by hierarchical constructions. This is achieved by two basic constructs, the direct sum and the direct product of vector spaces. In the following, we introduce these two in turn.

Direct sum

Consider two real vector spaces, V and W, of dimension n and m, respectively. The **direct sum** $V \oplus W$ is defined as the set of ordered pairs of elements of V and W, respectively,

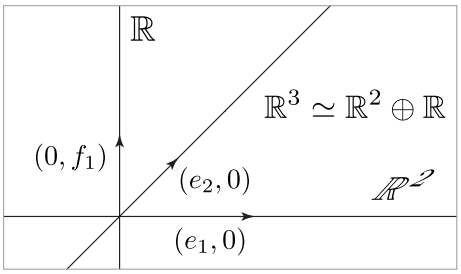
$$V \oplus W \equiv \{(v, w) \,|\, v \in V, w \in W\}. \tag{L249}$$

For these pairs, addition and scalar multiplication rules ($v, v' \in V$, $w, w' \in W$, $a \in \mathbb{R}$):

▷ $(v, w) + (v', w') = (v + v', w + w')$,

▷ $$a(v,w) = (av, aw), \tag{L250}$$

are declared to make $V \oplus W$ a real vector space. Given bases $\{e_i\}$ and $\{f_j\}$ of V and W, respectively, a generic element of $V \oplus W$ can be expressed as $\sum_i c^i(e_i, 0) + \sum_j d^j(0, f_j)$. This shows that the $n + m$ vectors $(e_i, 0)$ and $(0, f_j)$ form a basis of $V \oplus W$ and that $\dim(V \oplus W) = n+m$. Any element of $V \oplus W$ can be decomposed as $(v, w) = (v, 0)+(0, w)$ into a contribution of V and W, respectively. The sum $V \oplus W$ can therefore be imagined as a vector space in which V and W are embedded as natural subspaces. For example, $\mathbb{R}^3 = \mathbb{R}^2 \oplus \mathbb{R}$ may be considered as the direct sum of $\mathbb{R}^2$ and $\mathbb{R}$, see the figure. A component representation of vectors in $V \oplus W$ is obtained by concatenating the component vectors of V and W. In the example of $\mathbb{R}^3 = \mathbb{R}^2 \oplus \mathbb{R}$, two-dimensional vectors $(a, b)^T \in \mathbb{R}^2$ and one-dimensional vectors $c \in \mathbb{R}$ are concatenated to obtain a component representation $(a, b, c)^T$ of $\mathbb{R}^3$. Likewise, the basis vectors $e_1 = (1, 0)^T$ and $e_2 = (0, 1)^T$ of $\mathbb{R}^2$ and that, $f_1 = 1$, of $\mathbb{R}$ yield the three basis vectors $(e_1, 0) = (1, 0, 0)^T$, $(e_2, 0) = (0, 1, 0)^T$ and $(0, f_1) = (0, 0, 1)^T$ of $\mathbb{R}^3$.



The construction can be iterated to yield direct sums of higher order. For example, given three vector spaces, V, W, U with bases $\{e_i\}, \{f_j\}, \{g_k\}$, the direct sum $V \oplus W \oplus U$ may be obtained as $(V \oplus W) \oplus U = V \oplus (W \oplus U) \equiv V \oplus W \oplus U$ (why is this construction associative?), with basis vectors $(e_i, 0, 0), (0, f_j, 0)$ and $(0, 0, g_k)$. For example, the standard vector space $\mathbb{R}^n$ may be thought of as the direct sum of n copies of $\mathbb{R}$.

Tensor product

Besides the direct sum, there exists a second option to build a vector space from two constituent spaces V and W, the **direct product** or **tensor product**, $V \otimes W$ (Latin: *tendo* – I span). This space is defined as the set of real linear combinations $c_1 v_1 \otimes w_1 + c_2 v_2 \otimes w_2 + \ldots$ of pairs $v \otimes w$, $v \in V, w \in W$. Within the set of these formal linear combinations we declare the identifications ($v, v' \in V$, $w, w' \in W$, $a \in \mathbb{C}$):

▷ $$(v + v') \otimes w = v \otimes w + v' \otimes w,$$

▷ $$v \otimes (w + w') = v \otimes w + v \otimes w',$$

▷ $$(av) \otimes w = v \otimes (aw) \equiv a(v \otimes w).$$

These rules define addition and scalar multiplication in $V \otimes W$. Given bases e_i and f_j of V and W, they imply that each $v \otimes w$ can be decomposed as $v \otimes w = \sum_{ij} v^i w^j e_i \otimes f_j$, for example $(e_1 + 3e_2) \otimes (5f_4 + 2f_5) = 5e_1 \otimes f_4 + 2e_1 \otimes f_5 + 15e_2 \otimes f_4 + 6e_2 \otimes f_5$. This decomposition may be applied to each term in the sum, so that general elements of $V \otimes W$ afford a representation as $\sum_{ij} c^{ij} e_i \otimes f_j$:

$$V \otimes W = \left\{ \sum_{ij} c^{ij} e_i \otimes f_j \middle| c^{ij} \in \mathbb{R} \right\}. \tag{L251}$$

We conclude that $\{e_i \otimes f_j\}$ defines a basis of $V \otimes W$ and that the dimension of the latter is given by $n \times m$. However, unlike with the direct sum, there is no natural component representation of $V \otimes W$. For example, for $V = W = \mathbb{R}^3$, the nine-dimensional space $V \otimes W$ may be represented in terms of nine-component vectors, however, the connection between this representation and the component vectors of the spaces V and W is not particularly transparent. Relatedly, there is no intuitive graphical representation of $V \otimes W$, even for low-dimensional V and W; it is generally preferable to work with linear combinations in terms of basis vectors as in Eq. (L251). Finally notice – an important but easily forgotten fact – that not every element of $V \otimes W$ can be represented as a product $v \otimes w$. For example, $e_1 \otimes f_2 + e_2 \otimes f_1$ cannot.

As with the direct sum, the tensor product can be iterated to build tensor products of higher order: given three vector spaces, V, W, U with bases $\{e_i\}, \{f_j\}, \{g_k\}$, the tensor product $V \otimes W \otimes U$ may be obtained as the tensor product $(V \otimes W) \otimes U = V \otimes (W \otimes U) \equiv V \otimes W \otimes U$ (why is the product operation associative?) A basis is provided by the tensor products of basis vectors, $\{e_i \otimes f_j \otimes g_k\}$. The extension to products of higher order is obvious.

INFO Although tensor spaces are perhaps not easy to comprehend intuitively, they play a very important role in **physical applications**, notably in quantum mechanics. To appreciate why, consider once more the example of a particle on a lattice discussed on pp 118. There, we argued that the state of a particle moving in an N-site lattice chain is encoded in a vector $\psi \in V \equiv \mathbb{C}^N$. Now suppose that the particle is a physical electron. The electron is an elementary particle with a property called **spin**. Heuristically, we can think of spin in terms of a compass needle that may point only in one of two directions, say up and down. Following the principles of quantum mechanics the two alternatives correspond to the basis states of a two-dimensional vector space, for example spin up $\leftrightarrow s_1 \equiv (1,0)^T$ and spin down $\leftrightarrow s_2 \equiv (0,1)^T$. A general spin configuration of the particle is then described by a vector $\chi \in W \equiv \mathbb{C}^2$. For example, the state $\chi = \frac{1}{\sqrt{3}} s_1 + \frac{\sqrt{2}}{\sqrt{3}} s_2$ would describe a state where 'spin up' is realized with probability $(1/\sqrt{3})^2 = 1/3$ and 'spin down' with probability $2/3$.

Now consider the situation where the particle is free to move in the lattice, and may have arbitrary spin. The joint information is contained in states $\psi \in V \otimes W = \mathbb{C}^N \otimes \mathbb{C}^2$ that live in the tensor product[1] of the spaces V and W describing its position and spin, respectively. For example a spin-up electron at site i would be in state $e_i \otimes s_1$. However, the quantum particle may also be in a superposition state, for example an equal probability superposition $\frac{1}{\sqrt{2}} e_i \otimes s_1 + \frac{1}{\sqrt{2}} e_j \otimes s_2$ of spin up at i and spin down at j. A general configuration is described as

$$\sum_i \sum_{s_j} c^{ij} e_i \otimes s_j, \tag{L252}$$

i.e. an element of $\mathbb{C}^N \otimes \mathbb{C}^2$, where $c^{ij} \in \mathbb{C}$. The probability of a combined position/spin measurement is given by $|c^{ij}|^2$, subject to the condition $\sum_{ij} |c^{ij}|^2 = 1$, which enforces the requirement that with unit probability the particle is to be found at *some* lattice site with *some* spin projection.

This example illustrates how the mathematical structure of tensor products is tailored to the description of composite quantum systems. For a discussion at much greater conceptual and method-

[1] Tensor products of complex spaces are defined in analogy to the real case. The details are discussed in lecture courses in quantum mechanics and not essential for the present discussion.

ological depth we refer to lecture courses in quantum mechanics.

L11.2 Dual space

To each vector space V of dimension n there exists an intimately related partner space called its **dual space**, V^*. The dual space is defined as the set of all linear maps w of V into the real numbers,

$$w : V \to \mathbb{R}, \qquad v \mapsto w(v) \equiv wv, \tag{L253}$$

where linearity implies the properties $(v, v' \in V, a \in \mathbb{R})$

- ▷ $w(v + v') = wv + wv'$,
- ▷ $w(av) = a\, wv$.

Following the general convention to omit the brackets around the arguments of *linear* maps, the notation $wv \equiv w(v)$ is often used. Vector addition and multiplication by scalars, making V^* a *vector space*, are naturally defined as $(w + w')(v) = wv + w'v$ and $(aw)(v) = a\, wv$. The elements of V^* are called **dual vectors** or **covectors**.[2]

To understand the 'duality' $V \leftrightarrow V^*$ in more concrete terms, let $\{e_i\}$ be a basis of V. A corresponding basis of dual vectors, the so-called **dual basis**, $\{e^i\}$, (note the upper index!) is defined by the condition that

$$\forall j : \quad e^i(e_j) = e^i e_j \equiv \delta^i{}_j. \tag{L254}$$

This defines the action of e^i on a basis and hence fixes its action on a general vector $v = e_j v^j$ as $e^i v = e^i(e_j v^j) = e^i e_j v^j = v^i$, i.e. e^i maps v onto its ith component,

$$e^i v = v^i. \tag{L255}$$

A dual vector can be expanded as $w = w_i\, e^i$ in this basis, and its *co*variant components are given by

$$w_j = we_j. \tag{L256}$$

The action of w on v then yields

$$wv = (w_i e^i)(e_j v^j) = w_i v^i. \tag{L257}$$

Notice the apparent visual symmetry between vectors and dual vectors in this equation. Indeed, V^* is a vector space and one may ask what *its* dual is. Eq. (L254) suggests an interpretation of the vector $e_j \in V$ as a map $e_j : V^* \to \mathbb{R}$, $e^i \mapsto e^i e_j = \delta^i{}_j$. In spite of the unusual notation

[2] Alternative denotations include **linear functionals** or **one-forms**.

in which the symbol denoting the map, e_j, appears to the *right* of its argument, e^i, this is a valid interpretation. It shows that vectors $v \in V$ afford an interpretation of linear maps of V^* into the reals, and that

$$(V^*)^* = V, \tag{L258}$$

i.e. the dual of the dual space of V^* is V itself. The action of general vectors $v \in V$ on dual vectors $w \in V^*$ is again given by Eq. (L257), i.e. this equation can be read both as w-acts-on-v or v-acts-on-w.

This shows in what sense V and V^* are 'dual' to each other. Importantly, however, there exists no natural, or 'canonical' bijection assigning to elements $v \in V$ elements $w \in V^*$. The construction above, which assigned dual basis vectors e^i to basis vectors e_i, does define a map $V \to V^*$. However, this map requires the prior fixation of a basis, and hence is not canonical. (In a different basis, $\{f_i\}$, the prior basis vector e_i would be mapped onto a dual vector different from e^i; think about this point!) However, on p. 148 we will discuss how the presence of an inner product in V defines a very useful canonical identification $V \leftrightarrow V^*$.

Finally, it is sometimes useful to think about the connection between vector spaces and their duals in a **component representation**, where a basis is fixed and vectors $v \leftrightarrow (v^1, \ldots, v^n)^T$ are identified as column vectors or $n \times 1$ matrices. Eq. (L254) then suggest an identification $w \leftrightarrow (w_1, \ldots, w_n)$ of dual vectors as row vectors (the absence of the transposition symbol), or $1 \times n$ matrices. In this picture, the pairing $wv = w_i v^i$ is understood as the multiplication of an $1 \times n$ matrix with an $n \times 1$ matrix.

EXAMPLE In $V = \mathbb{R}^2$ consider a basis $e_1 = \binom{1}{1}$ and $e_2 = \binom{2}{3}$. To find a component representation of the dual basis vectors, e^1 and e^2, we express Eq. (L254) in the component representation (L257), $(e^i)_l (e_j)^l = \delta^i{}_j$. If we associate $(e^i)_l \equiv A^i{}_l$ with the components of an as yet unknown matrix, then $(e_j)^l = (A^{-1T})_j{}^l$ must be the transpose (cf. Eq. (L107)) of the inverse of that matrix, since $(e^i)_l (e_j)^l = A^i{}_l (A^{-1T})_j{}^l = A^i{}_l (A^{-1})^l{}_j = \delta^i{}_j$. Comparison with the given component representation of the basis vectors e_1 and e_2 yields $A^{-1T} = \left(\begin{smallmatrix} 1 & 1 \\ 2 & 3 \end{smallmatrix}\right)$. We transpose this matrix and compute the inverse to obtain $A = \left(\begin{smallmatrix} 3 & -2 \\ -1 & 1 \end{smallmatrix}\right)$. The rows of this matrix, $e^1 = (3, -2)$ and $e^2 = (-1, 1)$ define the sought-for dual vectors. Indeed one may double check to confirm that $e^1 e_1 = 1$, $e^1 e_2 = 0$, etc.

Co- and contravariant transformation

Suppose we choose a different basis, $e_i \mapsto e'_i \equiv e_j (T^{-1})^j{}_i$. The corresponding vector components transform as $v^i \mapsto v'^i = T^i{}_j v^j$, so that

$$v = e'_i v'^i = (e_j (T^{-1})^j{}_i)(T^i{}_k v^k) = e_j v^j$$

remains invariant. The dual vectors e'^i associated with the new basis vectors e'_i are defined as $e'^i(e'_j) = \delta^i{}_j$. This condition in turn implies that the expansion of the new dual basis vectors in the old dual basis reads as $e'^i = T^i{}_j e^j$ (show this!). The components of a dual vector must then transform as $w_i \mapsto w'_i = w_j (T^{-1})^i{}_j$, so as to leave $w = w_i e^i = w'_i e'^i$ invariant.

Observe that the co- or contravariance of an index fixes the **transformation behavior** of the object it refers to. Regardless of whether they represent vectors or coefficients, contravariant objects transform with T and covariant ones with T^{-1}. To summarize,

$$v^i \mapsto T^i{}_j v^j, \qquad e^i \mapsto T^i{}_j e^j, \qquad v_i \mapsto v_j (T^{-1})^j{}_i, \qquad w_i \mapsto w_j (T^{-1})^j{}_i. \tag{L259}$$

This transformation behavior ensures the invariance of all three types of 'contractions' encountered above, $v = e_i v^i$, $w = w_i e^i$ and $wu = w_i v^i$. Notice that the transformation under T is solely determined by the co- or contravariance of an index. Regardless of whether that index labels a component or a vector we have ($x^i = e^i, v^i$)

$$\boxed{x^i \mapsto T^i{}_j x^j, \qquad x_i \mapsto x_j (T^{-1})^j{}_i.} \tag{L260}$$

Although the placement of transformation matrix elements to the right of covariant objects is most natural, one may change the order by writing $x_i \mapsto (T^{-1T})_i{}^j x_j$.

INFO In physics there is a tendency to indiscriminately regard objects carrying single indices – forces, velocities, current densities, etc. – as 'vectors'. However, many of these objects afford a more natural interpretation as dual vectors. Consider the **example of mechanical force**. The force, F, acting on a particle is determined by measuring the work required to move the particle along small displacements. Work, W, is a scalar and displacements, $s \in \mathbb{R}^3$, are three-dimensional vectors, and the force is a function *defined* through the relation $F(s) = W$. Since the work required to go along to consecutive small segments $s + s'$ is additive, $F(s + s') = F(s) + F(s') = W + W'$, this function is linear. In other words, F is a dual vector, $F \in (\mathbb{R}^3)^*$. In a basis, the assignment of force to work reads $W = F_i s^i$, where F_i are the covariant components defining the force dual vector through work measurement. Another physics example of a dual vector is **angular momentum**, L. Describing the rotational motion of a body around a rotation center by a vector ω, where $|\omega|$ quantifies the frequency of the rotation, and $\omega/|\omega|$ the direction of the rotational axis, the number $\frac{1}{2} L_i \omega^i$ is the kinetic energy (a number) stored in the rotational motion. (Consider the motion of a point particle on a circle to convince yourself that this is so.) This shows that L is a map of vectors to numbers, a dual vector. Other examples of dual vectors in physics include the **electric and magnetic field**, E and H, and **mechanical momentum**, p. In all these cases, the dual vector identification follows from physical rather mathematical reasoning. The concept of dual vectors is as intuitive as that of vectors themselves and the all-is-vector culture of physics likely an artifact of traditional teaching.

If we accept that forces are more naturally described by dual vectors, the question presents itself how one may switch between the dual and the direct representation. In view of the fact that the passage between vector spaces and their duals is not canonical, it is not obvious how to translate from a dual F to a vectorial representative. The answer is that additional structure (viz. a metric, see the next section) is required. Depending on the context, the necessity to introduce extra structure may be harmless, or seriously obscure the natural interpretation of physical quantities.

Metric provides a canonical connection between space and dual space

The fact that the physics culture does not discriminate between vectors and dual vectors suggests that these objects must be intimately connected. A canonical identification of vectors

with dual vectors indeed exists for vector spaces with *scalar products*. (In all physics contexts where dual vectors are treated as vectors, a scalar product is available and implicitly used in the identification.) Formally, this identification is a linear map

$$J : V \to V^*, v \mapsto J(v), \tag{L261}$$

where the dual vector $J(v)$ is defined by through the condition,

$$\forall u \in V : \qquad J(v)u = g(v, u), \tag{L262}$$

and g should be the scalar product of V. This condition requires that the action of the dual vector $J(v)$ on any $u \in V$ should yield an image equal to the scalar product $g(v, u)$. To obtain a concrete expression for the covariant components $J(v)_i$, we fix a basis $\{e_i\}$ and its dual $\{e^i\}$.[3] We then have $J(v)_i = J(v)e_i = g(v, e_i) = v^j g_{ji} = v_i$, where in the last equality we used the index lowering convention (L51). The result

$$J(v)_i = v^j g_{ji} = v_i, \tag{L263}$$

affords a new interpretation of the previously formal index lowering operation:

> The covariant components, $v_i = v^j g_{ji}$, are the components of the dual vector $J(v)$ that is the image of the vector v with components v^j under the canonical mapping $J : V \to V^*$ induced by a metric, g, of V.

Not surprisingly, a few more index-changing operations can now be understood in more conceptual ways. We first note that the **inverse of** J is defined through the condition $J(J^{-1}(w))(u) = g(J^{-1}(w), u)$, where $w \in V^*$ and $u \in V$. The left-hand side yields $wu = w_j u^j$ and the right-hand side $J^{-1}(w)^l g_{lj} u^j$. This is implies the condition $w_j = J^{-1}(w)^l g_{lj}$, which can be inverted using g^{ji}, the inverse of the metric tensor (with $g_{lj} g^{ji} = \delta_l{}^i$), to yield

$$J^{-1}(w)^i = w_j g^{ji} = w^i. \tag{L264}$$

Thus, the contravariant components w^i obtained by raising the indices of the covariant components w_j via the inverse metric g^{ji} are the components of the image vector $J^{-1}(w)$ to which the dual vector w is mapped under the inverse isomorphism.

> Index lowering or raising is equivalent to passing from a vector space to its dual vector space or back, in a component language.

[3] The dual basis is again defined by the condition $e^i e_j = \delta^i{}_j$. Notice that the dual basis vector e^i assigned to e_i by this condition differs from the assignment $J(e_i)$, unless $\{e_i\}$ is an orthonormal basis, $g_{ij} = \delta_{ij}$. Indeed, Eq. (L263) implies that $J(e_i) = J(e_i)_l e^l = \delta_i{}^k g_{kl} e^l = g_{il} e^l$. This equals e_i, *iff* $g_{ij} = \delta_{ij}$.

We finally note that the isomorphism J defines a **metric of dual space**. The latter is defined as $g^* : V^* \times V^* \to \mathbb{R}, (w, w') \mapsto g^*(w, w')$ via the condition

$$g^*(w, w') = g(J^{-1}(w), J^{-1}(w')). \tag{L265}$$

(This can be equivalently formulated as $g^*(J(v), J(v')) = g(v, v')$.) Using a basis representation, and defining $(g^*)^{ij} = g^*(e^i, e^j)$, the left-hand side of Eq. (L265) yields $w_i(g^*)^{ij}w'_j$ and the right-hand side $g(e_k w^k, e_l w'^l) = w^k g_{kl} w'^l = w_i g^{ik} g_{kl} g^{lj} w'_j = w_i g^{ij} w'_j$, implying

$$(g^*)^{ij} = g^{ij}. \tag{L266}$$

Thus, the contravariant components of the canonical metric of dual space equal the components of the inverse of the metric tensor.

INFO In **physics**, the above connection between a vector space and its dual space is implicitly used when, e.g., the work along a line segment is calculated as the *scalar product* between the segment and a vector representing the force. In the previous section we argued that force is a dual vector with covariant components F_i. The work done along a segment with contravariant components s^i is then given by $W = F_i s^i$. Physics describes force by a vector with components F^i and the work by the scalar product $W = \langle F, s\rangle = g(F, s) = F^j g_{ji} s^j$. Comparison of the two descriptions shows that $F_i = g_{ij} F^j$. One may reason that the dual vector approach is more natural in that it (i) introduces force via a measurement protocol (cf. previous section), and (ii) does not require a scalar product for the computation of work. On the other hand, the usage of a metric required by the all-is-vector-approach is mostly harmless, which is why this tradition remains pervasive in physics. Exceptions include cases where the metric itself plays a key role (such as in the theory of gravity), or cases where it obscures physically important structures (such as in the understanding of topological structures).

L11.3 Tensors

Vectors and dual vectors are the basic elements from which all objects of linear algebra can be hierarchically built. The key to this construction is the **tensor product** of vector spaces introduced above. Of particular interest are tensor products built from a real vector space V and its dual V^*. Introducing the notation $\otimes^q V \equiv V \otimes \cdots \otimes V$ for the product of q identical spaces we define

$$T^q_{\ p}(V) \equiv (\otimes^q V) \otimes (\otimes^p V^*). \tag{L267}$$

This is the (tensor) product of the spaces $\otimes^q V$ and $\otimes^p V^*$, which in turn are q- and p-fold tensor products of the basic spaces, V and V^*, respectively. Elements $t \in T^q_{\ p}(V)$ are called tensors of contravariant degree q and covariant degree p. If a basis $\{e_i\}$ has been chosen, elements $t \in T^q_{\ p}$ can be represented by

$$\boxed{t = t^{i_1,\ldots,i_q}{}_{j_1,\ldots,j_p}\, e_{i_1} \otimes \ldots e_{i_q} \otimes e^{j_1} \otimes \cdots \otimes e^{j_p},} \tag{L268}$$

where $t^{i_1,\ldots,i_q}{}_{j_1,\ldots,j_p}$ are the **coefficients of the tensor** (think about this point). It is often useful to understand tensors as *multilinear maps*: much like a dual vector and a vector are maps of the vector space V and the dual space V^* into the reals, respectively, a general tensor $t \in T^q{}_p$ defines a multilinear[4] map assigning to q dual vectors and p vectors a number,

$$\begin{aligned} t: \quad & (\otimes^q V^*) \otimes (\otimes^p V) \longrightarrow \mathbb{R}, \\ & (w^1, \ldots, w^q, v_1, \ldots, v_p) \longmapsto t(w^1, \ldots, w^q, v_1, \ldots, v_p). \end{aligned} \tag{L269}$$

The image $t(w^1, \ldots, w^q, v_1, \ldots, v_p) \in \mathbb{R}$ of the action of t on a set of q dual vectors, $w^1, \ldots, w^q$, and p vectors, $v_1, \ldots, v_p$, is obtained by successive application of the q vectorial factors e_{i_k} in t on the corresponding dual-vector arguments, w^{i_k}, and the p dual-vectorial factors e^{j_l} on the corresponding vector arguments v_{j_l}, and multiplying the resulting factors:

$$t(w^1, \ldots, w^q; v_1, \ldots, v_p) = t^{i_1,\ldots,i_q}{}_{j_1,\ldots,j_p} \, (e_{i_1} w^1) \ldots (e_{i_q} w^q) \, (e^{j_1} v_1) \ldots (e^{j_p} v_p),$$

For example, for a tensor $t \in T^2{}_1(V)$ with component representation $t = t^{ij}{}_k e_i \otimes e_j \otimes e^k$ we have $t(w, w', v) = t^{ij}{}_k (e_i w) \otimes (e_j w') \otimes (e^k v) = t^{ij}{}_k w_i w'_j v^k$. Specifically, the action of a tensor on a set of basis/dual-basis vectors yields the components of the tensor in that basis:

$$t^{i_1,\ldots,i_q}{}_{j_1,\ldots,j_p} = t(e^{i_1}, \ldots, e^{i_q}, e_{j_1}, \ldots, e_{j_p}). \tag{L270}$$

Under a **transformation of bases**, $e_i \mapsto e_j T^j{}_i$, the coefficients of a tensor transform co- and contravariantly according to their degree.[5] For example, for $t \in T^1{}_2(V)$,

$$t^i{}_{jk} \mapsto T^i{}_{i'} \, t^{i'}{}_{j'k'} \, (T^{-1})^{j'}{}_j (T^{-1})^{k'}{}_k.$$

We finally note that a tensor can be applied to an incomplete set of arguments to produce a tensor of lowered rank. For example the application of $t = t^{ij}{}_k e_i \otimes e_j \otimes e^k \in T^2{}_1(V)$ to $(w, ., .)$ ($w \in V^*$, second and third argument left empty) yields $t(w, ., .) = (t^{ij}{}_k w_i) e_j \otimes e^k \in T^1{}_1$ which is a tensor of lower rank with components $t^{ij}{}_k w_i$. This exemplifies how the procedure yields tensors with fewer fixed co- or contravariant indices by pairing of indices with the indices of supplied arguments. An expression like $t^{ij}{}_k w_i$ is called a **contraction** of components of t against those of w. For further discussion of such operations, see section L11.8 below.

L11.4 Examples of tensor classes

Tensors of degree $(1, 0)$ and $(0, 1)$: vectors and dual vectors, respectively

The tensor spaces of lowest nontrivial degree[6] are $T^1{}_0 = V$ and $T^0{}_1 = V^*$, and the coefficients of these tensors are the contra- and covariant coefficients of **vectors** and **dual**

[4] A **multilinear map** is separately linear in each of its arguments, i.e. $t(\ldots av + a'v', \ldots) = at(\ldots v, \ldots) + a't(\ldots v', \ldots)$, $a, a' \in \mathbb{R}$. The properties of such maps define the subject of **multilinear algebra**.

[5] Do not confuse matrix elements of the transformation matrix, T^i_j with the denotation of the tensor space $T^q{}_p = T^q{}_p(V)$.

[6] The tensor space of zeroth degree is defined as $T^0{}_0 = \mathbb{R}$.

vectors, respectively. Eq. (L268) shows how vectors and dual vectors are the building blocks of more complex tensorial structures.

Tensors of degree $(1,1)$: matrices

Tensors of first contra- and covariant degree, $A \in T^1{}_1(V)$, can be expanded as $A = e_i \otimes e^j A^i{}_j$. Up to now, we have viewed the first degree co- and contravariant components $A^i{}_j$ as the components of **matrices**. The interpretation of A as a matrix (or linear map $V \to V$) becomes apparent upon application of the tensor to an incomplete set of arguments, $(.,v)$, where $v \in V$ is a vector, and the dual vector slot is left unspecified. This yields $A(.,v) = A^i{}_j v^j\, e_i \in V$, which is a vector whose components $A^i{}_j v^j$ are obtained by application of the matrix $A^i{}_j$ to the argument v. In this way, the tensor can be understood as a linear map $V \to V, v \mapsto A(.,v)$. However, the tensor formulation affords alternative interpretations of elements $A \in T^1{}_1(V)$. For example, we can think of A as a map $A(w,v) = A^i{}_j w_i v^j$ that assigns a number to a pair comprising a dual vector and vector. In conventional language, this would read $w^T A v$, where w^T is interpreted as a column vector with covariant components w_i. Or, we let act A on $(w,.)$ with vectorial argument left open, to obtain the dual vector $A(w,.) = A^i{}_j w_i e^j$, which in conventional language amounts the the action of the matrix A to the left as wA. Depending on the context, all these different views have advantages and they illustrate the versatility of the tensor formulation of linear algebra.

Finally note that under a basis transformation, the coefficients of the tensor transform as

$$A^i{}_j \mapsto T^i{}_{i'} A^{i'}{}_{j'} (T^{-1})^{j'}{}_j. \tag{L271}$$

In an index-free notation this reads as $A \mapsto TAT^{-1}$, in which we recognize the familiar transformation behavior of matrices.

INFO For every tensor $A \in V \otimes V^*$, we may define a corresponding **transpose**, $A^T \in V^* \otimes V$, as an element of a tensor product space in which the order of V and its dual V^* have been interchanged. As such the transpose can be expanded as $A^T = (A^T)_j{}^i e^j \otimes e_i$ and applied to a pair comprising a vector and dual vector, $(v,w) \in V \otimes V^*$, to yield the number $A^T(v,w) = (A^T)_j{}^i v^j w_i$. Given $A \in V \otimes V^*$, its transpose $A^T \in V^* \otimes V$ is *defined* by the condition that $A^T(v,w) = A(w,v)$ for arbitrary pairs (v,w). The component representation of this (invariant) condition reads $(A^T)_j{}^i v^j w_i = A^i{}_j w_i v^j$, implying $(A^T)_j{}^i = A^i{}_j$. In Eq. (L107) this relation served as a formal definition of a transposed matrix.

Tensors of degree $(0,2)$ or $(2,0)$: bilinear forms of V or V^*

Tensors of second covariant degree, $t \in T^0{}_2(V)$ are generally called **bilinear forms**. They can be understood as bilinear maps, $t : V \otimes V \to \mathbb{R}, (u,v) \mapsto t(u,v)$. A prominent example is the **metric**, g, of a vector space, cf. discussion in section L3.3. There, we defined a general scalar product of a vector space as $g(u,v) = u^i g_{ij} v^j$, through the set of coefficients g_{ij}. In tensor language, this is equivalent to the definition of a second-degree covariant tensor

$g = g_{ij} e^i \otimes e^j$. In physics, the set of coefficients $\{g_{ij}\}$ is often considered as a matrix. This can be a potent source of confusion, because under a change of basis, $e_i \mapsto e_j (T^{-1})^j{}_i$, the coefficients $g_{ij} \mapsto g_{i'j'} (T^{-1})^{i'}{}_i (T^{-1})^{j'}{}_j$ transform *differently* from a matrix (cf. (L271), or the previous subsection).

INFO Another prominent example of a bilinear form is the **inertia tensor**, I, of a rigid body. Describing the rotational motion of the body by a rotation vector ω, the kinetic energy stored in the rotation is given by $T = \frac{1}{2} I(\omega, \omega) = \frac{1}{2} I_{ij} \omega^i \omega^j$. Likewise, the components of the angular momentum are obtained as $L_i = I_{ij} \omega^j$.

L11.5 Alternating forms

We next introduce a subclass of tensors which is very important in applications and deserves a separate discussion: consider the space $T^0{}_p$, i.e. the set of multilinear maps of $\otimes^p V$ into the reals. Now define $\Lambda^p(V) \subset T^0{}_p$ [7] as

$$\Lambda^p(V) \equiv \{\phi : \otimes^p V \to \mathbb{R} \,|\, \phi \text{ multilinear \& alternating}\}, \tag{L272}$$

where 'alternating' means antisymmetry w.r.t. exchange of any of its vector arguments: $\phi(\dots, u, \dots, v, \dots) = -\phi(\dots, v, \dots, u, \dots)$. The elements of $\Lambda^p(V)$ are called **(alternating) forms of degree p**, or **p-form** for short. (When using the shorthand nomenclature be aware, however, that the general bilinear forms discussed earlier need not be alternating. For example, the metric $g(u, v) = g(v, u)$ is a symmetric bilinear form and therefore not a 2-form.)

EXAMPLE An example of a 2-form is $\phi = e^1 \otimes e^2 - e^2 \otimes e^1$. Applied to two vectors u and v it yields the antisymmetric combination $\phi(u, v) = u^1 v^2 - u^2 v^1$. The **triple product** discussed in section L4 is a 3-form in $\Lambda^3(\mathbb{R}^3)$: it maps three vectors onto a number and is antisymmetric under exchange of its arguments. The matrix **determinant** can be interpreted as an n-form in $\Lambda^n(\mathbb{R}^n)$: take an $n \times n$ matrix $A = (v_1, \dots, v_n)$ and consider it as a stack of n vectors $v_i \in \mathbb{R}^n$. We can then write $\det A = \det(v_1, \dots, v_n)$, where the latter representation is the image of the multilinear form $\det$, evaluated on n argument vectors v_i. The determinant is linear in each entry and antisymmetric under argument exchange, and this makes it an n-form. Expanded in a tensor basis the determinant assumes the form

$$\det = \sum_{P \in S_n} \operatorname{sgn}(P) e^{P(1)} \otimes e^{P(2)} \dots e^{P(n)}, \tag{L273}$$

where S_n is the permutation group of n objects and the sum runs over all permutations P.

[7] The notation where $\Lambda^p(V) \subset T^0{}_p$ carries the degree-index p upstairs is not ideal but standard and we will use it here too.

A general p-form can be expanded as

$$\boxed{\phi = \sum_{i_1<i_2<\cdots<i_p} \phi_{i_1,\ldots,i_p} \sum_{P\in S_p} \mathrm{sgn}(P) e^{i_{P1}} \otimes e^{i_{P2}} \ldots e^{i_{Pp}},} \tag{L274}$$

in basis forms. Here P is an element of the group of permutations of p objects. By definition, the coefficients of the expansion obey the antisymmetrization condition $\phi_{Pi_1,\ldots,Pi_p} = \mathrm{sgn}(P)\phi_{i_1,\ldots,i_p}$. For this reason, the sum over indices in (L274) may be limited to ordered index configurations $i_1 < i_2 < \cdots < i_p$. For example, the $p = 2$ forms in an $(n = 3)$-dimensional space afford the expansion

$$\phi = \phi_{12}(e^1 \otimes e^2 - e^2 \otimes e^1) + \phi_{23}(e^2 \otimes e^3 - e^3 \otimes e^2) + \phi_{31}(e^3 \otimes e^1 - e^1 \otimes e^3).$$

Terms with coinciding indices do not contribute due to antisymmetrization, ($\phi_{11}(e^1 \otimes e^1 - e^1 \otimes e^1) = 0$), and terms outside the ordering may be re-ordered to fit into the ordering scheme ($\phi_{21}(e^2 \otimes e^1 - e^1 \otimes e^2) = \phi_{12}(e^1 \otimes e^2 - e^2 \otimes e^1)$), where the antisymmetry $\phi_{21} = -\phi_{21}$ is essential. In the space $\Lambda^n(\mathbb{R}^n)$, where $p = n$, there is only one ordered configuration, $(i_1, \ldots, i_n) = (1, \ldots, n)$, hence forms in this space are characterized by a single number, $\phi_{1,\ldots,n}$. Applying the n-form with $\phi_{1,\ldots,n} = 1$ to a set of n vectors, $v_1, \ldots, v_n$, from $\mathbb{R}^n$ yields

$$\phi(v_1, \ldots, v_n) = \sum_{P\in S_n} \mathrm{sgn}(P) e^{P1} \otimes \ldots e^{Pn}(v_1, \ldots, v_n) = \sum_{P\in S_n} \mathrm{sgn}(P)(v_1)^{P1} \ldots (v_n)^{Pn}. \tag{L275}$$

Interpreting the n-tuple $(v_1, \ldots, v_n) \equiv A$ as a matrix with elements $A^i{}_j = (v_j)^i$, the value $\phi(v_1, v_2, \ldots, v_n) \equiv \phi(A)$ equals the determinant of A (cf. Eq. (L154)), i.e. $\phi(A) = \det(A)$, as mentioned above. In two and three dimensions, the corresponding top-forms are the determinants $\det(v_1, v_2)$ and $\det(v_1, v_2, v_3)$, which yield the area of the parallelogram or the volume of the parallelepiped spanned by their argument vectors, respectively (see p. 89). This generalizes to arbitrary dimensions: in $\mathbb{R}^n$ the top-form (L275) yields the geometric 'volume' of the n-dimensional parallelepiped spanned by its argument vectors, as will be explained in detail in Section V5.4.

In Eq. (L274), the product of the antisymmetric factor $\phi_{i_i,\ldots,i_p}$ and the antisymmetric sum over permutations is *symmetric* w.r.t. to all its indices. Therefore, one may choose to avoid the ordering condition in the sum and instead sum over *all* index combinations as

$$\phi = \frac{1}{p!} \sum_{i_1,i_2,\ldots,i_p} \phi_{i_1,\ldots,i_p} \sum_{P\in S_p} \mathrm{sgn}(P) e^{i_{P1}} \otimes e^{i_{P2}} \ldots e^{i_{Pp}}. \tag{L276}$$

The terms with coinciding indices vanish, and the redundant summation over un-ordered index pairs is compensated by the prefactor $1/p!$ (think about this point!).[8]

We conclude this section with a summary of the most important **mathematical properties of alternating forms**. They all follow immediately from our general discussion above.

[8] For example, for $p = 2$ we have a 2!-fold redundancy, $\sum_{ij} \phi_{ij}(e^i \otimes e^j - e^j \otimes^i) = \phi_{12}(e^1 \otimes e^2 - e^2 \otimes e^1) + \phi_{21}(e^2 \otimes e^1 - e^1 \otimes e^2) = 2\phi_{12}(e^1 \otimes e^2 - e^2 \otimes e^1)$, since both factors in the product are antisymmetric.

- ▷ The sum $\phi + \phi'$ of two alternating forms $\phi, \phi' \in \Lambda^p(V)$ is again an alternating form, i.e. $\Lambda^p(V)$ is a vector space.
- ▷ $\Lambda^1(V) = V^*$, the space of one-forms, is the dual vector space. We define $\Lambda^0(V) = \mathbb{R}$.
- ▷ For $\dim V = n$, $\Lambda^{p>n}(V) = \{\}$, in other words, an n-dimensional vector space does not support alternating p-forms if $p > n$. This is best seen by considering the action of forms $\phi(e_{i_i}, \dots, e_{i_p})$ on basis vectors. If $p > n$, identical basis vectors will appear repeatedly in the argument (because we have only n different ones). However, $\phi(\dots, e_i, \dots, e_i, \dots) = -\phi(\dots, e_i, \dots, e_i, \dots) = 0$ by antisymmetry.
- ▷ For $\dim V = n$, the dimension of the vector space of alternating p-forms is $\dim \Lambda^p(V) = \binom{n}{p}$. This follows since the number of ordered p-tuples $1 \leq i_1 < i_2 < \dots < i_p \leq n$ is $\binom{n}{p}$, and the sum in (L274) extends over as many basis forms.

L11.6 Visualization of alternating forms

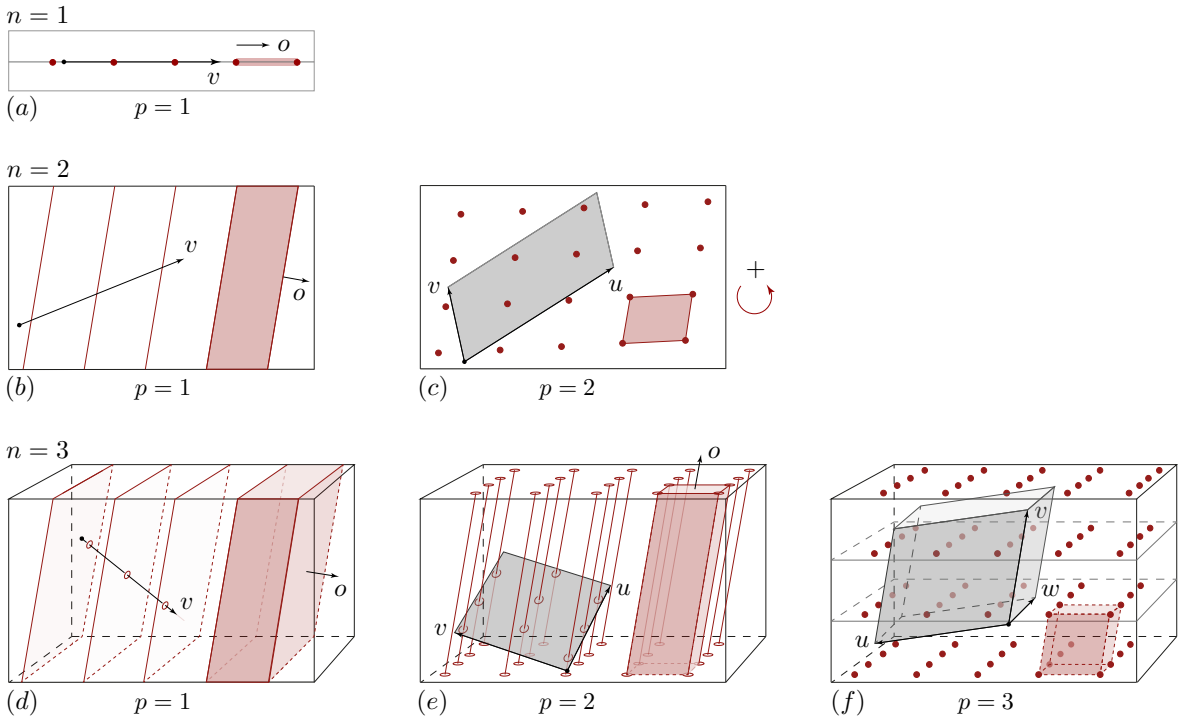
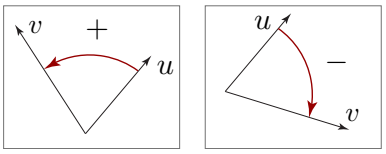


Figure L21: Visualization of alternating forms in (a) one-, (b,c) two- and (d-f) three-dimensional space. The periodically extended sub-units defining the graphical representation of forms are indicated in red shading. For a further discussion, see text.

Much as vectors can be visualized as arrows, alternating forms in low-dimensional spaces, $\dim(V) = 1, 2, 3$, too, afford pictorial representations. Although these are of limited use

for computations, they support the intuitive understanding of forms and are therefore worth discussing. Alternating p-forms in n-dimensional space are represented through periodically repeated patterns of $(n-p)$-dimensional linear structures, such as lines, planes, volumes, etc. These patterns are introduced such that they can be 'paired' with p vectors to yield the value of the form on the p argument vectors.

For example, a **one-form in two-dimensional space**, ϕ, is represented by a system of parallel lines of specified slope and inter-line spacing (cf. Fig. L21(b)). These lines define a pattern of strips (one is shown shaded) tiling the plane. The strips are given a sense of 'orientation' by choosing an 'upside' and a 'downside'. In the figure, this choice is indicated by an arrow labeled o pointing in the chosen 'upward' direction. The value of the form on a vector, $\phi(v)$, is now defined graphically as follows: The modulus, $|\phi(v)|$, equals the (generally fractional) number of strips cut by the arrow representing v (in the figure, this would be about 2.5). Note that this number is invariant under parallel translation of the arrow, as it should be. The sign of $\mathrm{sgn}(\phi(v))$ is positive/negative if v points in the upward/downward direction. It is straightforward to verify (do it!) that these rules are compatible with the linearity criteria defining differential forms. The algebraic coefficients, ϕ^i, defining the expansion of the form in a given dual basis, $\phi = \phi_1\, e^1 + \phi_2\, e^2$, are obtained by graphical evaluation of the form on corresponding basis vectors, $\phi^i = \phi(e_i)$.



In a similar manner, a **two-form in two-dimensional space**, ω, is defined by a lattice of unit cells (one is shown shaded in Fig. L21(c)) of arbitrary shape, but with a specified number of unit cells per unit area (this number can be fractional). An orientation is chosen by discriminating between anti-clockwise (mathematically positive) and clockwise (negative) orientated forms. The modulus of the form acting on two vectors, $|\omega(u,v)|$, is obtained by counting the (generally fractional) number of tiles covered by the parallelogram spanned by u and v (in this figure, this number would equal ca. 4.5). For an anti-clockwise orientated form, $\mathrm{sgn}(\omega(u,v))$ yields a positive sign when the orientation of v relative to u is anticlockwise (left panel), and a negative sign otherwise (right panel). For an clockwise oriented form the assignment is opposite. These rules are consistent with the linearity and antisymmetry criteria of differential two-forms. The algebraic coefficient, ω_{12}, defining the expansion of the form in a dual basis, $\omega = \omega_{12} e^1 \wedge e^2$, is obtained by graphical evaluation of $\omega(e_1, e_2)$ on the pair of corresponding basis vectors.

EXERCISE Discuss how a **one-form in one-dimensional space** can be defined through a periodic pattern of points on the real line, plus a sense of orientation, cf. Fig. L21(a). How is the value of the form on one-dimensional vector computed, and how is its expansion in a basis obtained?

A **one-form in three-dimensional space**, ϕ, is defined in conceptual analogy to the one-form in two-dimensional space, only that the strips are replaced by slabs defined by a system of equi-spaced parallel planes, cf. Fig. L21(d). As in the two-dimensional case the value of the form on a vector, $\phi(v)$, is obtained by determining the number of slabs pierced by v, where the sign follows from the alignment of v relative to that of an orienting direction, o. A **two-form**

in three-dimensional space, ϕ, may be represented by a lattice of parallel lines of specified direction, density of lines per unit area and orientation ('upwards' or 'downwards') along the lines, cf. Fig. L21(e). The lines define a pattern of parallel rods, and the absolute value, $|\phi(u,v)|$, of the form on a pair of vectors is obtained by counting the number of parallelogram-shaped inter-rod cross sections intersected by the parallelogram defined by u and v (about 5.5 in the figure). The sign of the form is positive/negative depending on whether the system (o,u,v) defined by a vector, o, pointing in upward direction and the two argument vectors define a right/left handed system. Finally a **three-form in three-dimensional space**, ϕ, can be defined through a lattice of points with specified density of points per unit volume, cf. Fig. L21(f). The points define a pattern of parallelepipeds, and $|\phi(u,v,w)|$ is obtained by counting how many of these are contained in the parallelepiped spanned by u, v and w.

In general, a ***p*-form in *n*-dimensional space** can be defined by pattern of identical $(n-p)$-dimensional linear structures.[9] The value of the form is obtained by determining how many of these are are covered by the generalized parallelepiped spanned by p vectors. For top-forms, $n-p=0$, the subunits have finite extent in all n dimensions, which explains why top-forms measure the geometric volume of n-dimensional parallelepipeds.

EXERCISE Think more about the pictures in Fig. L21 and make sure you are comfortable with the rules of assignment, the senses of orientation, the number of coefficients required to uniquely specify a form, etc. Explain how the fractional counting of lines or grid-areas implied by the procedures above can be avoided by reducing the separation between the points, lines or planes used to represent the various forms, respectively. Think how a graphical procedure in terms of an 'infinitely dense' pattern of lines or planes should be designed.

L11.7 Wedge product

Alternating forms can be multiplied with each other to yield alternating forms of higher degree. Given a p-form and a q-form we define their so-called **wedge product (exterior product)** as

$$\begin{aligned} &\wedge : \Lambda^p(V) \otimes \Lambda^q(V) \to \Lambda^{p+q}(V), \qquad (\phi,\psi) \mapsto \phi\wedge\psi, \\ &(\phi\wedge\psi)(v_1,\ldots,v_{p+q}) \equiv \frac{1}{p!q!} \sum_{P\in S_{p+q}} \operatorname{sgn} P\, \phi(v_{P(1)},\ldots,v_{P(p)})\psi(v_{P(p+1)},\ldots,v_{P(p+q)}). \end{aligned} \tag{L277}$$

Here, S_n is the permutation group of n objects and the sum runs over all permutations P. For example, for $p=q=1$, $(\phi\wedge\psi)(v,w) = \phi(v)\psi(w) - \phi(w)\psi(v)$. For $p=0$ and $q=1$, ϕ is a number and we define $\phi\wedge\psi(v) = \phi\psi(v)$. Important **properties of the wedge product** include ($\phi\in\Lambda^p(V), \psi\in\Lambda^q(V), \lambda\in\Lambda^r(V), c\in\mathbb{R}$):

[9] In the present context, a structure is called $(n-p)$-dimensional if it has infinite extent in $n-p$ dimensions. Examples of one-dimensional structures are the strips used to define one-forms in two-dimensional space $(n-p=2-1)$, and the rods used to define two-forms in three-dimensional space $(n-p=3-2)$.

- ▷ **bilinearity**, i.e. $(\phi_1 + \phi_2) \wedge \psi = \phi_1 \wedge \psi + \phi_2 \wedge \psi$ and $(c\phi) \wedge \psi = c(\phi \wedge \psi)$.
- ▷ **associativity**, i.e. $\phi \wedge (\psi \wedge \lambda) = (\phi \wedge \psi) \wedge \lambda \equiv \phi \wedge \psi \wedge \lambda$.
- ▷ **graded commutativity**, $\phi \wedge \psi = (-)^{pq}\, \psi \wedge \phi$.

The fact that the wedge product changes the degree of forms is motivation to define the direct sum of spaces

$$\Lambda(V) \equiv \bigoplus_{p=0}^{n} \Lambda^p(V), \tag{L278}$$

i.e. a space containing all spaces of fixed degree $0 \leq p \leq n$ as subspaces. This vector space has dimension $\dim(\Lambda(V)) = \sum_{p=0}^{n} \dim(\Lambda^p(V)) = \sum_{p=0}^{n} \binom{n}{p} = 2^n$, where in the last equality, we used the binomial formula. The most important feature of $\Lambda(V)$ is that it is more than a vector space, it is an *algebra*. An **algebra** is a vector space $(W, \cdot)$ endowed with a product operation, $u \cdot v = w$, $u, v, w \in W$, i.e. an operation that produces vectors by multiplication of other vectors (unlike the inner product which yields numbers). The space $(\Lambda(V), \wedge)$ is a vector space with an (associative) product operation, $\wedge$. It is therefore defines an algebra, the so-called **Grassmann algebra**, in the sense of the definition of p. L5.3.

INFO A (real) **algebra** is an $\mathbb{R}$-vector space W with a product operation

$$W \times W \to W, \qquad u, v \mapsto u \cdot v,$$

subject to the following conditions ($u, v, w \in W,\ c \in \mathbb{R}$):

- ▷ $(u + v) \cdot w = u \cdot w + v \cdot w$,
- ▷ $u \cdot (v + w) = u \cdot v + u \cdot w$,
- ▷ $c(v \cdot w) = (cv) \cdot w + v \cdot (cw)$.

For example, the space of $n \times n$ matrices $(\mathrm{mat}(\mathbb{R}, n), \cdot)$ forms an algebra, with matrix multiplication $A \cdot B = C$ as its product operation.

A natural basis of $\Lambda^p(V)$ is given by the set of forms

$$e^{i_1} \wedge \cdots \wedge e^{i_p}, \qquad 1 \leq i_1 < \cdots < i_p \leq n. \tag{L279}$$

To see this, notice (i) that these forms are alternating by construction, i.e. they belong to $\Lambda^p(V)$, (ii) that they are linearly independent, and (iii) that there are $\binom{n}{p}$ of them. For example, for $n = 3$ and $p = 2$, we have the $3 = \binom{3}{2}$ linearly independent forms, $e^1 \wedge e^2$, $e^2 \wedge e^3$, $e^3 \wedge e^1$.

The three criteria (i)-(iii) guarantee the basis property. Any p-form can be represented in the above basis as

$$\boxed{\phi = \sum_{i_1 < \cdots < i_p} \phi_{i_1, \ldots, i_p}\, e^{i_1} \wedge \cdots \wedge e^{i_p},} \tag{L280}$$

where the coefficients $\phi_{i_1,\ldots,i_p} \in \mathbb{R}$ are given by $\phi_{i_1,\ldots,i_p} = \phi(e_{i_1},\ldots,e_{i_p})$ and therefore are antisymmetric under exchange of index arguments (for example $\phi_{123} = -\phi_{213}$). Alternatively ϕ may be represented by an unrestricted sum with a compensating factor of $1/p!$ (cf. (L276)):[10]

$$\phi = \frac{1}{p!} \sum_{i_1,\ldots,i_p} \phi_{i_1,\ldots,i_p}\, e^{i_1} \wedge \cdots \wedge e^{i_p}. \tag{L281}$$

To illustrate Eq. (L280), we note that the $0,\ldots,3$-forms in $\mathbb{R}^3$ can be represented as

$$\begin{aligned} p=0: &\quad \phi = \phi_1, \\ p=1: &\quad \phi = \phi_1\, e^1 + \phi_2\, e^2 + \phi_3\, e^3, \\ p=2: &\quad \phi = \phi_{12}\, e^1 \wedge e^2 + \phi_{23}\, e^2 \wedge e^3 + \phi_{31}\, e^3 \wedge e^1, \\ p=3: &\quad \phi = \phi_{123}\, e^i \wedge e^2 \wedge e^3. \end{aligned} \tag{L282}$$

Notice that there are $8 = 2^3$ independent coefficients in all, and that the 1- and 2-forms are described by three coefficients each. The formulas above illustrate the importance of the wedge product: it allows us to build forms of arbitrary complexity from the much simpler 1-forms.

L11.8 Inner derivative

One can think of a p-form as a machine with p slots into which vectors are fed as arguments. It is sometimes useful to feed a p-form only one vector v to produce a form of lower degree, $p-1$. The corresponding map, denoted by $i_v : \Lambda^p(V) \to \Lambda^{p-1}(V)$, is called the **inner derivative** and defined by the relation

$$(i_v\phi)(v_1,\ldots,v_{p-1}) \equiv \phi(v, v_1,\ldots,v_{p-1}), \tag{L283}$$

where v, indicated as a subscript on the left, acts as additional argument to be supplied to the p-form ϕ, as indicated on the right. The components of $i_v\phi$ are obtained by 'contraction' of one of the components of ϕ with those of v (as follows from Eq. (L268)),

$$(i_v\phi)_{i_1,\ldots,i_{p-1}} = v^i \phi_{i,i_1,\ldots,i_{p-1}}.$$

Notice that in Eq. (L283) the seemingly ad hoc choice to feed v into the first argument slot of ϕ is inconsequential: due to the antisymmetry of ϕ, we have, e.g., $v^j\phi_{j,i_1,\ldots,i_{p-1}} = -v^j\phi_{i_1,j,\ldots,i_{p-1}}$, i.e. the contracted index can be permuted at the expense of, at most, a minus sign.

The inner derivative obeys the following properties, which are direct consequences of the definition:

▷ i_v is a linear map, $i_v(\phi+\phi') = i_v\phi + i_v\phi'$.

[10] For example, for $p=2$ we have $\sum_{ij}\phi_{ij}e^i\wedge e^j = \phi_{12}e^1\wedge e^2 + \phi_{21}e^2\wedge e^1 = 2\phi_{12}e^1\wedge e^2$, cf. [8].

- ▷ It is also linear in its 'parametric argument', $i_{v+w} = i_v + i_w$.
- ▷ i_v obeys the (graded) Leibniz rule:

$$i_v(\phi \wedge \psi) = (i_v\phi) \wedge \psi + (-)^p \phi \wedge (i_v)\psi, \qquad \phi \in \Lambda^p V^*. \tag{L284}$$

  Up to the minus sign, this resembles the product rule of differentiation, and because of this resemblance i_v is called a 'derivative'.
- ▷ The inner derivative is 'antisymmetric' in the sense that $i_v \circ i_w = -i_w \circ i_v$, in particular, $(i_v)^2 = 0$.

EXERCISE Gain familiarity with the **Leibniz rule** by computing the components of the inner derivative of a simple form, for example $i_v(e^1 \wedge e^2)$.

Let us illustrate the functioning of the inner derivative on the **example** of the three-form $\phi = e^1 \wedge e^2 \wedge e^3$ in $\mathbb{R}^3$. A quick calculation shows that

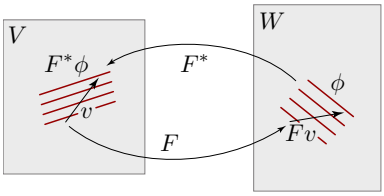
$$\begin{aligned} i_v(\phi) &= v^1 e^2 \wedge e^3 + v^2 e^3 \wedge e^1 + v^3 e^1 \wedge e^2, \\ i_w i_v(\phi) &= (v^2 w^3 - v^3 w^2)e^1 + (v^3 w^1 - v^1 w^3)e^2 + (v^1 w^2 - v^2 w^1)e^3, \\ i_u i_w i_v(\phi) &= \det(u, v, w). \end{aligned}$$

INFO The second of these lines contains an interesting message. The components of the one-form $i_w i_v(\phi)$ are those of the vector product $v \times w$. This is in line with our earlier observation that the vector product is not a real vector — it does not transform as a vector under linear transformation, but, as we now understand, as a one-form. In $d = 3$, we actually have three different objects characterized by three components: vectors $v = v^1 e_1 + v^2 e_2 + v^3 e_3$, one-forms $\phi = \phi_1 e^1 + \phi_2 e^2 + \phi_3 e^3$, and two-forms $\omega = \omega_{12} e^1 \wedge e^2 + \omega_{23} e^2 \wedge e^3 + \omega_{31} e^3 \wedge e^1$. In physics, they are all indiscriminately treated as vectors, while grudingly acknowledging the odd transformation behavior of one-forms by calling them '**pseudovectors**'. It would be better to accept one-forms as what they are, namely linear forms, but old habits are hard to change and physics culture will likely keep adhering to the misconception of calling them 'pseudovectors'.

L11.9 Pullback

Given a linear map, $F : V \to W$, between two vector spaces, a form, $\phi \in \Lambda^p(W)$, defined in W may be 'pulled back' by F to become a form $F^*(\phi) \in \Lambda^p(V)$ defined in V. The **pullback** operation is defined as,

$$\boxed{\begin{aligned} F^* : \Lambda^p(W) \to \Lambda^p(V), \qquad \phi \mapsto F^*\phi, \\ (F^*\phi)(w_1, \ldots, w_p) \equiv \phi(Fw_1, \ldots, Fw_p). \end{aligned}} \tag{L285}$$



The idea behind this definition is illustrated in the figure on the example of the pullback of one-forms between two-dimensional vector spaces: the action of $F^*\phi$ on vectors $v \in V$ is defined by the action of ϕ on the image $Fv \in W$: $(F^*\phi)(v) \equiv \phi(Fv)$. (The figure uses the visualization discussed in section **??**, where the value of a one-form on two-dimensional vectors is obtained by counting line-crossings.) Notice that the pullback operation imposes no conditions on F (besides linearity), nor on the dimensionality of V and W.

To understand what pullback means in a component language, we first consider the case of one-forms, $\phi \in \Lambda^1(W)$. Let $\{e_i\}$ and $\{f_j\}$ be bases of V and W, with dual bases $\{e^i\}$ and $\{f^j\}$, respectively. The map F is then described by a component matrix $\{F^i{}_j\}$ as $Fe_j = f_i F^i{}_j$. Now consider the pullback of a dual basis vector from $\Lambda^1(W)$, say f^j, to $\Lambda^1(V)$. We can find the components of F^*f^i w.r.t. the dual basis $\{e^j\}$ by acting with it on the basis vectors $\{e_j\}$ (cf. Eq. (L256)). We obtain $(F^*f^i)_j = (F^*f^i)(e_j) \overset{(L285)}{=} f^i(Fe_j) = f^i(f_l F^l{}_j) = F^i{}_j$, or

$$\boxed{F^*f^i = F^i{}_j e^j.} \tag{L286}$$

Notice how this formula parallels the one for contravariant basis change. In the particular case where $W = V$ and F *is* a change of bases, the pullback formula indeed describes the associated change of the dual basis vectors (think about this point). The action of F^* on forms of higher degree follows from the following general properties of the pullback operation:

- F^* is linear: $F^*(\phi + \psi) = F^*\phi + F^*\psi$.
- $F^*(\phi \wedge \psi) = (F^*\phi) \wedge (F^*\psi)$,
- $(F \circ G)^* = G^* \circ F^*$.

All three rules are immediate consequences of the definition, and the second may be applied to compute the pullback of general forms, as given by Eq. (L280): iterated application of the second identity to the expansion $\phi = \sum \phi_{i_1,\ldots,i_p} f^{i_1} \wedge \cdots \wedge f^{i_p}$ of a form $\phi \in \Lambda^p(W)$ leads to $F^*\phi = \sum \phi_{i_1,\ldots,i_p} (F^*f^{i_1}) \wedge \cdots \wedge (F^*f^{i_p})$. The pullbacks of the individual one-forms are obtained from Eq. (L286) and we obtain

$$F^*\phi = \sum_{i_1<\cdots<i_p} \phi_{i_1,\ldots,i_p} F^{i_1}{}_{j_1} \ldots F^{i_p}{}_{j_p} e^{j_1} \wedge \cdots \wedge e^{j_p}. \tag{L287}$$

Later on in chapters V5 and V6 we will understand that this operation is implicitly used in many routine operations of physics calculus, notably in the manipulation of integrals.

This concludes our survey of tensor algebra. Applications of the formalism will be discussed in chaptersV4 to V6.

PL Problems: Linear Algebra

The solutions to odd-numbered problems are given in part S, chapter SL. Lecturers can obtain the solutions to even-numbered problems from the publishers by request.

P.L1 Mathematics before numbers

The problems for chapter L1 are meant to help the reader gain familiarity with the notions of sets, maps, groups and fields. For further introductory examples we refer to lecture courses in mathematics.

P.L1.1 Sets and Maps

Become comfortable with the notation used to specify maps by doing the following problems on the composition of maps.

EL1.1.1 Composition of maps

Let $\mathbb{N}_0$ denote the set of all natural numbers including zero, and $\mathbb{Z}$ the set of all integers. Consider the following two maps:

$$A : \mathbb{Z} \to \mathbb{Z}, \qquad n \mapsto A(n) = n + 1,$$
$$B : \mathbb{Z} \to \mathbb{N}_0, \qquad n \mapsto B(n) = |n| \equiv n \cdot \mathrm{sign}(n).$$

(a) Find the composite map $C = B \circ A$, i.e. specify its domain, image and action on n.

(b) Which of the above maps A, B and C are surjective? Injective? Bijective?

PL1.1.2 Composition of maps

(a) Consider the set $S = \{-2, -1, 0, 1, 2\}$. Find its image, $T = A(S)$, under the map $n \mapsto A(n) = n^2$. Is the map $A : S \to T$ surjective? Injective? Bijective?

(b) Find the image, $U = B(T)$, of the set T from part (a) under the map $n \mapsto B(n) = \sqrt{n}$.

(c) Find the composite map $C = B \circ A$.

(d) Which of the above maps A, B and C are surjective? Injective? Bijective?

P.L1.2 Groups

To gain familiarity with the notion of a 'group operation' and the relations which it implies among the group elements, study the following elementary examples of groups. We particularly recommend the problems on permutations, L1.2.5 and L1.2.6, which set the stage for the discussion of determinants in chapter L6.

EL1.2.1 The group $\mathbb{Z}_2$

+	0	1
0	0	1
1	1	0

(a) Show that $\mathbb{Z}_2 \equiv (\{0,1\}, +)$, where the addition operation $+$ is defined by the adjacent composition table, is an abelian group.

(b) Construct a group isomorphic to $\mathbb{Z}_2$ using two integers as group elements and standard multiplication of integers as group operation. Set up the corresponding composition table.

PL1.2.2 The groups of addition modulo 5 and rotations by multiples of 72 deg

(a) Consider the set $\mathbb{Z}_5 = \{0,1,2,3,4\}$, endowed with the group operation

$$+ : \mathbb{Z}_5 \times \mathbb{Z}_5 \to \mathbb{Z}_5, \qquad (p,p') \mapsto p + p' \equiv (p+p') \bmod 5.$$

Set up the composition table for the group $(\mathbb{Z}_5, +)$. Which element is the neutral element? For a given $n \in \mathbb{Z}$, which element is the inverse of n?

(b) Let $r(\phi)$ denote a rotation by ϕ degrees about a fixed axis, with $r(\phi+360) = r(\phi)$. Consider the set of rotations by multiples of 72 deg, $\mathcal{R}_{72} = \{r(0), r(72), r(144), r(216), r(288)\}$, and the group $(\mathcal{R}_{72}, \bullet)$, where the group operation $\bullet$ involves two rotations in succession:

$$\bullet : \mathcal{R}_{72} \times \mathcal{R}_{72} \to \mathcal{R}_{72}, \qquad (r(\phi), r(\phi')) \mapsto r(\phi) \bullet r(\phi') \equiv r(\phi + \phi').$$

Set up the multiplication table for this group. Which element is the neutral element? Which element is the inverse of $r(\phi)$?

(c) Explain why the groups $(\mathbb{Z}_5, +)$ and $(\mathcal{R}_{72}, \bullet)$ are isomorphic.

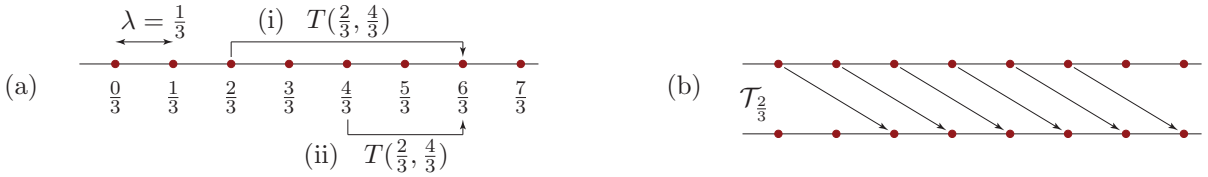
(d) Let $(\mathbb{Z}_n, +)$ denote the group of integer addition modulo n of the elements of the set $\mathbb{Z}_n = \{0, 1, \ldots, n-1\}$. Which group of discrete rotations is isomorphic to this group?

EL1.2.3 Group of discrete translations in one dimension

In this problem we show that discrete translations on an infinite, one-dimensional lattice form a group. The lattice $\mathbb{G}$ has lattice constant $0 < \lambda \in \mathbb{R}$ and consists of the set of all real numbers that are integer multiples of λ, thus $\mathbb{G} := \lambda\mathbb{Z} := \{x \in \mathbb{R} | \exists n \in \mathbb{Z} : x = \lambda \cdot n\}$, where $\cdot$ is the usual multiplication rule in $\mathbb{R}$. Note that for any given $x \in \mathbb{G}$, n is uniquely determined. On this lattice we define 'translation' by the composition rule

$$T : \quad \mathbb{G} \times \mathbb{G} \to \mathbb{G}, \quad (x,y) \mapsto T(x,y) \equiv x + y,$$

where $+$ denotes the usual addition of real numbers. Since this composition rule is symmetric, it can be visualized in two equivalent ways: $T(x, y)$ describes (i) a 'shift' or a 'translation' of lattice point x by the distance y, or (ii) a translation of lattice point y by the distance x. [Figure (a), where $\lambda = \frac{1}{3}$, shows both visualizations of $T(\frac{2}{3}, \frac{4}{3})$.]



(a) Show that $(\mathbb{G}, T)$ forms an abelian group.

(b) For a given $y \in \mathbb{G}$ we now define, in accordance with visualization (i), a 'translation' of the lattice by y, i.e. each lattice point x is 'shifted' by y:

$$\mathcal{T}_y : \quad \mathbb{G} \to \mathbb{G}, \quad x \mapsto \mathcal{T}_y(x) \equiv T(x, y).$$

[Figure (b), where $\lambda = \frac{1}{3}$, shows $\mathcal{T}_{\frac{2}{3}}$.] Now consider the set of all such translations, $\mathbb{T} := \{\mathcal{T}_y, y \in \mathbb{G}\}$. Show that $(\mathbb{T}, \boldsymbol{+})$ forms an abelian group, where $\boldsymbol{+}$ is defined as

$$\boldsymbol{+} : \quad \mathbb{T} \times \mathbb{T} \to \mathbb{T}, \quad (\mathcal{T}_x, \mathcal{T}_y) \mapsto \mathcal{T}_x \boldsymbol{+} \mathcal{T}_y \equiv \mathcal{T}_{T(x,y)}.$$

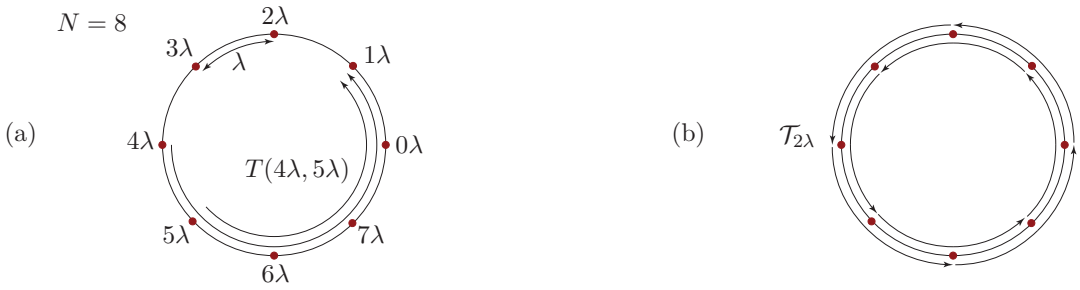
Remark: the set $\mathbb{T}$ underlying this group consists of maps (namely translations), illustrating that the set underlying a group need not be 'simple'.

PL1.2.4 Group of discrete translations on a ring

In this problem we show that discrete translations on a finite, one-dimensional lattice with periodic boundary conditions form a group. Consider a ring with radius $0 < R \in \mathbb{R}$ and lattice constant $\lambda = 2\pi R/N$ with $N \in \mathbb{N}$, thus $\mathbb{G} := \lambda(\mathbb{Z} \bmod N) := \{x \in \mathbb{R} | \exists n \in \{0, 1, \ldots, N-1\} : x = \lambda \cdot n\}$, where $\cdot$ is the usual multiplication rule in $\mathbb{R}$. Note that for any given $x \in \mathbb{G}$, n is uniquely determined. The ring forms a 'periodic' structure: when counting its sites, 0λ and $N\lambda$ describe the same lattice site, the same is true for 1λ and $(1+N)\lambda$, for 2λ and $(2+N)\lambda$, etc. On this lattice we define a composition rule, corresponding to a 'translation', using addition modulo N:

$$T : \quad \mathbb{G} \times \mathbb{G} \to \mathbb{G}, \quad (x, y) = (\lambda \cdot n_x, \lambda \cdot n_y) \mapsto T(x, y) \equiv \lambda \cdot ((n_x + n_y) \bmod N).$$

Here $+$ is the usual addition of integers, and $n \bmod N$ (spoken as 'n mod N') is defined as the integer remainder after division of n by N (e.g. $9 \bmod 8 = 1$). [For $N = 8$, figure (a) shows two visualizations of the translation $T(4\lambda, 5\lambda)$: as a 'shift' of the lattice site 4λ by the distance 5λ along the ring, or of the site 5λ by the distance 4λ.]



(a) Show that $(\mathbb{G}, T)$ forms an abelian group.

(b) For a given $y \in \mathbb{G}$ we now define a 'translation' of the lattice by y,

$$\mathcal{T}_y : \quad \mathbb{G} \to \mathbb{G}, \quad x \mapsto \mathcal{T}_y(x) \equiv T(x, y)$$

i.e. each site x is 'shifted' by y along the ring. [For $N = 8$, figure (b) shows the translation $\mathcal{T}_{2\lambda}$]. Now consider the set of all such translations, $\mathbb{T} := \{\mathcal{T}_y, y \in \mathbb{G}\}$. Show that $(\mathbb{T}, \mathbf{+})$ forms an abelian group, where $\mathbf{+}$ is defined as

$$\mathbf{+} : \quad \mathbb{T} \times \mathbb{T} \to \mathbb{T}, \quad (\mathcal{T}_x, \mathcal{T}_y) \mapsto \mathcal{T}_x \mathbf{+} \mathcal{T}_y \equiv \mathcal{T}_{T(x,y)}.$$

ᴇL1.2.5 The permutation group

A map which reorders n labelled objects is called a **permutation** of these objects. For example, $1234 \overset{[4312]}{\longmapsto} 4312$ is a permutation of the four numbers in the string 1234, where we use $[4312]$ as shorthand for the map $1 \mapsto 4$, $2 \mapsto 3$, $3 \mapsto 1$ and $4 \mapsto 2$. Similarly, if the same permutation is applied to the string 2314, it yields $2314 \overset{[4312]}{\longmapsto} 3142$. (In general, $[P(1)...P(n)]$ denotes the map $j \mapsto P(j)$, for $j = 1, ..., n$.) Two permutations performed in succession again yield a permutation. For example, acting on 1234 with $P = [4312]$ followed by $P' = [2413]$ yields $1234 \overset{[4312]}{\longmapsto} 4312 \overset{[2413]}{\longmapsto} 3124$, thus the resulting permutation is $P' \circ P = [3124]$.

The set of all possible permutations of n numbers is denoted by S_n. It contains $n!$ elements. Viewing $P' \circ P$ (perform first P, then P') as a group operation,

$$\circ : S_n \times S_n \to S_n, \qquad (P', P) \mapsto P' \circ P\,,$$

we obtain a group, $(S_n, \circ)$, the **permutation group**, usually denoted simply by S_n.

(a) Complete the adjacent composition table for S_3, in which the entries $P' \circ P$ are arranged such that those with fixed P' sit in the same row, those with fixed P in the same column.

$P' \circ P$	[123]	[231]	[312]	[213]	[321]	[132]
[123]	[123]	[231]	[312]	[213]	[321]	[132]
[231]		[312]	[123]	[321]	[132]	[213]
[312]			[231]	[132]	[213]	[321]
[213]					[312]	[231]
[321]						[312]
[132]						

(b) Which element is the neutral element of S_3? How can we see from the multiplication table that every element has a unique inverse?

(c) Is S_3 an abelian group? Justify your answer.

PL1.2.6 Decomposing permutations into sequences of pair permutations

Consider the permutation group S_n defined in the previous problem. Any permutation can be decomposed into a sequence of **pair permutations**, i.e. permuations which exchange just two objects, leaving the others unchanged. Examples:

$$
\begin{aligned}
123 &\overset{[321]}{\longmapsto} 321 \overset{[132]}{\longmapsto} 231 && \Rightarrow \quad [231] = [132] \circ [321].\\
1234 &\overset{[2134]}{\longmapsto} 2134 \overset{[3214]}{\longmapsto} 2314 && \Rightarrow \quad [2314] = [3214] \circ [2134],\\
1234 &\overset{[3214]}{\longmapsto} 3214 \overset{[1324]}{\longmapsto} 2314 && \Rightarrow \quad [2314] = [1324] \circ [3214],\\
1234 &\overset{[4231]}{\longmapsto} 4231 \overset{[1432]}{\longmapsto} 2431 \overset{[1243]}{\longmapsto} 2341 \overset{[4231]}{\longmapsto} 2314 && \Rightarrow \quad [2314] = [4231] \circ [1243] \circ [1432] \circ [4231].
\end{aligned}
$$

The last three lines illustrate that a given permutation can be pair-decomposed in several ways, and that these may or may not involve different numbers of pair exchanges. However, one may convince oneself (try it!) that all pair decompositions of a given permutation have the same **parity**, i.e. the number of exchanges is either always **even** or always **odd**.

To find a 'minimal' (shortest possible) pair decomposition of a given permutation, say $[2413]$, we may start from the naturally-ordered string 1234 and rearrange it to its desired form, 2413, one pair permutation at a time, bringing the 2 to the first slot, then the 4 to the second slot, etc. This yields $1234 \overset{[2134]}{\longmapsto} 2134 \overset{[4231]}{\longmapsto} 2431 \overset{[3214]}{\longmapsto} 2413$, hence $[2413] = [3214] \circ [4231] \circ [2134]$.

Find a minimal pair decomposition and the parity of each of the following permutations:

(a) $[132]$, (b) $[231]$, (c) $[3412]$, (d) $[3421]$, (e) $[15234]$, (f) $[31542]$.

P.L1.3 Fields

The number fields of most importance in physics are the real numbers and the complex numbers. The problems in this section focus on the latter, assuming you know the former from high school. The section's final problem L1.3.7 gives an example of a number field involving just four elements, included as an amusing curiosity.

EL1.3.1 Complex numbers – elementary computations

Consider the complex numbers $z_1 = 12 + 5\mathrm{i}$, $z_2 = -3 + 2\mathrm{i}$ and $z_3 = a - \mathrm{i}b$, with $a, b \in \mathbb{R}$. Compute (a) $\bar{z}_1$, (b) $z_1 + z_2$, (c) $z_1 + \bar{z}_3$, (d) $z_1 z_2$, (e) $\bar{z}_1 z_3$, and (f) z_1/z_2. (Present each answer in the form $x + \mathrm{i}y$.) Also compute (g) $|z_1|$, (h) $|z_1 + z_2|$ and (i) $|az_2 + 3z_3|$.

PL1.3.2 Complex numbers – elementary computations

Consider the complex numbers $z_1 = 3 + a\mathrm{i}$ and $z_2 = b - 2\mathrm{i}$ with $a, b \in \mathbb{R}$. Compute (a) $\bar{z}_1$, (b) $z_1 - z_2$, (c) $z_1\bar{z}_2$, and (d) $\bar{z}_1/z_2$. (Present each answer in the form $x + \mathrm{i}y$.) Also, compute (e) $|z_1|$ and (f) $|bz_1 - 3z_2|$. [Check your results for $a = 2$, $b = 3$: (a) $3 - 2\mathrm{i}$, (b) $4\mathrm{i}$, (c) $5 + 12\mathrm{i}$, (d) 1, (e) $\sqrt{13}$, (f) 12.]

EL1.3.3 Algebraic manipulations with complex numbers

For $z = x + \mathrm{i}y \in \mathbb{C}$, bring each of the following expressions into standard form, i.e. write them as (real part) + i(imaginary part):

(a) $z + \bar{z}$, (b) $z - \bar{z}$, (c) $z \cdot \bar{z}$, (d) $\dfrac{z}{\bar{z}}$,

(e) $\dfrac{1}{z} + \dfrac{1}{\bar{z}}$, (f) $\dfrac{1}{z} - \dfrac{1}{\bar{z}}$, (g) $z^2 + z$, (h) z^3.

[Check your results for $x = 2$, $y = 1$: (a) 4, (b) $\mathrm{i}2$, (c) 5, (d) $\frac{3}{5} + \mathrm{i}\frac{4}{5}$, (e) $\frac{4}{5}$, (f) $-\mathrm{i}\frac{2}{5}$, (g) $5 + \mathrm{i}5$, (h) $2 + \mathrm{i}11$.]

PL1.3.4 Algebraic manipulations with complex numbers

For $z = x + \mathrm{i}y \in \mathbb{C}$, bring each of the following expressions into standard form:

(a) $(z + \mathrm{i})^2$, (b) $\dfrac{z}{z + 1}$, (c) $\dfrac{\bar{z}}{z - \mathrm{i}}$.

[Check your results for $x = 1$, $y = 2$: (a) $-8 + \mathrm{i}6$, (b) $\frac{3}{4} + \mathrm{i}\frac{1}{4}$, (c) $-\frac{1}{2} - \mathrm{i}\frac{3}{2}$.]

EL1.3.5 Multiplying complex numbers – geometrical interpretation

(a) Let z_1 and z_2 be two complex numbers, with polar representations $z_j = (\rho_j \cos\phi_j, \rho_j \sin\phi_j)$. Show that multiplying them, $z_3 = z_1 z_2$, yields the relations $\rho_3 = \rho_1\rho_2$ and $\phi_3 = (\phi_1 + \phi_2) \mathrm{mod}(2\pi)$. [The $\mathrm{mod}(2\pi)$ is needed if polar angles are restricted to lie in the interval $\phi \in [0, 2\pi)$.] To this end, the following trigonometric identities are useful:
$\cos\phi_1 \cos\phi_2 - \sin\phi_1 \sin\phi_2 = \cos(\phi_1 + \phi_2)$, $\quad \sin\phi_1 \cos\phi_2 + \cos\phi_1 \sin\phi_2 = \sin(\phi_1 + \phi_2)$.

(b) For $z_1 = \sqrt{3} + \mathrm{i}$, $z_2 = -2 + 2\sqrt{3}\mathrm{i}$, compute the product $z_3 = z_1 z_2$, as well as $z_4 = 1/z_1$ and $z_5 = \bar{z}_1$. Find the polar representation [with $\phi \in [0, 2\pi)$] of all five complex numbers and sketch them in the complex plane (in one diagram). Is your result for z_3 consistent with (a)?

PL1.3.6 Multiplying complex numbers – geometrical interpretation

For $z_1 = \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{8}}\mathrm{i}$, $z_2 = \sqrt{3} - \mathrm{i}$, compute the product $z_3 = z_1 z_2$, as well as $z_4 = 1/z_1$ and $z_5 = \bar{z}_1$. Find the polar representation [with $\phi \in [0, 2\pi)$] of all five complex numbers and sketch them in the complex plane (in one diagram).

EL1.3.7 Field axioms for $\mathbb{F}_4$

For a field, the requirement that the addition and multiplication rules be distributive imposes powerful constraints on both composition rules. The present problem illustrates this fact for a discrete field involving just four elements.

Equip the set $\mathbb{F}_4 = \{0, 1, a, b\}$ with 'multiplication' and 'addition' rules chosen such that $(\mathbb{F}_4, +, \cdot)$ is a field, with 0 and 1 as neutral elements of addition and multiplication, respectively. To this end, complete the given composition tables in such a way that the properties of a field are fulfilled.

Hint: Start with the multiplication table!

$\cdot$	0	1	a	b
0				
1		1	a	b
a		a		
b		b		

$+$	0	1	a	b
0	0	1	a	b
1	1			
a	a			
b	b			

P.L2 Vector spaces

P.L2.4 Vector spaces: examples

EL2.4.1 Vector space axioms: rational numbers

(a) Show that the set $\mathbb{Q}^2 = \{\binom{x^1}{x^2} \,|\, x^1, x^2 \in \mathbb{Q}\}$, consisting of all pairs of rational numbers, forms a $\mathbb{Q}$-vector space over the field of rational numbers.

(a) Is it possible to construct a vector space from the set of all pairs of integers, $\mathbb{Z}^2 = \{\binom{x^1}{x^2} \,|\, x^1, x^2 \in \mathbb{Z}\}$? Justify your answer!

PL2.4.2 Vector space axioms: complex numbers

Show that the complex numbers $\mathbb{C}$ form a $\mathbb{R}$-vector space over the field of real numbers.

EL2.4.3 Vector space of real functions

Let $F \equiv \{f : \mathbb{R} \to \mathbb{R}, x \mapsto f(x)\}$ be the set of real functions. Show that $(F, +, \cdot)$ is an $\mathbb{R}$ vector space, where the addition of functions, and their multiplication by scalars, are defined as follows:

$$+ : F \times F \to F \quad (f, g) \mapsto f + g, \quad \text{with} \quad f + g : x \mapsto \big[f + g\big](x) \equiv f(x) + g(x) \tag{1}$$

$$\cdot : \mathbb{R} \times F \to F \quad (\lambda, f) \mapsto \lambda \cdot f, \quad \text{with} \quad \lambda \cdot f : x \mapsto \big[\lambda \cdot f\big](x) \equiv \lambda f(x) \tag{2}$$

Remark regarding notation: It is important to distinguish the 'name' of a function, f, from the 'function value', $f(x)$, which it returns when evaluated at the argument x. The sum of the functions f and g is a function named $f + g$. Eq. (1) states that its function value at x, denoted by $\big[f + g\big](x)$ (square brackets indicate the function name), is by definition equal to $f(x) + g(x)$, the sum of the function values of f and g at x. The product of the number c and the function f yields a function named $c \cdot f$. Eq. (2) states that its function value at x,

denoted by $\big[c \bullet f\big](x)$, is by definition equal to $cf(x)$, the product of c with the function value of f at x.

PL2.4.4 Vector space of polynomials of degree n

The vector space of all real functions is infinite-dimensional. However, if only functions of a prescribed form are considered, the corresponding vector space can be finite-dimensional. As an example, it is shown in this problem that the set of all polynomials of degree n form a vector space of dimension $n+1$, isomorphic to $\mathbb{R}^{n+1}$.
[Remark on the notation: In the context of the present problem on polynomials, x^k means "x to the power of k", and a_k is "the coefficient of x^k". This is in contrast to the notation that we have adopted elsewhere when discussing vectors, where x^k stands for the k-th component of the vector $\mathbf{x} = \sum_k \mathbf{v}_k x^k$ with respect to a basis of vectors $\{\mathbf{v}_k\}$. Every notational convention has exceptions!]

Let $p_\mathbf{a}$ denote a polynomial in the variable $x \in \mathbb{R}$ of degree n:

$$p_\mathbf{a} : \mathbb{R} \to \mathbb{R}, \qquad x \mapsto p_\mathbf{a}(x) \equiv a_0 x^0 + a_1 x^1 + \ldots a_n x^n. \tag{1}$$

$p_\mathbf{a}$ is uniquely specified by its $n+1$ real coefficients $a_0, a_1, \ldots, a_n$, which for notational brevity we arrange into a $(n+1)$-tuplet, $\mathbf{a} = (a_0, a_1, \ldots, a_n)^T \in \mathbb{R}^{n+1}$. Let $P_n = \{p_\mathbf{a} | \mathbf{a} \in \mathbb{R}^{n+1}\}$ denote the set of all such polynomials of degree n. The natural definitions for adding such polynomials, or multiplying them by a scalar $c \in \mathbb{R}$, are:

$$p_\mathbf{a} \boldsymbol{+} p_\mathbf{b} : \mathbb{R} \to \mathbb{R}, \qquad x \mapsto p_\mathbf{a}(x) + p_\mathbf{b}(x)\,, \tag{2}$$

$$c \bullet p_\mathbf{a} : \mathbb{R} \to \mathbb{R}, \qquad x \mapsto c\, p_\mathbf{a}(x)\,, \tag{3}$$

where on the right side the usual addition and multiplication in $\mathbb{R}$ is used.

(a) Show that the above addition and scalar multiplication imply the following composition rules in P_n,

$$\begin{aligned} &\text{Addition of polynomials:} && \boldsymbol{+} : && P_n \times P_n \to P_n, && (p_\mathbf{a}, p_\mathbf{b}) \mapsto p_\mathbf{a} \boldsymbol{+} p_\mathbf{b} \equiv p_{\mathbf{a}+\mathbf{b}}\,, \\ &\text{Multiplication by a scalar:} && \bullet : && \mathbb{R} \times P_n \to P_n, && (c, p_\mathbf{x}) \mapsto c \bullet p_\mathbf{a} \equiv p_{c\mathbf{a}}\,, \end{aligned}$$

where $\mathbf{a} + \mathbf{b}$ and $c\mathbf{a}$ denote the usual addition and scalar multiplication in $\mathbb{R}^{n+1}$.

(b) Show that $(P_n, \boldsymbol{+}, \bullet)$ is an $\mathbb{R}$ vector space, and that it is isomorphic to $\mathbb{R}^{n+1}$.

(c) Construct a set $n+1$ of polynomials, $\{p_{\mathbf{a}_0}, \ldots, p_{\mathbf{a}_n}\} \subset P_n$, that forms a basis for this vector space.

EL2.4.5 Vector space with unusual composition rule

The axioms that define a vector space can be satisfied in many different ways. These may involve unconventional definitions of vector addition and scalar multiplication. The purpose of the present problem is to illustrate this point.
For any $a \in \mathbb{R}$, let $V_a \equiv \{\mathbf{v}_x\}$ be a set whose elements $\mathbf{v}_x$, labelled by real numbers $x \in \mathbb{R}$, satisfy the following composition rules:

$$\begin{aligned} &\text{Addition:} && \boldsymbol{+}: && V_a \times V_a \to V_a, && (\mathbf{v}_x, \mathbf{v}_y) \mapsto \mathbf{v}_x \boldsymbol{+} \mathbf{v}_y \equiv \mathbf{v}_{x+y+a} \\ &\text{Multiplication by a scalar:} && \cdot: && \mathbb{R} \times V_a \to V_a, && (\lambda, \mathbf{v}_x) \mapsto \lambda \cdot \mathbf{v}_x \equiv \mathbf{v}_{\lambda x + a(\lambda-1)} \end{aligned}$$

The a and x labels, being real numbers, satisfy the usual addition and scalar multiplication rules of $\mathbb{R}$; e.g. in V_2 we have: $\mathbf{v}_3 \boldsymbol{+} \mathbf{v}_4 = \mathbf{v}_{3+4+2} = \mathbf{v}_9$ and $3 \cdot \mathbf{v}_4 = \mathbf{v}_{3\cdot 4+2(3-1)} = \mathbf{v}_{16}$. Show that the triple $(V_a, \boldsymbol{+}, \cdot)$ represents an $\mathbb{R}$-vector space, with $\mathbf{v}_{-a}$ and 1 being the neutral elements for addition and scalar multiplication, respectively, and $\mathbf{v}_{-x-2a}$ the additive inverse of $\mathbf{v}_x$.

PL2.4.6 Vector space with unusual composition rule

For any $\mathbf{a} \in \mathbb{R}^2$, let $V_{\mathbf{a}} \equiv \{\mathbf{v}_{\mathbf{x}}\}$ be a set whose elements $\mathbf{v}_{\mathbf{x}}$, labelled by vectors $\mathbf{x} \in \mathbb{R}^2$, satisfy the following composition rules:

$$\begin{aligned} &\text{Addition:} && \boldsymbol{+}: && V_{\mathbf{a}} \times V_{\mathbf{a}} \to V_{\mathbf{a}}, && (\mathbf{v}_{\mathbf{x}}, \mathbf{v}_{\mathbf{y}}) \mapsto \mathbf{v}_{\mathbf{x}} \boldsymbol{+} \mathbf{v}_{\mathbf{y}} \equiv \mathbf{v}_{\mathbf{x}+\mathbf{y}-\mathbf{a}} \\ &\text{Multiplication by a scalar:} && \cdot: && \mathbb{R} \times V_{\mathbf{a}} \to V_{\mathbf{a}}, && (\lambda, \mathbf{v}_{\mathbf{x}}) \mapsto \lambda \cdot \mathbf{v}_{\mathbf{x}} \equiv \mathbf{v}_{\lambda\mathbf{x} + f(\mathbf{a},\lambda)} \end{aligned}$$

Here $f(\mathbf{a}, \lambda)$ is a function of $\mathbf{a}$ and λ, whose form will be determined below.

(a) Show that $V_{\mathbf{a}}$, endowed with the composition rule $\boldsymbol{+}$, forms an abelian group, and specify the neutral element of addition and the additive inverse of $\mathbf{v}_{\mathbf{x}}$.

(b) Find the specific form of f that ensures that the triple $(V_{\mathbf{a}}, \boldsymbol{+}, \cdot)$ forms an $\mathbb{R}$-vector space.

(c) Would a similar construction work for $\mathbf{a}$, $\mathbf{x} \in \mathbb{R}^n$ (with n a positive integer) instead of $\mathbb{R}^2$?

P.L2.5 Basis and dimension

EL2.5.1 Linear Independence

(a) Are the vectors $\mathbf{v}_1 = (0, 1, 2)^T$, $\mathbf{v}_2 = (1, -1, 1)^T$ and $\mathbf{v}_3 = (2, -1, 4)^T$ linearly independent?

(b) Depending on whether your answer is yes or no, find a vector $\mathbf{v}_2'$ such that $\mathbf{v}_1$, $\mathbf{v}_2'$ and $\mathbf{v}_3$ are linearly dependent or independent, respectively, and show explicitly that they have this property.

PL2.5.2 Linear independence

(a) Are the vectors $\mathbf{v}_1 = (1,2,3)^T$, $\mathbf{v}_2 = (2,4,6)^T$ and $\mathbf{v}_3 = (-1,-1,0)^T$ linearly independent?

(b) Depending on whether your answer is yes or no, find a vector, $\mathbf{v}_2'$ such that $\mathbf{v}_1$, $\mathbf{v}_2'$ and $\mathbf{v}_3$ are linearly dependent or independent, respectively, and show explicitly that they have this property.

EL2.5.3 Einstein summation convention

Which of the following statements involving (a_1, a_2) and $\begin{pmatrix} b^1 \\ b^2 \end{pmatrix}$, formulated using the Einstein summation convention, are true and which are false? Justify your answers!

(a) $a_i b^i \stackrel{?}{=} b^j a_j$,

(b) $a_i \delta^i{}_j b^j \stackrel{?}{=} a_k b^k$,

(c) $a_i b^j a_j b^k \stackrel{?}{=} a_k b^l a_l b^i$,

(d) $a_1 a_i b^1 b^i + b^2 a_j a_2 b^j \stackrel{?}{=} (a_i b^i)^2$.

PL2.5.4 Einstein summation convention

Let $(a_1, a_2) = (1,2)$, $\begin{pmatrix} b^1 \\ b^2 \end{pmatrix} = \begin{pmatrix} -1 \\ x \end{pmatrix}$. Evaluate the following expressions, formulated using the Einstein summation convention, as functions of x:

(a) $a_i b^i$,

(b) $a_i a_j b^i b^j$,

(c) $a_1 a_j b^2 b^j$.

[Check your results for $x = 3$: (a) 5, (b) 25, (c) 15.]

P.L3 Euclidean geometry

P.L3.1 Scalar product of $\mathbb{R}^n$

P.L3.2 Normalization and orthogonality

EL3.2.1 Angle, orthogonal decomposition

(a) Find the angle between the vectors $\mathbf{a} = (3,4)^T$ and $\mathbf{b} = (7,1)^T$.

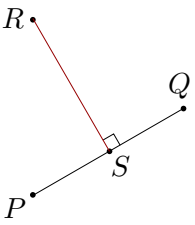
(b) Consider the vectors $\mathbf{c} = (3,1)^T$ and $\mathbf{d} = (-1,2)^T$. Decompose $\mathbf{c} = \mathbf{c}_\parallel + \mathbf{c}_\perp$ into components parallel and perpendicular to $\mathbf{d}$, respectively. Scetch all four vectors.

[Check your results: $\|\mathbf{c}_\parallel\| = \frac{1}{\sqrt{5}}$, $\|\mathbf{c}_\perp\| = \frac{7}{\sqrt{5}}$.]

PL3.2.2 Angle, orthogonal decomposition

(a) Find the angle between the vectors $\mathbf{a} = (2, 0, \sqrt{2})^T$ and $\mathbf{b} = (\sqrt{2}, 1, 1)^T$.

In the figure, the points P, Q and R have coordinate vectors $\mathbf{p} = (-1, -1)^T$, $\mathbf{q} = (2, 1)^T$ and $\mathbf{r} = (-1, -1 + 13a)^T$, with a a positive real number. The line RS is perpendicular to the line PQ.



(b) Find the coordinate vector $\mathbf{s}$ of S, expressed as a function of a.
Hint: Let $\mathbf{c}$ denote the vector from P to Q, and $\mathbf{d}$ the vector from P to R, then decompose $\mathbf{d} = \mathbf{d}_\parallel + \mathbf{d}_\perp$ into components parallel and perpendicular to $\mathbf{c}$.

(c) Find the distance $\overline{RS}$ from R to S and the distance $\overline{PS}$ from P to S.

[Check your results for $a = 1$: (b) $\mathbf{s} = (5, 3)^T$, (c) $\overline{RS}^2 + \overline{PS}^2 = 169$.]

P.L3.3 Inner product spaces

EL3.3.1 Inner product for vector space of continuous functions

This problem illustrates a particularly important example of an inner product: in the space of continuous functions, an inner product can be defined via integration.
Let V be the vector space of *continuous* real functions defined on an interval $I \in \mathbb{R}$, $f : I \to \mathbb{R}$, with the usual composition rules of vector addition and scalar multiplication:

$$\begin{aligned} &\forall f, g \in V : && f + g : I \to \mathbb{R}, && x \mapsto (f + g)(x) \equiv f(x) + g(x)), \\ &\forall f \in V, \lambda \in \mathbb{R} : && \lambda \cdot f : I \to \mathbb{R}, && x \mapsto \ (\lambda \cdot f)(x) \equiv \lambda\,(f(x))\,. \end{aligned}$$

(a) Show that the following map defines an inner product on V:

$$\langle \cdot, \cdot \rangle : V^2 \to \mathbb{R}, \qquad (f, g) \mapsto \langle f, g \rangle \equiv \int_I \mathrm{d}x\, f(x) g(x)\ .$$

(b) Now consider $I = [-1, 1]$. Compute $\langle f_1, f_2 \rangle$ for $f_1(x) \equiv \sin\left(\frac{x}{\pi}\right)$ and $f_2(x) \equiv \cos\left(\frac{x}{\pi}\right)$.

PL3.3.2 Unconvential inner product

The defining properties of an inner product on $\mathbb{R}^n$ are of course satisfied not only by the 'standard' definition, $\langle \mathbf{x}, \mathbf{x} \rangle = \sum_{i=1}^n (x^i)^2$; there are infinitely many other bilinear forms that do so, too. The present problem illustrate this with a simple example. Show that the following map defines an inner product on the vector space $\mathbb{R}^2$:

$$\langle \cdot, \cdot \rangle \colon \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}, \qquad \big(\mathbf{x}, \mathbf{y}\big) \mapsto x_1 y_1 + x_1 y_2 + x_2 y_1 + 3 x_2 y_2\,.$$

EL3.3.3 Projection onto an orthonormal basis

(a) Show that the vectors $\mathbf{e}'_1 = \frac{1}{\sqrt{2}}(1,1)^T$, $\mathbf{e}'_2 = \frac{1}{2}(1,-1)^T$ form an orthonormal basis for $\mathbb{R}^2$.

(b) Express the vector $\mathbf{w} = (-2,3)^T$ in the form $\mathbf{w} = \mathbf{e}'_1 w^1 + \mathbf{e}'_2 w^2$, by computing its components w^i with respect to the basis $\{\mathbf{e}'_i\}$ through projection onto the basis vectors. [Check your results: $\sum_{i=1}^{2} w^i = -2\sqrt{2}$.]

PL3.3.4 Projection onto an orthonormal basis

(a) Show that the vectors $\mathbf{e}'_1 = \frac{1}{9}(4,-1,8)^T$, $\mathbf{e}'_2 = \frac{1}{9}(-7,4,4)^T$ and $\mathbf{e}'_3 = \frac{1}{9}(-4,-8,1)^T$ form an orthonormal basis in $\mathbb{R}^3$.

(b) Let $\mathbf{w} = \mathbf{e}'_i w^i$ be the decomposition of $\mathbf{w} = (1,2,3)^T$ in this basis. Find the components w^i. [Check your results: $\sum_{i=1}^{3} w^i = \frac{22}{9}$.]

EL3.3.5 Non-orthonormal basis vectors and metric

Consider the vectors $\hat{\mathbf{v}}_1 = \binom{2}{0}$ and $\hat{\mathbf{v}}_2 = \binom{1}{1}$, written as column vectors in the standard basis of $\mathbb{R}^2$. (In this problem we use the notation of section **??**: vectors in the inner product space $\mathbb{R}^2$ carry a caret, e.g. $\hat{\mathbf{x}}$, and their components w.r.t. a given basis do not, e.g. $\mathbf{x}$.)

(a) Write the standard basis vector $\hat{\mathbf{e}}_1 = \binom{1}{0}$ as a linear combination of $\hat{\mathbf{v}}_1$ and $\hat{\mathbf{v}}_2$. Ditto for $\hat{\mathbf{e}}_2 = \binom{0}{1}$. Do $\{\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2\}$ form a basis for $\mathbb{R}^2$?

(b) Let $\hat{\mathbf{x}} = \hat{\mathbf{v}}_1 x^1 + \hat{\mathbf{v}}_2 x^2$ and $\hat{\mathbf{y}} = \hat{\mathbf{v}}_1 y^1 + \hat{\mathbf{v}}_2 y^2$ be two vectors in $\mathbb{R}^2$, whose components w.r.t. $\hat{\mathbf{v}}_1$ and $\hat{\mathbf{v}}_2$ are given by $\mathbf{x} = (x^1, x^2)^T = (3,-4)^T$ and $\mathbf{y} = (y^1, y^2)^T = (-1,3)^T$ respectively. Express $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ as column vectors in the standard basis of $\mathbb{R}^2$ and compute their scalar product $\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_{\mathbb{R}^2}$.

(c) If the scalar product $\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_{\mathbb{R}^2}$ is expressed through the components x^i of $\hat{\mathbf{x}}$ and y^i of $\hat{\mathbf{y}}$ w.r.t. the non-orthogonal basis $\{\hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2\}$, then it takes the form of an inner product with a metric: $\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_{\mathbb{R}^2} = \langle \mathbf{x}, \mathbf{y} \rangle_g = x^i g_{ij} y^j$, with $g_{ij} = \langle \hat{\mathbf{v}}_i, \hat{\mathbf{v}}_j \rangle_{\mathbb{R}^2}$. Compute the components of the metric explicitly (concretely: find g_{11}, g_{12}, g_{21} and g_{22}).

(d) The inner product from (c) can be written as $\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_{\mathbb{R}^2} = (x^i g_{ij}) y^j = x_j y^j$, with $x_j = x^i g_{ij}$, thus "hiding" the metric by absorbing it into the definition of covariant components (with subscript indices). Compute $\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_{\mathbb{R}^2}$ in this manner, by first finding x_1 and x_2. [Check: is the result consistent with that from (b)?]

PL3.3.6 Non-orthonormal basis vectors and metric

Consider the vectors $\hat{\mathbf{v}}_1 = (2,1,2)^T$, $\hat{\mathbf{v}}_2 = (1,0,1)^T$, and $\hat{\mathbf{v}}_3 = (1,1,0)^T$, written as column vectors in the standard basis of $\mathbb{R}^3$. (In this problem we use the notation of section **??**: vectors in the inner product space $\mathbb{R}^3$ carry a caret, e.g. $\hat{\mathbf{x}}$, and their components w.r.t. a given basis do not, e.g. $\mathbf{x}$.)

(a) Write the standard basis vector $\hat{\mathbf{e}}_1 = (1,0,0)^T$ as a linear combination of $\hat{\mathbf{v}}_1$, $\hat{\mathbf{v}}_2$ and $\hat{\mathbf{v}}_3$. Ditto for $\hat{\mathbf{e}}_2 = (0,1,0)^T$ and $\hat{\mathbf{e}}_3 = (0,0,1)^T$. Do $\hat{\mathbf{v}}_1$, $\hat{\mathbf{v}}_2$ and $\hat{\mathbf{v}}_3$ form a basis for $\mathbb{R}^3$?

(b) Let $\hat{\mathbf{x}} = \hat{\mathbf{v}}_1 x^1 + \hat{\mathbf{v}}_2 x^2 + \hat{\mathbf{v}}_3 x^3$ and $\hat{\mathbf{y}} = \hat{\mathbf{v}}_1 y^1 + \hat{\mathbf{v}}_2 y^2 + \hat{\mathbf{v}}_3 y^3$ be two vectors in $\mathbb{R}^3$, whose components w.r.t. $\hat{\mathbf{v}}_1$, $\hat{\mathbf{v}}_2$ and $\hat{\mathbf{v}}_3$ are given by $\mathbf{x} = (x^1, x^2, x^3) = (2,-5,3)^T$ and $\mathbf{y} = (y^1, y^2, y^3) = (4,-1,-2)^T$, respectively. Express $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ as column vectors in the standard basis of $\mathbb{R}^3$ and compute their scalar product $\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_{\mathbb{R}^3}$.

(c) Find the components of the metric $g_{ij} = \langle \hat{\mathbf{v}}_i, \hat{\mathbf{v}}_j \rangle_{\mathbb{R}^3}$ explicitly.

(d) Now calculate the scalar product of $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ using the formula $\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_{\mathbb{R}^3} = \langle \mathbf{x}, \mathbf{y} \rangle_g = x^i g_{ij} y^j = x_j y^j$, with $x_j = x^i g_{ij}$, and carry out the sum over i and j explicitly. [Check: is the result consistent with that from (b)?]

EL3.3.7 Gram-Schmidt orthonormalization

Apply the Gram-Schmidt procedure to the following set of linearly independent vectors $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ to construct an orthonormal set $\{\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3\}$ with the same span and with $\mathbf{e}'_1 || \mathbf{v}_1$.

$$\mathbf{v}_1 = (1,-2,1)^T, \qquad \mathbf{v}_2 = (1,1,1)^T, \qquad \mathbf{v}_3 = (0,1,2)^T.$$

PL3.3.8 Gram-Schmidt orthonormalization

Apply the Gram-Schmidt procedure to each of the following sets of linearly independent vectors $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ to construct an orthonormal set $\{\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3\}$ with the same span and with $\mathbf{e}'_1 || \mathbf{v}_1$.

(a) $\mathbf{v}_1 = (-2,0,2)^T$, $\mathbf{v}_2 = (2,1,0)^T$, $\mathbf{v}_3 = (3,6,5)^T$.

(b) $\mathbf{v}_1 = (1,1,0,0)^T$, $\mathbf{v}_2 = (0,0,1,1)^T$, $\mathbf{v}_3 = (0,1,1,0)^T$.

P.L3.4 Complex scalar product

P.L4 Vector product

P.L4.2 Algebraic formulation

EL4.2.1 Elementary computations with vectors

Given the vectors $\mathbf{a} = (4,3,1)^T$ and $\mathbf{b} = (1,-1,1)^T$.

(a) Calculate $\|\mathbf{b}\|$, $\mathbf{a}-\mathbf{b}$, $\mathbf{a}\cdot\mathbf{b}$ and $\mathbf{a}\times\mathbf{b}$.

(b) Decompose $\mathbf{a}$ into a vector $\mathbf{a}_\parallel$ parallel to $\mathbf{b}$ and a vector $\mathbf{a}_\perp$ perpendicular to $\mathbf{b}$.

(c) Calculate $\mathbf{a}_\parallel\cdot\mathbf{b}$, $\mathbf{a}_\perp\cdot\mathbf{b}$, $\mathbf{a}_\parallel\times\mathbf{b}$ and $\mathbf{a}_\perp\times\mathbf{b}$. Do these results match your expectations?

[Check your results: (a) $\mathbf{a}\cdot\mathbf{b}+\sum_i(\mathbf{a}\times\mathbf{b})^i=-4$, (b) $\sum_i(\mathbf{a}_\parallel)^i=\frac{2}{3}$, $\sum_i(\mathbf{a}_\perp)^i=7\frac{1}{3}$.]

PL4.2.2 Elementary computations with vectors

Given the vectors $\mathbf{a}=(2,1,5)^T$ and $\mathbf{b}=(-4,3,0)^T$.

(a) Calculate $\|\mathbf{b}\|$, $\mathbf{a}-\mathbf{b}$, $\mathbf{a}\cdot\mathbf{b}$ and $\mathbf{a}\times\mathbf{b}$.

(b) Decompose $\mathbf{a}$ into a vector $\mathbf{a}_\parallel$ parallel to $\mathbf{b}$ and a vector $\mathbf{a}_\perp$ perpendicular to $\mathbf{b}$.

(c) Calculate $\mathbf{a}_\parallel\cdot\mathbf{b}$, $\mathbf{a}_\perp\cdot\mathbf{b}$, $\mathbf{a}_\parallel\times\mathbf{b}$ and $\mathbf{a}_\perp\times\mathbf{b}$. Do these results match your expectations?

[Check your results: (a) $\mathbf{a}\cdot\mathbf{b}+\sum_i(\mathbf{a}\times\mathbf{b})^i=-30$, (b) $\sum_i(\mathbf{a}_\parallel)^i=\frac{1}{5}$, $\sum_i(\mathbf{a}_\perp)^i=7\frac{4}{5}$.]

EL4.2.3 Levi-Civita tensor

(a) Is the statement $a^ib^j\epsilon_{ij2}\stackrel{?}{=}-a^k\epsilon_{k2l}b^l$ true or false? Justify your answer.

Express the following k-sums over products of two Levi-Civita tensors in terms of Kronecker delta functions. Check your answers by also writing out the k-sums explicitly and evaluating each term separately.

(b) $\epsilon_{1ik}\epsilon_{kj1}$, (c) $\epsilon_{1ik}\epsilon_{kj2}$.

PL4.2.4 Levi-Civita tensor

(a) Is the statement $a^ia^j\epsilon_{ij3}\stackrel{?}{=}b^mb^n\epsilon_{mn2}$ true or false? Justify your answer.

Express the following k-sums over products of two Levi-Civita tensors in terms of Kronecker delta functions.

(b) $\epsilon_{1ik}\epsilon_{23k}$, (c) $\epsilon_{2jk}\epsilon_{ki2}$, (d) $\epsilon_{1ik}\epsilon_{k3j}$.

P.L4.3 Further properties of the vector product

EL4.3.1 Grassmann identity (BAC-CAB) and Jacobi identity

(a) Prove the Grassmann (or BAC-CAB) identity for arbitrary vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c} \in \mathbb{R}^3$:

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = \mathbf{b}(\mathbf{a} \cdot \mathbf{c}) - \mathbf{c}(\mathbf{a} \cdot \mathbf{b}).$$

Hint: Expand the three vectors in an orthonormal basis, e.g. $\mathbf{a} = \mathbf{e}_i a^i$, and use the identity $\epsilon_{ijk}\epsilon_{mnk} = \delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}$ for the Levi-Civita-tensor. If you prefer, you may equally well write all indices downstairs, e.g. $\mathbf{a} = \mathbf{e}_i a_i$, since in an orthonormal basis $a_i = a^i$.

(b) Use the Grassmann identity to derive the Jacobi identity:

$$\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) + \mathbf{b} \times (\mathbf{c} \times \mathbf{a}) + \mathbf{c} \times (\mathbf{a} \times \mathbf{b}) = \mathbf{0}\,.$$

(c) Check both identities explicitly for $\mathbf{a} = (1, 1, 2)^T$, $\mathbf{b} = (3, 2, 0)^T$ and $\mathbf{c} = (2, 1, 1)^T$ by separately computing all terms they contain.

PL4.3.2 Lagrange identity

(a) Prove the Lagrange identity for arbitrary vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$, $\mathbf{d} \in \mathbb{R}^3$:

$$(\mathbf{a} \times \mathbf{b}) \cdot (\mathbf{c} \times \mathbf{d}) = (\mathbf{a} \cdot \mathbf{c})(\mathbf{b} \cdot \mathbf{d}) - (\mathbf{a} \cdot \mathbf{d})(\mathbf{b} \cdot \mathbf{c}).$$

Hint: Work in an orthonormal basis and use the properties of the Levi-Civita tensor.

(b) Use (a) to compute $\|\mathbf{a} \times \mathbf{b}\|$ and express the result in terms of $\|\mathbf{a}\|$, $\|\mathbf{b}\|$ and the angle ϕ between $\mathbf{a}$ and $\mathbf{b}$.

(c) Check the Lagrange identity explicitly for the vectors $\mathbf{a} = (2, 1, 0)^T$, $\mathbf{b} = (3, -1, 2)^T$, $\mathbf{c} = (3, 0, 2)^T$, $\mathbf{d} = (1, 3, -2)^T$, by separately computing all its terms.

EL4.3.3 Scalar triple product

This problem illustrates an important relation between the scalar triple product and the question whether three vectors in $\mathbb{R}^3$ are linearly independent or not.

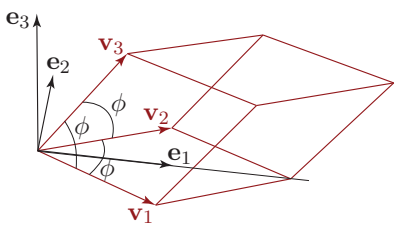
(a) Compute the scalar triple product $S(y)$ of $\mathbf{v}_1 = (1, 0, 2)^T$, $\mathbf{v}_2 = (3, 2, 1)^T$ and $\mathbf{v}_3 = (-1, -2, y)^T$ as a function of the variable y. [Check your result: $S(1) = -4$].

(b) By solving the vector equation $\mathbf{v}_i a^i = \mathbf{0}$, find that value of y for which $\mathbf{v}_1$, $\mathbf{v}_2$ are $\mathbf{v}_3$ *not* linearly independent.

(c) What is the value of $S(y)$ for the value of y found in (b)? Interpret your result!

PL4.3.4 Scalar triple product

Compute the volume $V(\phi)$ of the parallelepiped spanned by three unit vectors $\mathbf{v}_1$, $\mathbf{v}_2$ and $\mathbf{v}_3$, each pair of which encloses a mutual angle of ϕ (with $0 \leq \phi \leq \frac{2}{3}\pi$; why is this restriction needed?).
Check your results: (i) What do you expect for $V(\frac{\pi}{2})$ and $V(\frac{2}{3}\pi)$? (ii): $V(\frac{\pi}{3}) = \frac{1}{\sqrt{2}}$.



Hint: Choose the orientation of the parallelepiped such that $\mathbf{v}_1$ and $\mathbf{v}_2$ both lie in the plane spanned by $\mathbf{e}_1$ and $\mathbf{e}_2$, and that $\mathbf{e}_1$ bisects the angle between $\mathbf{v}_1$ and $\mathbf{v}_2$ (see figure).

P.L5 Matrices I: general theory

P.L5.1 Linear maps

P.L5.2 Matrices

P.L5.3 Matrix multiplication

EL5.3.1 Matrix multiplication

Compute all possible products of pairs of the following matrices, including their squares, where possible:

$$P = \begin{pmatrix} 4 & -3 & 1 \\ 2 & 2 & -4 \end{pmatrix}, \quad Q = \begin{pmatrix} 3 & 0 & 1 \\ 1 & 2 & 5 \\ 1 & -6 & -1 \end{pmatrix}, \quad R = \begin{pmatrix} 3 & 0 \\ 1 & 2 \\ 1 & -6 \end{pmatrix}.$$

[Check your results: the sum of all elements of the first column of the following matrix products is: $\sum_i (PQ)_{i1} = 14$, $\sum_i (PR)_{i1} = 14$, $\sum_i (QR)_{i1} = 16$, $\sum_i (RP)_{i1} = 12$, $\sum_i (QQ)_{i1} = 16$.]

PL5.3.2 Matrix multiplication

Compute all possible products of pairs of the following matrices, including their squares, where possible:

$$P = \begin{pmatrix} 2 & 0 & 3 \\ -5 & 2 & 7 \\ 3 & -3 & 7 \\ 2 & 4 & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} -3 & 1 \\ -1 & 0 \\ 2 & 1 \end{pmatrix}, \quad R = \begin{pmatrix} 6 & -1 & 4 \\ 4 & 4 & -4 \\ -4 & -4 & 6 \end{pmatrix}.$$

[Check your results: the sum of all elements of the first column of the following matrix products is: $\sum_i (PQ)_{i1} = 25$, $\sum_i (PR)_{i1} = -44$, $\sum_i (RQ)_{i1} = -5$, $\sum_i (RR)_{i1} = 8$.]

EL5.3.3 Spin $\frac{1}{2}$ matrices

The following matrices are used to describe quantum mechanical particles with spin $\frac{1}{2}$:

$$S_x = \tfrac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S_y = \tfrac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad S_z = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

(a) Compute $\mathbf{S}^2 = S_x^2 + S_y^2 + S_z^2$.

(b) Compute the commutators $[S_x, S_y]$, $[S_y, S_z]$ and $[S_z, S_x]$, and express each result in terms of one of the matrices given above. *Remark:* $[A, B] = AB - BA$.

(c) The results from (b) can be compactly summarized in an equation of the form $[S_i, S_j] = a_{ijk}S_k$ for $\{i, j, k\} \in \{x, y, z\}$ (with summation over k). Find the tensor a_{ijk}.

PL5.3.4 Spin 1 matrices

The following matrices are used to describe quantum mechanical particles with spin 1:

$$S_x = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad S_y = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \qquad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

(a) Compute $\mathbf{S}^2 = S_x^2 + S_y^2 + S_z^2$.

(b) Comute the commutators $[S_x, S_y]$, $[S_y, S_z]$ and $[S_z, S_x]$, and express each result through one of the matrices given above. *Remark:* $[A, B] = AB - BA$.

EL5.3.5 Matrix multiplication

Let A and B be $N \times N$ matrices with matrix elements $A^i{}_j = A_j\delta^i{}_m$ and $B^i{}_j = B_i\delta^i{}_j$. *Remark:* Since the indices i and j are specified on the left, they are *not* summed over on the right even though in the expression for $B^i{}_j$ the index i appears twice on the right.

(a) For $N = 3$ and $m = 2$, write these matrices explicitly in the usual matrix representation and calculate the matrix product AB explicitly.

(b) Calculate the product AB for arbitrary $N \in \mathbb{N}$ and $1 \leq m \leq N$. [Check your result: the sum of the diagonal elements yields: $\sum_{i=1}^{N}(AB)_{ii} = A_m B_m$.]

PL5.3.6 Matrix multiplication

Let A and B be $N \times N$ matrices with matrix elements $A^i{}_j = A_i\delta^i{}_{N+1-j}$ and $B^i{}_j = B_i\delta^i{}_j$. *Remark:* Since the indices i and j are specified on the left, they are *not* summed over on the right even though the index i appears twice in $B^i{}_j$ on the right.

(a) For $N = 3$ and $m = 2$, write these matrices explicitly in the usual matrix representation and calculate the matrix product AB explicitly.

(b) Calculate the product AB for arbitrary $N \in \mathbb{N}$ and $1 \leq m \leq N$. [Check your result: if N is odd, the sum of the diagonal elements yields: $\sum_{i=1}^{N}(AB)_{ii} = A_{\frac{N+1}{2}} B_{\frac{N+1}{2}}$.]

P.L5.4 The inverse of a matrix

EL5.4.1 Gaussian elimination and matrix inversion

(a) Solve the following system of linear equations using Gaussian elimination.

$$\begin{array}{rcrcrcr} 3x^1 & + & 2x^2 & - & x^3 & = & 1, \\ 2x^1 & - & 2x^2 & + & 4x^3 & = & -2, \\ -x^1 & + & \frac{1}{2}x^2 & - & x^3 & = & 0. \end{array}$$

[Check your result: the norm of $\mathbf{x}$ is $\|\mathbf{x}\| = 3$.]

(b) How does the solution change when the last equation is removed?

(c) What happens if the last equation is replaced by $-x^1 + \frac{2}{7}x^2 - x^3 = 0$?

(d) This system of equations can also be expressed in the form $A\mathbf{x} = \mathbf{b}$. Calculate the inverse A^{-1} of the 3×3 Matrix A using Gaussian elimination, and verify your answer to (a) using $\mathbf{x} = A^{-1}\mathbf{b}$.

PL5.4.2 Gaussian elimination and matrix inversion

Consider the linear system of equations $A\mathbf{x} = \mathbf{b}$, with

$$A = \begin{pmatrix} 8-3a & 2-6a & 2 \\ 2-6a & 5 & -4+6a \\ 2 & -4+6a & 5+3a \end{pmatrix}. \tag{1}$$

(a) For $a = \frac{1}{3}$, use Gaussian elimination to compute the inverse matrix A^{-1}. (*Remark:* It is advisable to avoid the occurrence of fractions until the left side has been brought into row echelon form.) Use the result to find the solution $\mathbf{x}$ for $\mathbf{b} = (4, 1, 1)^T$. [Check your result: the norm of $\mathbf{x}$ is $\|\mathbf{x}\| = \sqrt{117}/18$.]

(b) For which values of a can the matrix A *not* be inverted?

(c) If A can be inverted, the system of equations $A\mathbf{x} = \mathbf{b}$ has a unique solution for every $\mathbf{b}$, namely $\mathbf{x} = A^{-1}\mathbf{b}$. If A cannot be inverted, then either the solution is not unique, or no solution exists at all – it depends on $\mathbf{b}$ which of these two cases arises. Decide this for $\mathbf{b} = (4, 1, 1)^T$ and the values for a found in (b), and determine $\mathbf{x}$, if possible.

EL5.4.3 Matrix inversion

Let M_n be an $n \times n$ matrix with matrix elements $(M_n)^i{}_j = \delta^i{}_j m + \delta^1{}_j$, with $i, j = 1, \ldots, n$.

(a) Find the inverse matrices M_2^{-1} and M_3^{-1}. Verify in both cases that $M_n^{-1} M_n = \mathbb{1}$.

(b) Use the results from (a) to formulate a guess at the form of the inverse matrix M_n^{-1} for arbitrary n. Check your guess by calculating $M_n^{-1} M_n$.

(c) Give a compact formula for the matrix elements $(M_n^{-1})^i{}_j$. Check its validity by showing that $\sum_l (M_n^{-1})^i{}_l (M_n)^l{}_j = \delta^i{}_j$ holds, by explicitly performing the sum on l.

PL5.4.4 Matrix inversion

Let M_n be an $n \times n$ matrix with matrix elements $(M_n)^i{}_j = m\,\delta_{ij} + \delta_{i+1,j}$, with $i, j = 1, \ldots, n$.

(a) Find the inverse matrices M_2^{-1} and M_3^{-1}. Verify in both cases that $M_n^{-1} M_n = \mathbb{1}$.

(b) Use the results from (a) to formulate a guess at the form of the inverse matrix M_n^{-1} for arbitrary n. Check your guess by calculating $M_n^{-1} M_n$.

(c) Give a compact formula for the matrix elements $(M_n^{-1})^i{}_j$. Check its validity by showing that $\sum_l (M_n^{-1})^i{}_l (M_n)^l{}_j = \delta^i{}_j$ holds, by explicitly performing the sum over l.

P.L5.5 General linear maps and matrices

EL5.5.1 Two-dimensional rotation matrices

A rotation in two dimensions is a linear map, $R : \mathbb{R}^2 \to \mathbb{R}^2$, that rotates every vector by a given angle about the origin without changing its length.

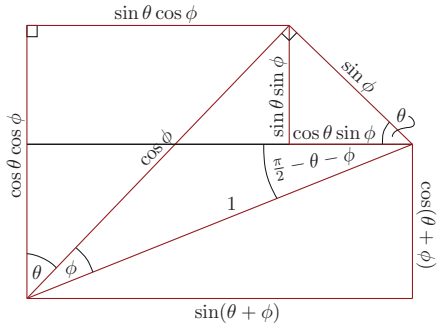
(a) Find the 2×2 dimensional rotation matrix R_θ describing a rotation by the angle θ by proceeding as follows: Make a sketch that illustrates the effect $\mathbf{e}_j \overset{R_\theta(\mathbf{e}_i)}{\longrightarrow} \mathbf{e}'_j$ of the rotation about the i axis on the three basis vectors $\mathbf{e}_j$ $(j = 1, 2, 3)$ (eg. for $\theta = \frac{\pi}{6}$). The image vectors $\mathbf{e}'_j$ of the basis vectors $\mathbf{e}_j$ yield the columns of R_θ.

(b) Write down the matrix R_{θ_i} for the angles $\theta_1 = 0, \theta_2 = \pi/4, \theta_3 = \pi/2$ and $\theta_4 = \pi$. Compute the action of R_{θ_i} $(i = 1, 2, 3, 4)$ on $\mathbf{a} = (1, 0)^T$ and $\mathbf{b} = (0, 1)^T$, and make a scetch to visualize the results.

(c) The composition of two rotations again is a rotation. Show that $R_\theta R_\phi = R_{\theta+\phi}$.

Hint: Utilize the following 'addition theorems':

$$\cos(\theta+\phi) = \cos\theta\cos\phi - \sin\theta\sin\phi\,,$$
$$\sin(\theta+\phi) = \sin\theta\cos\phi + \cos\theta\sin\phi\,.$$



Remark: A geometric proof of these theorems (not requested here) follows from the figure by inspecting the three right-angled triangles with diagonals of length 1, $\cos\phi$ and $\sin\phi$.

(d) Show that the rotation of an arbitrary vector $\mathbf{r} = (x, y)^T$ by the angle θ does not change its length, i.e. that $D_\theta\mathbf{r}$ has the same length as $\mathbf{r}$.

PL5.5.2 Three-dimensional rotation matrices

Rotations in three dimensions are represented by 3×3 dimensional matrices. Let $R_\theta(\mathbf{n})$ be the rotation matrix that describes a rotation by the angle θ about an axis whose direction is given by the unit vector $\mathbf{n}$.

(a) Find the three rotation matrices $R_\theta(\mathbf{e}_i)$ for rotations about the three coordinate axes $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ explicitly, by proceeding as follows: Make a separate sketch for each of $j = 1, 2$ and 3 that illustrates the effect $\mathbf{e}_j \xrightarrow{R_\theta(\mathbf{e}_i)} \mathbf{e}'_j$ of a rotation about the i axis on the three basis vectors $\mathbf{e}_j$ $(j = 1, 2, 3)$ (e.g. for $\theta = \frac{\pi}{6}$). The image vectors $\mathbf{e}'_j$ of the basis vectors $\mathbf{e}_j$ yield the columns of the sought rotation matrix R_θ.

(b) It can be shown that for a general direction $\mathbf{n} = (n_1, n_2, n_3)^T$ of the axis of rotation, the matrix elements have the following form:

$$(R_\theta(\mathbf{n}))^i{}_j = \delta_{ij}\cos\theta + n_i n_j(1-\cos\theta) - \epsilon_{ijk}\,n_k\sin\theta \qquad (\epsilon_{ijk} = \text{Levi-Civita-Tensor})\,.$$

Use this formula to find the three rotation matrices $R_\theta(\mathbf{e}_i)$ $(i = 1, 2, 3)$ explictly. Are your results consistent with those from (a)?

(c) Write down the following rotation matrices explicitly, and compute and scetch their effect on the vector $\mathbf{v} = (1, 0, 1)^T$:

(i) $A = R_\pi(\mathbf{e}_3)$, (ii) $B = R_{\frac{\pi}{2}}(\frac{1}{\sqrt{2}}(\mathbf{e}_3 - \mathbf{e}_1))$.

(d) Rotation matrices form a group. Use A and B from (c) to illustrate that this group is not commutative (in contrast to the two-dimensional case!).

(e) Show that a general rotation matrix R satisfies the relation $\mathrm{Tr}(R) = 1 + 2\cos\theta$, where the 'trace' of a matrix R is defined by $\mathrm{Tr}(R) = \sum_i (R)^i{}_i$.

(f) The product of two rotation matrices is again a rotation matrix. Consider the product $C = AB$ of the two matrices from (c), and find the corresponding unit vector $\mathbf{n}$ and rotation angle θ. *Hint:* these are uniquely defined only up to an arbitrary sign, since $R_\theta(\mathbf{n})$

and $R_{-\theta}(-\mathbf{n})$ describe the same rotation. (To be concrete, fix this sign by choosing the component n_2 positive.) $|\theta|$ and $|n_i|$ are fixed by the trace and the diagonal elements of the rotation matrix, respectively; their relative sign is fixed by the off-diagonal elements. [Check your result: $n_2 = 1/\sqrt{3}$.]

P.L5.6 Matrices describing coordinate changes

ᴇL5.6.1 Basis transformations and linear maps in $\mathbb{E}^2$

Remark on notation: For this problem we denote vectors in euclidean space $\mathbb{E}^2$ using hats (e.g. $\hat{\mathbf{e}}_j$, $\hat{\mathbf{x}}$, $\hat{\mathbf{y}} \in \mathbb{E}^2$. Their components with respect to a given basis are vectors in $\mathbb{R}^2$ and are written without hats (e.g. $\mathbf{x}$, $\mathbf{y} \in \mathbb{R}^2$).

Consider two bases for the Euclidean vector space $\mathbb{E}^2$, one old $\{\hat{\mathbf{e}}_j\}$, and one new $\{\hat{\mathbf{e}}'_i\}$, with

$$\hat{\mathbf{e}}_1 = \tfrac{3}{4}\hat{\mathbf{e}}'_1 + \tfrac{1}{3}\hat{\mathbf{e}}'_2\,, \quad \hat{\mathbf{e}}_2 = -\tfrac{1}{8}\hat{\mathbf{e}}'_1 + \tfrac{1}{2}\hat{\mathbf{e}}'_2\,.$$

(a) The relation $\hat{\mathbf{e}}_j = \hat{\mathbf{e}}'_i T^i{}_j$ expresses the old basis in terms of the new basis. Find the transformation matrix $T = (T^i{}_j)$.

(b) Find the matrix T^{-1}, and use the inverse transformation $\hat{\mathbf{e}}'_j = \hat{\mathbf{e}}_i (T^{-1})^i{}_j$ to express the new basis in terms of the old basis.

(c) Let $\hat{\mathbf{x}}$ be a vector with components $\mathbf{x} = (1,2)^T$ in the old basis. Find its components $\mathbf{x}'$ in the new basis. [Check your result: $\mathbf{x}' = (\frac{1}{2}, \frac{4}{3})^T$.]

(d) Let $\hat{\mathbf{y}}$ by a vector with components $\mathbf{y}' = (\frac{3}{4}, \frac{1}{3})^T$ in the new basis. Find its components $\mathbf{y}$ in the old basis.

(e) Let $\hat{A}$ be the linear map defined by $\hat{\mathbf{e}}'_1 \overset{\hat{A}}{\mapsto} 2\hat{\mathbf{e}}'_1$ and $\hat{\mathbf{e}}'_2 \overset{\hat{A}}{\mapsto} \hat{\mathbf{e}}'_2$. First find the matrix representation A' of this map in the new basis, then use a basis transformation to find its matrix representation A in the old basis. [Check your result: $(A)^2{}_1 = -\frac{3}{5}$.]

(f) Let $\hat{\mathbf{z}}$ be the image vector onto which the vector $\hat{\mathbf{x}}$ is mapped by $\hat{A}$, i.e. $\hat{\mathbf{x}} \overset{\hat{A}}{\mapsto} \hat{\mathbf{z}}$. Find its components $\mathbf{z}'$ with respect to the new basis by using A', and its components $\mathbf{z}$ with respect to the old basis by using A. Are your results for $\mathbf{z}'$ and $\mathbf{z}$ consistent?

(g) Now make the choice $\hat{\mathbf{e}}_1 = 3\tilde{\mathbf{e}}_1 + \tilde{\mathbf{e}}_2$ and $\hat{\mathbf{e}}_2 = -\frac{1}{2}\tilde{\mathbf{e}}_1 + \frac{3}{2}\tilde{\mathbf{e}}_2$ for the old basis, where $\tilde{\mathbf{e}}_1 = (1,0)^T$ and $\tilde{\mathbf{e}}_2 = (0,1)^T$ are the basis vectors of the standard basis of $\mathbb{E}^2$. What are the components of $\hat{\mathbf{e}}'_1$, $\hat{\mathbf{e}}'_2$, $\hat{\mathbf{x}}$ and $\hat{\mathbf{z}}$ in the standard basis $\mathbb{E}^2$? [Check your results: $\|\hat{\mathbf{e}}'_1\| = 4$, $\|\hat{\mathbf{e}}'_2\| = 3$, $\|\hat{\mathbf{x}}\| = 2\sqrt{5}$, $\|\hat{\mathbf{z}}\| = 4\sqrt{2}$.]

(h) Make a sketch (with $\tilde{\mathbf{e}}_1$ and $\tilde{\mathbf{e}}_2$ as unit vectors in the horizontal and vertical directions respectively), showing the old and new basis vectors, as well as the vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{z}}$. Are the coordinates of these vectors, discussed in (c) and (f), consistent with your sketch?

PL5.6.2 Basis transformations and linear maps in $\mathbb{E}^2$

Remark on notation: For this problem we denote vectors in euclidean space $\mathbb{E}^2$ using hats (e.g. $\hat{\mathbf{e}}_j$, $\hat{\mathbf{x}}$, $\hat{\mathbf{y}} \in \mathbb{E}^2$). Their components with respect to a given basis are vectors in $\mathbb{R}^2$ and are written without hats (e.g. $\mathbf{x}$, $\mathbf{y} \in \mathbb{R}^2$).

Consider two bases for the Euclidean vector space $\mathbb{E}^2$, one old $\{\hat{\mathbf{e}}_j\}$, and one new $\{\hat{\mathbf{e}}'_i\}$, with

$$\hat{\mathbf{e}}_1 = \tfrac{1}{5}\hat{\mathbf{e}}'_1 + \tfrac{3}{5}\hat{\mathbf{e}}'_2\,, \quad \hat{\mathbf{e}}_2 = -\tfrac{6}{5}\hat{\mathbf{e}}'_1 + \tfrac{2}{5}\hat{\mathbf{e}}'_2\,.$$

(a) The relation $\hat{\mathbf{e}}_j = \hat{\mathbf{e}}'_i T^i{}_j$ expresses the old basis in terms of the new basis. Find the transformation matrix $T = (T^i{}_j)$.

(b) Find the matrix T^{-1}, and use the inverse transformation $\hat{\mathbf{e}}'_j = \hat{\mathbf{e}}_i (T^{-1})^i{}_j$ to express the new basis in terms of the old basis.

(c) Let $\hat{\mathbf{x}}$ be a vector with components $\mathbf{x} = (2, -\frac{1}{2})^T$ in the old basis. Find its components $\mathbf{x}'$ in the new basis.

(d) Let $\hat{\mathbf{y}}$ by a vector with components $\mathbf{y}' = (-3, 1)^T$ in the new basis. Find its components $\mathbf{y}$ in the old basis.

(e) Let $\hat{A}$ be the linear map defined by $\hat{\mathbf{e}}_1 \overset{\hat{A}}{\mapsto} \frac{1}{3}(\hat{\mathbf{e}}_1 - 2\hat{\mathbf{e}}_2)$ and $\hat{\mathbf{e}}_2 \overset{\hat{A}}{\mapsto} -\frac{1}{3}(4\hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_2)$. First find the matrix representation A of this map in the old basis, then use a basis transformation to find its matrix representation A' in the new basis. [Check your result: $(A')^2{}_1 = \frac{2}{3}$.]

(f) Let $\hat{\mathbf{z}}$ be the image vector onto which the vector $\hat{\mathbf{x}}$ is mapped by $\hat{A}$, i.e. $\hat{\mathbf{x}} \overset{\hat{A}}{\mapsto} \hat{\mathbf{z}}$. Find its components $\mathbf{z}$ with respect to the old basis by using A, and its components $\mathbf{z}'$ with respect to the new basis by using A'. Are your results for $\mathbf{z}$ and $\mathbf{z}'$ consistent? [Check your result: $\mathbf{z}' = \frac{1}{3}(5, 1)^T$.]

(g) Now make the choice $\hat{\mathbf{e}}_1 = \tilde{\mathbf{e}}_1 + \tilde{\mathbf{e}}_2$ and $\hat{\mathbf{e}}_2 = 2\tilde{\mathbf{e}}_1 - \tilde{\mathbf{e}}_2$ for the old basis, where $\tilde{\mathbf{e}}_1 = (1, 0)^T$ and $\tilde{\mathbf{e}}_2 = (0, 1)^T$ are the basis vectors of the standard basis of $\mathbb{E}^2$. What are the components of $\hat{\mathbf{e}}'_1$, $\hat{\mathbf{e}}'_2$, $\hat{\mathbf{x}}$ and $\hat{\mathbf{z}}$ in the standard basis $\mathbb{E}^2$? [Check your results: $\|\hat{\mathbf{e}}'_1\| = \frac{\sqrt{41}}{4}$, $\|\hat{\mathbf{e}}'_2\| = \frac{\sqrt{89}}{4}$, $\|\hat{\mathbf{x}}\| = \|\hat{\mathbf{z}}\| = \frac{\sqrt{29}}{2}$.]

(h) Make a sketch (with $\tilde{\mathbf{e}}_1$ and $\tilde{\mathbf{e}}_2$ as unit vectors in the horizontal and vertical directions respectively), showing the old and new basis vectors, as well as the vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{z}}$. Are the coordinates of these vectors, discussed in (c) and (f), consistent with your sketch?

EL5.6.3 Basis transformations

Consider the following three transformations in $\mathbb{R}^3$, using the standard basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$:

A : Rotation about the third axis by the angle $\theta_3 = \frac{\pi}{4}$, in the right-hand positive direction. *Hint:* Use the compact notation $\cos\theta_3 = \sin\theta_3 = s$.

B : Dilation (stretching) of the first axis by the factor $s_1 = 3$;

C : Rotation about the second axis by the angle $\theta_2 = \frac{\pi}{2}$, in the right-hand positive direction.

Hint: To understand what 'right-hand positive' means, imagine wrapping your right hand around the axis of rotation, with your thumb pointing in the positive direction. Your other fingers will be curled in the direction of 'positive rotation'.

(a) Find the matrix representations (with respect to the standard basis) of A, B and C.

(b) What is the image $\mathbf{y} = B\mathbf{x}$ of the vector $\mathbf{x} = (1, 1, 1)^T$ under the dilation B?

(c) What is the image $\mathbf{z} = D\mathbf{x}$ of $\mathbf{x}$ under the composition of all three maps, $D = C \cdot B \cdot A$? [Check your result: $z^2 = \sqrt{2}$.]

(d) Now consider a new basis $\{\mathbf{e}'_j\}$, defined by a rotation of the standard basis by A, i.e. $\mathbf{e}_j \overset{A}{\mapsto} \mathbf{e}'_j$. Draw the new and old basis vectors in the same figure. Find the transformation matrix T, and specify the matrix elements of the transformation between the old and the rotated bases using $\mathbf{e}_j = \mathbf{e}'_i t^i{}_j$.

(e) In the $\{\mathbf{e}'_i\}$ basis let the vectors $\mathbf{x}$ and $\mathbf{y}$ be represented by $\mathbf{x} = \mathbf{e}'_i x'^i$ and $\mathbf{y} = \mathbf{e}'_i y'^i$. Find the corresponding components $\mathbf{x}' = (x'^1, x'^2, x'^3)^T$ and $\mathbf{y}' = (y'^1, y'^2, y'^3)^T$. [Check your results: $x'^1 = \sqrt{2}$, $y'^3 = 1$.]

(f) Let B' denote the dilation B in the rotated basis. Find B' by the appropriate transformation of the matrix B, and use the result to calculate the image $\mathbf{y}'$ of $\mathbf{x}'$ under B'. [Does the result match that from (e)?]

▹L5.6.4 Basis transformations and linear maps

Consider the following three linear transformations in $\mathbb{R}^3$, using the standard basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$.

A : Rotation around the first axis by the angle $\theta_1 = -\frac{\pi}{3}$ in the right-handed sense, i.e. a left-handed rotation. *Hint:* Use the compact notation $\cos\theta_1 = c$, $\sin\theta_1 = s$.

B : Dilation of the first and second axes by the factors $s_1 = 2$ and $s_2 = 4$ respectively.

C : A reflection in the 2,3-plane.

(a) Find the matrix representations (using the standard basis) of A, B, C. Which of these transformations commute with each other (i.e. for which pairs of matrices does $T_1 T_2 = T_2 T_1$)?

(b) What is the image $\mathbf{y} = CA\mathbf{x}$ of the vector $\mathbf{x} = (1, 1, 1)^T$ under the transformation CA?

(c) Find the vector $\mathbf{z}$, whose image under the composition of all three transformations , $D = C \cdot B \cdot A$, gives y. [Hint: $D^{-1} = A^{-1}B^{-1}C^{-1}$.] [Check your result: $z^3 = \frac{1}{16}(7 - 3\sqrt{3})$.]

(d) Now consider a new basis $\{\mathbf{e}'_i\}$, defined by a rotation and reflection CA of the standard basis, $\mathbf{e}'_i \overset{CA}{\mapsto} \mathbf{e}_i$. [*Caution:* in the sample the order was reversed!] Sketch the old and new bases in the same picture. [*Note:* The new basis vectors are a left handed system! Why?] Find the transformation matrix T, and specify the matrix elements of the transformation between the old and the new basis, with $\mathbf{e}_j = \mathbf{e}'_i T^i{}_j$.

(e) In the $\{\mathbf{e}'_i\}$-Basis let the vectors $\mathbf{z}$ and $\mathbf{y}$ be represented by $\mathbf{z} = \mathbf{e}'_i z'^i$ and $\mathbf{y} = \mathbf{e}'_i y'^i$. Find the corresponding components $\mathbf{z}' = (z'^1, z'^2, z'^3)^T$ and $\mathbf{y}' = (y'^1, y'^2, y'^3)^T$. [Check your results: $z'^3 = \frac{1}{2}(1-\sqrt{3})$, $y'^2 = \frac{1}{2}(-1+\sqrt{3})$.]

(f) Let D' denote the representation of D in the new Basis. Find D' by an appropriate Transformation of the Matrix D, and use the result to find the image $\mathbf{y}'$ of $\mathbf{z}'$ under D'. [Does the result match the one from (e)?].

P.L6 Matrices II: determinants

P.L6.1 Determinant

EL6.1.1 Calculating determinants

Compute the determinants of the following matrices by expanding them along an arbitrary row or column. *Hint:* The more zeros it contains, the easier the calculation.

$$A = \begin{pmatrix} 2 & 1 \\ 5 & -3 \end{pmatrix}, \quad B = \begin{pmatrix} 3 & 2 & 1 \\ 4 & -3 & 1 \\ 2 & -1 & 1 \end{pmatrix}, \quad C = \begin{pmatrix} a & a & a & 0 \\ a & 0 & 0 & b \\ 0 & 0 & b & b \\ a & b & b & 0 \end{pmatrix}.$$

[Check your result: for $a = 1$, $b = 2$ one has $\det C = -4$.]

PL6.1.2 Calculating determinants

(a) Compute the determinant of the matrix $D = \begin{pmatrix} 1 & c & 0 \\ d & 2 & 3 \\ 2 & 2 & e \end{pmatrix}$. [Check your result: for $c = 1$, $d = 3$, $e = 2$, one has $\det C = -2$.]

(i) Which values must c and d have to ensure that $\det D = 0$ for all values of e?

(ii) Which values must d and e have to ensure that $\det D = 0$ for all values of c?

Could you have found the results of (i,ii) *without* explicitly calculating $\det D$?

Now consider the two matrices $A = \begin{pmatrix} 2 & -1 & -3 & 1 \\ 0 & 1 & 5 & 5 \end{pmatrix}$ and $B = \begin{pmatrix} 2 & 1 \\ 6 & 6 \\ -2 & 8 \\ -2 & -2 \end{pmatrix}$.

(b) Compute the product AB, as well as its determinant $\det(AB)$ and inverse $(AB)^{-1}$.

(c) Compute the product BA, as well as its determinant $\det(BA)$ and inverse $(BA)^{-1}$.

Is it possible to calculate the determinant and the inverse of A and B?

P.L7 Matrices III: diagonalizing a matrix

P.L7.3 Characteristic polynomial

P.L7.4 Matrix diagonalization

EL7.4.1 Diagonalising real 2×2 matrices

For the following real matrices, find the eigenvalues $\lambda_j \in \mathbb{R}$, eigenvectors $\mathbf{v}_j \in \mathbb{R}^2$ and the similarity transformation S, as well as its inverse, S^{-1}, for which $S^{-1}AS$ is diagonal:

(a) $A = \begin{pmatrix} -1 & 6 \\ -2 & 6 \end{pmatrix}$, (b) $A = \frac{1}{5}\begin{pmatrix} 11 & -8 \\ -8 & -1 \end{pmatrix}$.

[Check your result: verify that $S^{-1}AS$ contains the eigenvalues on the diagonal.]

PL7.4.2 Diagonalising real 2×2 matrices

For the following real matrices, find the eigenvalues $\lambda_j \in \mathbb{R}$, eigenvectors $\mathbf{v}_j \in \mathbb{R}^2$ and the similarity transformation S, as well as its inverse, S^{-1}, for which $S^{-1}AS$ is diagonal:

(a) $A = \begin{pmatrix} 4 & -6 \\ 3 & -5 \end{pmatrix}$, (b) $A = \frac{1}{10}\begin{pmatrix} -19 & 3 \\ 3 & -11 \end{pmatrix}$.

[Check your result: verify that $S^{-1}AS$ contains the eigenvalues on the diagonal.]

EL7.4.3 Diagonalising complex 2×2 matrices

For the following complex matrices, find the eigenvalues $\lambda_j \in \mathbb{C}$, eigenvectors $\mathbf{v}_j \in \mathbb{C}^2$ and the similarity transformation S, as well as its inverse, S^{-1}, for which $S^{-1}AS$ is diagonal:

(a) $A = \begin{pmatrix} -\mathrm{i} & 0 \\ 2 & \mathrm{i} \end{pmatrix}$, (b) $A = \begin{pmatrix} 1 & \mathrm{i} \\ -\mathrm{i} & 1 \end{pmatrix}$.

[Check your result: verify that $S^{-1}AS$ contains the eigenvalues on the diagonal.]

PL7.4.4 Diagonalising complex 3×3 matrices

For the following complex matrices, find the eigenvalues $\lambda_j \in \mathbb{C}$, eigenvectors $\mathbf{v}_j \in \mathbb{C}^3$ and the similarity transformation S, as well as its inverse, S^{-1}, for which $S^{-1}AS$ is diagonal:

(a) $A = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2\mathrm{i} & 0 \\ 1 & 0 & 1 \end{pmatrix}$, (b) $A = \begin{pmatrix} 1 & 0 & -\mathrm{i} \\ 0 & 1 & 0 \\ \mathrm{i} & 0 & 1 \end{pmatrix}$.

[Check your result: verify that $S^{-1}AS$ contains the eigenvalues on the diagonal.]

EL7.4.5 Diagonalising a matrix that depends on a variable

Consider the matrix $A = \begin{pmatrix} x & 1 & 0 \\ 1 & 2 & 1 \\ 3-x & -1 & 3 \end{pmatrix}$, which depends on the variable $x \in \mathbb{R}$. Find the eigenvalues λ_j and eigenvectors $\mathbf{v}_j \in \mathbb{R}^3$ of A, with $j = 1, 2, 3$.
Hints: One of the eigenvalues is $\lambda = x$. (Of course the other results, too, can depend on x.) Avoid fully multiplying out the characteristic polynomial; try instead to directly bring it to a completely factorized form! [Check your results: for $x = 4$, two of the (unnormalized) eigenvectors are given by $(1, -2, -1)^T$ and $(1, -1, -2)^T$.]

PL7.4.6 Diagonalizing a matrix depending on two variables: qubit

A qubit (for "quantum bit" = quantum version of a classical bit) is a manipulable two-level quantum systems. The simplest version of a qubit is described by the matrix $H = \begin{pmatrix} B & \overline{\Delta} \\ \Delta & -B \end{pmatrix}$, with $B \in \mathbb{R}$ and $\Delta \in \mathbb{C}$.

(a) Calculate the eigenvalues E_j (choose $E_1 < E_2$) and normalized eigenvectors $\mathbf{v}_1$ and $\mathbf{v}_2$ of H as a function of B, Δ and $X \equiv [B^2 + |\overline{\Delta}|^2]^{1/2}$.

(b) Show that the eigenvectors can be brought to the form $\mathbf{v}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} -\sqrt{1-Y} \\ e^{i\phi}\sqrt{1+Y} \end{pmatrix}$ and $\mathbf{v}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1+Y} \\ e^{i\phi}\sqrt{1-Y} \end{pmatrix}$, where $e^{i\phi}$ is the phase factor of $\Delta \equiv |\Delta| e^{i\phi}$. How does Y scale as a function of B and X? On three diagrams arranged below each other, each showing two curves, sketch first E_1 and E_2, second, the square of the absolute values of the components $|v^1{}_1|^2$ and $|v^2{}_1|^2$ of the eigenvector $\mathbf{v}_1$, and third the square of the absolute values of the components of $|v^1{}_2|^2$ and $|v^2{}_2|^2$ of the eigenvector $\mathbf{v}_2$, all as functions of $B/|\Delta| \in \{-\infty, \infty\}$ for fixed $|\Delta|$.

Background information: The first sketch shows the so called "avoided crossing", a typical trait of a quantum bit. The second and third sketches show that the eigenvectors "exchange their roles" if B/Δ goes from $-\infty$ to $+\infty$. Both these properties have been detected in many experiments.

EL7.4.7 Inertia tensor

The inertia tensor of a rigid body composed of point masses is defined as

$$\widetilde{I}_{ij} = \sum_a m_a \widetilde{I}_{ij}(\mathbf{r}_a, \mathbf{r}_a) \,, \quad \text{with} \quad \widetilde{I}_{ij}(\mathbf{r}, \mathbf{r}') \equiv \delta_{ij} \mathbf{r} \cdot \mathbf{r}' - (\mathbf{e}_i \cdot \mathbf{r})(\mathbf{e}_j \cdot \mathbf{r}') \,,$$

where m_a and $\mathbf{r}_a = (r^1{}_a, r^2{}_a, r^3{}_a)^T$ are, respectively, the mass and position of point mass a. The eigenvalues of the inertia tensor are known as the rigid body's *moments of inertia*.
Consider a rigid body consisting of three point masses $m_1 = 4$, $m_2 = M$ and $m_3 = 1$ at positions $\mathbf{r}_1 = (1, 0, 0)^T$, $\mathbf{r}_2 = (0, 1, 2)^T$ and $\mathbf{r}_3 = (0, 4, 1)^T$, respectively. Determine its inertia tensor $\widetilde{I}$ and moments of inertia as functions of M. (Eigenvectors are not required.) [Check your results: if $M = 5$, then $\lambda_1 = 42$, $\lambda_2 = 39$, $\lambda_3 = 11$.]

PL7.4.8 Inertia tensor

Consider a rigid body consisting of two point masses, $m_1 = \frac{2}{3}$ and $m_2 = 3$, at positions $\mathbf{r}_1 = (2, 2, -1)^T$ and $\mathbf{r}_2 = \frac{1}{3}(2, -1, 2)^T$, respectively.

(a) Show that its inertia tensor has the following form: $\widetilde{I} = \begin{pmatrix} 5 & -2 & 0 \\ -2 & 6 & 2 \\ 0 & 2 & 7 \end{pmatrix}$.

(b) Find the moments of inertia (eigenvalues). (*Hint:* One eigenvalue is $\lambda = 3$.)

(c) Construct matrices S and S^{-1} that diagonalize the inertia tensor.

EL7.4.9 Degenerate eigenvalue problem

For the matrix $A = \begin{pmatrix} 2 & -1 & 2 \\ -1 & 2 & -2 \\ 2 & -2 & 5 \end{pmatrix}$, find the eigenvalue λ_j, the normalized eigenvectors $\mathbf{v}_j \in \mathbb{R}^3$, and the similarity transformation S, as well as its inverse, S, such that $S^{-1}AS$ is diagonal. *Hint:* One eigenvalue is $\lambda_1 = 1$. [Check your result: verify that $S^{-1}AS$ contains the eigenvalues on the diagonal.]

PL7.4.10 Degenerate eigenvalue problem

Consider the following matrices:

$$A = \begin{pmatrix} 15 & 6 & -3 \\ 6 & 6 & 6 \\ -3 & 6 & 15 \end{pmatrix}, \qquad B = \begin{pmatrix} -1 & 0 & 0 & 2\mathrm{i} \\ 0 & 7 & 2 & 0 \\ 0 & 2 & 4 & 0 \\ -2\mathrm{i} & 0 & 0 & 2 \end{pmatrix}.$$

(a) One of the eigenvectors $\mathbf{v}_j \in \mathbb{R}^3$ of the matrix A is $\mathbf{v}_3 = \frac{1}{\sqrt{3}}(1, 1, 1)^T$. Find all eigenvalues λ_j of A. (*Hint:* Two of them form a degenerate pair.) Construct an orthonormal basis $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3\}$ of $\mathbb{R}^3$ consisting of eigenvectorss of A. Find a similarity transformation S, and its inverse S^{-1}, for which $S^{-1}AS$ is diagonal.

(b) One of the eigenvectors $\mathbf{v}_j \in \mathbb{C}^4$ of the matrix B is $\mathbf{v}_3 = \frac{1}{\sqrt{5}}(0, 1, -2, 0)^T$. Find all eigenvalues λ_j of B. (*Hint:* Two of them form a degenerate pair.) Construct an orthonormal basis $\{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \mathbf{v}_4\}$ of $\mathbb{C}^4$ consisting of eigenvectors of B. Find a similarity transformation S, and its inverse S^{-1}, for which $S^{-1}BS$ is diagonal.

EL7.4.11 Determinant equals product of eigenvalues

If A is an $n \times n$ matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$, then $\det A = \prod_{j=1}^{n} \lambda_j$, i.e. the determinant is equal to the product of the eigenvalues. Prove this for the case that A is diagonalizable.

PL7.4.12 Trace of a matrix

The trace of an $n \times n$ matrix, $\mathrm{Tr}\, A$, is defined as the sum of all diagonal elements, $\mathrm{Tr}\, A = \sum_{j=1}^{n} A_{jj}$. Show the following properties of the trace:

(a) $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ for any $n \times n$ matrices A and B.

(b) $\mathrm{A} = \mathrm{Tr}(S^{-1}AS)$ for any $n \times n$ matrices A and S, where S is invertible.

(c) If A has the eigenvalues $\lambda_1, \ldots, \lambda_n$, then $\mathrm{Tr}\, A = \lambda_1 + \ldots + \lambda_n$. You may assume that A is diagonalizable.

P.L7.5 Functions of matrices

EL7.5.1 Functions of matrices

The purpose of this problem is to gain familiarity with the concept of a 'function of a matrix'. Let f be an analytic function, with Taylor series $f(x) = \sum_{l=0}^{\infty} c_l x^l$, and $A \in \mathrm{mat}(\mathbb{R}, n, n)$ a square matrix, then $f(A)$ is defined as $f(A) = \sum_{l=0}^{\infty} c_l A^l$, with $A^0 = \mathbb{1}$.

(a) A matrix A is called 'nilpotent' if an $l \in \mathbb{N}$ exists such that $A^l = 0$. Then the Taylor series of $f(A)$ ends after l terms. Example: Compute e^A for $A = \begin{pmatrix} 0 & a \\ 0 & 0 \end{pmatrix}$.

(b) If $A^2 \propto \mathbb{1}$, then $A^{2m} \propto \mathbb{1}$ and $A^{2m+1} \propto A$, and the Taylor series for $f(A)$ has the form $f_0\mathbb{1} + f_1 A$. Example: Compute e^A explicitly for $A = \theta\tilde{\sigma}$, with $\tilde{\sigma} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.
[Check your result: if $\theta = -\frac{\pi}{6}$, then $\mathrm{e}^A = \frac{1}{2}\begin{pmatrix} \sqrt{3} & 1 \\ -1 & \sqrt{3} \end{pmatrix}$.]

(c) If A is diagonalizable, then $f(A)$ can be expressed in terms of its eigenvalues. Let S be the similarity transformation that diagonalizes A, with diagonal matrix $D = S^{-1}AS$ and diagonal elements $D = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Show that the following relations then hold:

$$f(A) = Sf(D)S^{-1} = S \begin{pmatrix} f(\lambda_1) & 0 & \cdots & 0 \\ 0 & f(\lambda_2) & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & f(\lambda_n) \end{pmatrix} S^{-1}\,.$$

Remark: Both equalities are to be established independently of each other.

(d) Now compute the matrix function e^A from (b) using diagonalization, as in (c).

PL7.5.2 Functions of matrices

Express each of the following matrix functions explicitly in terms of a matrix:

(a) e^A, with $A = \begin{pmatrix} 0 & a & 0 \\ 0 & 0 & b \\ 0 & 0 & 0 \end{pmatrix}$.

(b) e^B, with $B = b\sigma_1$ and $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, using the Taylor series of the exponential function.
[Check your result: if $b = \ln 2$, then $\mathrm{e}^B = \frac{1}{4}\begin{pmatrix} 5 & 3 \\ 3 & 5 \end{pmatrix}$.]

(c) The same function as in (b), now by diagonalizing B.

(d) e^C, with $C = \mathrm{i}\theta\,\Omega$, where $\Omega = n_j S_j$, while $\mathbf{n} = (n_1, n_2, n_3)^T$ is a unit vector ($\|\mathbf{n}\| = 1$) and S_j are the spin-$\frac{1}{2}$ matrices: $S_1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $S_2 = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$, $S_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
Hint: Start by computing Ω^2 (for this, the property $S_iS_j + S_jS_i = \frac{1}{2}\delta_{ij}\mathbb{1}$ of the spin-$\frac{1}{2}$ matrices is useful), and then use the Taylor series of the exponential function.
[Check your result: if $\theta = -\pi/2$ and $n_1 = -n_2 = n_3 = \frac{1}{\sqrt{3}}$, then $\mathrm{e}^C = \frac{1}{\sqrt{6}}\begin{pmatrix} \sqrt{3}-\mathrm{i} & 1-\mathrm{i} \\ -1-\mathrm{i} & \sqrt{3}+\mathrm{i} \end{pmatrix}$.]

Remark: The exponential form e^C is a representation of SU(2) transformations, the group of all special unitary transformations in $\mathbb{C}^2$. Its elements are characterized by three continuous real parameters (here θ, n_1 and n_2, with $n_3 = \sqrt{1-n_1^2-n_2^2}$). The S_j matrices are 'generators' of these transformations; they satisfy the SU(2) algebra, i.e. their commutators yield $[S_i, S_j] = \mathrm{i}\epsilon_{ijk}S_k$.

ᴇL7.5.3 Exponential representation of 2-dimensional rotation matrix

The matrix $R_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$ describes a rotation by the angle θ in $\mathbb{R}^2$. Use the following 'infinite product decomposition' to find an exponential representation of this matrix:

(a) A rotation by the angle θ can be represented as a sequence of m rotations, each by the angle θ/m: $R_\theta = [R_{(\theta/m)}]^m$. For $m \to \infty$ we have $\theta/m \to 0$, thus the matrix $R_{(\theta/m)}$ can be written as $R_{(\theta/m)} = \mathbb{1} + (\theta/m)\tilde{\sigma} + \mathcal{O}\big((\theta/m)^2\big)$ Find the matrix $\tilde{\sigma}$.

(b) Now use the identity $\lim_{m\to\infty}[1 + x/m]^m = \mathrm{e}^x$ to show that $R_\theta = \mathrm{e}^{\theta\tilde{\sigma}}$.
Remark: Justification for this identity: We have $\mathrm{e}^x = [\mathrm{e}^{x/m}]^m = [1+x/m+\mathcal{O}\big((x/m)^2\big)]^m$. In the limit $m \to \infty$ the terms of order $\mathcal{O}\big((x/m)^2\big)$ can be neglected.

[Check your result: does the Taylor series for $\mathrm{e}^{\theta\tilde{\sigma}}$ reproduce the matrix for R_θ given above?]

Remark: The procedure illustrated here, by which an infinite sequence of identical, infinitesimal transformations is exponentiated, is a cornerstone of the theory of 'Lie groups', whose elements are associated with continuous parameters (here the angle θ). In this context the above matrix $\tilde{\sigma}$ is called the 'generator' of the rotation.

ᴘL7.5.4 Exponential representation 3-dimensional rotation matrix

In $\mathbb{R}^3$, a rotation by an angle θ, about an axis whose direction is given by the unit vector $\mathbf{n} = (n_1, n_2, n_3)$, is represented by a 3×3 matrix that has the following matrix elements:

$$(R_\theta(\mathbf{n}))_{ij} = \delta_{ij}\cos\theta + n_i n_j(1-\cos\theta) - \epsilon_{ijk}\,n_k\sin\theta \qquad (\epsilon_{ijk} = \text{Levi-Civita-Tensor})\,. \quad (1)$$

The goal of the following steps is to supply a justification for Eq. (1).

(b) Consider first the three matrices $R_\theta(\mathbf{e}_j)$ for rotations by the angle θ about the three coordinate axes $\mathbf{e}_j$, with $j = 1, 2, 3$. Elementary geometrical considerations yield:

$$R_\theta(\mathbf{e}_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}, \quad R_\theta(\mathbf{e}_2) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}, \quad R_\theta(\mathbf{e}_3) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

For each of these matrices, use an infinite product decomposition of the form $R_\theta(\mathbf{n}) = \lim_{m\to\infty}[R_{\theta/m}(\mathbf{n})]^m$ to obtain an exponential representation of the form $R_\theta(\mathbf{e}_i) = \mathrm{e}^{\theta\tau_i}$. Find the three 3×3 matrices τ_1, τ_2 and τ_3. [Check your results: The τ_i commutators yield $[\tau_i, \tau_j] = \epsilon_{ijk}\tau_k$. This is the so-called SO(3) algebra, which underlies the representation theory of 3-dimensional rotations. Moreover, $\tau_1^2 + \tau_2^2 + \tau_3^2 = -2\mathbb{1}$.]

(c) Now consider a rotation by the angle θ about an arbitrary axis $\mathbf{n}$. To find an exponential representation for it using an infinite product decomposition, we need an approximation for $R_{\theta/m}(\mathbf{n})$ up to first order in the small angle θ/m. It has the following form:

$$R_{(\theta/m)}(\mathbf{n}) = R_{(n_1\theta/m)}(\mathbf{e}_1)R_{(n_2\theta/m)}(\mathbf{e}_2)R_{(n_3\theta/m)}(\mathbf{e}_3) + \mathcal{O}\big((\theta/m)^2\big). \tag{2}$$

Intuitive justification: If the rotation angle θ/m is sufficiently small, the rotation can be performed in three substeps, each about the direction $\mathbf{e}_j$, by the 'partial' angle $n_j\theta/m$. The prefactors n_j ensure that for $\mathbf{n} = \mathbf{e}_j$ (rotation about a coordinate axis j) only *one* of the three factors in (2) is different from $\mathbb{1}$, namely the one that yields $R_{(\theta/m)}(\mathbf{e}_j)$; for example, for $\mathbf{n} = \mathbf{e}_2 = (0, 1, 0)^T$: $R_{(0\theta/m)}(\mathbf{e}_1)R_{(1n_2\theta/m)}(\mathbf{e}_2)R_{(0\theta/m)}(\mathbf{e}_3) = R_{(n_2\theta/m)}(\mathbf{e}_2)$.

Show that such a product decomposition of $R_\theta(\mathbf{n})$ yields the following exponential representation:

$$R_\theta(\mathbf{n}) = \mathrm{e}^{\theta\Omega}, \qquad \Omega = n_i\tau_i = \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix}, \qquad (\Omega)_{ij} = -\epsilon_{ijk}n_k\,. \tag{3}$$

(d) Show that Ω, the 'generator' of the rotation, has the following properties:

$$(\Omega^2)_{ij} = n_in_j - \delta_{ij}, \qquad \Omega^l = -\Omega^{l-2} \quad \text{for } 3 \le l \in \mathbb{N}. \qquad \text{[Cayley-Hamilton theorem]} \tag{4}$$

Hint: First compute Ω^2 and Ω^3, then the form of $\Omega^{l>3}$ will be obvious.

(e) Show that the Taylor expansion of $R_\theta(\mathbf{n}) = \mathrm{e}^{\theta\Omega}$ yields the following expression,

$$R_\theta(\mathbf{n}) = \mathbb{1} + \Omega\sin\theta + \Omega^2(1 - \cos\theta), \tag{5}$$

and that its matrix elements correspond to Eq. (1).

P.L8 Orthogonality and unitarity

P.L8.1 Orthogonal and unitary maps

P.L8.2 Orthogonal and unitary matrices

EL8.2.1 Orthogonal and unitary matrices

(a) Is the matrix A as given below an orthogonal matrix? Is B unitary?

$$A = \begin{pmatrix} \sin\theta & \cos\theta \\ -\cos\theta & \sin\theta \end{pmatrix}, \qquad B = \frac{1}{1-i}\begin{pmatrix} 2 & 1+\mathrm{i} & 0 \\ 1+\mathrm{i} & -1 & 1 \\ 0 & 2 & \mathrm{i} \end{pmatrix}$$

(b) Let $\mathbf{x} = (1, 2)^T$. Calculate $\mathbf{a} = A\mathbf{x}$ explicitly, as well as the norm of $\mathbf{x}$ and $\mathbf{a}$. Does the action of A on $\mathbf{x}$ conserve its norm?

(c) Let $\mathbf{y} = (1, 2, \mathrm{i})^T$. Calculate $\mathbf{b} = B\mathbf{y}$ explicitly, and also the norm of $\mathbf{y}$ and $\mathbf{b}$. Does the action of B on $\mathbf{y}$ conserve its norm?

PL8.2.2 Orthogonal and unitary matrices

(a) Determine if whether the following matrices are orthogonal or unitary:

$$A = \begin{pmatrix} 0 & 3 & 0 \\ 2 & 0 & 1 \\ -1 & 0 & 2 \end{pmatrix}, \quad B = \frac{1}{3}\begin{pmatrix} 1 & 2 & -2 \\ -2 & 2 & 1 \\ 2 & 1 & 2 \end{pmatrix}, \quad C = \frac{1}{\sqrt{2}}\begin{pmatrix} \mathrm{i} & 1 \\ -1 & -\mathrm{i} \end{pmatrix}$$

(b) Let $\mathbf{x} = (1, 2, -1)^T$. Calculate $\mathbf{a} = A\mathbf{x}$ and $\mathbf{b} = B\mathbf{x}$ explicitly. Also, calculate the norm of $\mathbf{x}$, $\mathbf{a}$ and $\mathbf{b}$. Which of these norms should be equal? Why?

(c) Let $\mathbf{y} = (1, \mathrm{i})^T$. Calculate $\mathbf{c} = C\mathbf{y}$ explicitly, and also determine the norm of $\mathbf{y}$ and $\mathbf{c}$. Should the norms be equal? Why?

P.L8.3 Special unitary and special orthogonal matrices

P.L8.4 Orthogonal and unitary basis changes

P.L9 Hermiticity and symmetry

P.L9.2 Hermitian and symmetric matrices

P.L9.3 Relation between Hermitian and unitary matrices

C

Calculus

Part C of this book introduces the elements of calculus[1] required in the first years of the physics curriculum. We start with a recapitulation of one-dimensional differentiation and integration. Although this may be material familiar to many readers, we will provide interpretations of differentiation and integration not normally emphasized in school. We then turn to higher dimensions and discuss how differentiation can be applied to understand the behavior of functions depending on several parameters. The second part of the chapter discusses the integration of multi-dimensional functions and functions defined on higher-dimensional geometric domains, such as spheres. The generalized concepts of differentiation and integration are the basis for the advanced elements of calculus discussed in later parts of the chapter, including differential equations, Fourier analysis, functional calculus, and the calculus of functions depending on complex variables.

The mathematics of physics is all about differentiating and integrating. The reasons for this are deeply rooted in the foundations of our science. To understand why, consider the situation before the age of enlightenment. At that time scientific knowledge was accumulated empirically, for example through the tabulation of the motion of celestial bodies. Although people were aware that a complete tabulation of all planets and stars is out of the question no alternative method was known. The situation changed when it became understood that a more rewarding approach was to monitor small incremental *changes* in the motion of celestial bodies. For example, an interesting quantity to study were the changes, $\mathbf{v}(t+\delta)-\mathbf{v}(\delta)$, accumulated in a body's velocity during small increments of time, δ. For sufficiently small δ this change is approximately proportional to δ, and it made sense to shift the focus of attention to the study of the rate-change, or *derivative*, of the velocity, $\mathbf{v}'(t) \equiv \lim_{\delta\to 0}\delta^{-1}(\mathbf{v}(t+\delta)-\mathbf{v}(t))$. The great step forward came with the observation that these incremental changes were *universal* and could be described through relatively simple physical laws equally applicable to all bodies. This realization, which found its quantitative expression in Newton's famous laws of mechanical motion, defined the starting point of modern physics. From then on the laws of nature were often encoded in 'differential relations' describing rate changes of physical quantities. From such laws the actual behavior of a physical object, for example, the full time dependent profile, $\mathbf{v}(t)$, of a planet's velocity, could be reconstructed through the twin sister of differentiation, integration, to be discussed in section C2.

In the next chapter we introduce the concept of differentiation on the important example of one-dimensional functions familiar from high school. However, we will do so in a manner that differs from the school approach in that it affords straightforward generalization to the case of more complex function.

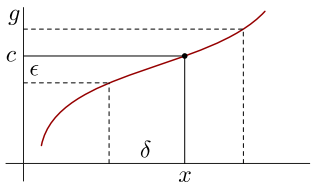
[1] Although '**analysis**' maytion a shade more rigorous than '**calculus**' the almost synonymous with each other.

C1 Differentiation of one-dimensional functions

In school, differentiation is often introduced as a tool to describe slope of a function defined on a one-dimensional interval. However, differentiation is a concept much more general than that: much like the surface of earth looks flat when viewed locally, even very complicated functions assume a simple (linear) appearance if we 'zoom in' closely and look at them from close up. For example, what has been said above amounts to the statement that for short time differences, δ, the velocity is a function linear in δ, $\mathbf{v}(t+\delta) \simeq \mathbf{v}(t) + \delta\,\mathbf{v}'(t)$. More generally, the overarching objective of differentiation is to describe functions locally in terms of simple linear approximations. In this chapter we introduce this idea on the example of one-dimensional functions familiar from high school. This will set the stage for the generalization to more complicated functions discussed in later chapters.

C1.1 Definition of differentiability

We start by recapitulating the definition of differentiability as it is usually taught in school. Heuristically, a function $f : \mathbb{R} \to \mathbb{R}$, $x \mapsto f(x)$ is differentiable at x if it may be approximated by a well defined tangent, and if that tangent does not have infinite slope, see Fig. C1.



The construction of a tangent effectively monitors the changes of the function in the limit of small increments of its arguments. As a first step towards a more rigorous definition, we need to discuss what is meant by the term '**limit**'. Intuitively, g approaches the limit $g(x) = c$, if deviations off the value c become arbitrarily small for arguments y sufficiently close to x. In this case we write $\lim_{y\to x} g(y) = c$, or $\lim_{\delta\to 0} g(x+\delta) = g(x)$ and say that the limit exists. An equivalent formulation is to say that g converges to $g(x) = c$ in the limit $y \to x$.

INFO There are various ways to turn the intuitive formulation into a rigorous **definition of a limit**. Referring for in-depth discussions to lecture courses in mathematics, we mention the Weierstrass-Jordan (also known as ϵ-δ criterion) which says that g converges to $g(x) = c$ if for any $\epsilon > 0$ there exists a $\delta > 0$ such that for all arguments y which are δ-close to x, $|y - x| < \delta$ the function values $g(y)$ are ϵ-close to $g(x)$, $|g(y) - g(x)| < \epsilon$ (see the figure.)

We now define a function $f : \mathbb{R} \to \mathbb{R}$, $x \mapsto f(x)$ to be **differentiable** if the **difference**

quotient $\frac{1}{\delta}\big[f(x+\delta)-f(x)\big]$ has a well defined limit $\delta \to 0$. In this case, it probes the local slope of f at x and the limit

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} \equiv \lim_{\delta\to 0} \frac{1}{\delta}\big[f(x+\delta)-f(x)\big], \tag{C1}$$

is called the **derivative** of f at x. The limiting form of the difference quotients on the r.h.s. is sometimes called **differential quotient**. Alternative denotations of the derivative include

$$f'(x) = \frac{\mathrm{d}f(x)}{\mathrm{d}x} = \frac{\mathrm{d}f(y)}{\mathrm{d}y}\Big|_{y=x} = \frac{\mathrm{d}}{\mathrm{d}x}f(x) = \mathrm{d}_x f(x) = f_x(x).$$

However, all these notations are defined in the same way by the r.h.s. of Eq. (C1). Before continuing to discuss the properties of the 'differential quotients' defined through Eq. (C1) it is worthwhile to understand the conditions under which the limits $\delta \to 0$ exist. A first, if not sufficient existence condition is the *continuity* of f at x.

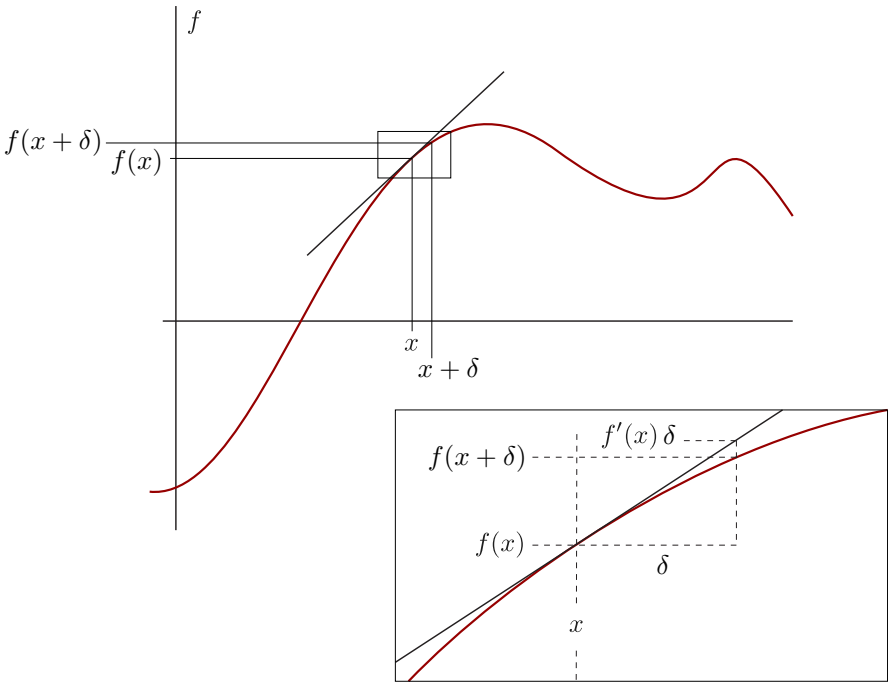


Figure C1: Differentiation of a function. Discussion, see text.

Continuity and differentiability of functions

The existence of the differential quotient in Eq. (C1) requires that f have no 'jumps' at x which in mathematical terminology is called the absence of discontinuities. For example, the function shown in the left panel of Fig. C2 has a unit jump at zero, implying the divergence of the limit of $\delta^{-1}(f(0+\delta)-f(0)) = \delta^{-1}$. **Continuity** is a necessary (but not sufficient, see discussion below) prerequisite for differentiability. Using the above terminology of limits, a

function is continuous at x if $\lim_{y\to x} f(y) = f(x)$, i.e. if it converges to $f(x)$ for arguments approaching x.

To understand that **continuity does not necessarily imply differentiability** consider the second panel of Fig. C2. It shows a function which *is* continuous, but not differentiable at $x = 0$. The reason is the presence of an 'edge', i.e. $f(x) = +x$ for any $x > 0$ and $f(x) = -x$ for $x < 0$. For *positive* values of δ we then have $\delta^{-1}\big[f(\delta) - f(0)\big] = \delta^{-1}[+\delta - 0] = 1$, while for negative values $\delta^{-1}\big[f(\delta) - f(0)\big] = \delta^{-1}[-\delta - 0] = -1$. This means that the limit is not unambiguously defined, and therefore the differentiability criterion fails. Another thing that may go wrong is that 'infinitely strong' slopes appear (third panel.) For example, the function $f(x) = 3x^{1/3}$ has the derivative (see below for a summary of differentiation rules) $f'(x) = x^{-2/3}$ and this does not exist at $x = 0$ where the function crosses the x axis with 'infinite slope'. Finally, functions such as that shown in the fourth panel have well defined tangents everywhere and therefore are differentiable.

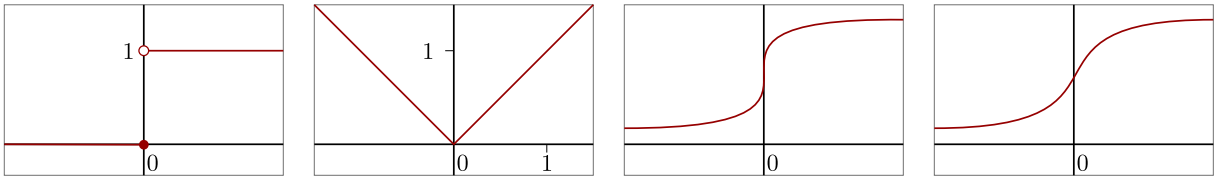


Figure C2: Left: a function that is not continuous at $x = 0$. The solid dot indicates that $f(0) = 0$. For all strictly positive values $x > 0$, $f(x) = 1$. Center: a function that is continuous but not differentiable at $x = 0$. Right: a smooth function that is differentiable throughout its domain of definition.

In this text, we often require global differentiability and for this reason we generally consider functions defined on **open intervals**, $I \equiv (a, b)$ (cf. the discussion of openness on p. 16.) Openness is required to safeguard the existence of the differential quotient throughout the entire interval: by definition, an interval I is open if any $x \in U \subset I$ lies in a neighborhood $U = \{y||y - x| \leq \epsilon\} \subset I$ entirely contained in I. The differential quotient can then be computed within U. By contrast, the differential quotient cannot be computed at the boundary points of a closed interval, $[a, b]$, because for any $\delta > 0$, $b + \delta$ is outside $[a, b]$ and $f(b + \delta)$ is not defined.

Interpretation of the derivative

In school it is often emphasized that the derivative, $f'(x)$, determines the slope (Steigung) of f at x. This view adequately applies the situation with one-dimensional functions but is too narrow to capture the meaning of derivatives in more general contexts. A more versatile interpretation is as follows: before taking the limit $\delta \to 0$, consider a fixed but very small value of δ. The right-hand side of (C1) will then be a very good approximation to the derivative, i.e. $\frac{1}{\delta}\big[f(x + \delta) - f(x)\big] \simeq f'(x)$. Now rewrite this equation as

$$\boxed{f(x + \delta) \simeq f(x) + f'(x)\,\delta.} \qquad \text{(C2)}$$

This tells us that in the immediate neighborhood of x, the function f can be approximated by a function[1] which is linear in δ, namely $f(x) + f'(x)\,\delta$ (see Fig. C1). We may set $x + \delta \equiv y$ to formulate the linear approximation as

$$f(y) \simeq f(x) + f'(x)\,(y - x).$$

However, it has to be understood that this equation holds only for arguments y very close to the fixed value x where the derivative is taken. Summarizing, we understand that

Derivatives provide local approximations to functions by linear functions.

We will soon see that this interpretation carries over to more general contexts, including situations where the notion of 'slope' is not defined. By contrast, the approximation-by-linear-functions view is generally valid and provides the key to understanding even the most involved derivative operations.

INFO The approximate equality (C2) is often applied to actually compute derivatives. To illustrate this principle, consider the function $f(x) = x^3$. Then $f(x+\delta) = (x+\delta)^3 = f(x) + 3x^2\,\delta + 3x\delta^2 + \delta^3$. Now, δ is assumed to be very small, hence δ^2 is even smaller, and δ^3 smaller still. For example, for $\delta = 10^{-2}$ we have $\delta^2 = 10^{-4}$ and $\delta^3 = 10^{-6}$. This illustrates that for δ approaching zero, terms beyond linear order become negligible compared to the linear ones. It is standard to represent this smallness as

$$f(x + \delta) = f(x) + 3x^2\delta + \mathcal{O}(\delta^2),$$

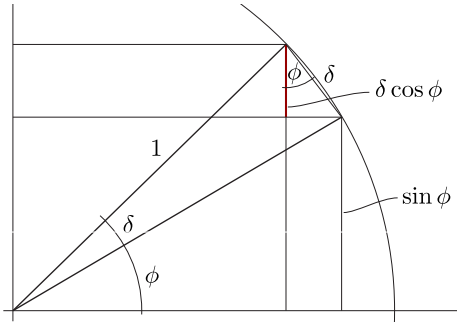
where the notation $\mathcal{O}(\delta^2)$ (spoken 'order-δ^2') indicates that terms of order δ^2 and higher are neglected.[2] Rearranging terms we have $\delta^{-1}(f(x+\delta) - f(x)) = 3x^2 + \delta^{-1} \times \mathcal{O}(\delta^2)$. In the limit $\delta \to 0$ the second term on the right hand side vanishes and comparison with (C2) leads to the identification $\mathrm{d}_x x^3 = 3x^2$.

Notice that we did not take the limit $\delta \to 0$ in the expansion above — that would have yielded a trivial equation, $f(x) = f(x)$. Instead, we took δ to be nonzero but 'arbitrarily small'. Variables, δ, assuming values smaller than any other in a specific mathematical context are sometimes referred to as **infinitesimally small** quantities. The attribute **infinitesimal** usually implies that a limit $\delta \to 0$ will eventually be taken. Still, it can be advantageous to keep the variable temporarily finite and use its smallness as an aid in computations (ignoring terms of $\mathcal{O}(\delta^2)$, etc.)

[1] A function $g(x)$ is called linear in x if it is of the form $x \mapsto g(x) = ax + b$, $a, b \in \mathbb{R}$. This should be distinguished from the slightly more restrictive definition $x \mapsto ax$ of linear *maps* used in chapter L.

[2] The mathematically precise definition of the symbol $\mathcal{O}$ is as follows: given two functions, $g(x), h(x)$, we write $g(x) = \mathcal{O}(h(x))$ in the limit $x \to 0$, if there exists a constant, c, such that $|g(x)| < c|h(x)|$ for sufficiently small x. For example, $x^2 + 3x^3$ is $\mathcal{O}(x^2)$ because $|x^2 + 3x^3|/|x^2| < c$, for $c > 1$ and x sufficiently small. The notation always makes reference to a limit which, however, need not be 0. For example, $1/(x^2 + x^3)$ is $\mathcal{O}(x^{-2})$ in the limit $x \to \infty$.

As an instructive example, a geometric construction may be applied to show that the derivative of the sine function is given by $\mathrm{d}_\phi \sin(\phi) = \cos(\phi)$. To this end, apply geometric reasoning to verify that an infinitesimal increment of the argument of the sine function changes its value from $\sin(\phi)$ to $\sin(\phi+\delta) \simeq \sin\phi + \delta\cos\phi$.



Derivatives of higher order and smoothness

Derivatives of higher order are defined by the iteration of ordinary derivatives. For example, the second derivative of a function is defined as

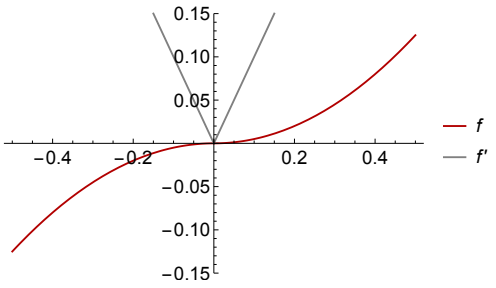
$$\frac{\mathrm{d}^2 f(x)}{\mathrm{d}x^2} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}f(x)}{\mathrm{d}x}\right). \tag{C3}$$

One sometimes says that a derivative is taken by 'applying the derivative operator $\frac{\mathrm{d}}{\mathrm{d}x}$ to a function'. The mathematical formulation of this statement reads

$$\frac{\mathrm{d}^n f(x)}{\mathrm{d}x^n} \equiv \frac{\mathrm{d}^n}{\mathrm{d}x^n} f(x) \equiv \underbrace{\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}}{\mathrm{d}x}\cdots\left(\frac{\mathrm{d}}{\mathrm{d}x} f(x)\right)\right)}_{n \text{ factors}}. \tag{C4}$$

For example,

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}x}(x^2\sin(x)) &= 2x\sin(x) + x^2\cos(x),\\
\frac{\mathrm{d}^2}{\mathrm{d}x^2}(x^2\sin(x)) &= (2-x^2)\sin(x) + 4x\cos(x),\\
\frac{\mathrm{d}^3}{\mathrm{d}x^3}(x^2\sin(x)) &= (-6x)\sin(x) + (6-x^2)\cos(x),\\
&\vdots \qquad \vdots
\end{aligned}$$



Functions that can be differentiated infinitely many times are called **smooth functions**. Examples of such functions include polynomials, or trigonometric functions. By contrast, the function defined by

$$f(x) = \frac{1}{2}\begin{cases} +x^2, & x \geq 0,\\ -x^2, & x < 0, \end{cases}$$

is differentiable at $x = 0$, but not smooth. Indeed, $f'(x) = |x|$ and this cannot be differentiated at zero, i.e. the function above is differentiable, but not two-fold differentiable. Although it looks smooth the function is not smooth in the

mathematical sense. We finally note that higher-order derivatives are sometimes represented in terms of the alternative **notation**

$$f^{(n)}(x) \equiv \mathrm{d}_x^n f(x) \equiv \frac{\mathrm{d}^n}{\mathrm{d}x^n} f(x), \tag{C5}$$

which indicates the order of differentiation as a superscript. It is imperative to put the latter in parentheses, $f^{(n)}$, to avoid confusion with the n-th power, f^n, of the function f.

C1.2 Differentiation rules

We here summarize the most important rules of differentiation. These identities may be familiar from high school and they are routinely proven in introductory courses in mathematics. In the following, $f, g : \mathbb{R} \to \mathbb{R}$ are smooth functions, and $a \in \mathbb{R}$.

▷ **Product rule**

$$\boxed{\frac{\mathrm{d}(fg)}{\mathrm{d}x} = \frac{\mathrm{d}f(x)}{\mathrm{d}x} g(x) + f(x) \frac{\mathrm{d}g(x)}{\mathrm{d}x}.} \tag{C6}$$

▷ **Chain rule**

$$\boxed{\frac{\mathrm{d}f\big(g(x)\big)}{\mathrm{d}x} = \frac{\mathrm{d}f(y)}{\mathrm{d}y}\Big|_{y=g(x)} \frac{\mathrm{d}g(x)}{\mathrm{d}x}.} \tag{C7}$$

The essence of the chain rule is that the rate of change of the function $f(g(x))$ is determined by that of the function $f(y)$ at $y = g(x)$, multiplied by that of $g(x)$ with x. It is worth taking a moment to understand this statement in intuitive terms.

In particular, $\frac{\mathrm{d}f(ax)}{\mathrm{d}x} = a \frac{\mathrm{d}f(y)}{\mathrm{d}y}|_{y=ax}$ and

$$\frac{\mathrm{d}}{\mathrm{d}x} \frac{1}{g(x)} = -\frac{1}{\big(g(x)\big)^2} \frac{\mathrm{d}g(x)}{\mathrm{d}x},$$

where the latter identity follows from the choice $f(y) = 1/y$, and $\mathrm{d}_y(1/y) = -1/y^2$.

▷ **Derivative of inverse functions**. Let f^{-1} be the **inverse function**[3] of f, i.e. $f^{-1}\big(f(x)\big) = x$. Then,

$$\frac{\mathrm{d}f^{-1}(y)}{\mathrm{d}y} = \frac{1}{\frac{\mathrm{d}f(x)}{\mathrm{d}x}\Big|_{x=f^{-1}(y)}}. \tag{C8}$$

[3] The inverse function of a function f is usually denoted by f^{-1} and this must not be confused with the inverse of the function value $f^{-1}(x) = 1/f(x)$. (For example, $f(x) = x^2$ has the inverse function $f^{-1}(y) = \sqrt{y}$, different from $f^{-1}(x) = 1/x^2$.) Which quantity is meant should generally be evident from the context.

For example,

$$\frac{\mathrm{d}}{\mathrm{d}y}\ln(y) = \frac{1}{\exp'(x)\big|_{x=\ln(y)}} = \frac{1}{\exp(x)\big|_{x=\ln(y)}} = \frac{1}{y}.$$

INFO Differentiation formulae such as the chain rule, or the derivative of inverse functions can always be derived by application of the basic rule (C2). Let us illustrate this idea on a heuristic **proof of the chain rule, Eq.** (C7). Using the abbreviation $g(x) = y$, Eq. (C2) may be applied to to linearize first g, then f, and obtain

$$f(g(x+\delta)) \simeq f(g(x) + g'(x)\,\delta) = f(y + g'(x)\,\delta) \simeq f(y) + f'(y)\,g'(x)\,\delta. \tag{C9}$$

In the second equality we noted that for infinitesimally small δ the product $g'(x)\delta$ is likewise small. The function f may therefore be linearized in it as indicated. Rearranging terms and dividing by δ we obtain $\delta^{-1}\,[f(g(x+\delta)) - f(g(x))] \simeq f'(y)\,g'(x)$. Remembering the definition of the derivative, Eq. (C1), we arrive at the chain rule. Use similar reasoning to derive the (simpler!) product rule.

C1.3 Derivatives of selected functions

For reference we list below the derivatives of a number of functions frequently occurring in practice.

▷ **Power functions**

$$\frac{\mathrm{d}x^\alpha}{\mathrm{d}x} = \alpha x^{\alpha-1}. \tag{C10}$$

The formula also applies to fractional powers, e.g. for $\alpha = 1/3$ we have $\frac{\mathrm{d}x^{1/3}}{\mathrm{d}x} = \frac{1}{3}x^{-2/3}$.

▷ **Trigonometric functions**

$$\sin'(x) = \cos(x), \qquad \cos'(x) = -\sin(x), \qquad \tan'(x) = \frac{1}{\big(\cos(x)\big)^2}. \tag{C11}$$

▷ **Exponential function and logarithm**

$$\exp'(x) = \exp(x), \qquad \ln'(x) = \frac{1}{x}. \tag{C12}$$

▷ **Hyperbolic functions**[4]

$$\sinh'(x) = \cosh(x), \quad \cosh'(x) = \sinh(x), \quad \tanh'(x) = \frac{1}{(\cosh(x))^2}. \tag{C14}$$

[4] The hyperbolic sine, cosine and tangent functions are defined as:

$$\sinh(x) = \tfrac{1}{2}(\mathrm{e}^x - \mathrm{e}^{-x}), \qquad \cosh(x) = \tfrac{1}{2}(\mathrm{e}^x + \mathrm{e}^{-x}), \qquad \tanh(x) = \frac{\sinh x}{\cosh x}. \tag{C13}$$

▷ **Inverse trigonometric and hyperbolic functions** are differentiated using (C8):

$$\arcsin'(x) = \frac{1}{\sqrt{1-x^2}}, \quad \arccos'(x) = -\frac{1}{\sqrt{1-x^2}}, \quad \arctan'(x) = \frac{1}{1+x^2}, \tag{C15}$$

$$\operatorname{arcsinh}'(x) = \frac{1}{\sqrt{1+x^2}}, \quad \operatorname{arccosh}(x)' = \frac{1}{\sqrt{x^2-1}}, \quad \operatorname{arctanh}'(x) = \frac{1}{1-x^2}. \tag{C16}$$

Derivatives of more complicated functions can be computed with the help of the product and chain rules. For example,

$$\frac{\mathrm{d}}{\mathrm{d}x} x^2 \exp(3x) = 2x \exp(3x) + 3x^2 \exp(3x), \qquad \frac{\mathrm{d}}{\mathrm{d}x} \ln(x^2+5) = \frac{1}{x^2+5} 2x.$$

Practice computing derivatives by doing problems C1.3.1-2. Problems C1.3.3-4 deal with verifying the formulas (C15) and (C16) for the derivatives of inverse trigonometric and hyperbolic functions.

C1.4 Summary and Outlook

In this introductory chapter we have reviewed the basic idea of differentiation on the example of one-dimensional real valued functions. We discussed why differentiation is so important to physics and emphasized its interpretation as a linear approximation of smooth functions. In this way of thinking it is frequently useful to keep the infinitesimal parameter δ entering the construction of the differential quotient (C1) finite and to work with effectively linearized representations of functions as in (C2). The utility of such representations became evident in a number of cases, including the explicit computation of derivatives via the manipulation of difference quotients with finite δ. We also discussed various more technical aspects of differentiation including continuity requirements, differentiation rules, and the derivatives of various important classes of functions. Although these concepts have been discussed within the framework of one-dimensional functions they are of general relevance and will play an important role in our subsequent discussion of multi-dimensional functions, starting in chapter C3.1

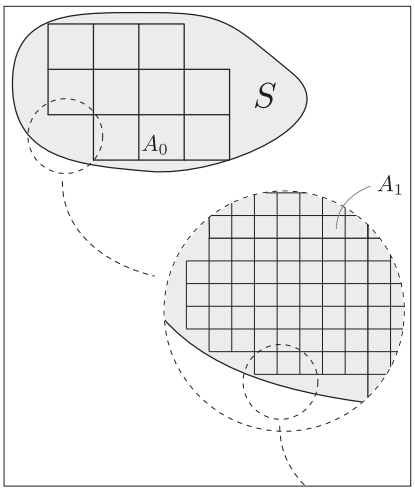
However, before generalizing to the multi-dimensional case, we first introduce the twin-operation of differentiation, integration. Following the same logics as above, we begin with the case of one-dimensional functions, once more staying at a level familiar to many readers from high school. This will allow us to keep the intimate connection between integration and differentiation in sight when we advance to higher dimensions.

C2 Integration of one-dimensional functions

Integration is as important to physics as differentiation. Whereas incremental changes in physical quantities are monitored by differentiation, integration is applied to *sum* over small increments. For example, once the incremental change in the coordinates of a stellar body has been understood, an integration procedure needs to be applied to sum over increments and obtain the change of the observable over finite time spans. This simple analogy already indicates that, quite generally, differentiation and integration are mutually inverse operations.

In the following, we adopt a strategy similar to that of the previous chapter and introduce the concept of integration on the example of one-dimensional real functions. The technical aspects of this operation will be familiar to many readers from high school. However, we stress an interpretation of integration which is not usually emphasized in school and which extends to the integrals over more complex functions to be discussed in later chapters.

C2.1 The concept of integration



In school, integration is introduced as an operation to determine the area under a function. However, only a small minority of the integrals encountered in physics can be interpreted in this way. A more general view is to think of integrals as generalized *sums*. Let us introduce this interpretation on a simple example: suppose we are given a two-dimensional painted surface, S, and want to determine its geometric area, A. A practical approach to solving this task would first choose a reference shape of known area A_0, a square say. One might then count the number, $N(A_0)$, of squares fitting into the area (see figure). An estimate of A would then be given by

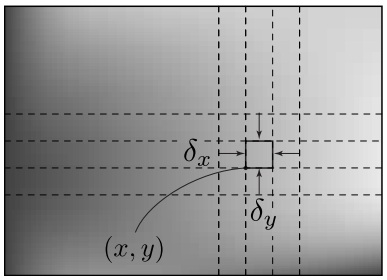
$$A \simeq \sum_{\ell=1}^{N(A_0)} A_0 = N(A_0)A_0,$$

where the index ℓ enumerates the squares. Of course, this estimate generally contains an error because parts of the area remain uncovered. However, the accuracy may be refined by turning

to squares of smaller area, A_1, and counting the number, $N_1 > N_0$, of squares required to cover S in this refined way. This leaves less uncovered excess area and leads to the improved estimate

$$A \simeq \sum_{\ell=1}^{N(A_1)} A_1 = N(A_1)A_1.$$

In principle, the procedure may be iterated down to 'infinitely many' squares of infinitesimally small area and in this limit the true value of A will be recovered. The limiting operation is called an 'integral'. All integrals have in common that they can be interpreted as limits of sums conceptually similar to that considered above.



It is straightforward to generalize the above procedure to more complicated settings. For example, consider a surface, S, coated with an inhomogeneous distribution of a massive substance, cf. the figure where darker/lighter areas represent regions of stronger/weaker coverage. We describe the system through two cartesian coordinates (x, y) and a **mass distribution function**, $\rho(x, y)$, defined in such a way that $\rho(x, y)\delta_x\delta_y$ equals the weight of the substance present in a small rectangle of area $\delta_x\delta_y$ at the coordinate point (x, y).

An estimate for the total mass, M, of the substance may be obtained by discretizing the total area, A, of the surface into a system of $N(\delta_x\delta_y) \propto A/\delta_x\delta_y$ infinitesimal rectangles at points (x_ℓ, y_ℓ), where the index ℓ enumerates the rectangles. Summing over the respective weights we obtain the estimate $M \simeq \delta_x\delta_y \sum_{\ell=1}^{N(\delta_x\delta_y)} \rho(x_\ell, y_\ell)$. We may now proceed to finer and finer discretizations to generate a sequence[1] of increasingly accurate estimates, which in the limit of infinitely small discretization areas, $\delta_x\delta_y \to 0$,approaches the true value of M:

$$M = \lim_{\delta_x\delta_y\to 0} \delta_x\delta_y \sum_{\ell=1}^{N(\delta_x\delta_y)} \rho(x_\ell, y_\ell) \equiv \int_S \mathrm{d}x\mathrm{d}y\, \rho(x, y).$$

Here, the symbolic notation appearing on the r.h.s. of the equation is *defined* by the expression in the center: the **integral** symbol $\int$ stands for an infinitely refined sum carried out over the area S, indicated as a subscript. That the summation is over a set of two-dimensional 'surface elements' $\delta_x\delta_y$, built with reference to coordinates (x, y), is indicated by the symbol $\mathrm{d}x\mathrm{d}y$. However, we repeat that all this notation is 'implicit' in the sense that the actual definition of the integral is given by the sequence of sums on the l.h.s. of the equation. Each of these sums

[1] An (infinite) **sequence**, $(a_n)_{n\in\mathbb{N}} = (a_0, a_1, \dots)$ is an infinite and sequentially ordered collection of objects. For example, $a_n = 1/n$ defines the sequence $(1, 1/2, 1/3, \dots)$. The sequence converges to a **limit**, $\lim_{n\to\infty} a_n \equiv a$, if for increasing n the values a_n converge to the value a. For example, the sequence $a_n = 1/n$ converges to 0. **Convergence** means that for any $\epsilon > 0$ there exists a threshold $n_\epsilon \in \mathbb{N}$ such that for $n > n_\epsilon$ $|a_n - a| < \epsilon$.

can be computed in concrete ways, either manually, or on a computer, and at any desired level of accuracy. The important and general statement conveyed by this discussion above is that[2]

> Almost any integral encountered in physics can be represented as the limit of a sequence of finite sums, each of which can be computed by 'conventional techniques'.

The sequences of sums representing integrals are generally called **Riemann sums**. All Riemann sums have the structure

$$\text{Riemann sum} = \lim_{\delta\to 0} \delta \sum_{\ell=1}^{N(\delta)} X_\ell, \qquad \text{(C17)}$$

where X_ℓ is the quantity to be summed and the index ℓ enumerates subdivisions of a summation domain that has been divided into $N(\delta) \propto \delta^{-1}$ compartments. This proportionality ensures that the smallness of δ is balanced by the increase in the number of summation steps. In the following we will discuss various concrete examples of Riemann summation procedures.

Bernhard Riemann (1826-1866)

A German mathematician who made breakthrough contributions to analysis, number theory and differential geometry. Riemann gave the concept of integration a precise meaning. He also introduced various foundations of modern geometry, including the concept of Riemannian manifolds fundamental to the later formulation of general relativity.

C2.2 One-dimensional integration

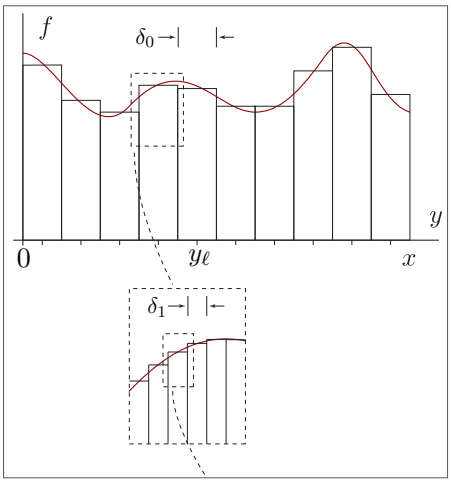
In this section, we apply the program outlined above to one-dimensional functions $f : \mathbb{R} \to \mathbb{R}$, $y \mapsto f(y)$. The quantities to be summed up now are the values $f(y)\delta y$ obtained by multiplying function values with small increments in the argument variable. We observe that $f(y)$ plays a role analogous to that of the mass distribution discussed in the previous section. In the present one-dimensional context the result of the summation procedure will be the geometric area enclosed by the function graph and the abscissa (see the figure below.) We begin by discussing how the summation procedure is made quantitative.

One-dimensional Riemann sums

In the one-dimensional case, the integration domain (i. e. the analog of the area S in our example above) is a real interval, say $[0, x]$. Proceeding in analogy to the previous discussion, the domain is partitioned into $N(\delta_0) \equiv x/\delta_0$ intervals of small width δ_0. For finite δ_0 these increment intervals are sometimes called **bins** and we will use this denotation for convenience. Let $f_\ell \equiv f(y_\ell)$, with $\ell = 1, \ldots, N(\delta_0)$, be the value of f at a point y_ℓ somewhere in the ℓth bin.

[2] We write 'almost any' because there are rare cases of integrals which cannot be computed along the lines of our construction above. For further comments on this point, see section C2.2.

The corresponding area is then approximately given by $\delta_0 f_\ell$, and summation leads to the estimate



$$F(x) \simeq \delta_0 \sum_{\ell=1}^{N(\delta_0)} f_\ell,$$

for the total area. Note that for finite δ_0 the value of this estimate depends on the arbitrary choice of the readout point y_ℓ within the ℓth bin — left edge, right edge, center? — and therefore contains arbitrariness. However, as is indicated by the figure, the dependence of the individual strip areas on the positioning of y_ℓ diminishes upon passing to bins of higher resolution. In fact, this statement holds true even for functions containing isolated singularities,[3] and we will revisit it in more detail and generality on p. 430.

The limiting case of an infinitely refined sum is called the **integral** of the function:

$$\boxed{F(x) = \lim_{\delta\to 0} \delta \sum_{\ell=1}^{x/\delta} f_\ell \equiv \int_0^x \mathrm{d}y\, f(y).} \tag{C18}$$

The interpretation in terms of sums also shows how **integration and differentiation are 'inverse' operations**. To understand this point, let us ask how $F(x)$ varies as a function of x. An approximate answer can be found by considering its Riemann sum at a small but fixed value of δ:

$$F(x+\delta) = \delta \sum_{\ell=1}^{\frac{x}{\delta}+1} f_\ell = \delta \sum_{\ell=1}^{\frac{x}{\delta}} f_\ell + \delta f_{\frac{x}{\delta}+1} = F(x) + \delta \cdot f(x),$$

where in the last step we conveniently put the readout position to the left of the bin, $f_{\frac{x}{\delta}+1} = f(x)$. (Why is the arbitrariness of this choice inessential?) We divide by δ and take the limit $\delta \to 0$ to obtain

$$\frac{\mathrm{d}F(x)}{\mathrm{d}x} \equiv \lim_{\delta\to 0} \frac{1}{\delta}\big[F(x+\delta) - F(x)\big] = f(x)$$

[3] For a bin containing an isolated singularity, the value $\delta_0 f_\ell$ of course depends crucially on whether the readout coordinate lies to the left or the right of the singularity. However, no matter what is chosen, the 'error' will be of $\mathcal{O}(\delta_0)$ and as long as the number of singularities is finite the sum will contain a finite number of these errors. In the limit $\delta_0 \to 0$ the defective contribution goes to zero. Perhaps, think more about this point.

This confirms that the rate at which an integral $F(x) = \int_0^x \mathrm{d}y f(y)$ changes under variation of the integration boundary, x, is given by the value of the integrand at the boundary, $f(x)$. The reciprocity between integration and differentiation is summarized by the **fundamental theorem of calculus**:

$$\boxed{F(x) = \int_0^x \mathrm{d}y\, f(y) \quad \Rightarrow \quad \frac{\mathrm{d}F(x)}{\mathrm{d}x} = f(x).} \tag{C19}$$

Later in the text, we will see that similar relations hold for more general classes of integrals and derivatives. They all follow from the interpretation of integrals as sums and of derivatives as measures of small increments.

Definite and indefinite integrals

Any function, $F(x)$, whose derivative equals $f(x)$, $\frac{\mathrm{d}}{\mathrm{d}x}F(x) = f(x)$, is called a **primitive function**primitive functions or **anti-derivative** of f. The terminology anti–derivative emphasizes that passing from f to F is the opposite of passing from f to f'. We write 'a' instead of 'the' primitive function because for any constant C the function $F(x) + C$ is an equally valid primitive function, $\frac{\mathrm{d}}{\mathrm{d}x}(F(x) + C) = f(x)$.

Even in the higher dimensional integration theory to be discussed in later sections actual calculations come down to successions of one-dimensional integrals. Eq. (C19) indicates that primitive functions are the key to the computation of these integrals and this explains their general importance. The connection between integrals and the primitive function is underpinned by the notation

$$\int \mathrm{d}x\, f(x) \equiv F(x) + C, \tag{C20}$$

where the symbol on the l.h.s. is called an **indefinite integral**. The indefinite integral is just a another denotation for the whole class of primitive functions with unspecified **integration constant**, C. For example, $\int \mathrm{d}x\, x^4 = \frac{1}{5}x^5 + C$, since $\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{1}{5}x^5 + C\right) = x^4$, irrespective of the value of C. In integral tables the additive constant is often omitted, although its presence is implicitly assumed.

Knowing a primitive function, the value of a **definite integral**, i.e. an integral over a definite interval $[a, b]$ is obtained as

$$\int_a^b \mathrm{d}y\, f(y) = F(b) - F(a) \equiv F(x)\Big|_a^b \equiv \Big[F(x)\Big]_b^a. \tag{C21}$$

This relation follows from Eq. (C19) and the observation that $\int_a^b \mathrm{d}y\, f = \int_0^b \mathrm{d}y\, f - \int_0^a \mathrm{d}y\, f$, i.e. the summed area from a to b equals that from 0 to b minus that from 0 to a. Note that in the difference on the r.h.s. the integration constant drops out and there is no arbitrariness in the definite integral. The general consistency of the additivity of integrals with Eq. (C21) is seen from relations such as $\int_a^b \mathrm{d}y\, f(y) = \int_a^c \mathrm{d}y\, f(y) + \int_c^b \mathrm{d}y\, f(y)$, which is compatible with $F(b) - F(a) = [F(b) - F(c)] + [F(c) - F(a)]$.

When doing an integral over a definite interval, $[a, b]$, the first step usually is to 'compute the indefinite integral' and find a primitive function of the integrand. However, unlike with the derivative of functions, not every integral can be solved in closed form — sometimes it is just not possible to find a suitable primitive function. Nevertheless, there exists a huge body of solution strategies (analytical, approximate, or numerical) and satisfactory solutions to most integration problems can be found. Some general rules and hints in this regard are summarized in section C2.4.

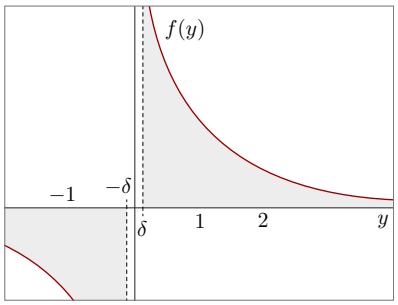
We finally note that the **integral over an open interval**, (a, b), gives the same result as that over its closure, $[a, b]$. The reason is that the estimate of the bin width entering the Riemann sum construction does not depend on the presence or absence of the isolated endpoints, a, b, in which the two intervals differ. (In fact, the notation $\int_a^b \mathrm{d}x f(x)$ does not even distinguish between the two cases.) As mentioned previously, we will mostly work with open intervals in this text. However, where integration is concerned the difference between 'open' and 'closed' is conveniently irrelevant.

EXERCISE In the formulas above on definite integrals, $\int_a^b \mathrm{d}y f(y)$ we tacitly assumed $a < b$. However, convince yourself that all relations remain valid if we define

$$\int_b^a \mathrm{d}y\, f(y) = -\int_a^b \mathrm{d}y\, f(y) \tag{C22}$$

Although integrals with lower boundaries exceeding the upper boundary do not really make sense, expressions with sign inverted boundaries sometimes appear at intermediate step, and the above relation can be used to convert them to 'ordinary integrals'.

Integrability



Not all integrals are well-defined. Much like a function can vary too rapidly to be differentiable, it can diverge too strongly to be 'summable'. More precisely, an integral over a specified interval is said to 'exist' if and only if the Riemann sum (C18) converges to a finite value in the limit $\delta \to 0$. If it does not, we say that the integral 'does not exist' or that the integrand is not **Riemann integrable**.[4] For example, consider the function $f(y) = 1/y$, which has a **singularity** (i.e. a point of divergence) at $y = 0$. The integral $\int_1^2 \mathrm{d}y\, y^{-1} = \ln(y)\big|_1^2 = \ln(2)$ exists, but $\int_0^2 \mathrm{d}y\, y^{-1} = \ln(y)\big|_0^2$ does not because the primitive function, $F(y) = \ln(y)$, diverges at zero (see figure). Note that the divergence of an integrand at a singularity does not necessarily imply the non-existence of its

[4] There exist more general integration schemes – the relevant keyword is **Lebesgue integrability** – often discussed in advanced lecture courses of calculus. However in view of the rarity of functions which are Lebesgue- but not Riemann-integrable we do not address this generalization here.

integral. For example $y^{-1/2}$ has a singularity at $y = 0$, however, the integral $\int_0^1 \mathrm{d}y\, y^{-1/2} = 2y^{1/2}\big|_0^1 = 2$ does exist. This is an example of an **integrable singularity**. More generally, any power, $y^{-\alpha}$, $\alpha < 1$ has the primitive function $-\frac{1}{\alpha-1}y^{-(\alpha-1)}$ which is well behaved at $y = 0$. However, $y^{-\alpha}, \alpha \geq 1$ are examples of **non-integrable singularities**.

Finally, there are integrals that trick one into believing that they are Riemann-doable, although they are not. As an example, consider the integral $\int_{-3}^{2} \mathrm{d}y y^{-1}$. A naive evaluation through the primitive function $F(y) = \ln(y)$ yields the result $\ln(2) - \ln(-3)$. This looks like the difference of two finite numbers. However, the appearance of the (ill-defined) logarithm of a negative real number makes the result questionable. Indeed, the integrand contains a **non-integrable singularity** at $y = 0$, whereas the application of Eq. (C18) requires integrability throughout the entire domain of integration.

One one may make sense of an integral with an **isolated singularity** at y_0 by considering the expression

$$P\int_a^b \mathrm{d}y\, f(y) \equiv \lim_{\delta\to 0}\left(\int_a^{y_0-\delta} + \int_{y_0+\delta}^b \mathrm{d}y\right) f(y),$$

For finite δ the singularity is avoided by removal of a region of around it. If the limit $\delta \to 0$ of an infinitesimally small cutout region exists, $P\int_a^b \mathrm{d}y\, f(y)$ is called the **principal value integral** of the function around the singularity. This expression must not be identified with the integral of the function $f(y)$, which does not even exist if the limits $\lim_{\delta\to 0}\int_a^{y_0-\delta} f$ and $\lim_{\delta\to 0}\int_{y_0+\delta}^b f$ do not exist separately. (If the limits exist, then $P\int \mathrm{d}y f = \int \mathrm{d}y f$ by construction.) Principal value integrals can be finite if the diverging contributions to an integral from the left and the right of a singularity almost cancel each other. For example, the principle value integral (see the figure above for an illustration):

$$P\int_a^b \frac{\mathrm{d}y}{y} = \lim_{\delta\to 0}\left[\int_a^{-\delta}\frac{\mathrm{d}y}{y} + \int_\delta^b \frac{\mathrm{d}y}{y}\right] = \lim_{\delta\to 0}\left[-\int_\delta^{-a}\frac{\mathrm{d}y'}{y'} + \int_\delta^b \frac{\mathrm{d}y}{y}\right] =$$
$$= \lim_{\delta\to 0}\left[-\ln(-a) + \ln\delta + \ln b - \ln\delta\right] = \ln\left(\frac{b}{|a|}\right),$$

$a < 0 < b$, is finite. In the second equality we used a substitution $y' = -y$[5] and in the third noted that the contribution of the interval $[\delta, 2]$ to the two integrals cancels. We will discuss applications of principal value integrals in chapter C9.

As a corollary we note that a **criterion for the integrability of a function**, f, is the integrability of its *modulus*, $|f|$. The integral $\int \mathrm{d}y|f(y)| \geq \left|\int \mathrm{d}y f(y)\right|$ is an upper bound for the modulus of an integral (why?) and if it exists, the integral of f exists with certainty. In the integral of the modulus, potential singularities are all counted with equal sign and a spurious cancellation mechanism as discussed above will not go undetected.

[5] Readers not familiar with variable substitutions in integrals from high school find the concept explained in the next section.

C2.3 Integration rules

The fundamental theorem of calculus Eq. (C19) is called 'fundamental' for a reason: from it, other integration identities can be derived with little effort. In the following, we discuss two important secondary identities, the rule of integration by parts, and that of substitution of variables.

Integration by parts

Consider the function $F(x) = u(x)v(x)$ where u and v are differentiable functions. The product rule of differentiation, Eq. (C6), then states that $F' = u'\,v + u\,v'$ where we omitted the arguments for clarity. This means that

$$F(b) - F(a) = \int_a^b \mathrm{d}x\, F'(x) = \int_a^b \mathrm{d}x \big[u'(x)\,v(x) + u(x)\,v'(x)\big].$$

Rearranging terms we obtain the formula for **integration by parts**

$$\boxed{\int_a^b \mathrm{d}x\, u(x)\,v'(x) = \Big[u(x)\,v(x)\Big]_a^b - \int_a^b \mathrm{d}x\, u'(x)\,v(x)\,.} \tag{C23}$$

This rule is often formulated without explicit reference to boundaries:

$$\int \mathrm{d}x\, u(x)\,v'(x) = u(x)\,v(x) - \int \mathrm{d}x\, u'(x)\,v(x)\,. \tag{C24}$$

This relation is useful in cases where the integral on the right is easier to do than that on the left (→ C2.3.1-2).

EXAMPLE Consider the integral $\int \mathrm{d}x\, x\mathrm{e}^x$. With $u(x) = x$ and $v(x) = \exp(x)$ we have $u' = 1$ and $v = (\exp(x))'$. Integration by parts then yields

$$\int \mathrm{d}x\, x\,\mathrm{e}^x = -\int \mathrm{d}x\, \mathrm{e}^x + x\,\mathrm{e}^x = \mathrm{e}^x(x-1)\,.$$

As a check, we note that differentiating the result indeed reproduces the integrand, $x\mathrm{e}^x$.

Substitution of variables

Much like Eq. (C23) follows from the product rule of differentiation, an integration formula for changes of variables follows from the chain rule (C7): Consider a function $f(y) \equiv \mathrm{d}_y F(y)$. Let $y(x)$ be a *monotonically increasing* differentiable function of the variable x. Then $b > a$ implies $y(b) > y(a)$, and application of the fundamental theorem yields $F(y(b)) - F(y(a)) = \int_{y(a)}^{y(b)} \mathrm{d}y \mathrm{d}_y F(y) = \int_{y(a)}^{y(b)} \mathrm{d}y f(y)$. On the other hand, we may consider $F(y(x))$ as a function

of x. Applying the fundamental theorem once more, but this time with reference to the variable x, we obtain $F(y(b)) - F(y(a)) = \int_a^b \mathrm{d}x\, \mathrm{d}_x F(y(x)) = \int_a^b \mathrm{d}x\, \mathrm{d}_y F\big|_{y(x)} \mathrm{d}_x y(x) = \int_a^b \mathrm{d}x\, f(y(x)) \mathrm{d}_x y(x)$. Equating the two results yields the rule of **substitution of variables**,

$$\boxed{\int_a^b \mathrm{d}x\, \frac{\mathrm{d}y(x)}{\mathrm{d}x} f(y(x)) = \int_{y(a)}^{y(b)} \mathrm{d}y\, f(y).} \tag{C25}$$

EXAMPLE Consider the integral $\int \mathrm{d}x\, x\, \mathrm{e}^{-x^2}$. Define $y(x) = x^2$ and write it as $\frac{1}{2} \int \mathrm{d}x\, \frac{\mathrm{d}y(x)}{\mathrm{d}x} \mathrm{e}^{-y(x)} = \frac{1}{2} \int \mathrm{d}y\, \mathrm{e}^{-y} = -\frac{1}{2}\mathrm{e}^{-y} = -\frac{n}{2}\mathrm{e}^{-x^2}$. Check the formula by differentiation.

For a monotonically *decreasing* function y the same construction yields

$$\int_a^b \mathrm{d}x\, \frac{\mathrm{d}y(x)}{\mathrm{d}x} f(y(x)) = -\int_{y(b)}^{y(a)} \mathrm{d}y\, f(y),$$

where now $y(b) < y(a)$. Since the derivative of a decreasing function is negative, we may absorb the minus sign by writing $-\mathrm{d}_x y = |\mathrm{d}_x y|$. Both variants may therefore be subsumed in single equation, known as the **indefinite version of the rule of substitutions of variables**,

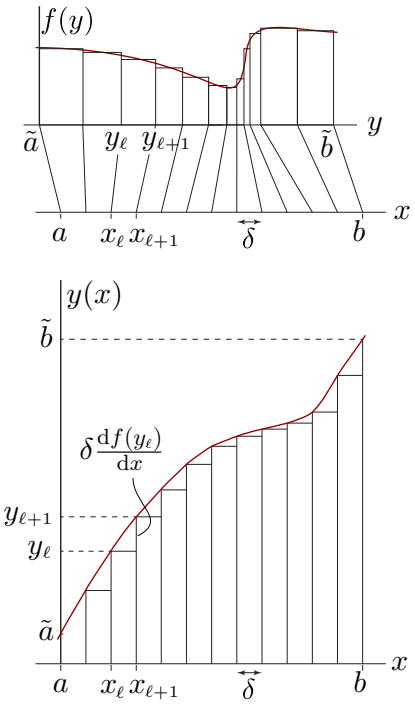
$$\boxed{\int \mathrm{d}x\, \left|\frac{\mathrm{d}y(x)}{\mathrm{d}x}\right| f(y(x)) = \int \mathrm{d}y\, f(y).} \tag{C26}$$

INFO Consider the substitution rule (C25). Formulae describing the change of variables in integrals generally contain derivative factors such as $\frac{\mathrm{d}y}{\mathrm{d}x}$ above. The following **dirty trick** is a mnemonic for remembering the placement of such factors: suppose $\mathrm{d}x$ and $\mathrm{d}y$ were ordinary 'variables' and $\frac{\mathrm{d}y}{\mathrm{d}x}$ an ordinary ratio. The structure '$\mathrm{d}x \frac{\mathrm{d}y}{\mathrm{d}x} = \mathrm{d}y$' would then be an ordinary formula for fractions. The mathematically precise formulation of this mnemonic is discussed in chapter V5.

Study problems C2.3.3-4 to gain practice with performing integrals by substitution. Problems C2.3.5-8 provide guidance to performing certain standard classes of integrals using **trigonometric or hyperbolic substitutions**.

INFO Above we provided a formal proof of the rule of substitution of variables by application of the fundamental theorem. However, variable substitutions appear very frequently, not just in one-dimensional contexts, and it is well to understand the meaning of Eq. (C25) intuitively. To this end, let us return to the description of integration as sums over increasingly fine discretization 'grids'. The point to notice now is that these grids need not be evenly spaced. The freedom to choose discretizations of varying width is the **principle behind all variable substitution rules** of integration.

Consider a function $f : [\tilde{a}, \tilde{b}] \to \mathbb{R}$, $y \mapsto f(y)$ for which regions of rapid variation alternate with ones where changes are slow (see the figure). In this case, it might make sense to introduce a system of bins of varying width: rapid changes would call for a finer discretization through a large number of narrow bins, while fewer and wider bins would suffice to describe regions of modest variation. (On a computer such flexible sampling leads to higher efficiency and saves memory without sacrificing accuracy.)



A variant of the Riemann sum over N bins, $[y_\ell, y_{\ell+1}]$, of varying width, $y_{\ell+1} - y_\ell$, reads

$$\int_{\tilde{a}}^{\tilde{b}} \mathrm{d}y f(y) = \lim_{N\to\infty} \sum_{\ell=0}^{N-1} [y_{\ell+1} - y_\ell] f(y_\ell). \tag{C27}$$

To compute the sum (C27) in concrete terms we need to specify the points y_ℓ. To this end, we introduce an interval $[a, b]$ and a *monotonically increasing* function

$$y : [a, b] \to [\tilde{a}, \tilde{b}], \qquad x \mapsto y(x), \tag{C28}$$

where $y(a) = \tilde{a}$, $y(b) = \tilde{b}$. This function is defined such that for a *uniform* discretization of $[a, b]$ into N points $x_\ell = a + \ell\delta$, with $\delta = (b - a)/N$ and $\ell = 0, \ldots, N - 1$, the values $y_\ell \equiv y(x_\ell)$ define the the points of the desired discretization. For example (see figure), a region of rapid variation of $y(x)$ leads to widely spaced points y_ℓ, and hence wide bins $y_{\ell+1} - y_\ell$.

Using $y_{\ell+1} - y_\ell = y(x_\ell + \delta) - y(x_\ell) \simeq \delta \frac{\mathrm{d}y(x_\ell)}{\mathrm{d}x}$, we now represent the Riemann sum as

$$\begin{aligned}\int_{\tilde{a}}^{\tilde{b}} \mathrm{d}y\, f(y) &= \lim_{N\to\infty} \sum_{\ell=0}^{N-1} \big[y(x_\ell + \delta) - y(x)\big] f(y(x_\ell)) \\ &\overset{\text{(C2)}}{\simeq} \lim_{N\to\infty} \sum_{\ell=0}^{N-1} \delta \frac{\mathrm{d}y(x_\ell)}{\mathrm{d}x} f(y(x_\ell)) = \int_a^b \mathrm{d}x \frac{\mathrm{d}y}{\mathrm{d}x} f(y(x))\,.\end{aligned}$$

Here, the factor $\frac{\mathrm{d}y}{\mathrm{d}x}$ describes the way in which the uniform x-grid gets distorted to generate the non-uniform y-grid. For example, regions where $\frac{\mathrm{d}y}{\mathrm{d}x}$ is large contribute to the x-integral with increased weight because they correspond to wide grid spacings in the original y-representation. Recalling that $\tilde{a} = y(a)$ and $\tilde{b} = y(b)$ we recognize the rule of substitution of variables, Eq. (C25) above.

Later in the text, we will meet various other identities describing the change of variables in integrals. However, all these formulae rely on constructions similar to that discussed above. It may be a good idea to spend a little time and let the geometric interpretation sink in, both in the discrete and the continuum representation.

C2.4 Practical remarks on one-dimensional integration

Although there exists no general recipe to compute the primitive function for arbitrary f, the majority of integrals encountered in the physics curriculum involve standard functions — polynomials, exponentials, logarithms, trigonometric functions, etc. With time and practice the integrals of these functions will become familiar. A number of important examples of such 'basic' integrals are implicit in the derivatives listed in section C1.3, we just need to read the equations from right to left. For example,

$$(\ln(x))' = \frac{1}{x} \Leftrightarrow \int \mathrm{d}x \frac{1}{x} = \ln(x).$$

How do we approach integrals if the solution is not immediately obvious? The following list contains a number of useful procedures and guiding principles:

- ▷ It often helps to start from an **educated guess** for the primitive $F(x)$. Sometimes one just needs to play around a little to improve an initially not-quite-correct guess and arrive at a function satisfying $\frac{\mathrm{d}}{\mathrm{d}x}F(x) = f(x)$.
- ▷ If the integrand contains functions whose derivative looks more inviting than the function itself **try to integrate by parts** (→ C2.3.1-2). For example,

$$\begin{aligned}\int \mathrm{d}x\, x \ln(x) &= \int \mathrm{d}x\, \frac{1}{2}\frac{\mathrm{d}x^2}{\mathrm{d}x} \ln(x) \overset{(C24)}{=} \frac{1}{2}x^2 \ln(x) - \frac{1}{2}\int \mathrm{d}x\, x^2 \frac{\mathrm{d}\ln(x)}{\mathrm{d}x} \\ &= \frac{1}{2}x^2 \ln(x) - \frac{1}{2}\int \mathrm{d}x\, x^2 \frac{1}{x} = \frac{x^2}{2}\left(\ln(x) - \frac{1}{2}\right).\end{aligned}$$

- ▷ If an integral contains terms more complicated than the elementary functions listed in section C1.3 **try substitutions** (→ C2.3.3-**??**). An expression containing $\mathrm{d}x\frac{1}{x}$, might call for the substitution $y = \ln(x)$, which results in $\mathrm{d}y = \mathrm{d}x\frac{1}{x}$. For example,

$$\int \mathrm{d}x \frac{1}{x}\frac{1}{a + \ln(x)} = \int \mathrm{d}y \frac{1}{a + y} = \ln(a + y).$$

  Similarly, the combination $\mathrm{d}x\, x$ suggests the substitution $y = x^2$, with $\mathrm{d}x\, x = \frac{1}{2}\mathrm{d}y$.
- ▷ There are families of functions whose integrals look complicated but are known to be doable. An important example are the **rational functions**, i.e. functions $f(x) = P(x)/Q(x)$ which can be written as a ratio of two polynomials. These can be integrated using a technique called **partial fraction decomposition** (→ C2.3.9-12). Other examples of integrable families include **rational functions of trigonometric functions** (ratios of polynomials in the functions $\sin(x), \cos(x)$ and $\tan(x)$), and **polynomials in exponential functions**. For the corresponding integration strategies we refer to textbooks on calculus. Try to memorize the families of functions mentioned above to be able to recognize their integrals as doable when you meet them.

- **Computer algebra** packages such as Mathematica® or Maple® can be powerful aids for solving even very complex integration problems. However, we suggest not to use these packages excessively: integrals encountered in physics often have a structure that 'reflects' the underlying physics, and if one lets a computer do the job one looses touch with this structure. On the same note, the 'manual' struggling with an integral usually is rewarded with added insight into the problem. It is therefore good practice to seriously try to solve integrals by hand before turning to a computer.

- As a compromise between the manual and the fully automated solution of integrals one may use **integral tables**. The primary reference in this context is I.S.Gradshteyn and I.M. Ryzhik, *Table of Integrals, Series, and Products*, Academic Press, 7th edition, 2007. This book tabulates thousands of integrals.

- No matter how the primitive function has been obtained, *always* check it by differentiation.

- **Many integrals are not expressible through elementary functions**. For example, the Gaussian function, $\exp(-x^2)$, does not have an elementary primitive. In cases where an 'important' function cannot be integrated to elementary functions, its primitive *defines* a what is called a **special function**. For example, the integral of the Gaussian function defines the so-called **error function**

$$\int_0^y \mathrm{d}x\, \mathrm{e}^{-x^2} \equiv \frac{\sqrt{\pi}}{2}\mathrm{erf}(y).$$

  Mathematica® or Maple® can be powerful aids for solving even very complex integration problems. However, we suggest not to use these packages excessively: integrals encountered in physics often have a structure that 'reflects' the underlying physics, and if one lets a computer do the job one looses touch with this structure. On the same note, the 'manual' struggling with an integral usually is rewarded with added insight into the problem. It is therefore good practice to seriously try to solve integrals by hand before turning to a computer.

- For some types of **definite integrals**, there exists methods which avoid the need to find the primitive function, and some of these will be discussed in section C9.5 on complex calculus. Such shortcuts are helpful in cases where the indefinite integrals cannot be expressed in elementary terms. For example, the **Gaussian integral**,

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-x^2} = \sqrt{\pi}, \tag{C29}$$

  can be computed (→ C2.3.13-14) without reference to its indefinite integral, the error function. Other integrals in the same league include the exponential integrals $\int_0^\infty \mathrm{d}x\, x^n\, \mathrm{e}^{-x}$ (→ C2.3.15) and general Gaussian integrals $\int_0^\infty \mathrm{d}x\, x^{2n}\, \mathrm{e}^{-x^2}$ (→ C2.3.16).

- Any (Riemann integrable) function can be integrated **numerically** on a computer. In this case, a computer is employed to evaluate the Riemann discretizations. The accuracy of the results can be increased by lowering the discretization steps, and/or turning to non-uniform

discretizations (cf. info section on p. 211) adjusted to the profile of the integrand. For the discussion of discretization grids tailored to obtain rapid convergence, etc., we refer to textbooks on numerical integration.

C2.5 Summary and Outlook

In this chapter we introduced the idea of integration as a refined way of summation on the example of one-dimensional functions. Many aspects of this discussion, notably the 'reciprocity' of integration and differentiation, carry over to the generalized integrals addressed in later chapters. For example, the substitution rule has various higher dimensional generalizations. Although these may look a little more complicated than the one-dimensional one, the constructions principles always reflect the discussion of the info section on p. 211. We also discussed various integration techniques specific to one-dimensional functions. These, too, continue to play an important role in more general contexts: higher dimensional integrals are usually broken down to successions of one-dimensional ones, which then need to be processed by the methods reviewed above.

We have now reached a good basis to turn to the generalize the concepts of differentiation and integration to functions defined in higher dimensional spaces, and this is the subject to which we turn next.

C3 Partial differentiation

Consider a function depending on more than one variable, such as the water depth, $D(\mathbf{r})$, beneath a boat at position $\mathbf{r} = (x, y)$ on a lake, or the air pressure, $P(T, V)$, in a container of volume V at temperature T. One may ask how these quantities change if only *one* of the variables is varied: how does the water depth vary if the boat moves in x-direction at fixed y? Or how does the pressure in the container change upon increasing temperature at fixed volume? The present chapter introduces **partial derivatives** as the mathematical tools to adress such questions.

C3.1 Partial derivative

Consider a function $f : \mathbb{R}^d \to \mathbb{R}$, $\mathbf{x} \mapsto f(\mathbf{x}) = f(x^1, \ldots, x^d)$ depending on d variables $x^1, \ldots, x^d$. The **partial derivative** of f with respect to x^i probes how $f(\mathbf{x})$ changes if only the single variable x^i is varied. It is defined as the ordinary derivative of f w.r.t. to x^i taken at fixed values of the other variables:

$$\boxed{\frac{\partial f(\mathbf{x})}{\partial x^i} \equiv \lim_{\delta \to 0} \frac{1}{\delta} \Big[f(x^1, \ldots, x^i + \delta, \ldots, x^d) - f(x^1, \ldots, x^i, \ldots, x^d) \Big].} \tag{C30}$$

The symbol ∂ indicates that this is a *partial* derivative of a multi-dimensional function, in contrast to the ordinary derivative (written as d) of a one-dimensional function. Other frequently used notations include[1]

$$\frac{\partial f(\mathbf{x})}{\partial x^i} \equiv \partial_{x^i} f(\mathbf{x}) \equiv \partial_i f(\mathbf{x}).$$

EXAMPLE The examples below are partial derivatives written in different notations:

$$\partial_1 \big[(x^1)^2 x^2 + x^3 \big] = 2 x^1 x^2,$$

[1] In **covariant notation** where component indices are written as superscripts (x^i), the symbol ∂_i carries a subscript. The rationale behind this convention will be discussed in chapter V5. However, an easy way to memorize it is to note that $\partial / \partial x^i$ is an object carrying a superscript symbol in the *denominator*. Much as with a double fraction $(1/(1/5) = 5)$ this corresponds to a symbol with inverted index position in the numerator, $\partial / \partial x^i = \partial_i$.

$$\partial_{x^2}\big[(x^1)^2 x^2\cos(x^2)+x^3\big] = (x^1)^2\big[\cos(x^2)-x^2\sin(x^2)\big],$$
$$\partial_y\big[(x^2+y^3)\sin(x+y^2)\big] = 3y^2\sin(x+y^2)+(x^2+y^3)2y\cos(x+y^2).$$

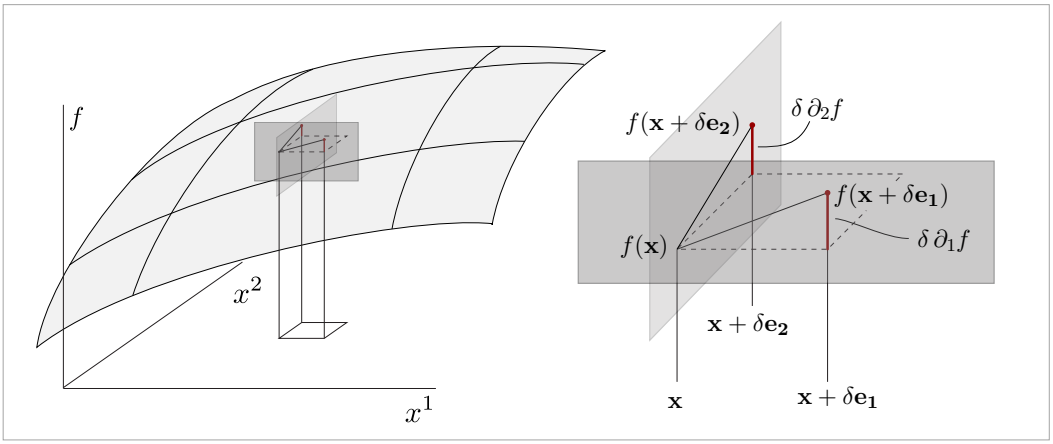


Figure C3: Partial derivatives illustrated for a function $f:\mathbb{R}^2\to\mathbb{R}$.

It is sometimes useful to write Eq. (C30) in a vectorial notation where the variables x^i define a vector as $\mathbf{x}=\sum_i^d \mathbf{e}_i x^i$. We then have

$$\frac{\partial f(\mathbf{x})}{\partial x^i} = \lim_{\delta\to 0}\frac{1}{\delta}\big(f(\mathbf{x}+\delta\,\mathbf{e}_i)-f(\mathbf{x})\big). \tag{C31}$$

Fig. C3 illustrates the interpretation of the partial derivative on a two-dimensional example. The shaded planes indicate how one variable is kept constant in the process. The variation of the other variable yields the partial derivative as an ordinary derivative taken in the direction of the corresponding coordinate axis.

Since partial derivatives are ordinary derivatives taken w.r.t. one out of d variables they are as easy to take as one-dimensional derivatives (→ C3.1.1-2). All differentiation rules discussed in Section C1.2 directly carry over to partial differentiation. For example, the product rule reads:

$$\partial_i\big(f(\mathbf{x})\,g(\mathbf{x})\big) = \big(\partial_i f(\mathbf{x})\big)\,g(\mathbf{x}) + f(\mathbf{x})\,\big(\partial_i g(\mathbf{x})\big).$$

C3.2 Multiple partial derivatives

Just as with multiple ordinary derivatives (cf. Eq. (C4)) **multiple partial derivatives** are obtained by repeatedly taking single derivatives. For example, the symbols $\partial^2_{x^i,x^j}$ or just $\partial^2_{i,j}$ indicate a double partial derivative in which one first differentiates in the variable x^j, and

then the result in x^i. If $i = j$ this is an ordinary second order derivative in x^i and generally abbreviated as $\partial^2_{x^i,x^i} \equiv \partial^2_{x^i} \equiv \partial^2_i$. For example, with $x^1 \equiv x$ and $x^2 \equiv y$

$$\partial_x^2\big(x^3y^2\big) = \partial_x\big(3x^2y^2\big) = 6xy^2, \qquad \partial_y^2\big(x^3y^2\big) = \partial_y\big(2x^3y\big) = 2x^3.$$

Mixed derivatives in different variables generally are to be taken in the order specified by the notation:

$$\partial^2_{i,j} f(\mathbf{x}) \equiv \partial^2_{x^i,x^j} f(\mathbf{x}) \equiv \partial_{x^i}\partial_{x^j} f(\mathbf{x}) \equiv \partial_{x^i}\big(\partial_{x^j} f(\mathbf{x})\big).$$

However, for smooth functions **Schwarz' theorem** states that the order in which partial derivatives are taken does not matter:[2]

$$\partial^2_{i,j} f(\mathbf{x}) = \partial_{x^i}\partial_{x^j} f(\mathbf{x}) = \partial_{x^j}\partial_{x^i} f(\mathbf{x}) = \partial^2_{j,i} f(\mathbf{x}), \qquad (f \text{ 'smooth'}). \tag{C32}$$

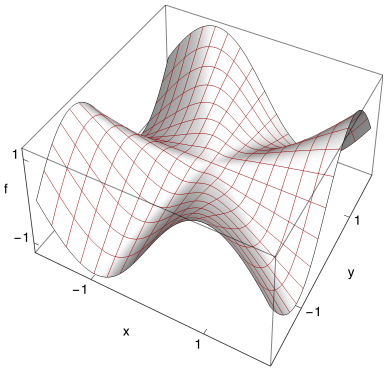
For example (→ C3.2.1-2),

$$\partial^2_{x,y} \cos(x\mathrm{e}^y) = \partial_x\big(-\sin(x\mathrm{e}^y)x\mathrm{e}^y\big) = -\cos(x\mathrm{e}^y)x\mathrm{e}^{2y} - \sin(x\mathrm{e}^y)\mathrm{e}^y,$$
$$\partial^2_{y,x} \cos(x\mathrm{e}^y) = \partial_y\big(-\sin(x\mathrm{e}^y)\mathrm{e}^y\big) = -\cos(x\mathrm{e}^y)x\mathrm{e}^{2y} - \sin(x\mathrm{e}^y)\mathrm{e}^y.$$

In physics, multiple partial derivatives appear frequently and changes in the order of derivatives are applied to simplify calculations or even prove statements. However, it is important to remember that such operations rely on the smoothness condition and that there exist (few) treacherous functions which look smooth but are not (in the sense of the definition on p. 199). In such cases, the exchange of derivatives may be invalid:

EXAMPLE Consider the function

$$f(x,y) = \begin{cases} \frac{xy(x^2-y^2)}{x^2+y^2}, & (x,y) \neq (0,0), \\ 0, & (x,y) = (0,0), \end{cases}$$



The function looks smooth and is partially differentiable everywhere. However, at $(x,y) = (0,0)$ the partial derivatives do not commute: $\partial_x\partial_y f\big|_{(0,0)} \neq \partial_y\partial_x f\big|_{(0,0)}$ (check this). This signifies that the smoothness conditions required by Schwarz' theorem are not given. In mathematics, it is good practice to check the required criteria *before* a derivative is carried out. Physicists tend to be more cavalier and assume the commutativity of derivatives. This approach becomes dangerous in the (admittedly very rare) cases where functions look smooth, but are not in a mathematical sense. Premature differentiation may then lead to errors, which, however, are generally easy to track.

[2] Actually, Schwarz' theorem does not require smoothness but the weaker condition that all second order partial derivatives $\partial^2_{i,j} f$ be *continuous* at $\mathbf{x}$.

C3.3 Chain rule for functions of several variables

In physics one frequently encounters situations in which a multivariate function $f(\mathbf{g}) = f(g^1, \ldots, g^d)$ depends on a parameter variable, x, indirectly via the dependence $g^i = g^i(x)$ of its arguments on x. For example, the pressure, $P(V,T)$, of a gas in a piston depends on the available volume, V, and temperature, T. This dependence may become time dependent, $P(t) = P(V(t), T(t))$, if temperature, $T(t)$, and pressure, $P(t)$, vary in time. In such cases, it is natural to ask how the composite function $f\big(\mathbf{g}(x)\big)$ varies with x. The answer to this question is provided by a generalization of the chain rule to be introduced in this section.

An auxiliary relation

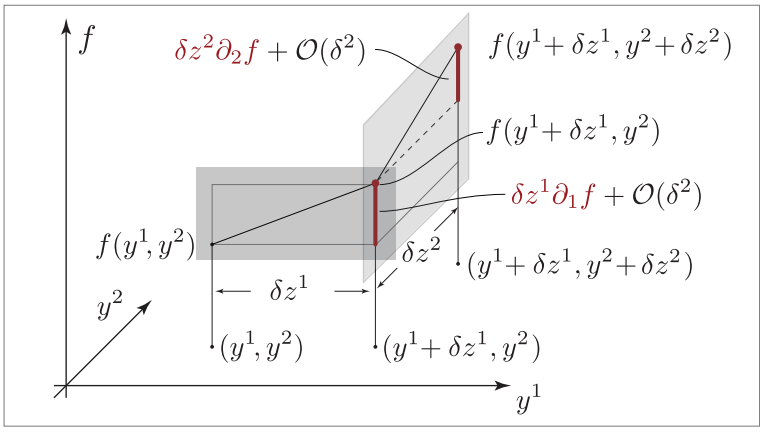


Figure C4: The qualitative picture behind the relation (C35), illustrated in $d = 2$ dimensions. Discussion, see text.

We first ask how a function $f(\mathbf{y}) = f(y^1, \ldots, y^d)$ changes under the simultaneous variation of *all* its arguments, $\mathbf{y} \to \mathbf{y} + \delta\mathbf{z}$, where $\mathbf{z} \in \mathbb{R}^d$ is arbitrary and δ is infinitesimal. Before answering this question in general, let us consider a function depending on just two arguments, $d = 2$. In this case, the rate of change is described by the difference quotient, $\frac{1}{\delta}\left[f(y^1 + \delta z^1, y^2 + \delta z^2) - f(y^1, y^2)\right]$. We aim to reduce this expression to one containing the more familiar difference quotients of ordinary derivatives in single variables. This can be achieved by the insertion of $0 = -f(y^1 + \delta z^1, y^2) + f(y^1 + \delta z^1, y^2)$. In this way, the difference quotient becomes

$$\begin{aligned}
&\frac{1}{\delta}\left[f(y^1 + \delta z^1, y^2 + \delta z^2) - f(y^1, y^2)\right] \\
&= \frac{1}{\delta}\left[f(y^1 + \delta z^1, y^2 + \delta z^2) - f(y^1 + \delta z^1, y^2)\right] + \frac{1}{\delta}\left[f(y^1 + \delta z^1, y^2) - f(y^1, y^2)\right] \\
&\overset{(C30)}{\simeq} z^2 \frac{\partial f(y^1 + \delta z^1, y^2)}{\partial y^2} + z^1 \frac{\partial f(y^1, y^2)}{\partial y^1} \xrightarrow{\delta \to 0} z^2 \frac{\partial f(y^1, y^2)}{\partial y^2} + z^1 \frac{\partial f(y^1, y^2)}{\partial y^1}.
\end{aligned} \tag{C33}$$

Here, the second term probes the function's increment when its first argument y^1 changes to $y^1+\delta z^1$, at fixed y^2. Similarly, the first term probes the function's increment when its second argument y^2 changes to $y^2+\delta z^2$, at fixed $y^1+\delta z^1$. Figure C4 visualizes this decomposition of the full increment into two separate contributions, indicated by thick vertical lines.

In the first equality of the third line, the two increments are expressed by the corresponding partial derivatives, taken at $y^1+\delta z^1$ and y^2, respectively. Finally, f was assumed to be smooth, and so $\partial_{y^2} f$ is likewise smooth. In particular, it is continuous. This implies $\lim_{\delta\to 0}\partial_{y^2} f(y^1+\delta z^1, y^2) = \partial_{y^2} f(y^1, y^2)$, i.e. in the limit of infinitesimal δ the slight shift in the evaluation point of the partial derivative does not matter, and this point is made in the final equality. Similar lines of reasoning will be applied in several other cases below. Before reading on, make sure that you understand the logic of the construction above well.

The construction immediately generalizes to functions depending on more than two arguments and the result then reads

$$\boxed{\lim_{\delta\to 0}\frac{1}{\delta}\big[f(\mathbf{y}+\delta\,\mathbf{z})-f(\mathbf{y})\big]=\sum_{j=1}^{d}\frac{\partial f(\mathbf{y})}{\partial y^j}z^j.} \tag{C34}$$

This identity states that the net change of the function is obtained by computing its partial derivatives, ∂_{y^i}, in the directions of the individual variables, weighting each with the component of the increment vector, z^i, and adding up.

A version of this formula describing the 'linearization' of f in small yet not necessarily infinitesimal variations of δ reads

$$f(\mathbf{y}+\delta\,\mathbf{z})-f(\mathbf{y})\simeq\sum_{j=1}^{d}\frac{\partial f(\mathbf{y})}{\partial y^j}\delta z^j. \tag{C35}$$

Notice how relation this equation embodies the essence of differentiation: the local structure of a function, i.e. the difference of function values between nearby points on the l.h.s., can is approximately described by a function that is linear in the argument displacements, $\propto \delta z^i$. The linearization on the r.h.s. is the higher-dimensional analogue of the straight line of figure C1.

Chain rule

Let us now turn back to the setting mentioned in the beginning of the section and consider the composite function (cf. Fig. C5)

$$f\circ\mathbf{g}:\mathbb{R}\to\mathbb{R},\quad x\mapsto f\big(\mathbf{g}(x)\big)=f\big(g^1(x),\ldots,g^d(x)\big)\equiv f(x),$$

where $\mathbf{g}:\mathbb{R}\to\mathbb{R}^d$, $x\mapsto\mathbf{g}(x)=\big(g^1(x),\ldots,g^d(x)\big)$ defines the dependence of the arguments on a single parameter x. Notice that the dependence $x\mapsto f(x)$ defines an ordinary real-valued function of a single variable and so it must be possible to compute the derivative $\mathrm{d}_x f(x)$. We compute this derivative by explicit linearization of the functions involved in the process:

$$\frac{\mathrm{d}f\big(\mathbf{g}(x)\big)}{\mathrm{d}x}=\lim_{\delta\to 0}\frac{1}{\delta}\Big[f\big(\mathbf{g}(x+\delta)\big)-f\big(\mathbf{g}(x)\big)\Big]=\lim_{\delta\to 0}\frac{1}{\delta}\Big[f\big(\mathbf{g}(x)+\delta\,\mathrm{d}_x\mathbf{g}(x)\big)-f\big(\mathbf{g}(x)\big)\Big],$$

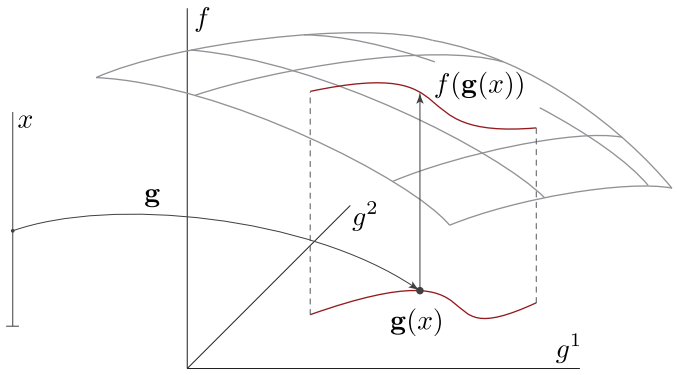


Figure C5: Geometric description relevant to the discussion of the chain rule illustrated for $n = 2$. Discussion, see text.

where in the last step we used $g^j(x+\delta) = g^j(x)+\delta\,\frac{g^j(x)}{\mathrm{d}x}$, and introduced the shorthand notation $\mathrm{d}_x\mathbf{g} \equiv \left(\frac{\mathrm{d}g^1}{\mathrm{d}x}, \ldots, \frac{\mathrm{d}g^d}{\mathrm{d}x}\right)^T$. We may now apply Eq. (C34) with the identifications $\mathbf{y} = \mathbf{g}(x)$ and $\mathbf{z} = \mathrm{d}_x\mathbf{g}(x)$ to obtain

$$\boxed{\frac{\mathrm{d}f\big(\mathbf{g}(x)\big)}{\mathrm{d}x} = \sum_{j=1}^{d} \frac{\partial f(\mathbf{y})}{\partial y^j}\Big|_{\mathbf{y}=\mathbf{g}(x)} \frac{\partial g^j(x)}{\mathrm{d}x} = \sum_{j=1}^{d} \frac{\partial f\big(\mathbf{g}(x)\big)}{\partial g^j} \frac{\partial g^j(x)}{\mathrm{d}x},} \tag{C36}$$

where the right-most expression defines a shorthand for the middle one. This is one of various versions of a **chain rule for a function of several variables**. The rationale underlying this formula is similar to that of the ordinary chain rule Eq. (C7):

> The change of a function $f\big(\mathbf{g}(x)\big)$ under variations of the argument x multiplicatively depends on both the change of $f(\mathbf{g})$ with g^j and the change of $g^j(x)$ with x. The total rate changes in the different variables, $\partial_{g^j} f \partial_x g^j$, need to be added to obtain the full variation as in Eq. (C36).

EXAMPLE Chain rules appear frequently in **physical applications**. Consider, for example, a mobile particle in a volume with nontrivial temperature profile, $T(\mathbf{x})$. The trajectory of the particle is described by a curve $\mathbf{r}(t)$ and the instantaneous ambient temperature 'felt' by the particle at time t is $T(\mathbf{r}(t))$. The rate of change in temperature with time is described by the derivative $\frac{\mathrm{d}T(\mathbf{r}(t))}{\mathrm{d}t}$, for which Eq. (C36) yields

$$\frac{\mathrm{d}T(\mathbf{r}(t))}{\mathrm{d}t} = \sum_{j=1}^{3} \frac{\partial_j T(\mathbf{r}(t))}{\partial r^j} \frac{\mathrm{d}r^j(t)}{\mathrm{d}t}.$$

Generalized chain rules

The chain rule has two extensions which straightforwardly follow from Eq. (C36). The **first generalization** replaces the scalar function f by a vectorial function

$$\mathbf{f} : \mathbb{R}^d \to \mathbb{R}^m, \qquad \mathbf{y} \mapsto \mathbf{f}(\mathbf{y}) = \big(f^1(\mathbf{y}), \ldots, f^m(\mathbf{y})\big).$$

This function may be composed with the function $\mathbf{g}(x)$ to yield $\mathbf{f} \circ \mathbf{g} : \mathbb{R} \to \mathbb{R}^m, x \mapsto \mathbf{f}(\mathbf{g}(x))$. The chain rule (C36) applies to each component $f^i(\mathbf{g}(x))$ separately. Using the vectorial notation

$$\frac{\mathrm{d}\mathbf{f}}{\mathrm{d}x} \equiv \left(\frac{\mathrm{d}f^1}{\mathrm{d}x}, \ldots, \frac{\mathrm{d}f^m}{\mathrm{d}x}\right)^T, \qquad \frac{\partial \mathbf{f}}{\partial y_j} \equiv \left(\frac{\partial f^1}{\partial y_j}, \ldots, \frac{\partial f^m}{\partial y_j}\right)^T, \tag{C37}$$

etc., we may the generalized chain rule as

$$\boxed{\frac{\mathrm{d}\mathbf{f}(\mathbf{g}(x))}{\mathrm{d}x} = \sum_{j=1}^{d} \frac{\partial \mathbf{f}(\mathbf{g})}{\partial g^j} \frac{\mathrm{d}g^j(x)}{\mathrm{d}x}.} \tag{C38}$$

To formulate the **second generalization** we introduce a function $\mathbf{g}(\mathbf{x})$ of $n > 1$ variables x^k,

$$\mathbf{g} : \mathbb{R}^n \to \mathbb{R}^d, \qquad \mathbf{x} \mapsto \mathbf{g}(\mathbf{x}) = \big(g^1(x^1, \ldots, x^n), \ldots g^d(x^1, \ldots, x^n)\big)^T,$$

and compose it with $\mathbf{f}$ to yield

$$\mathbf{f} \circ \mathbf{g} : \mathbb{R}^n \to \mathbb{R}^m, \qquad \mathbf{x} \mapsto \mathbf{f}\big(\mathbf{g}(\mathbf{x})\big) = \mathbf{f}\big(g^1(x^1, \ldots, x^n), \ldots, g^d(x^1, \ldots, x^n)\big)\,.$$

We may now ask how the component f^i changes if one variable x^k is varied while all others are kept fixed. By definition, this amounts to taking the partial derivative $\partial_{x^k} f^i$. Remembering that this is just an ordinary derivative in x^k taken at fixed $x^{l \neq k}$ Eq. (C38) may be applied to obtain (→ C3.3.1-2)

$$\boxed{\frac{\partial \mathbf{f}\big(\mathbf{g}(\mathbf{x})\big)}{\partial x^k} = \sum_{j=1}^{d} \frac{\partial \mathbf{f}\big(\mathbf{g}(\mathbf{x})\big)}{\partial g^j} \frac{\partial g^j(\mathbf{x})}{\partial x^k}\,.} \tag{C39}$$

INFO As an **example application** consider a jet engine whose output power $W(T, P)$ depends on both the temperature, T, and the pressure, P, in the combustion chamber. These two quantities in turn depend on the fuel injection rate, κ, and the chamber volume, V. The task is to optimize the function $W(T(\kappa, V), P(\kappa, V))$ with respect to κ and V. To this end, one needs to know the partial derivatives $\partial_\kappa W$ and $\partial_V W$ (here $m = 1$, $n = 2$, $d = 2$). Application of Eq. (C39) yields

$$\partial_\kappa W = \partial_T W\, \partial_\kappa T + \partial_P W\, \partial_\kappa P, \qquad \partial_V W = \partial_T W\, \partial_V T + \partial_P W\, \partial_V P,$$

where we have used shorthand notations for the partial derivatives, $\partial_T = \frac{\partial}{\partial_T}$, etc. An optimization procedure would now seek points where these derivatives vanish, i.e. configurations where the adjustable parameters are such that the engine output is at an extremum.

EXERCISE Consider the two functions

$$\mathbf{f}(y^1, y^2) = \begin{pmatrix} y^1 \cos(y^2) \\ y^1 \sin(y^2) \end{pmatrix}, \qquad \mathbf{g}(x^1, x^2) = \begin{pmatrix} ((x^1)^2 + (x^2)^2)^{1/2} \\ \arctan(x^2/x^1) \end{pmatrix}.$$

Show that $\dfrac{\partial f^i(g^1(x^1, x^2), g^2(x^1, x^2))}{\partial x^j} = \delta^i{}_j$. How would you interpret this result?

C3.4 Summary and Outlook

In this chapter we introduced partial differentiation as a means to probe the variation of multivariate functions. Partial derivatives monitor the rate at which such functions change if just one of their arguments is varied, and all others are kept fixed. All rules of ordinary differentiation are equally applicable to partial derivatives. The same goes for the interpretation of derivatives as effective linearizations of functions. The application of this idea to functions with indirect variable dependences led to higher-dimensional variants of the chain rule, the most general one being Eq. (C39). These rules are required to describe the change of functions depending on multiple, mutually correlated variables.

Partial derivatives are the workhorses used to break down even very complex derivatives down to manageable 'ordinary derivatives' in individual scalar variables. They are easy to get used to, not least because they appear on a daily basis in the work of any physicist. Much like ordinary derivatives are 'dual' to integrals over single variables, partial derivatives are dual to repeated integrations over several variables. In the next chapter, we introduce this first extension of one-dimensional integrals, which will then become the basis of the more general multi-dimensional integrals discussed in later parts of the text.

C4 Multi-dimensional integration

In physics, one often needs to integrate ('sum') over the values of functions defined in higher-dimensional spaces. A cartoon of the general situation has been discussed in section C2.1 where we asked how the total mass carried by a surface coated with a substance of a given 'mass density' can be obtained. More generally, integration problems arise when the many incremental changes accumulated by a function in a given context (differentiation) need to be resummed (integration) to obtain the change of the function at large. In one dimensional contexts, this task is achieved by the highschool variant of integration which effectively samples the area enclosed by the graph of a function. Building on the understanding of this procedure we here discuss the extension of integration to higher dimensions.

Higher-dimensional integration theory is a subject of considerable depth and needs to be introduced with an appropriate level of care. At the same time, many beginning physics students face the situation that multi-dimensional integration techniques are required early on in the (experimental) physics curriculum. We have therefore decided to include a fast track to integration into this chapter. It provides a pragmatic introduction to the integrals generally required by first and second term experimental physics lecture courses, integration over functions defined in two-dimensional and three-dimensional space, and on two-dimensional surfaces. These integrals are under control after the reading of sections C4.1 and the first subsection in each of C4.2, C4.3 and C4.4 respectively. However, we emphasize that these text snippets do not treat integration at the level of depth required in later stages of the curriculum; students should return to reading the chapter in full after they went through the crash course.

C4.1 Cartesian area and volume integrals

Integrals over higher-dimensional structures can always be reduced to successions of one-dimensional integrals. This reduction is best introduced on the example of 'cuboids' — rectangles in two-dimensional space, boxes in three-dimensional space, etc. Once the principles are understood, the extension to the more complex integrals discussed in later parts of the chapter will be straightforward.

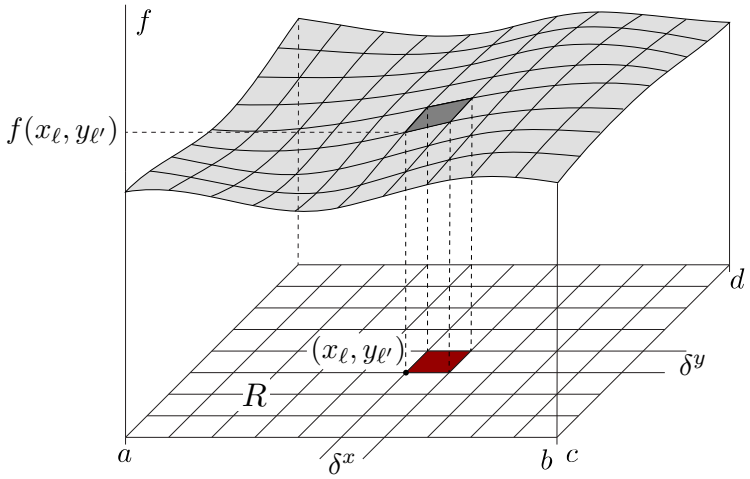


Figure C6: On the concept of two-dimensional integration over a function.

Integration over rectangles

Consider a function of two variables defined on a rectangle, $R = [a, b] \times [c, d]$:[1]

$$f : [a, b] \times [c, d] \subset \mathbb{R}^2 \to \mathbb{R}, \qquad (x, y)^T \mapsto f(x, y) : \tag{C40}$$

In physical applications, f will usually represent some kind of 'density'. For example, it might be a mass density in the sense that $f(x, y)\delta^x\delta^y$ represents the mass of a substance contained in a small rectangle with area $\delta^x\delta^y$ at the point $(x, y)^T$. In this case, the integral would compute the total mass contained in the full rectangle R. In the visualization in Fig. C6, the mass contained in such a small is represented by the volume of the column above that rectangle, and the total mass by the volume under the floating surface defined by $f(x, y)$.

Following the discussion of section C2.1, we tile the rectangle R by a set of infinitesimal rectangular cells and then sum the contributions of all cells. The summation procedure is set up by dividing the interval $[a, b]$ into N_x bins of infinitesimal width $\delta^x = (b-a)/N_x$, and similarly for the interval $[c, d]$, with $\delta^y = (d-c)/N_y$. Next, the function values are read out as $f(x_\ell, y_{\ell'})$ where x_ℓ and $y_{\ell'}$ lie in the ℓth x-bin and ℓ'th y-bin, respectively. The exact positioning of these coordinates within the bins is not essential (cf. the analogous discussion in section C2.2). For example, $x_\ell = \ell\delta^x$ with $\ell = 0, \ldots, N_x-1$, and $y_{\ell'} = \ell'\delta^y$ with $\ell' = 0, \ldots, N_y-1$, will do the job. One may now sum over $f(x_\ell, y_{\ell'})\delta^x\delta^y$ and in the limit $\delta^x, \delta^y \to 0$ obtains the **two-dimensional integral** as

$$\boxed{\int_R \mathrm{d}x\mathrm{d}y\, f(x, y) \equiv \lim_{\delta^x, \delta^y \to 0} \delta^x\delta^y \sum_\ell \sum_{\ell'} f(x_\ell, y_{\ell'}).} \tag{C41}$$

[1] Referring to the definition of Cartesian products of sets Eq. (L1), the rectangle is defined as the set of points $[a, b] \times [c, d] \equiv \{(x, y) | x \in [a, b], y \in [c, d]\}$.

This construction not only defines the integral but also contains the recipe for its **practical computation**: In the limit $\delta^y \to 0$, at fixed δ^x and fixed first coordinate x_ℓ the integral converges to a one-dimensional integral of the function $f(x_\ell, y)$ over y,

$$\lim_{\delta^y \to 0} \delta^y \sum_{\ell'} f(x_\ell, y_{\ell'}) = \int_c^d \mathrm{d}y\, f(x_\ell, y) \equiv I(x_\ell),$$

whose value $I(x_\ell)$ depends on the value of x_ℓ. The insertion of $I(x_\ell)$ into the remaining sum, followed by a limit $\delta^x \to 0$ leads to another one-dimensional integral, now over x: $\lim_{\delta^x \to 0} \delta^x \sum_\ell I(x_\ell) = \int_a^b \mathrm{d}x\, I(x)$. We conclude that the area integral is given by

$$\int_R \mathrm{d}x\, \mathrm{d}y\, f(x,y) = \int_a^b \mathrm{d}x \int_c^d \mathrm{d}y\, f(x,y) = \int_c^d \mathrm{d}y \int_a^b \mathrm{d}x\, f(x,y), \tag{C42}$$

where $\int \mathrm{d}y f(x,y)$ means 'integrate $f(x,y)$ over the second argument, y, at a fixed value of the first argument, x'. The second equality holds since the construction above could have been formulated in the reverse order — first integrate over x, then over y.

EXAMPLE As an example, consider the function $f : [0,2] \times [0,1] \to \mathbb{R}, (x,y) \mapsto f(x,y) = xy + y^2$. It can be integrated in either order to obtain identical results:

$$\int_0^2 \mathrm{d}x \int_0^1 \mathrm{d}y\, f(x,y) = \int_0^2 \mathrm{d}x \Big[\tfrac{1}{2}y^2 x + \tfrac{1}{3}y^3\Big]_0^1 = \int_0^2 \mathrm{d}x \Big(\tfrac{1}{2}x + \tfrac{1}{3}\Big) = \Big[\tfrac{1}{4}x^2 + \tfrac{1}{3}x\Big]_0^2 = \tfrac{5}{3},$$
$$\int_0^1 \mathrm{d}y \int_0^2 \mathrm{d}x\, f(x,y) = \int_0^1 \mathrm{d}y \Big[\tfrac{1}{2}x^2 y + xy^2\Big]_0^2 = \int_0^1 \mathrm{d}y \Big(2y + 2y^2\Big) = \Big[y^2 + \tfrac{2}{3}y^3\Big]_0^1 = \tfrac{5}{3}.$$

The fact that the order of integration does not matter is known as **Fubini's theorem**. Generally speaking, integrals are defined as Riemann sums over the cells tiling the integration domains. Due to the commutativity of addition the order in which one sums over these is arbitrary. This statement holds for all types of integrals to be discussed in subsequent chapters.

INFO Apart from rare exceptions, Fubini's theorem holds if the double integral over a function, performed in either order, exists. More precisely, the **condition granting Fubini interchangeability** is that $\int_R \mathrm{d}x\mathrm{d}y|f(x,y)|$, i.e. the integral over the *modulus* of the function must exist. To appreciate the relevance of the modulus, consider the function $f(x,y) = (x^2 - y^2)/(x^2 + y^2)^2$. It is straightforward to verify that

$$\int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \frac{x^2 - y^2}{(x^2 + y^2)^2} = \frac{\pi}{4}.$$

However, the integral done in reverse order yields the negative value, $-\pi/4$. To understand what is happening here, notice that for x, y approaching zero while $x > y$ the integrand contains a strong positive divergence. For $x < y$ the divergence is negative. The integrals over the respective regions, $1 \geq x > y \geq 0$ and $0 \leq x < y \leq 1$, do not exist. Likewise, the integral of the modulus $|f(x,y)|$

over the full square, $0 \leq x, y \leq 1$ does not exist either (because in this case the two singularities add). However, doing the double integral over the function itself, we obtain a result of $\infty - \infty$ type, where the two ∞'s come from $x > y$ and $x < y$, respectively. The naive evaluation of the integral tricks one into believing that the difference of the two infinities is finite, either $\pi/4$ or $-\pi/4$, depending on the order in which the x- and y-integrals are performed. However, the sign discrepancy is a manifestation of the fact that the difference of two ∞'s is actually not well defined. While the double integrals make formal sense, they do not represent a well-defined *area* integral.

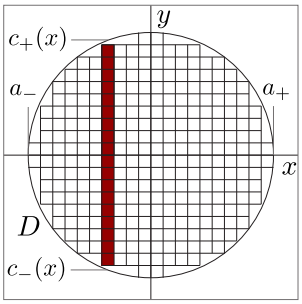
The general message is that before doing an integral one should check that the integral over the modulus of the integrated function exists (cf. discussion on p. 209). If not, one is generally working with an ill-defined expression.

The tiling construction described above can readily be generalized to **integrals over higher-dimensional cuboids**. For example, consider a function $f(x, y, z)$ on $C = [a, b] \times [c, d] \times [e, f] \subset \mathbb{R}^3$. The separate discretization along each dimension divides C into a large number of small cubicles. In the limit, the Riemann sum over all these leads to the triple integral

$$\int_C \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\, f(x, y, z) = \int_a^b \mathrm{d}x \int_c^d \mathrm{d}y \int_\mathrm{e}^f \mathrm{d}z\, f(x, y, z), \tag{C43}$$

where the order of integrations is again arbitrary. The extension to cuboids of higher dimension should be obvious.

Integration over domains with spatially varying boundaries



Many functions of practical interest are defined on non-rectangular domains. Integrals over such functions can often be computed by straightforward adaption of the above strategy: the integration domain is tiled by infinitesimal rectangular cells (or boxes in three-dimensional settings). However, the number of cells in one direction may now depends on the cell index in other directions. For a two-dimensional example, consider the circular disk, D, shown in the figure. In this case, the number of cells in y-direction is largest close to the center of the x-axis at $x_\ell \simeq 0$. As a consequence, the lower and upper summation thresholds for $y_{\ell'}$ now depend on x_ℓ. Let us denote them by $c_-(x_\ell)$ and $c_+(x_\ell)$, respectively, and the lower and upper thresholds for x_ℓ by a_- and a_+. The discrete approximation of the integral then assumes the form

$$\delta^x \delta^y \sum_{a_- \leq x_\ell < a_+} \sum_{c_-(x_\ell) \leq y_{\ell'} < c_+(x_\ell)} f(x_\ell, y_{\ell'}).$$

We take the limit $\delta^x, \delta^y \to 0$ to obtain the integral representation

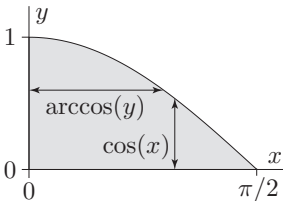
$$\int_D \mathrm{d}x\,\mathrm{d}y\, f(x, y) \equiv \int_{a_-}^{a_+} \mathrm{d}x \int_{c_-(x)}^{c_+(x)} \mathrm{d}y\, f(x, y).$$

Here, the integration boundaries of the 'inner' y-integral, $I(x) = \int_{c_-(x)}^{c_+(x)} \mathrm{d}y\, f(x,y)$, depend on the integration variable of the 'outer' x-integral. However, this is no cause for concern — one simply integrates over y to find $I(x)$, and subsequently over x to obtain $\int_{a_-}^{a_+} \mathrm{d}x\, I(x)$ (→ C4.1.1-6).

EXAMPLE Consider a **disk of radius** R and let us determine its area, A, by integration. In this case, the boundaries $a_\pm = \pm R$ are set by the disk radius and $c_\pm(x) = \pm\sqrt{R^2 - x^2}$. This gives

$$A = \int_{-R}^{R} \mathrm{d}x \int_{-\sqrt{R^2-x^2}}^{\sqrt{R^2-x^2}} \mathrm{d}y\, 1 = 2\int_{-R}^{R} \mathrm{d}x\, \sqrt{R^2 - x^2} = \left[x\sqrt{R^2 - x^2} + R^2 \arctan\left(\frac{x}{\sqrt{R^2 - x^2}} \right) \right]_{-R}^{R}.$$

(The integral can be done using the substitution $x = R\cos u$. Verify the last equality by differentiating the result of the integration.) For $x = \pm R$ the first term on the right vanishes while the argument of the $\arctan$ assumes the value $\pm\infty$. Since $\arctan(\pm\infty) = \pm\frac{\pi}{2}$ we arrive at the expected result $A = \pi R^2$, i.e. the familiar area enclosed by a circle of radius R. Note that the computation appears to be unwieldy; there should be easier ways to obtain the surface of a disk, and we will introduce them in the next section.



Fubini's theorem on the interchangeability of integration orders extends to non-cuboidal integration domains. For example, the above construction for the disk could have been organized in such a way that the integration over x is performed first and that over y second. The freedom to choose the order of integration order becomes relevant when one order is more convenient than the other. As an example, let us apply two-dimensional integration to compute the area enclosed between the curve $y = \cos(x)$ and the x- and y-axes (see figure). Integrating first over y, then x, turns out to be easier than the reverse order:

$$A = \int_0^{\pi/2} \mathrm{d}x \int_0^{\cos(x)} \mathrm{d}y = \int_0^{\pi/2} \mathrm{d}x \cos(x) = \Big[\sin(x)\Big]_0^{\pi/2} = 1,$$
$$A = \int_0^{1} \mathrm{d}y \int_0^{\arccos(y)} \mathrm{d}x = \int_0^{1} \mathrm{d}y \arccos(y) = \Big[-\sqrt{1-y^2} - y\arccos(y)\Big]_0^{1} = 1.$$

C4.2 Curvilinear area integrals

The integration procedure described in the preceding section uses Cartesian coordinates. However, these coordinates are not ideal for the description of integration domains possessing rotational or other symmetries. This is illustrated by the above example, where the integration over a disk in Cartesian coordinates led to cumbersome expressions. In this section we introduce more powerful techniques and learn how to integrate over two-, three- and higher-dimensional structures in arbitrary coordinates.

Describing areas by curvilinear coordinates

REMARK Knowledge of sections V2.1 to V2.4 on curvilinear coordinates is required for this section.

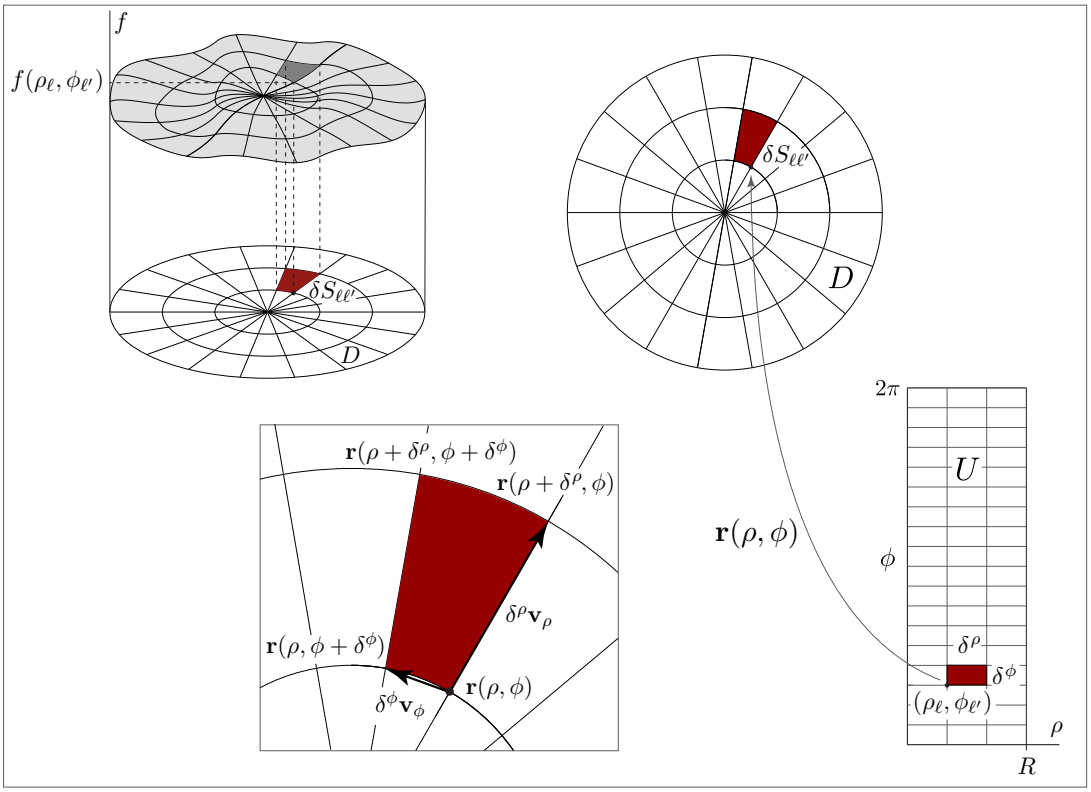


Figure C7: Integration in two dimensions using polar coordinates. A rectangular coordinate domain U (bottom right) is used to parametrize the disk D (top right). This leads to area elements $\delta S_{\ell\ell'}$ shaped like distorted rectangles (bottom left). The integration of a function $f(\rho, \phi)$ over the disk amounts to the summation over these shapes, weighted with the product of the base areas $|\delta S_{\ell\ell'}|$ and the heights $f(\rho_\ell, \phi_{\ell'})$ (top left). The arrows shown in the bottom left panel are defined in Eq. (C46).

Let us turn back to the example of **integration over a circular disk**, D. Again, we start by introducing a discretization grid, however, this time it will be defined such that the symmetries of the integration domain are taken into account. To this end, consider the representation of D in terms of the polar coordinates introduced in section V2.1,

$$\mathbf{r} : U \equiv (0, R) \times (0, 2\pi) \to D, \qquad \mathbf{y} \equiv (\rho, \phi)^T \mapsto \mathbf{r}(\rho, \phi) \equiv (\rho \cos\phi, \rho \sin\phi)^T. \tag{C44}$$

Observe that the circular domain of integration, D, is now parameterized by the rectangular coordinate domain, $U = (0, R) \times (0, 2\pi)$.

INFO As always with curvilinear coordinate descriptions, we take the coordinate domain to be **open**.

This is done to ensure global differentiability of the map, cf. the discussion at the end of section V2.1 (p. 390). The **openness of the coordinate intervals** often implies that an integration domain can be *almost*, but not *fully* covered by a single coordinate map. For example, the image of the map above does not cover the boundary of the disk, where $R = 1$, nor the intersection of the disk with the positive real axis, where $\phi = 0$. However, these excluded regions are of dimension lower than two and their exclusion does not affect a two-dimensional integral over a continuous functions. The heuristic picture behind this statement is that an 'infinitely thin' line does not contribute to the summation over areas. A more formal justification of this statement will be given in the context of Eq. (C52) below. In the following, what we mean when we say that a d-dimensional integration domain, M, is covered by a system of coordinates is that the coordinates parameterize all of M, except perhaps for subsets of lower dimension. For completeness, we mention that situations where the full coverage of a domain by coordinates is essential are addressed in chapter **??**.

We now introduce a set of points, $\{(\rho_\ell, \phi_{\ell'})^T\}$, $\rho_\ell = \ell\delta^\rho$, $\phi_{\ell'} = \ell'\delta^\phi$, $0 \le \ell \le R/\delta^\rho$, $0 \le \ell' \le 2\pi/\delta^\phi$, defining the corners of a system of rectangular cells of area $\delta^\rho\delta^\phi$ covering U. The coordinate map $\mathbf{r}(\rho, \phi)$ sends this rectangular grid onto a 'distorted grid' of image points, $\mathbf{r}(\rho_\ell, \phi_{\ell'})$, whose corners define a set of area elements, $\delta S_{\ell\ell'}$, in D. These have the shape of 'distorted rectangles' tiling D in a spider-web pattern, as illustrated in Fig. C7. The covering generated in this fashion reflects the rotational symmetry of the disk — a key advantage relative to the Cartesian grid of p. 227.

Geometrically distorted area elements

The strategy just described is not limited to polar coordinates. Integration over non-rectangular domains often starts with a coverage generated by curvilinear coordinates. All steps that follow then are of general nature and it therefore makes sense to introduce them for a generic two-dimensional coordinate system, $\mathbf{r} : U \to M$, $\mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$. In the end of the section we will turn back to polar coordinates, $\mathbf{y} = (\rho, \phi)^T$ and $M = D$, and do specific integrals over the disk.

Let us denote the points of a tiling grid in U by $\mathbf{y}_{\ell\ell'} \equiv (y^1_\ell, y^2_{\ell'})^T \equiv (\ell\delta^1, \ell'\delta^2)^T$ and let $\mathbf{r}(\mathbf{y}_{\ell\ell'})$ define the induced grid in M. The integral of a function, $f : M \to \mathbb{R}$, $\mathbf{r} \mapsto f(\mathbf{r})$ over M is then define as the Riemann sum over the area elements,

$$\int_M \mathrm{d}S\, f(\mathbf{r}) \equiv \lim_{\delta^1, \delta^2 \to 0} \sum_{\ell\ell'} |\delta S_{\ell\ell'}| f(\mathbf{y}_{\ell\ell'}), \tag{C45}$$

where the notation $f(\mathbf{y}) \equiv f(\mathbf{r}(\mathbf{y}))$ is used and $|\delta S_{\ell\ell'}|$ is the geometric area of the surface element $\delta S_{\ell\ell'}$. If f represents the density of a quantity such as mass, then the summand $|\delta S_{\ell\ell'}| f(\mathbf{y}_{\ell\ell'})$ gives the amount of this quantity associated with that area element.

Eq. (C45) remains formal as long as the dependence of the area elements $|\delta S_{\ell\ell'}|$ on the coordinate points $\mathbf{y}_{\ell\ell'}$ has not been specified. To this end, we temporarily suppress the indices ℓ, ℓ' and note that an element δS labeled by $\mathbf{y}$ is defined by the four corner points $\mathbf{r}(y^1, y^2)$, $\mathbf{r}(y^1 + \delta^1, y^2)$, $\mathbf{r}(y^1 + \delta^1, y^2 + \delta^2)$ and $\mathbf{r}(y^1, y^2 + \delta^2)$. These points are connected by the corresponding coordinate lines (see Fig. C7). What simplifies the computation of the enclosed

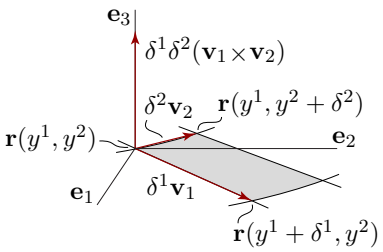
area is the proximity of the corner points to each other: in the limit of infinitesimally small δ^1 and δ^2, the curvature of the coordinate lines between the points becomes negligibly small and the shape of δS approaches that of a *parallelogram* spanned by the two vectors

$$\begin{aligned}\mathbf{r}(y^1+\delta^1,y^2)-\mathbf{r}(y^1,y^2) &\simeq \delta^1\,\partial_{y^1}\mathbf{r}(\mathbf{y}) = \delta^1\,\mathbf{v}_1(\mathbf{y}),\\ \mathbf{r}(y^1,y^2+\delta^2)-\mathbf{r}(y^1,y^2) &\simeq \delta^2\,\partial_{y^2}\mathbf{r}(\mathbf{y}) = \delta^2\,\mathbf{v}_2(\mathbf{y}).\end{aligned} \tag{C46}$$

In the last equalities of each line we noted that (cf. section V2.3) the tangent vectors to the coordinate lines, $\partial_{y^i}\mathbf{r}$, equal the basis vectors, $\mathbf{v}_i$, of the coordinate basis. The vectors spanning δS are thus given by the scaled basis vectors $\delta^1\mathbf{v}_1$ and $\delta^2\mathbf{v}_2$ and $|\delta S|$ is the area of the corresponding parallelogram.

There are three different ways to describe the geometric area of this particular parallelogram. All have advantages and we will discuss them in turn. The first approach is based on elementary geometry and suffices for a first introduction to the subject. The other two formulations are more general and distinctly more powerful. They are introduced in the next subsection, where integration in two dimensions is discussed from a general perspective.

Area element from geometric construction



The first approach describes the **area element by geometric construction**. The area of the parallelogram spanned by two vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ enclosing an angle $\angle(\mathbf{v}_1,\mathbf{v}_2)$ is given by $A(\mathbf{v}_1,\mathbf{v}_2) = \|\mathbf{v}_1\|\|\mathbf{v}_2\|\sin(\angle(\mathbf{v}_1,\mathbf{v}_2))$. Using Eq. (L73), this may be rewritten as $\|\mathbf{v}_1\times\mathbf{v}_2\|$. (The latter notation implicitly assumes that the vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ span a two-dimensional plane in three-dimensional space, see the figure. Their cross product, $\mathbf{v}_1\times\mathbf{v}_2$, then points in the 3-direction perpendicular to the plane and its norm gives the required parallelogram area.) In this notation, the area of δS is expressed as

$$|\delta S| \simeq \delta^1\delta^2\,A(\mathbf{v}_1,\mathbf{v}_2) = \delta^1\delta^2\,\|\mathbf{v}_1\times\mathbf{v}_2\| = \delta^1\delta^2\,\|\partial_{y^1}\mathbf{r}(\mathbf{y})\times\partial_{y^2}\mathbf{r}(\mathbf{y})\|. \tag{C47}$$

It remains to substitute this expression into Eq. (C45) and perform the summation over indices ℓ,ℓ'. In the limit of an infinitely fine discretization, each sum $\delta\sum_\ell \to \int \mathrm{d}y$ becomes an integral over a coordinate interval. The Riemann sum thus assumes the form of a double integral,

$$\int_M \mathrm{d}S\,f(\mathbf{r}) = \int_U \mathrm{d}y^1\mathrm{d}y^2\,\|\partial_{y^1}\mathbf{r}(\mathbf{y})\times\partial_{y^2}\mathbf{r}(\mathbf{y})\|\,f(\mathbf{y}). \tag{C48}$$

Note that the final integral extends over a rectangular coordinate domain and hence falls into the category of integrals discussed in the previous chapter. The geometric distortion of the coordinate lines in the image domain, M, enters through the factor $\|\partial_{y^1}\mathbf{r}\times\partial_{y^2}\mathbf{r}\|$. This factor mediates between the *rectangular* shape of the coordinate cells in U (convenient for integration) and the *distorted* shape of the image cells in M (convenient for tiling a general integration area). The formal expression

$$\mathrm{d}S = \mathrm{d}y^1\mathrm{d}y^2\,\|\partial_{y^1}\mathbf{r}(\mathbf{y})\times\partial_{y^2}\mathbf{r}(\mathbf{y})\| \tag{C49}$$

is sometimes called the **area element** or the **integration measure** of two-dimensional integration. The latter terminology refers to the right-hand side of the defining equation as a 'measure' of geometric areas in the integration domain.[2] In the following, we will refer to both $\mathrm{d}S$ and its finite analogue δSas 'area elements'.

The result (C48) also shows why the **assumed openness of the coordinate domain** does not matter. For a rectangular open domain $U = (a, b) \times (c, d)$, the double integral becomes $\int_U \mathrm{d}y^1 \mathrm{d}y^2 = \int_a^b \mathrm{d}y^1 \int_c^d \mathrm{d}y^2$. However, as discussed in section C2.2, integrals over open and closed intervals yield the same values, i.e. the same expression would be obtained for the integration over product of intervals, $[a, b] \times [c, d]$ parameterizing a closed coordinate domain.

Integration in polar coordinates

Let us now return to **polar coordinates** and evaluate the expressions above in that concrete context. Eq. (C47) applied to the coordinate basis vectors (V28) of the polar coordinate system, $\mathbf{v}_\rho = \partial_\rho \mathbf{r} = \mathbf{e}_\rho$ and $\mathbf{v}_\phi = \partial_\phi \mathbf{r} = \mathbf{e}_\phi \rho$, yields

$$\|\partial_{y^1} \mathbf{r}(\mathbf{y}) \times \partial_{y^2} \mathbf{r}(\mathbf{y})\| = \|\mathbf{v}_\rho \times \mathbf{v}_\phi\| = \rho, \tag{C50}$$

and the **polar area element**

$$\boxed{\mathrm{d}S = \rho \, \mathrm{d}\rho \, \mathrm{d}\phi.} \tag{C51}$$

The proportionality to ρ means that the area element *increases* in the radial direction. The geometric reason is that the extension of δS in the ϕ-direction, given by $\rho \, \delta^\phi$, increases linearly with the radial coordinate (see Fig. C7). Substituting this result into Eq. (C48), we obtain

$$\int_D \mathrm{d}S \, f(\mathbf{r}) = \int_0^R \mathrm{d}\rho \int_0^{2\pi} \mathrm{d}\phi \, \rho \, f(\rho, \phi) \tag{C52}$$

as a formula for the **integration in polar coordinates** over the disk D.

EXAMPLE Turning back to the example on p. 228, the **geometric area of a circular disk** of radius R is now simply obtained by integrating the constant function $f(\mathbf{r}) = 1$ over the disk D:

$$A = \int_0^R \rho \, \mathrm{d}\rho \int_0^{2\pi} \mathrm{d}\phi \, 1 = \int_0^R \rho \, \mathrm{d}\rho \, 2\pi = \pi R^2.$$

This computation is simpler and more elegant than its Cartesian counterpart of p. 228. The independence of the integration domains of ϕ and ρ implies that the integrals over these variables factorize. This is the essential advantage of polar coordinates over Cartesian coordinates and it is owed to the fact that the former are adjusted to the rotational symmetry of the disk. Polar representations are particularly well-suited for integrating functions which are rotationally symmetric and hence depend

[2] The mathematically precise definition of measures is a subject of 'measure theory'. However, we do not enter this discussion here.

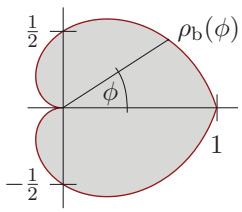
only on the radial coordinate, $f(\rho,\phi) = f(\rho)$. Consider, for example, a surface carrying a mass density increasing quadratically with the distance from the origin, $\rho_{\mathrm{m}}(\rho) = \kappa\rho^2$, where κ is a constant. The total mass carried by the surface is obtained by integration:

$$M = \int_D \mathrm{d}S\, \rho_{\mathrm{m}}(\rho) = \int_0^R \rho\,\mathrm{d}\rho \int_0^{2\pi} \mathrm{d}\phi\, \kappa\rho^2 = \int_0^R \rho\,\mathrm{d}\rho\,(2\pi\kappa\rho^2) = \tfrac{1}{2}\pi\kappa R^4.$$

The analogous calculation in Cartesian coordinates would be significantly harder.

The result (C52) may be straightforwardly generalized to the **integration over domains without rotational symmetry** (→ C4.2.1-2). For example, the integral of a function $f(\mathbf{r})$ over the quarter of a disc, parameterized as $\{\mathbf{r}(\rho,\phi)\,|\,\rho\in(0,R),\phi\in(0,\pi/2)\}$, is given by

$$\int_0^R \rho\,\mathrm{d}\rho \int_0^{\pi/2} \mathrm{d}\phi\, f(\rho,\phi).$$



EXAMPLE As a less trivial example, consider the heart-shaped area shown in the figure. For any given angle, $\phi\in(-\pi,\pi)$ the distance from the origin to the boundary of the heart is given by $\rho_{\mathrm{b}}(\phi) = \big(1-|\phi|/\pi\big)$. This means that its area is given by

$$A = \int_{-\pi}^{\pi}\mathrm{d}\phi \int_0^{\rho_{\mathrm{b}}(\phi)} \rho\,\mathrm{d}\rho\, 1 = \int_{-\pi}^{\pi}\mathrm{d}\phi\, \tfrac{1}{2}\rho_{\mathrm{b}}^2(\phi) = \tfrac{1}{2}\int_{-\pi}^{\pi}\mathrm{d}\phi \left[1-\frac{|\phi|}{\pi}\right]^2 = \tfrac{1}{3}\pi.$$

Jacobian and metric representations of area element

REMARK Requires chapter L6.1 on matrix determinants.

Above we applied geometric reasoning to obtain the area of the surface element δS. We here introduce two different approaches to the same problem which will lead to alternative representations of the area integral. Depending on the context, application of either of these methods can be favorable. An important feature of the procedures introduced in this section is that they afford transparent generalizations to integrals in arbitrary dimensions.

The second method expresses the **area element as a matrix determinant**. To this end assume the presence of a Cartesian basis $\{\mathbf{e}_a\}$ in the integration domain. Adopting the notation of section V2.3, the coordinate image points can then be expanded as $\mathbf{r}(\mathbf{y}) = \mathbf{e}_a x^a(\mathbf{y})$ where the Cartesian expansion coefficients $x^a(\mathbf{y})$ are functions of the coordinates $\mathbf{y}$. The partial derivative of $\mathbf{r}(\mathbf{y})$ in the coordinates y^i yields the expansion of the coordinate basis vectors as $\mathbf{v}_j(\mathbf{y}) = \mathbf{e}_a v^a{}_j(\mathbf{y})$ with components $v^a{}_j = \frac{\partial x^a}{\partial y^j}$, cf. Eq. (V22). The advantage of this Cartesian representation is that the area spanned by the coordinate basis vectors can be expressed through the determinant formula Eq. (L158) (which assumes an expansion in a

Cartesian basis): the area spanned by $\mathbf{v}_1$ and $\mathbf{v}_2$ is given by $A(\mathbf{v}_1, \mathbf{v}_2) = |\det J|$, where the 2×2 matrix $J = (\mathbf{v}_1, \mathbf{v}_2)$ contains the components ${v^a}_j = (\mathbf{v}_j)^a$ as columns. In the present context, where ${v^a}_j = \frac{\partial x^a}{\partial y^j}$, this is often expressed through the suggestive notation

$$\boxed{J \equiv \frac{\partial \mathbf{x}}{\partial \mathbf{y}} \equiv \frac{\partial(x^1, x^2)}{\partial(y^1, y^2)} \equiv \begin{pmatrix} \frac{\partial x^1}{\partial y^1} & \frac{\partial x^1}{\partial y^2} \\ \frac{\partial x^2}{\partial y^1} & \frac{\partial x^2}{\partial y^2} \end{pmatrix},} \tag{C53}$$

where $\mathbf{x}_j = (x^1, x^2)^T$ is the component vector representing $\mathbf{r}$ in the Cartesian basis $\{\mathbf{e}_a\}$. (Keep in mind that all these quantities are functions of the generalized coordinates, $\mathbf{x} = \mathbf{x}(\mathbf{y})$, etc.)

The matrix J is called the **Jacobi matrix** (or just **Jacobian**) of the map $\mathbf{r} : U \to M$, $\mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$. (Confusingly, the determinant $|\det J| = |\det \frac{\partial \mathbf{x}}{\partial \mathbf{y}}|$ is likewise called the **Jacobian** of the map. In cases where unambiguous phrasing is required we will refer to it as the **Jacobi determinant**.) Comparison with Eq. (C47) shows that the area element is given by

$$|\delta S| = \delta^1\delta^2 |\det J| = \delta^1\delta^2 \left|\det\left(\frac{\partial(x^1, x^2)}{\partial(y^1, y^2)}\right)\right| = \delta^1\delta^2 \left|\frac{\partial x^1}{\partial y^1}\frac{\partial x^2}{\partial y^2} - \frac{\partial x^1}{\partial y^2}\frac{\partial x^2}{\partial y^1}\right|. \tag{C54}$$

A straightforward check shows that for polar coordinates, Eq. (C50) is indeed reproduced.

The third approach expresses the **area element via the metric tensor**. Here, the starting point is Eq. (L40) for the parallelogram area,

$$A(\mathbf{v}_1, \mathbf{v}_2) = |\langle \mathbf{v}_1, \mathbf{v}_1\rangle\langle \mathbf{v}_2, \mathbf{v}_2\rangle - \langle \mathbf{v}_1, \mathbf{v}_2\rangle^2|^{1/2} = |g_{11}g_{22} - g_{12}g_{21}|^{1/2} = |\det(g(\mathbf{y}))|^{1/2}, \tag{C55}$$

where in the second step we noted that the scalar products $\langle \mathbf{v}_i, \mathbf{v}_j\rangle \overset{(V24)}{=} g_{ij}(\mathbf{y})$ define the metric tensor, and $\det(g)$ is the determinant of the matrix $\{g_{ij}\}$. We thus obtain

$$|\delta S| = \delta^1\delta^2 |\det(g(\mathbf{y}))|^{1/2}. \tag{C56}$$

This formula expresses the area element through the metric tensor defined by the coordinate basis vectors, $g(\mathbf{y})$. For example, in polar coordinates, Eq. (V25) yields $\sqrt{\det(g(\rho, \phi))} = \sqrt{g_{\rho\rho}g_{\phi\phi}} = \rho$, so that we again arrive at Eq. (C50).

Generally speaking, the metric determinant is the 'strongest' of the three representations discussed above. Unlike the Jacobi determinant, it does not make reference to Cartesian representations of the vectors $\mathbf{v}_1$ and $\mathbf{v}_2$. We will also see in section C4.4 generalizes to integrals for which no Jacobian determinant exists. On the other hand, there are situations where the Jacobian, or the elementary geometric procedure are more convenient than others; it is certainly good to know all three.

Two dimensional area integrals – summary

Summarizing, we now have three representations for the area spanned by $\mathbf{v}_1$ and $\mathbf{v}_2$, and this implies three alternative representations for the integral of a function, Eq. (C48):

$$\int_M \mathrm{d}S\, f(\mathbf{r}) = \int_U \mathrm{d}y^1\mathrm{d}y^2 \left\{ \begin{array}{l} \|\partial_{y^1}\mathbf{r}(\mathbf{y}) \times \partial_{y^2}\mathbf{r}(\mathbf{y})\| \\ \left|\det\left(\frac{\partial(x^1,x^2)}{\partial(y^1,y^2)}\right)\right| \\ |\det(g(\mathbf{y}))|^{1/2} \end{array} \right\} f(\mathbf{r}(\mathbf{y})). \tag{C57}$$

Each of these expresses the curvilinear integration of f over M in terms of

- ▷ an integral over the underlying **coordinate domain**, U,
- ▷ of the **function evaluated in curvilinear coordinates**, $f(\mathbf{r}(\mathbf{y}))$, and
- ▷ any of the **rescaling factors**, $\|\partial_1\mathbf{r} \times \partial_2\mathbf{r}\|$, $\left|\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right|$, $|\det(g(\mathbf{y}))|^{1/2}$, which all represent the geometric area in the integration domain corresponding to an infinitesimal area $\delta^1\delta^2$ in the coordinate domain. This area element generally varies as a function of $\mathbf{y}$.

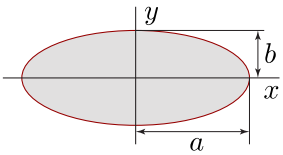
EXAMPLE As an instructive application of the second line of Eq. (C57), consider the integral

$$I \equiv \int_{\mathbb{R}^2} \mathrm{d}x\mathrm{d}y\, f\big((x/a)^2 + (y/b)^2\big)\,.$$

The integrand depends on the Cartesian coordinates $\mathbf{x} \equiv (x, y)^T$ only via the combined variable $\mu^2 \equiv (x/a)^2 + (y/b)^2$. This suggests a coordinate transformation, $\mathbf{x}(\mathbf{y}) = (x(\mathbf{y}), y(\mathbf{y}))^T = (a\mu\cos\phi, b\mu\sin\phi)^T$, to 'generalized polar coordinates', $\mathbf{y} \equiv (\mu, \phi)^T$. Its Jacobi matrix is[3]

$$\frac{\partial \mathbf{x}}{\partial \mathbf{y}} = \frac{\partial(x,y)}{\partial(\mu,\phi)} = \begin{pmatrix} \frac{\partial x}{\partial \mu} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial \mu} & \frac{\partial y}{\partial \phi} \end{pmatrix} = \begin{pmatrix} a\cos\phi & -a\mu\sin\phi \\ b\sin\phi & b\mu\cos\phi \end{pmatrix},$$

with Jacobi determinant $\left|\det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right)\right| = \mu ab$. We may now pass to a (μ, ϕ) integration as



$$I = \int_0^\infty \mathrm{d}\mu\,(\mu ab) \int_0^{2\pi} \mathrm{d}\phi\, f(\mu^2),$$

where the integration boundaries are chosen such that $M = \mathbb{R}^2$ is covered. This integral is easier to compute than the original expression. For example, consider the function $f(\mu^2) = 1$ for $\mu^2 \leq 1$ and 0 else, so that the integrand assumes the value one on the ellipsoidal area shown in the figure, and vanishes elsewhere. The integral I should then yield the area, πab, of an ellipse with semi-axes a and b. Doing the integral, we indeed obtain $I = \int_0^1 \mathrm{d}\mu(\mu ab) \int_0^{2\pi} = \pi ab$.

[3] Notice that for generalized polar coordinates the coordinate basis vectors $\mathbf{v}_\mu = \partial_\mu \mathbf{r}$ and $\mathbf{v}_\theta = \partial_\theta \mathbf{r}$ are not orthogonal. This coordinate system thus has non-orthogonal coordinate lines.

Jacobian vs. metric determinant

The considerations discussed above imply the **equality of the Jacobian and metric expressions** for the area element,

$$\boxed{\left|\det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right)\right| = |\det(g(\mathbf{y}))|^{1/2}.} \tag{C58}$$

We have established this equality in two dimensions by geometric reasoning. However, the final formula does not make visible reference to the two-dimensionality of the vectors and one may suspect that it is of more general validity.

That this is indeed the case can be shown by algebraic reasoning: the invariance of the determinant under transposition, $\det J \overset{(L170)}{=} \det J^T$, implies that $(\det J)^2 = (\det J^T)(\det J) \overset{(L178)}{=} \det(J^T J)$. Now observe that the matrix elements of $J^T J$ are given by $(J^T J)_{ij} = (J^T)_i{}^a (J)^a{}_j \overset{(L107)}{=} v^a{}_i v^a{}_j = \langle \mathbf{v}_i, \mathbf{v}_j \rangle = g_{ij}(\mathbf{y})$. This shows that $\det(J)^2 = \det(g)$. Taking the square root of the modulus of this equation we obtain Eq. (C58). The beauty of this construction is that it does not make reference to two dimensions and generalizes to higher-dimensional situations.

C4.3 Curvilinear volume integrals

The concepts developed above are straightforwardly generalized to higher dimensions. Of particular importance to applications are integrals over three-dimensional space, or volume integrals. For example, the mass of a three-dimensional structure is obtained by integrating a mass density function over its volume. This section explain how to do integrals of this type.

Geometric representation of the volume element

Three-dimensional volumes, $V \subset \mathbb{R}^3$, such as balls, cylinders, or the general structure shown in Fig. C8, can be described by a three-dimensional extension of the curvilinear coordinates discussed in the previous section. We define coordinates, $\mathbf{y} \equiv (y^1, y^2, y^3)^T$, on a domain, U, and a smooth map, $\mathbf{r} : U \to V, \mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$, parameterizing the integration domain in these coordinates. For example, the **unit radius ball**, $B \equiv \{\mathbf{r} \in \mathbb{R}^3 \,|\, \|\mathbf{r}\| \leq 1\}$, is conveniently described in spherical coordinates, Eq. (V41a), through a map $U \to B, \mathbf{y} = (r, \theta, \phi)^T \mapsto \mathbf{r}(r, \theta, \phi)$.

Once a system of good coordinates has been established, volume integrals may be constructed in analogy to the one- and two-dimensional integrals discussed above (cf. Fig. C8). Let us assume that the coordinate domain is given by the Cartesian product of three intervals, $U = (a^1, b^1) \times (a^2, b^2) \times (a^3, b^3)$ as in $U = (0, 1) \times (0, \pi) \times (0, 2\pi)$ for the spherical coordinates (r, θ, ϕ). The domain U is partitioned into a large number of boxes with corner points at $\mathbf{y}_{\boldsymbol{\ell}} \equiv (y^1_{\ell_1}, y^2_{\ell_2}, y^3_{\ell_3})^T$, $y^i_{\ell_i} \equiv \ell_i \delta^i$ ($i = 1, 2, 3$, no summation) and volume $\delta^1 \delta^2 \delta^3$. The indices enumerating these points run in the ranges $0 \leq \ell_i \leq (b^i - a^i)/\delta^i$, and $\boldsymbol{\ell}$ is a shorthand for $\boldsymbol{\ell} = (\ell_1, \ell_2, \ell_3)^T$. Under the coordinate map $\mathbf{r}(\mathbf{y})$ these boxes get sent onto distorted volume

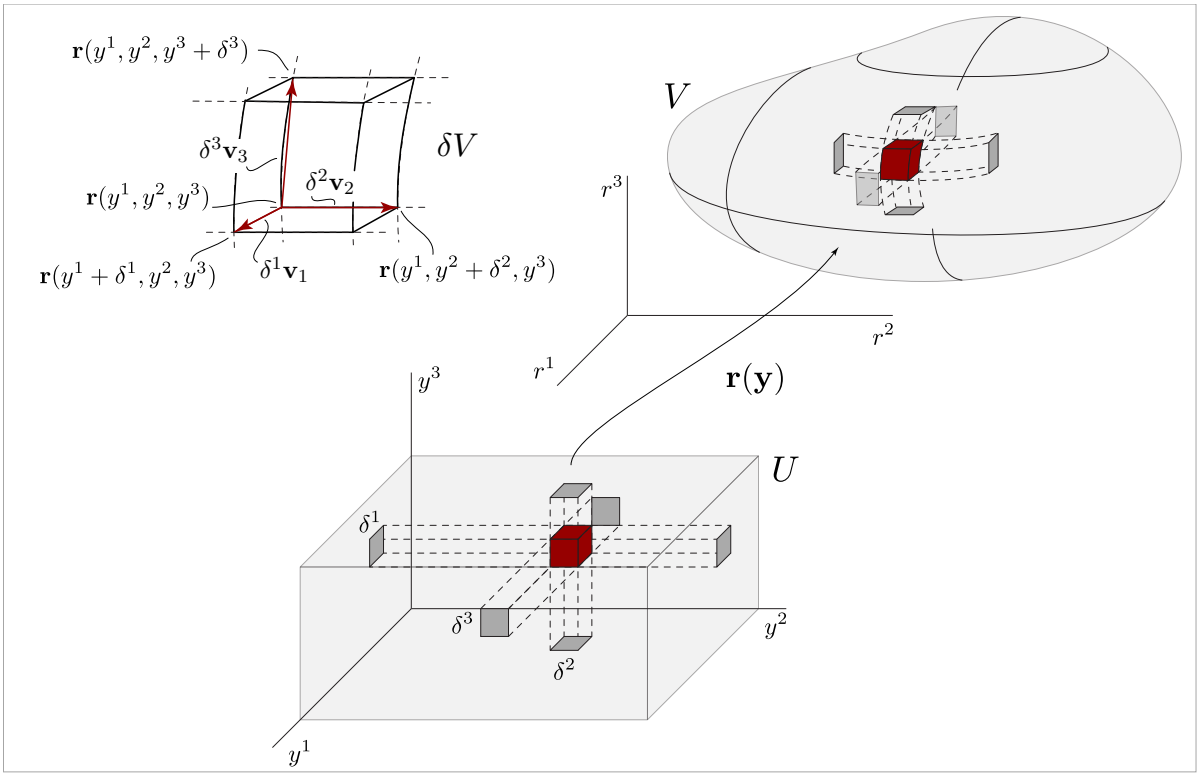


Figure C8: On the definition of three-dimensional volume integrals.

elements, $\delta V_{\boldsymbol{\ell}}$, in V bounded by the coordinates lines running through the corners $\mathbf{r}(\mathbf{y}_{\boldsymbol{\ell}})$ (see Fig. C8).

By construction, the system of volume elements $\{\delta V_{\boldsymbol{\ell}}\}$ covers the target volume. The integral of a function $f : V \to \mathbb{R}$, $\mathbf{r} \mapsto f(\mathbf{r})$, may thus be defined as the sum

$$\int_V \mathrm{d}V f \equiv \lim_{\delta^i \to 0} \sum_{\boldsymbol{\ell}} |\delta V_{\boldsymbol{\ell}}|\, f(\mathbf{y}_{\boldsymbol{\ell}}), \tag{C59}$$

where $f(\mathbf{y}) \equiv f(\mathbf{r}(\mathbf{y}))$ and $|\delta V_{\boldsymbol{\ell}}|$ is the geometric volume of $\delta V_{\boldsymbol{\ell}}$. This formula is the three-dimensional analogue of the two-dimensional Eq. (C45).

Next we need a formula for the volume elements. Proceeding in analogy to the two-dimensional case, and suppressing the box index $\boldsymbol{\ell}$ for brevity, we note that for small δ^i, δV can be approximated by a parallelepiped spanned by the vectors $\delta^i\, \partial_{y_i}\mathbf{r}(\mathbf{y}) = \delta^i\, \mathbf{v}_i$ ($i = 1, 2, 3$, no summation), cf. Fig. C8. Its volume can be computed by a **geometric construction** similar to that applied in the two-dimensional case: according to Eq. (L89), the volume of the parallelepiped spanned by the vectors $\mathbf{v}_1$, $\mathbf{v}_2$ and $\mathbf{v}_3$ is given by the triple product $|(\mathbf{v}_1 \times \mathbf{v}_2) \cdot \mathbf{v}_3|$. The volume of δV thus equals

$$|\delta V| = \delta^1\delta^2\delta^3 |(\mathbf{v}_1 \times \mathbf{v}_2) \cdot \mathbf{v}_3| = \delta^1\delta^2\delta^3 \left| \left(\partial_{y^1}\mathbf{r}(\mathbf{y}) \times \partial_{y^2}\mathbf{r}(\mathbf{y})\right) \cdot \partial_{y^3}\mathbf{r}(\mathbf{y}) \right| .$$

This expression is the three-dimensional analogue of Eq. (C47) for the two-dimensional area

element $|\delta S|$. Substituting it into the Riemann sum (C59) and taking the limit we obtain

$$\boxed{\int_V \mathrm{d}V\, f(\mathbf{r}) = \int_U \mathrm{d}y^1\mathrm{d}y^2\mathrm{d}y^3 \left|(\partial_{y^1}\mathbf{r} \times \partial_{y^2}\mathbf{r}) \cdot \partial_{y^3}\mathbf{r}\right| f(\mathbf{y}),} \tag{C60}$$

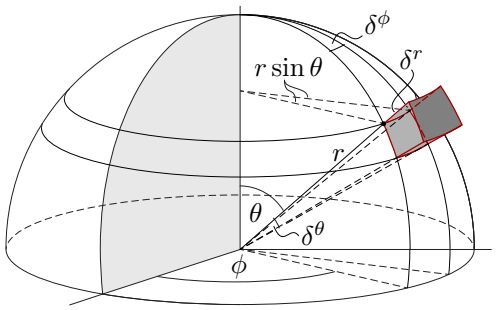
for the three-dimensional volume integral. The combination

$$\mathrm{d}V \equiv \mathrm{d}y^1\mathrm{d}y^2\mathrm{d}y^3 |(\partial_{y^1}\mathbf{r} \times \partial_{y^2}\mathbf{r}) \cdot \partial_{y^3}\mathbf{r}| \tag{C61}$$

is called the **volume element** or **integration measure** of the integral.

EXAMPLE The coordinate basis vectors in **spherical coordinates** are given by (cf. Eq. (V42)) $\mathbf{v}_r = \mathbf{e}_r$, $\mathbf{v}_\theta = \mathbf{e}_\theta\, r$, $\mathbf{v}_\phi = \mathbf{e}_\phi\, r\sin\theta$. The orthonormality of the *local* spherical basis vectors, $\mathbf{e}_i$, implies $|(\mathbf{e}_r \times \mathbf{e}_\theta) \cdot \mathbf{e}_\phi| = 1$. By Eq. (C61), the **volume element in spherical coordinates** is given by

$$\boxed{\mathrm{d}V = r^2\, \mathrm{d}r\, \sin\theta\, \mathrm{d}\theta\, \mathrm{d}\phi.} \tag{C62}$$



Here, the factor $r^2\sin\theta$ reflects the fact that the dimensions of the distorted box δV in θ- and ϕ-directions are given by $r\,\delta^\theta$ and $r\sin\theta\,\delta^\phi$, respectively. The factor $\sin\theta$ is best understood by exploring how the volume element shrinks upon approaching the north and south pole of the sphere, respectively (think about this point).

For example, the integral of a function over a ball, B, of radius R has the form

$$\int_B \mathrm{d}V\, f(\mathbf{r}) = \int_0^R r^2\mathrm{d}r \int_0^\pi \sin\theta\mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, f(r,\theta,\phi).$$

For $f = 1$ this integral yields the result $\frac{4}{3}\pi R^3$, the well-known formula for the volume of the ball (→ C4.3.1-6).

EXERCISE Verify that the **volume element in cylindrical coordinates** is given by

$$\boxed{\mathrm{d}V = \rho\, \mathrm{d}\rho\, \mathrm{d}\phi\, \mathrm{d}z.} \tag{C63}$$

Jacobian and metric representations of volume element

Above we applied geometric reasoning to express the volume $|\delta V|$ of the element δV as a triple product. Proceeding in analogy to section C4.2 we now introduce alternative representations of the same quantity as a Jacobian and a metric determinant, respectively.

As in our previous discussion the Jacobian representation of the volume element is based on a Cartesian expansion of the coordinate vectors, $\mathbf{v}_j = \mathbf{e}_a v^a{}_j$, where $v^a{}_j = \frac{\partial x^a}{\partial y^j}$. Recalling Eq. (L159), the volume of the parallelepiped spanned by these vectors may be represented as $V(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3) = |\det J|$, where the 3×3 matrix $J = (\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$ contains the Cartesian component representations, $(\mathbf{v}_j)^a = v^a{}_j = \frac{\partial x^a}{\partial y^j}$, of these vectors as columns. As in the two-dimensional case, this motivates the definition of the **Jacobi matrix** as $J = \frac{\partial \mathbf{x}}{\partial \mathbf{y}} \equiv \frac{\partial(x^1,x^2,x^3)}{\partial(y^1,y^2,y^3)}$ such that $|\delta V| = \delta^1\delta^2\delta^3 \det(J)$.

The third representation is based on Eq. (C58) which we saw holds in arbitrary dimensions. Hence, $|\det J| = |\det g|^{1/2}$, where $g_{ij}(\mathbf{y}) = \langle \mathbf{v}_i, \mathbf{v}_j \rangle$, is the **metric tensor** in the coordinate basis. We have thus obtained two more representations for the volume element,

$$|\delta V| = \delta^1\delta^2\delta^3 \left| \det \left(\frac{\partial(x^1,x^2,x^3)}{\partial(y^1,y^2,y^3)} \right) \right| = \delta^1\delta^2\delta^3 \left| \det(g(\mathbf{y})) \right|^{1/2}.$$

In conceptual analogy to Eq. (C57), a volume integral can now be represented by any of the three formulae

$$\boxed{\int_V \mathrm{d}V f(\mathbf{r}) = \int_U \mathrm{d}y^1\mathrm{d}y^2\mathrm{d}y^3 \left\{ \begin{array}{l} \left| (\partial_{y^1}\mathbf{r} \times \partial_{y^2}\mathbf{r}) \cdot \partial_{y^3}\mathbf{r} \right| \\ \left| \det \left(\frac{\partial(x^1,x^2,x^3)}{\partial(y^1,y^2,y^3)} \right) \right| \\ \left| \det(g(\mathbf{y})) \right|^{1/2} \end{array} \right\} f(\mathbf{y}).} \tag{C64}$$

For later reference we note that the determinants of the metric tensor in **cylindrical and spherical coordinates** are given by (cf. Eqs. (V42) and (V36))

$$\begin{aligned} \text{cylindrical:} \quad & \sqrt{\det(g(\rho,\phi,z))} = \sqrt{g_{\rho\rho}g_{\phi\phi}g_{zz}} = \rho, \\ \text{spherical:} \quad & \sqrt{\det(g(r,\theta,\phi))} = \sqrt{g_{rr}g_{\theta\theta}g_{\phi\phi}} = r^2 \sin\theta. \end{aligned} \tag{C65}$$

These formulae lead back to Eqs. (C63) and (C62), as they should. As an instructive exercise, re-derive them from the Jacobian perspective.

C4.4 Curvilinear integration in arbitrary dimensions

REMARK Requires chapter L6.1 on matrix determinants.

In this section we consider integrals over generic d-dimensional objects embedded in n-dimensional space. Once more, the construction of these integrals is based on a suitable integration 'measure'. The definition of these measures in turn relies on the metric and the ensuing integrals will be generalized variants of the third representations in Eqs. (C57) and (C64), respectively.

Consider a smooth subset of n-dimensional space, $M \subset \mathbb{R}^n$. By 'smooth' we mean that M is the image of a smooth map $U \to M \subset \mathbb{R}^n$, $\mathbf{r} : U \to M$, $\mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$, where $U \subset \mathbb{R}^d$ is a d-dimensional coordinate domain.[4] In this case, d coordinates $\mathbf{y} = (y^1, \ldots, y^d)^T$ are required to parameterize M and we call it a 'd-dimensional' structure. For example, a sphere of unit radius is a $(d=2)$-dimensional object embedded in $(n=3)$-dimensional $\mathbb{R}^3$ which can be parameterized by two spherical coordinates (θ, ϕ). Without loss of generality, we assume $U = (a^1, b^1) \times \cdots \times (a^d, b^d)$ to be a d-dimensional cuboid.

Consider U discretized by a d-dimensional lattice of coordinate points as discussed on p. 236, only that the index i now runs from 1 to d. The assignment $\mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$ maps this lattice onto a distorted lattice of image points in M. These define the corners of generalized d-dimensional volume elements covering M. Each element δV can be approximated by a d-dimensional parallelepiped spanned by the d vectors $\delta^i \partial_{y^i} \mathbf{r}(\mathbf{y}) = \delta^i \mathbf{v}_i \in \mathbb{R}^n$ $(i = 1, \ldots, d,$ no summation).

Next we need formulae for the volume, $|\delta V|$, of these generalized parallelepipeds. As a warmup to the discussion of general n and d, let us discuss an instructive example:

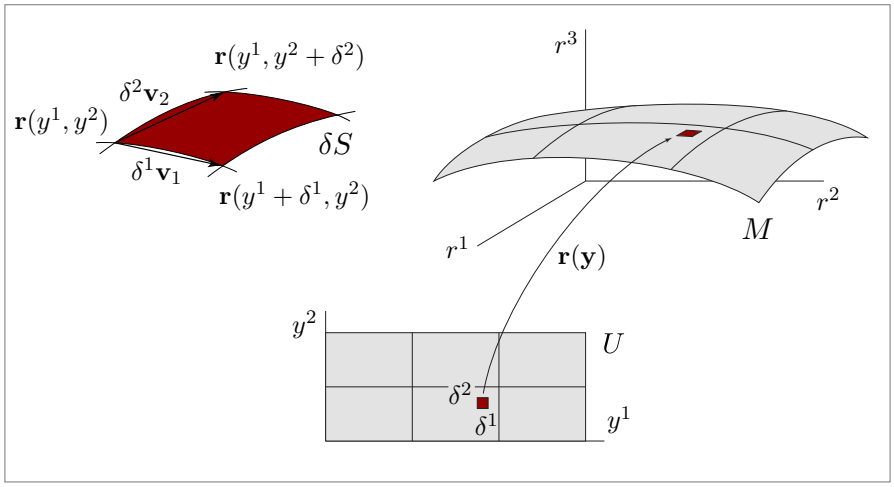


Figure C9: Integral over a two-dimensional surface in three-dimensional space.

Example: integration over a two-dimensional surface in three-dimensional space

In practice, one often needs to integrate over an $(d = 2)$-dimensional surface, M, embedded in $(n = 3)$-dimensional space, $\mathbb{R}^3$, see Fig. C9. The 'volume elements' then actually are *surface* elements, δS, embedded in $\mathbb{R}^3$. They are spanned by the pair of three-dimensional vectors $\delta^1 \partial_{y^1} \mathbf{r} = \delta^1 \mathbf{v}_1$ and $\delta^2 \partial_{y^2} \mathbf{r} = \delta^2 \mathbf{v}_2$. We know two expressions for the geometric area of such parallelograms: the norm of their vector product Eq. (C47), and Eq. (L40) which in the present context assumes the form of Eq. (C55). The area of the surface element δS is therefore given

[4] Again, we tolerate the presence of 'defects' of dimension $< d$ in M which are not in the image $\mathbf{r}(U)$.

as

$$|\delta S| = \delta^1\delta^2 \|\partial_{y^1}\mathbf{r} \times \partial_{y^2}\mathbf{r}\| = \delta^1\delta^2 |\det(g(\mathbf{y}))|^{1/2}. \tag{C66}$$

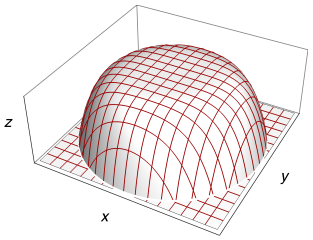
This in turn means that the integral over a two-dimensional surface M embedded in $\mathbb{R}^3$ is defined as

$$\boxed{\int_M \mathrm{d}S\, f(\mathbf{r}) = \int_U \mathrm{d}y^1\mathrm{d}y^2 \left\{ \begin{array}{c} \|\partial_{y^1}\mathbf{r} \times \partial_{y^2}\mathbf{r}\| \\ |\det(g(\mathbf{y}))|^{1/2} \end{array} \right\} f(\mathbf{r}(\mathbf{y})).} \tag{C67}$$

The first of these two representations is often encountered in introductory texts. It utilizes the vector product, and is therefore limited to the present situation of dimensions, $d = 2$, $n = 3$. The second representation, however, holds for a $(d = 2)$-dimensional surface embedded in a space of arbitrary dimension $n \geq 2$. This can be traced to the fact that the formula for the area element, Eq. (C55), is valid for any n. Also notice that the surface integral does not afford a representation in terms of a Jacobian $\det(\partial\mathbf{x}/\partial\mathbf{y})$, the reason being that Jacobians can be defined only for $d = n$. These observations suggest that integral formulae based on the metric determinant may be the 'most general' representations. This impression will be corroborated by the discussion of the general case below.

EXAMPLE Let us use Eq. (C67) to compute the area of a **two-dimensional sphere in three-dimensional space**. We apply (V41a) with $r = R$ to parameterize a sphere of radius R by spherical coordinates $(y^1, y^2) = (\theta, \phi)$. From Eq. (V42) we find $\partial_{y^1}\mathbf{r} = \partial_\theta\mathbf{r} = \mathbf{v}_\theta = \mathbf{e}_\theta R$ and $\partial_{y^2}\mathbf{r} = \partial_\phi\mathbf{r} = \mathbf{v}_\phi = \mathbf{e}_\phi R\sin\theta$ for the curvilinear velocities, and $g_{\theta\theta} = R^2$, $g_{\phi\phi} = \sin^2(\theta)R^2$, $g_{\theta\phi} = g_{\phi\theta} = 0$ for the elements of the metric tensor. Both $\|\mathbf{v}_\theta \times \mathbf{v}_\phi\|$ and $|\det(g)|^{1/2}$ yield $R^2\sin(\theta)$. We thus obtain the area as ($\rightarrow$ C4.4.1)

$$A = \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, R^2\sin(\theta) = 4\pi R^2. \tag{C68}$$



EXERCISE As another example consider the surface shown in the figure. It is radially symmetric in the xy-plane, and the Cartesian height coordinate is given by $z = \frac{1}{3}(a^3 - (x^2+y^2)^{3/2})$ for $x^2 + y^2 < a^2$. We aim to compute the geometric area of this surface. To this end, we introduce polar coordinates, $\mathbf{y} = (\rho, \phi)^T$, in the xy-plane and obtain the parameterization $\mathbf{r}(\mathbf{y}) = (x, y, z)^T(\mathbf{y}) = (\rho\cos\phi, \rho\sin\phi, \frac{1}{3}(a^3 - \rho^3))^T$. Show that the metric determinant reads as

$$\det(g(\mathbf{y}))^{1/2} = \rho(1+\rho^4)^{1/2}.$$

Use this result to confirm that the area is given by $A = \frac{\pi}{2}(a^2\sqrt{1+a^4} + \mathrm{arcsinh}(a^2))$. Discuss the results in the limit $a \gg 1$ and $a \ll 1$, respectively ($\rightarrow$ C4.4.2-4).

Integration over objects of arbitrary dimension: metric tensor

We now turn to the generic case $d \leq n$. We need the volume of a d-dimensional parallelepiped, $\delta V \subset \mathbb{R}^n$, spanned by the vectors $\delta^i \mathbf{v}_i$, with $i = 1, \ldots, d$. Referring to section **??** for a general argument, we state that this volume is given by the metric determinant

$$|\delta V| = (\delta^1 \ldots \delta^d)\, \det(g(\mathbf{y}))^{1/2}, \tag{C69}$$

where $g_{ij} = \langle \mathbf{v}_i, \mathbf{v}_j \rangle$ is computed using the standard scalar product of the embedding space $\mathbb{R}^n$. The integral over M is thus defined as

$$\boxed{\int_M \mathrm{d}V\, f(\mathbf{r}) = \int_U \mathrm{d}y^1 \ldots \mathrm{d}y^d \left[\det(g(\mathbf{y}))\right]^{1/2} f(\mathbf{r}(\mathbf{y})).} \tag{C70}$$

All multi-dimensional integration formulae descend from this powerful result. It holds for arbitrary $d \leq n$ and encompasses all the special cases discussed so far. To recapitulate, the application of this formula requires

- ▷ a parameterization of the integration domain, M, by a coordinate map, $\mathbf{r}(\mathbf{y})$,
- ▷ computation of the partial derivative vectors, $\mathbf{v}_i = \partial_{y^i}\mathbf{r}$, the elements of the metric tensor, $g_{ij}(\mathbf{y}) = \langle \mathbf{v}_i, \mathbf{v}_j \rangle$, and its determinant $\det(g(\mathbf{y}))$, and finally
- ▷ the computation of the integral over the coordinate domain U.

Integration over d-dimensional volumes in d-dimensional space: Jacobian

In the special case $d = n$ there exists an alternative representation of the volume element in terms of a Jacobian. Although this case, too, is covered by Eq. (C70), the Jacobian formulation is widely used and we discuss it for completeness. The **Jacobi matrix** of the coordinate map $\mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$ generalizes Eq. (C53): it is defined as the matrix, $J(\mathbf{v}_1, \ldots, \mathbf{v}_d)$, whose columns contain the Cartesian coordinates $\{v^a{}_j\} = \{\frac{\partial x^a}{\partial y^j}\}$ of the vectors, $\mathbf{v}_j = \partial_{y^j}\mathbf{r}(\mathbf{y})$:

$$\boxed{\frac{\partial \mathbf{r}}{\partial \mathbf{y}} \equiv \frac{\partial(x^1, \ldots, x^d)}{\partial(y^1, \ldots, y^d)} \equiv \begin{pmatrix} \frac{\partial x^1}{\partial y^1} & \frac{\partial x^1}{\partial y^2} & \cdots & \frac{\partial x^1}{\partial y^d} \\ \frac{\partial x^2}{\partial y^1} & \frac{\partial x^2}{\partial y^2} & \cdots & \frac{\partial x^2}{\partial y^d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial x^d}{\partial y^1} & \frac{\partial x^d}{\partial y^2} & \cdots & \frac{\partial x^d}{\partial y^d} \end{pmatrix}.} \tag{C71}$$

From Eq. (C58) we know that $\left|\det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right)\right| = |\det(g(\mathbf{y}))|^{1/2}$, and this implies the representation

$$\boxed{\int_M \mathrm{d}V\, f(\mathbf{r}) = \int_U \mathrm{d}y^1 \ldots \mathrm{d}y^d \, \frac{\partial(x^1, \ldots, x^d)}{\partial(y^1, \ldots, y^d)}\, f(\mathbf{r}(\mathbf{y})).} \tag{C72}$$

Notice the structural similarity of this formula to the one-dimensional substitution rule (C26). In the next section we discuss how Eqs. (C26) and (C72) can be understood as special cases of a general formula describing variable changes in integrals of arbitrary dimensionality.

C4.5 Changes of variables in higher-dimensional integration

Eq. (C72) affords an interesting interpretation as a generalization of the one-dimensional substitution rule (**??**). To understand this, consider an integral over a d-dimensional volume, M, in d-dimensional space. Assume that $\mathbf{r}(\mathbf{x}) = \mathbf{e}_a x^a$ has been parameterized by a Cartesian coordinate system. In this case, the basic integration formulae of section C4.1 may be applied to represent the integral as

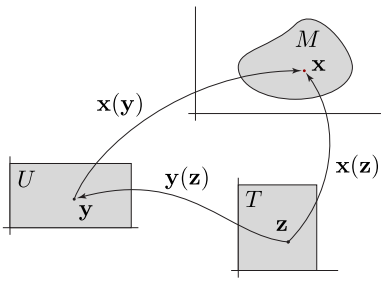
$$\int_M \mathrm{d}V f(\mathbf{r}) = \int_M \mathrm{d}x^1 \dots \mathrm{d}x^d \, f(\mathbf{x}),$$

where the boundaries of the x^a-integrals must be chosen so as to obtain a full coverage of M. Alternatively we may introduce a map, $\mathbf{x} : U \to M$, $\mathbf{y} \mapsto \mathbf{x}(\mathbf{y})$, to cover M by a different system of coordinates, $\mathbf{y}$, and represent the integral through Eq. (C72). The equality of the two representations leads to the formula

$$\boxed{\int_M \mathrm{d}x^1 \dots \mathrm{d}x^d \, f(\mathbf{x}) = \int_U \mathrm{d}y^1 \dots \mathrm{d}y^d \left| \det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right) \right| f(\mathbf{x}(\mathbf{y})).} \tag{C73}$$

This formula is valid independent of the geometric context in which it has been derived. In particular, it does not rely on an interpretation of $\mathbf{x}$ as a *Cartesian* coordinate vector. It describes, rather, a **change of integration variables**, $\mathbf{x} \to \mathbf{x}(\mathbf{y})$, in general d-dimensional integrals and extends the one-dimensional formula (C26) to higher dimensions. The notation $\mathbf{x} \to \mathbf{x}(\mathbf{y})$ is a shorthand for saying: 'a reparameterization of variables, $\mathbf{y} \mapsto \mathbf{x}(\mathbf{y})$, is applied to convert an integral over $\mathbf{x}$ to an identical integral over $\mathbf{y}$'. The appearance of the Jacobian in this formula may be remembered from the dirty mnemonic $\mathrm{d}x \leftrightarrow \mathrm{d}\not{y} \det\left(\frac{\partial \mathbf{x}}{\partial \not{\mathbf{y}}}\right)$, which has a status similar to that of the trick mentioned after Eq. (C26).

Equation Eq. (C73) motivated from a different perspective



To obtain a better understanding of the generality of formula (C73), consider another change of variables (cf. the figure),$\mathbf{y} : T \to U$, $\mathbf{z} \mapsto \mathbf{y}(\mathbf{z})$. One now has two options to express Eq. (C73) as an integral over $\mathbf{z}$. The first is to parametrize $\mathbf{x}$ through $\mathbf{z}$ via the composite map, $\mathbf{x} \circ \mathbf{y} : T \to M$, $\mathbf{z} \mapsto \mathbf{x}(\mathbf{y}(\mathbf{z})) \equiv \mathbf{x}(\mathbf{z})$. Application of Eq. (C73) to $\mathbf{x} \to \mathbf{x}(\mathbf{z})$ then yields

$$\int_M \mathrm{d}x^1 \dots \mathrm{d}x^d \, f(\mathbf{x}) = \int_T \mathrm{d}z^1 \dots \mathrm{d}z^d \left| \det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}}\right) \right| f(\mathbf{x}(\mathbf{z})).$$

The second is to apply the variable change $\mathbf{y} \to \mathbf{y}(\mathbf{z})$ to the integral on the r.h.s. of Eq. (C73):

$$\int_U \mathrm{d}y^1 \dots \mathrm{d}y^d \left| \det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right) \right| f(\mathbf{x}(\mathbf{y})) = \int_T \mathrm{d}z^1 \dots \mathrm{d}z^d \left| \det\left(\frac{\partial \mathbf{y}}{\partial \mathbf{z}}\right) \right| \left| \det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right) \right|_{\mathbf{y}(\mathbf{z})} f(\mathbf{x}(\mathbf{y}(\mathbf{z}))),$$

where the notation emphasizes that in the integral on the right, all functions have to be expressed through the $\mathbf{z}$-coordinates.

Since the preceding two equations represent the same integral, we conclude that the Jacobian determinants occuring therein must satisfy the relation

$$\left|\det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{z}}\right)\right| = \left|\det\left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right)\Big|_{\mathbf{y}(\mathbf{z})}\right| \left|\det\left(\frac{\partial \mathbf{y}}{\partial \mathbf{z}}\right)\right| . \tag{C74}$$

Indeed, the validity of Eq. (C74) follows from an important property of the Jacobi matrix: application of the chain rule (C39) (with the identification $f^i = x^i$, $g^j = y^j$, $x^k = z^k$) gives

$$\frac{\partial x^i(\mathbf{y}(\mathbf{z}))}{\partial z^k} = \frac{\partial x^i(\mathbf{y})}{\partial y^j}\Big|_{\mathbf{y}(\mathbf{z})} \frac{\partial y^j(\mathbf{z})}{\partial z^k}.$$

This formula has the suggestive short-hand notation $\frac{\partial x^i}{\partial z^k} = \frac{\partial x^i}{\partial y^j}\frac{\partial y^j}{\partial z^k}$, or just

$$\boxed{\frac{\partial \mathbf{x}}{\partial \mathbf{z}} = \frac{\partial \mathbf{x}}{\partial \mathbf{y}}\frac{\partial \mathbf{y}}{\partial \mathbf{z}}.} \tag{C75}$$

Eq. (C75) states that Jacobi matrices are multiplicative: the Jacobian of the transformation $\mathbf{x} \to \mathbf{x}(\mathbf{z})$ equals the product of those of $\mathbf{x} \to \mathbf{x}(\mathbf{y})$ and $\mathbf{y} \to \mathbf{y}(\mathbf{z})$, respectively. The matrix product identity for determinants, $\det(AB) = \det(A)\det(B)$, then directly implies Eq. (C74).

To summarize, Eq. (C73) is the generalization of the one-dimensional substitution rule (C26) to changes of variables in generic higher-dimensional integrals.

C4.6 Summary and Outlook

In this chapter we introduced the higher dimensional integration techniques required in the early physics curriculum. Building on the general understanding of integration as generalized (Riemann) summation, we began with a straightforward construction of integrals over cuboidal domains, line segments, rectangles, boxes, etc. We then moved on to the important subject of integration over more general structures, where the usage of problem adjusted coordinates became vital. In all cases integration turned out to be an algorithm of three consecutive steps: i) the coverage of the integration domain by suitable coordinates, preferably defined on a cuboidal coordinate domain. ii) Determination of the geometric distortion factors by which the cuboidal line, surface, volume elements of the coordinate domain differ from the distorted line, surface, volume elements defined by the coordinate map in the integration domain. This step really is at the heart of the matter of all integration and we provided three alternative solutions, each tailored to different situations. Finally, iii) doing the integral over the coordinate domain weighted over a function of interest and said distortion factor.

We discussed various types of integrals distinguished by the dimension of the integration domain (the number of coordinates required to parameterize it) and the dimensionality of

the space in which the domain is embedded. This led to a perhaps somewhat overwhelming multitude of integrals all of which, however, all are of granted relevance in practice. In the later chapter V5.4 we will introduce a more geometric perspective of integration and demonstrate that the integrals introduced above are not so different as they might seem. However, for the time being we leave the subject of integration and turn back to the 'local' analysis of functions by advanced techniques of differentiation.

C5 Taylor series

Depending on the type of information they encode, mathematical functions may be simple or complicated. Sometimes they are defined 'implicitly',[1] or they may be the results of measurements in which case no analytic representation exists. While the description of a function in full generality may be a difficult task, it is often sufficient to understand its behavior in the vicinity of a specific point of interest.

INFO For example, the binding potentials stabilizing a chemical molecule such as O_2 are complicated functions $V(r)$ of the inter-atomic distances, r. However, at temperatures far below those where the molecule disintegrates, the inter-atomic separations are close to an equilibrium value $r = a$. Much of the observable physics of the molecule can then be understood from the profile of $V(r)$ for values of r close to a.

In this chapter we introduce methodology capable of describing the 'local' structure of functions even if the global structure is not known. In the next chapter, we then take a complementary point of view and introduce concepts to characterize the global profile of functions.

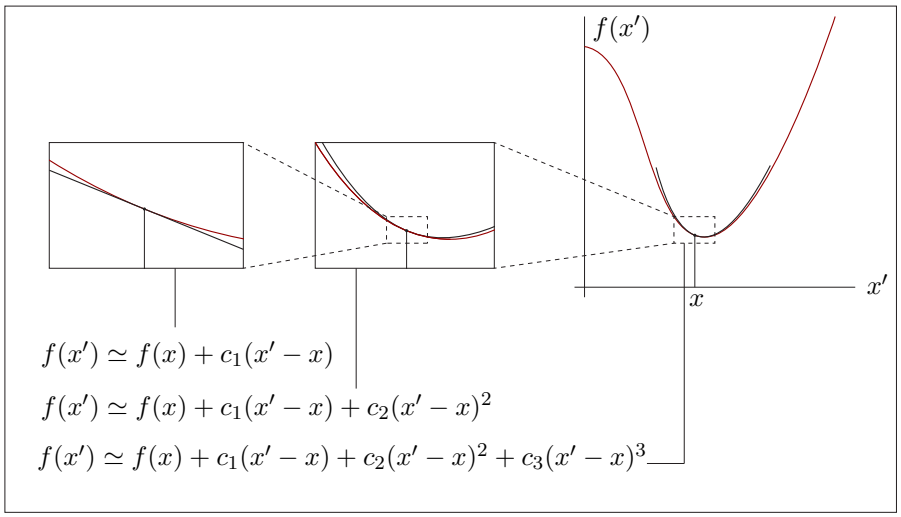


Figure C10: Schematic on the interpretation of a Taylor series expansion. Discussion, see text.

[1] For example, the function might be the result of an integral $\int^x \mathrm{d}x\, f(x)$ for which no closed representation is known.

C5.1 Approximating functions by polynomials

In chapter C1 we discussed how the derivative of a function $f(x)$ yields a local approximation in terms of a linear function. This is made explicit in Eq. (C2), $f(x+\delta) \simeq f(x)+\delta\, f'(x)$, where the $\simeq$ sign indicates that the quality of the approximation depends on the range over which it is applied. The reason is that even for small δ, $f(x+\delta)$ generally is not linear in δ but may depend on arbitrary powers, δ, δ^2 ,δ^3, ... However, for δ small, say, $\delta = 10^{-9}$, these terms rapidly decrease as $10^{-9}, 10^{-18}, 10^{-27}$, and this explains why for very small δ a linear approximation may be good enough. For larger δ, however, we should consider an 'expansion' of the form

$$f(x+\delta) = c_0 + c_1\delta + c_2\delta^2 + c_3\delta^3 + \ldots, \tag{C76}$$

where $c_0 = f(x)$, $c_1 = f'(x)$, and $c_{i\geq 2}$ are coefficients that need to be determined. Alternatively, we may define $x' \equiv x+\delta$ and write

$$f(x') = c_0 + c_1(x'-x) + c_2(x'-x)^2 + c_3(x'-x)^3 + \cdots = \sum_{n=0}^{\infty} c_n (x'-x)^n\,. \tag{C77}$$

This equation defines a representation of the function f in the vicinity of a fixed argument x in terms of an power series in $(x'-x)$. If only a finite number of terms of this series are kept, one obtains an approximation of f in terms of a polynomial in $(x'-x)$ of finite order. For increasing $|x'-x|$ an increasing number of terms of the series needs to be kept to obtain an accurate representation of f. The situation is illustrated in Fig. C10. On the smallest scales (left panel), the function looks nearly linear and can be approximated by a linear polynomial (a straight line). At somewhat larger scales (middle panel), the curvature of f becomes noticeable and a local representation in terms of a quadratic polynomial (corresponding to a generalized parabola) becomes appropriate. On yet larger scales (right panel), a cubic polynomial representation is required, etc.

C5.2 Taylor expansion

The concrete values of the expansion coefficients characterizing a function f in the neighborhood of a point x are easy to determine. The nth coefficient, c_n, is obtained by differentiating Eq. (C77) n times w.r.t. x' at the point $x' = x$. To see how this works, we note that on the l.h.s. side the differentiation yields $\frac{\mathrm{d}^n f(x')}{\mathrm{d}x'^n}\big|_{x'=x} = \frac{\mathrm{d}^n f(x)}{\mathrm{d}x^n}$, which is nth derivative of the function f at x. We assume that this derivative can be computed analytically (or perhaps numerically if the function is the result of a measurement). Turning to the r.h.s., we note that only the contribution of nth order to the series yields a non-vanishing contribution to the derivative: for $l < n$, we have $\mathrm{d}^n_{x'}(x'-x)^l = 0$, and for $l > n$, $\mathrm{d}^n_{x'}(x'-x)^l = \mathrm{const}\times(x'-x)^{l-n}$, which vanishes at $x' = x$. The surviving terms yields $\mathrm{d}^n_{x'}(x'-x)^n c_n = 1\cdot 2\cdots(n-1)\cdot n c_n \equiv n! c_n$, where we defined the **factorial** of a number as

$$n! \equiv 1\cdot 2\cdots(n-1)\cdot n, \qquad . \tag{C78}$$

for positive integers $n \in \mathbb{N}^+$, and $0! \equiv 1$ We thus have the identification $c_n = \frac{1}{n!}\frac{\mathrm{d}^n f(x)}{\mathrm{d}x^n}$, and so the expansion (C77) can be written as

$$\boxed{f(x') = \sum_{n=0}^{\infty} \frac{1}{n!}\frac{\mathrm{d}^n f(x)}{\mathrm{d}x^n}(x'-x)^n.} \tag{C79}$$

This series representation is called the **Taylor series expansion** of the function f around x.

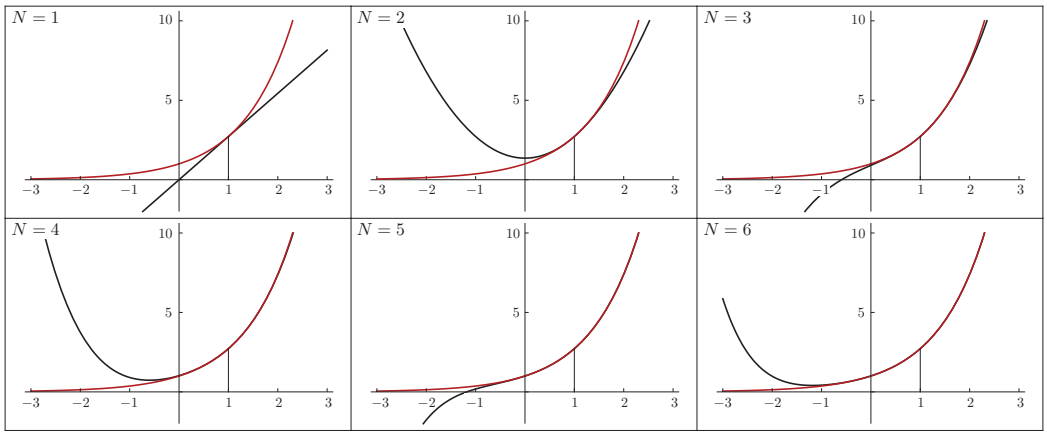


Figure C11: The function $\exp(x)$ (red curves) and the first six approximate representations around $x = 1$. For large N the approximate representation of $\exp(x)$ becomes increasingly accurate over wider intervals around $x = 1$.

Examples of Taylor series

Consider, for example, the function $f(x) = \exp(x)$. The derivatives of this function are easy to evaluate, $\exp^{(n)}(x) \equiv \frac{\mathrm{d}^n \exp(x)}{\mathrm{d}x^n} = \exp(x)$. We thus obtain

$$\exp(x') = \exp(x)\sum_{n=0}^{\infty} \frac{(x'-x)^n}{n!}. \tag{C80}$$

The contributions of the first few terms of this series, up to sixth order, are shown in the panels of Fig. C11. Setting $x = 0$, we obtain the famous **exponential series**

$$\boxed{\exp(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!}\,.} \tag{C81}$$

Notice that this series converges for all x: no matter how large its value, the factorial $n!$ in the denominator grows more rapidly with n than the power law x^n in the numerator[2] so that

[2] For large n, the coefficients $r_n \equiv x^n/n!$ rapidly converge to zero. This is because they are ratios of products $x \cdot x \cdots$ in the numerator, and the much larger products $n \cdot (n-1) \cdots$ in the denominator. Equivalently, one may note that the ratio of two consecutive values $r_{n+1}/r_n = x/n + 1 \ll 1$ becomes arbitrarily small. The sum over all these values remains finite.

sum over n converges to a finite value. Referring for a more substantial discussion to the next subsection, we say that the 'radius of convergence' of the series is infinite.
Taylor series representations are often applied to describe the local profile of functions. However, they may also contain information on global structures. To illustrate this point, let us consider the Taylor expansion of the **sine and cosine functions**, $\sin(x)$ and $\cos(x)$ at $x = 0$. The elementary properties $\sin(0) = 0$, $\cos(0) = 1$, $\mathrm{d}_x \sin(x) = \cos(x)$ and $\mathrm{d}_x \cos(x) = -\sin(x)$ readily lead to the following general expressions for higher order derivatives at $x = 0$: $\sin^{(2n)}(0) = 0$ (vanishing even-order derivatives), $\sin^{(2n+1)}(0) = (-1)^n$ (odd-order derivatives), and $\cos^{(2n)}(0) = (-1)^n$, $\cos^{(2n+1)}(0) = 0$. We thus obtain the Taylor expansions:

$$\boxed{\sin(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1}, \qquad \cos(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n}.} \tag{C82}$$

Again, these series have coefficients of $\mathcal{O}(x^n/n!)$ and therefore infinite radius of convergence.

If a Taylor series does exist, it need not necessarily converge for all values of x'. Consider, for example, the function $f(x) = \frac{1}{1-x}$. Differentiating this function at $x = 0$ we obtain $f^{(n)}(0) = n!$ and this leads to the so-called **geometric series**,

$$\boxed{\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n.} \tag{C83}$$

The convergence of the right hand side is limited to values $|x| < 1$. This reflects the fact that for $x \nearrow 1$,[3] we hit the divergence of the left hand side.

As another important example, we consider the logarithm, $f(x) = \ln(1-x)$. Since $f'(x) = -(1-x)^{-1}$, its series expansion is closely related to that of the geometric series. Indeed, it is straightforward to verify that the **logarithmic series** assumes the form

$$\boxed{\ln(1-x) = -\sum_{n=0}^{\infty} \frac{1}{n} x^n.} \tag{C84}$$

Again the radius of convergence is finite and convergence is lost for $|x| > 1$.

Complex Taylor series I: Convergence

Above we have seen that a Taylor series need not converge for all values of x'. The interval of values x' within which a series converges is called its **radius of convergence**. The functions $\exp, \sin$, and $\cos$ have infinite radius of convergence, the functions $1/(1-x)$ and $\ln(1-x)$ do not. In the latter cases the radius of convergence depends on the point around which one expands.[4]

[3] The symbol $\nearrow$ indicates that x approaches 1 from below, with $x < 1$ throughout the limiting process. Similarly, $x \searrow -1$ would indicate that x approaches -1 from above, with $x > -1$.

[4] For example, for $x = 1 + \delta$, $\delta > 0$, the radius of convergence is set by δ.

Brook Taylor (1685-1731)

A British mathematician best known for introducing the concept of Taylor series to mathematics. The series appeared as part of his work on generalizing infinitesimal calculus to a calculus of finite differences (the precise description how a function changes upon finite changes of the argument). The importance of this line of thinking remained unrecognized until four decades after Taylor's death when Lagrange understood its powers.

The existence of a Taylor series requires a function to be infinitely differentiable. A function satisfying this criterion throughout its entire domain of definition is called an **entire function** (ganze Funktion). For example, the exponential function, and the trigonometric functions $\sin$ and $\cos$, are entire on the real axis and can be Taylor expanded around arbitrary points. Most functions, however, contain singularities (such as the function $1/x$ at $x = 0$), or lack differentiability (e.g. the function $|x|$ at $x = 0$), or can only be differentiated a finite number of times (e.g. $x^{3/2}$ at $x = 0$). In such cases no Taylor series representation exists around the points violating the condition of infinite differentiability.

Compared to real functions, **functions of a complex variable** possess much stronger mathematical properties which will be addressed in detail in chapter C9. At this point we just note that the concept of Taylor series can be effortlessly extended to complex functions. One of several benefits of that extension is that the important question of series convergence is much better understood in that context. To construct the Taylor series of a function $f : \mathbb{C} \to \mathbb{C}, z \mapsto f(z)$ we first need to define a **complex derivative**, $f'(z)$. This derivative is defined in analogy to the derivative of a real function, Eq.(C1),

$$\frac{\mathrm{d}f(z)}{\mathrm{d}z} = \lim_{\delta_z \to 0} \frac{1}{\delta_z} \big[f(z + \delta_z) - f(z) \big]. \tag{C85}$$

If the limit exists, i.e. if the same limiting value is obtained *independent* of the way in which δ_z is sent to zero, the function is called 'complex differentiable'. If they exist, higher-order derivatives are defined by repeated differentiation, e.g. $\mathrm{d}_z^2 f(z) = \mathrm{d}_z f'(z)$, etc. For example, the function $1/(1 - z)$ is complex differentiable around $z = 0$ and its first two derivatives are given by $\mathrm{d}_z(1/(1 - z)) = 1/(1 - z)^2$, and $\mathrm{d}_z^2(1/(1 - z)) = 2/(1 - z)^3$, respectively. This example illustrates the general rule that complex derivatives are computed like real derivatives; all differentiation rules familiar from the real case carry over to the complex case.

For a function which is infinitely differentiable at z' its **complex Taylor series** may now be defined as

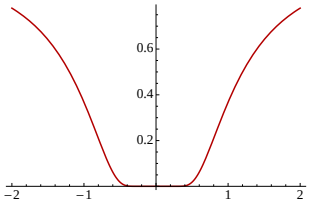
$$\boxed{f(z') = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{\mathrm{d}^n f(z)}{\mathrm{d}z^n} (z' - z)^n.} \tag{C86}$$

As in the real case, the validity of this representation is shown by n-fold differentiation of the both sides at $z' = z$. For example, the complex generalization of the geometric series reads as

$$\frac{1}{1 - z} = \sum_{n=0}^{\infty} z^n. \tag{C87}$$

Comparison to the real case (C83) shows that the complex series is obtained by complex generalization $x \to z$ in the latter. Indeed it is good practice to

> Always think of Taylor series as complex series. The restriction to real series is then obtained by the substitution $z = x + \mathrm{i}y \to x$.



EXAMPLE As an example illustrating how complex Taylor series are superior to real ones, consider the function

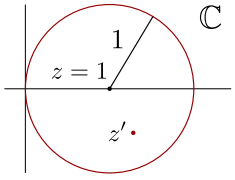
$$f(x) = \mathrm{e}^{-1/x^2}. \tag{C88}$$

The function f is infinitely differentiable at $x = 0$ and all its derivatives vanish, $f^{(n)}(0) = 0$. The Taylor series expansion thus predicts $f(x) = \sum_n 0 \cdot (x^n/n!) = 0$. However, this is incorrect, since f is clearly different from the zero function.

This frustrating ambiguity – whether or not one can tell in advance if the series is equal to the function – disappears if f is interpreted as the restriction of the complex function $f(z) = \exp -1/z^2$, with $z \in \mathbb{C}$, to the real axis, where $z = x$. To see this, let us briefly digress to discuss the differentiability of complex functions (for an in-depth discussion, see chapter C9).

At $z = 0$, the function $\exp(-1/z^2)$ is not differentiable. (To see why, explore the limiting behavior of $\exp(-1/z^2)$ for $z = \delta$ and $z = \mathrm{i}\delta$, respectively, when the real number δ is sent to zero. Two different limiting values are obtained, in violation of the differentiability criterion which requires the existence of a unique limiting value.) Consequently, a series representation of $\exp(-1/z^2)$ around $z = 0$ does not exist.

This explains why the real function $\exp(-1/x^2)$ of Eq. (C88) does not have a Taylor series expansion around $x = 0$, although all its derivatives w.r.t. to x do exist. The function is the real restriction, $\exp(-1/z^2) = \exp(-1/(x+iy)^2) \to \exp(-1/x^2)$, of a complex function which does not have a series expansion around $z = 0$. Although a rigorous discussion of Taylor series convergence is best undertaken within the framework of functions of a complex variable, pathologies such as the one above are rare. In most cases, the convergence of a real Taylor series can be addressed within a real framework.



Complex Taylor series are defined in the *plane* of complex numbers. The maximum value, R, such that the Taylor series converges for all z' inside the complex circle $|z' - z| < R$ is called its **radius of convergence** around z. For example, the complex geometric series (C87) has radius of convergence $R = 1$ around $z = 1$. For all $|z' - 1| < R$ the powers $|z - z'|^n < r^n$, where $r < R = 1$ is smaller than unity. This makes the series convergent. The 'radius of convergence' of the real series (C83) is the width of the interval $|x' - 1| < 1$ defined by the intersection of the complex disk of convergence with the real numbers.

Complex Taylor series II: Relation between functions

Complex Taylor series representations can be applied to reveal connections between functions which are difficult to understand otherwise. As an example, consider the series

$$\exp(z) = \sum_{n=0}^{\infty} \frac{z^n}{n!}, \tag{C89}$$

generalizing the real series (C81) to the complex plane. As in the real case, its radius of convergence is infinity. Now substitute the argument $z = \mathrm{i}x$, $x \in \mathbb{R}$ to obtain

$$\exp(\mathrm{i}x) = \sum_{m=0}^{\infty} \frac{(\mathrm{i}x)^m}{m!} = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n} + \mathrm{i} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1},$$

where in the second equality we split the summation into even ($m = 2n$) and odd ($m = 2n+1$) powers of x, and used $\mathrm{i}^{2n} = (\mathrm{i}^2)^n = (-1)^n$. Comparison with (C82) shows that the even and odd parts of the series coincide with the $\cos$- and the $\sin$-series, respectively. All series involved here have infinite radius of convergence and therefore can be considered as equivalent to the functions they represent (i.e. substituting an arbitrary argument into $\exp(x)$ or into its series representation leads to identical results). Equating the series to their respective functions then leads to the conclusion

$$\boxed{\exp(\mathrm{i}x) = \cos(x) + \mathrm{i}\sin(x).} \tag{C90}$$

Leonhard Euler (1707-1783)

A swiss mathematician and physicist. Euler played a pioneering role in the development of modern analysis, but also contributed to number theory, graph theory, and applied mathematics. In physics he worked on problems of mechanics, fluid dynamics, astronomy, and others. Euler is generally considered one of the greatest mathematicians of all time. An exclamation by a famous contemporary mathematician:'Read Euler, read Euler, he is the master of us all!'

Eq. (C90) is known as the **Euler formula**. Remarkably, this very simple relation between three elementary functions is not straightforward to prove by means other than series expansion. At the same time, the Euler formula is immensely useful in applications. For example, it can be used to reformulate the 'polar representation' of complex numbers, Eq. (L11), as

$$\boxed{z = |z|\mathrm{e}^{\mathrm{i}\phi},} \tag{C91}$$

i.e. as a decomposition in terms of the modulus $|z|$ and the **phase**, ϕ (i.e. the angle enclosed by the point z in the complex plane). This representation plays an important role in numerous applications in physics and engineering.

INFO It is worthwhile to list a few important **corollaries of the Euler formula**: taking the real and imaginary parts of the relation we obtain

$$\boxed{\sin(x) = \frac{1}{2\mathrm{i}}\left(\mathrm{e}^{\mathrm{i}x} - \mathrm{e}^{-\mathrm{i}x}\right), \qquad \cos(x) = \frac{1}{2}\left(\mathrm{e}^{\mathrm{i}x} + \mathrm{e}^{-\mathrm{i}x}\right).} \tag{C92}$$

At the particular values $x = 2\pi n$, $n \in \mathbb{Z}$, the relation reduces to the identity

$$\mathrm{e}^{\mathrm{i}2\pi n} = 1, \tag{C93}$$

which we will see plays an important role within the framework of Fourier calculus, section C6.2 Similarly, inserting $x = \pi$ into Eq. (C90) leads to

$$\mathrm{e}^{\mathrm{i}\pi} + 1 = 0, \tag{C94}$$

a remarkably simple relation between five of the most important numbers in mathematics, 0, 1, π, e and i.

EXERCISE Compute the Taylor series expansion of the functions $\sinh(x)$ and $\cosh(x)$ around $x = 0$ and use the result to verify that

$$\exp(x) = \cosh(x) + \sinh(x). \tag{C95}$$

Formulate the complex extension of the $\sin$- and $\cos$-series, Eq. (C82) to verify that

$$\sinh(x) = \mathrm{i}\sin(-\mathrm{i}x), \qquad \cosh(x) = \cos(-\mathrm{i}x).$$

C5.3 Finite-order expansion

Taylor expansions of finite order are often applied to approximate a function f in the neighborhood of a point x by

$$f_N(x') \equiv \sum_{n=0}^{N} \frac{f^{(n)}(x)}{n!}(x' - x)^n\,, \tag{C96}$$

i.e. a polynomial comprising the the first $N + 1$ terms of the Taylor expansion of f about x. The advantage of such a representation is that the information on the local behavior of even a very complicated function is now encoded in $N + 1$ *numbers*, the derivatives $f^{(n)}(x)$. On the other hand we need to understand the accuracy of the approximation, which depends on the order, N, on the range, $|x - x'|$, and on the local profile of f. It should be evident that a rapidly varying function is less easy to approximate than slowly varying one.

The accuracy of a finite-order Taylor expansion is determined by the magnitude of the difference $|f(x') - f_N(x')|$. Quantitative bounds for approximation errors are derived in lecture courses of mathematics and we here restrict ourselves to stating a principal result: let $I \subset \mathbb{R}$ be an interval on which the function's nth derivative is bounded, up to a multiplicative constant α, by the nth power of some constant C, i.e. assume that constants α and C exist such that

$$|f^{(n)}(x')| < \alpha C^n, \qquad \forall x' \in I, n \in \mathbb{N}. \tag{C97}$$

The error made by approximating $f(x')$ by $f_N(x')$ is then bounded as

$$|f(x') - f_N(x')| < \alpha \frac{(C|x' - x|)^{N+1}}{(N+1)!}.$$

Since the factorial function grows more rapidly than the exponential function, [2] the right-hand side vanishes in the limit of large N and the Taylor series converges to f. We also observe that the magnitude of the function derivatives, which are a measure of the speed of its variation, enter the estimate.

INFO If functions violate the above convergence criterion it is often possible to find an 'optimal' N for which the finite series represents an approximation with the least error. For such functions, truncating the series at either larger or smaller values of N will produce worse results. The systematic discussion of these so-called **asymptotic expansions** is beyond the scope of this text.

C5.4 Solving equations by Taylor expansion

Taylor expansions can be applied to find approximate solutions of equations which are too complicated to be solved in closed form. To introduce the idea let us consider the example of an equation that *can* be solved exactly:

$$y^2 - 2\epsilon y - 1 = 0. \tag{C98}$$

Considered as an equation for y, this quadratic equation has the exact solution

$$y(\epsilon) = \epsilon \pm (1 + \epsilon^2)^{1/2}, \tag{C99}$$

where the notation indicates that the solution for y depends on ϵ. Now, if ϵ is small, it is possible to find an approximate solution for $y(\epsilon)$ without knowing the exact solution. The advantage of such an approximate scheme is that it also works for equations so complicated that it is difficult or impossible to find the exact solution.

For $\epsilon = 0$, Eq. (C98) is trivially solved by $y = \pm 1$, hence we anticipate that for $|\epsilon| \ll 1$, the solution $y(\epsilon)$ will remain close to $y(0) = \pm 1$. To find the solution up to and including order $\mathcal{O}(\epsilon^2)$, say, we thus express it in terms of a series ansatz of the form

$$y(\epsilon) = c_0 + c_1\epsilon + c_2\epsilon^2 + \mathcal{O}(\epsilon^3), \tag{C100}$$

where $c_0 = \pm 1$ and the higher coefficients need to be determined. To this end we substitute the series into Eq. (C98), retaining only terms up to $\mathcal{O}(\epsilon^2)$, to obtain

$$\left[c_0^2 + 2c_0c_1\epsilon + (c_1^2 + 2c_0c_2)\epsilon^2\right] + -2\epsilon(c_0 + c_1\epsilon) - 1 + \mathcal{O}(\epsilon^3) = 0\,,$$

or, rearranged to group terms with the same power of ϵ together,

$$(c_0^2 - 1) + (2c_0c_1 - 2c_0)\epsilon + (c_1^2 + 2c_0c_2 - 2c_1)\epsilon^2 + \mathcal{O}(\epsilon^3) = 0.$$

The left-hand side is a polynomial in ϵ, and we require it to vanish identically for arbitrary ϵ. The only way to satisfy this condition is that all coefficients of the polynomial (the expressions in brackets) vanish individually. This leads to the system of equations

$$\begin{aligned} &c_0^2 - 1 = 0\,, \\ &2c_0c_1 - 2c_0 = 0\,, \\ &c_1^2 + 2c_0c_2 - 2c_1 = 0\,. \end{aligned} \tag{C101}$$

Notice that the coefficients c_n appear successively: the first equation contains c_0, the second c_0 and c_1, the third all coefficients up to c_2, etc. Also observe that each time a new coefficient $c_{n\geq 1}$ appears, it enters the corresponding equation *linearly*. These two properties do not depend on the particular form of our equation, but are general features of the solution strategy of solving an equation using a series ansatz (think about this point). They allow us to solve the equations (C101) iteratively, determining first c_1 in terms of c_0, then c_2 in terms of c_0 and c_1, etc. This yields

$$c_0 = \pm 1, \qquad c_1 = 1, \qquad c_2 = \pm\tfrac{1}{2},$$

and hence

$$y(\epsilon) = \pm 1 + \epsilon \pm \tfrac{1}{2}\epsilon^2 + \mathcal{O}(\epsilon^3).$$

This agrees with the Taylor expansion of the exact solution up to quadratic order(C99).

Let us conclude with a few **general remarks on the procedure**. First, we built the approach on the *a priori* assumption that the solution can be expanded in ϵ. If this assumption turns out to be illegitimate, the equations will signal it by a breakdown of the hierarchical construction. For example, the simple equation $\big(y(\epsilon)\big)^2 = \epsilon$ cannot be expanded in ϵ. This can be understood by inspection of its exact solution, $y(\epsilon) = \pm\sqrt{\epsilon}$, which cannot be Taylor expanded around $\epsilon = 0$ (why?). Attempting a series ansatz as above, one readily finds that no solvable hierarchy of equations ensues.[5]

For equations whose solutions *can* be expanded in some small parameter, ϵ, the procedure above generally works. To repeat the three-step algorithm, consider an equation $F(y, \epsilon) = 0$ and assume that for $\epsilon = 0$ the solution of the equation $F(y, 0) = 0$ is known as $y = c_0$. To find an approximate solution for small $\epsilon \neq 0$, one proceeds as follows:

[5] Explicitly: inserting the Ansatz $y(\epsilon) = c_0 + c_1\epsilon + \mathcal{O}(\epsilon^2)$ into $y^2 = \epsilon$ yields $c_0^2 + 2c_0c_1\epsilon + (c_1\epsilon)^2 + \mathcal{O}(\epsilon^2) = \epsilon$. Equating coefficients with the same power of ϵ yields $c_0 = 0$ and $c_0c_1 = 1$, which would imply $c_1 = \infty$.

- ▷ Start by substituting the power series ansatz $y(\epsilon) = \sum_{n=0} c_n \epsilon^n$ into the equation.
- ▷ Expand the resulting expression $F\left(\sum_n c_n \epsilon^n, \epsilon\right) = 0$ in powers of ϵ^n to obtain another power series in ϵ, of the form $\sum_n a_n(c_0, \ldots, c_n)\epsilon^n = 0$. Here each coefficient a_n is linear in c_n and in general can depend on all $c_{i \leq n}$.
- ▷ This power series must vanish for all ϵ, implying that each of its coefficients must vanish identically, $a_n = 0$. Solving these equations iteratively yields the sought-after coefficients c_n.

Iterative solution strategies of this type are called **perturbative solutions**. The procedure is 'perturbative' in the sense that for small ϵ the solution is weakly deformed from its $\epsilon = 0$ value, y_0.

INFO Perturbative solutions of algebraic equations, and of the differential equations to be discussed later, play an enormously important role in physics. The reason is that physical problems generally present themselves in the form of equations. We often encounter situations where an equation contains a 'small' parameter, ϵ, and becomes simpler if it is expanded in powers of ϵ. For example, let $y = I$ be the electric current flowing through a metal in response to the application of a voltage $\epsilon = V$. For $V = 0$ no current will flow, i.e. $I = 0$ in this case. Since an external electric field is generally small in comparison to the internal fields that hold the metal together, it may be considered a 'small perturbation'. We may thus expand the current to linear order in this small perturbation, writing it as $I = 0 + gV$, where the unknown coefficient, g, is to be interpreted as the (linear) conductance of the system. Computing the linear coefficient g for a real solid can still be complicated, but it is much easier than computing the full form of the function $I(V)$ for general V. Such perturbative expansions turn out to be very usefull – indeed, there exists a plethora of different types of **perturbation theory**, which play an important role in almost all sub-disciplines of physics. The discussion of advanced types of perturbation theory is a subject of lecture courses in theoretical physics and beyond the scope of this text.

C5.5 Higher-dimensional Taylor expansion

REMARK Requires section **??**. The physical understanding of the example contained in this section requires basic familiarity with electrostatics.

The concept of local approximations by Taylor expansion is not limited to functions of one argument. Its generalization to the expansion of a multi-dimensional function $f : \mathbb{R}^m \to \mathbb{R}$ in the vicinity of a fixed argument $\mathbf{x} \in \mathbb{R}^m$ reads

$$f(\mathbf{x}') = \sum_{n=0}^{\infty} \frac{1}{n!}((\mathbf{x}' - \mathbf{x}) \cdot \boldsymbol{\nabla})^n f(\mathbf{x}), \tag{C102}$$

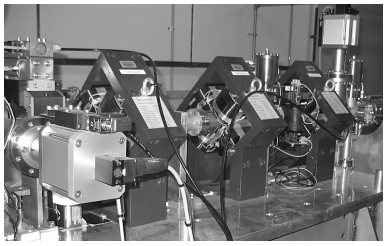


Figure C12: Taylor expansions of electric and magnetic fields play an important role in applications. For example, the focusing of particle beams in **accelerators** relies on magnetic fields designed in such a way that the first-order Taylor expansions of the local magnetic field strengths vanish. Magnets for which this is the case are called quadrupole or octupole magnets, respectively, and their construction is a task of great importance (the image shows a quadrupole magnet employed in the Australian synchrotron, a $3\mathrm{GeV}$ synchrotron accelerator).

where $\mathbf{y}\cdot\boldsymbol{\nabla}\equiv\sum_{i=1}^{m}y^i\partial_{x_i}$. For example, the expansion up to second order is given by

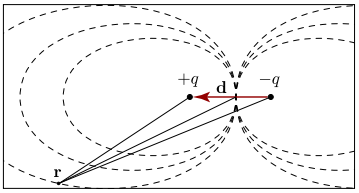
$$f(\mathbf{x}')\simeq f(\mathbf{x})+\sum_i(x'-x)^i\partial_{x^i}f(\mathbf{x})+\tfrac{1}{2}\sum_{ij}(x'-x)^i(x'-x)^j\partial^2_{x^i,x^j}f(\mathbf{x}). \tag{C103}$$

To prove Eq. (C102) one proceeds as in the one dimensional case Eq. (C79). An n-fold partial derivative $\partial^n_{x'^{i_1},\ldots,x'^{i_n}}\big|_{\mathbf{x}'=\mathbf{x}}$ is applied to both the left and the right hand side, where $i_1,\ldots,i_n\in\{1,\ldots,m\}$ are arbitrarily chosen indices. On the l.h.s. of the equation this yields $\partial^n_{x^{i_1},\ldots,x^{i_n}}f(\mathbf{x})$. On the r.h.s. the derivatives act on the factors x'^i multiplying the derivative operators. For $n=2$ it is straightforward to verify by inspection of Eq. (C103) that the resulting expression coincides with the l.h.s. Some more bookkeeping is required to do the calculation for general n, however the principal procedure remains the same.

However, unlike with the infinitely-extended Taylor series discussed in the previous sections, multi-dimensional expansions are usually truncated after the first few orders. The reason is that the bookkeeping required to keep the variable indices x^i under control quickly becomes unmanageably complicated.

EXAMPLE The electric potential created by a point particle at $\mathbf{r}_0$ carrying positive charge q is given by $\varphi(\mathbf{r})=\frac{q}{|\mathbf{r}-\mathbf{r}_0|}$. (We are working in so-called CGS units here.) At the point $\mathbf{r}$ this potential creates an electric field

$$\mathbf{E}\equiv-\boldsymbol{\nabla}\varphi(\mathbf{r})=q\frac{\mathbf{r}-\mathbf{r}_0}{|\mathbf{r}-\mathbf{r}_0|^3}.$$



Consider now an **electric dipole**, i.e. a system of two opposite electric charges, $\pm\mathbf{q}$, sitting at positions $\pm\mathbf{a}$ relative to the origin of a coordinate system. When observed from a remote point, $\mathbf{r}$, with $r\equiv|\mathbf{r}|\gg|\mathbf{a}|$, the electric potentials generated by these charges, $\varphi_\pm(\mathbf{r})=\pm q/|\mathbf{r}\mp\mathbf{a}|\simeq\pm q/|\mathbf{r}|$, largely cancel out. However, the cancellation is not perfect. The residual contribution is captured by a first-order Taylor

expansion of the function $(1/|\mathbf{r}-\mathbf{a}|)$ in the offset $\mathbf{a}$ around $\mathbf{a}=0$. Using $\partial_i(1/|\mathbf{r}|) = -x_i/|\mathbf{r}|^3$, we find

$$\varphi_\pm(\mathbf{r}) = \frac{q}{|\mathbf{r}\mp\mathbf{a}|} = \pm\frac{q}{|\mathbf{r}|} + \frac{q\mathbf{a}\cdot\mathbf{r}}{|\mathbf{r}|^3} + \mathcal{O}(\mathbf{a}^2).$$

The potential created by the two charges, $\varphi(\mathbf{r}) = \varphi_+(\mathbf{r}) + \varphi_-(\mathbf{r})$, is thus given by

$$\varphi(\mathbf{r}) \simeq \frac{2q\mathbf{a}\cdot\mathbf{r}}{|\mathbf{r}|^3} \equiv \frac{\mathbf{d}\cdot\mathbf{n}}{r^2}.$$

Here we introduced the unit vector $\mathbf{n} \equiv \mathbf{r}/r$, and defined the **dipole moment**, $q\mathbf{d} = q(2\mathbf{a})$, as a vector connecting the positions of the two opposite charges, multiplied by their magnitude. The contour lines of the dipole potential (i.e. lines along which the potential remains constant) are indicated in the figure above.

Dipole fields appear in many different contexts. For example, biological membranes often comprise layers of molecules stacked in such a way that the membrane does not carry a net charge but does create a dipole potential.

Verify that the **dipole electric field**, $\mathbf{E} = -\boldsymbol{\nabla}\varphi$, is given by

$$\mathbf{E}(\mathbf{r}) \simeq \frac{3(\mathbf{d}\cdot\mathbf{n})\mathbf{n} - \mathbf{d}}{r^3}.$$

Discuss the spatial profile of this field.

C6 Fourier calculus

In the previous chapter we have introduced tools to describe the 'local' profile of functions. We now take a complementary perspective and turn to the description of 'global' properties. Our first step will be the introduction of a rather special 'function' which will later serve as a diagnostic tool to probe the properties of generic functions.

C6.1 δ-Function

For a fixed number $y \in \mathbb{R}$, consider a 'function' $\delta_y : \mathbb{R} \to \mathbb{R}$ obeying the condition that for any continuous function $f : \mathbb{R} \to \mathbb{R}$

$$\boxed{\int \mathrm{d}x\, \delta_y(x) f(x) = f(y).} \tag{C104}$$

This so-called δ-**function** clearly is a strange object. The condition states that for every function f the integral of f multiplied by δ_y projects out the function value $f(y)$. A moment's thought shows that the function $\delta_y(x)$ must vanish for all values of x except for $x = y$, cf. Fig. C13.[1] On the other hand we may consider the particular 'test function' $f = 1$ to obtain the normalization condition

$$\int_{\mathbb{R}} \mathrm{d}x\, \delta_y(x) = 1.$$

We are thus dealing with a 'function' that vanishes everywhere except at one point, $x = y$, and at the same time integrates to unity, i.e. has unit 'weight'. This means that $\delta_y(y)$ must be 'infinitely large' to compensate for the 'vanishingly narrow width' of the 'function':

$$\delta_y(x) = \begin{cases} 0, & x \neq y, \\ \infty, & x = y. \end{cases} \tag{C105}$$

This extreme behavior implies that the δ-'function' cannot be a function in an ordinary sense.

However, much like $0 = \lim_{\epsilon \to 0} \epsilon$ can be thought of as a limiting value, we may try to construct a family of well-defined functions $\delta_y^{(\epsilon)}$ such that for any finite ϵ, $\delta_y^{(\epsilon)}$ is a regular function and only in the limit $\lim_{\epsilon \to 0} \delta_y^{(\epsilon)} = \delta_y$ the extreme behavior of δ_y is approached. In the next sections we introduce concrete realizations of such constructions.

[1] If $\delta_y(x)$ were non-vanishing for $x \neq y$, it would be possible to devise functions $f(y)$ such that $\int \mathrm{d}x, \delta_y(x) f(x) \neq f(y)$. Think about this point.

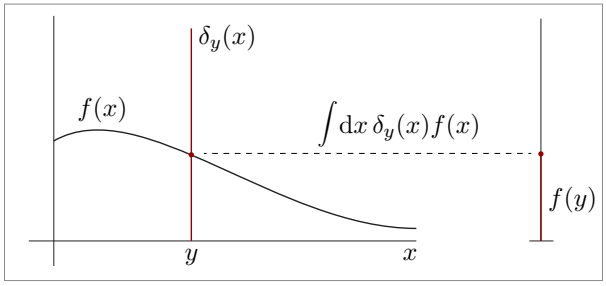
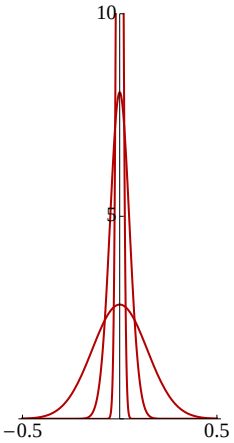


Figure C13: On the definition of the δ-function. A function with the required property (C104) must be vanishing for all values of x except for $x = y$ where it has to be 'infinitely large'.

Construction of the δ-function

It is not difficult to define a family of functions $\delta^{(\epsilon)}$ satisfying the required convergence criterion. Consider, for example, the **Gaussian functions**

$$\delta_y^{(\epsilon)}(x) \equiv \frac{1}{\epsilon\sqrt{\pi}} \mathrm{e}^{-(x-y)^2/\epsilon^2}.$$



These functions are defined such that, irrespective of the value of ϵ, the normalization condition $\int_{-\infty}^{\infty} \mathrm{d}x\, \delta_y^{(\epsilon)}(x) = 1$ is satisfied. For decreasing values of ϵ the support[2] of $\delta_y^{(\epsilon)}$ shrinks to a narrow region of width ϵ centered around y: $\lim_{\epsilon\to 0} \delta_y^{(\epsilon)}(x) = 0$ for $x \neq y$. On the other hand, the function values at y diverge, $\lim_{\epsilon\to 0} \delta_y^{(\epsilon)}(y) = \infty$, in such a manner that the normalization remains constant. The figure illustrates this behavior for the three values $\epsilon = 0.2, 0.07, 0.02$, respectively.

We conclude that we may write $\lim_{\epsilon\to 0} \delta_y^{(\epsilon)} = \delta_y$, since in this limit the defining criteria of Eq. (C105) are all satisfied. Also notice that the parameter y and the argument x appear in $\delta_y^{(\epsilon)}(x)$ in the combination $y - x$, i.e. the function depends only on the distance between the argument x and the reference point y. In particular we have $\delta_y^{(\epsilon)}(x) = \delta_0^{(\epsilon)}(x-y) \equiv \delta^{(\epsilon)}(x-y)$, where $\delta_0^{(\epsilon)} \equiv \delta^{(\epsilon)}$ is centered around 0 and the reference to that special center is usually omitted in the notation. This leads to the alternative representation

$$\delta^{(\epsilon)}(x - y) \equiv \frac{1}{\epsilon\sqrt{\pi}} \mathrm{e}^{-(x-y)^2/\epsilon^2}. \tag{C106}$$

In a similar manner, we write $\delta_y(x) \equiv \delta(x - y)$, where $\delta(x - y) \equiv \lim_{\epsilon\to 0} \delta^{(\epsilon)}(x - y)$.

To summarize, we **constructively define the δ-function** as the limit,

$$\delta(x) \equiv \lim_{\epsilon\to 0} \delta^{(\epsilon)}(x), \tag{C107}$$

[2] The **support** (Träger), $\mathrm{supp}(f) \equiv \{x \in \mathbb{R} | f(x) \neq 0\}$, of a function $f : \mathbb{R} \to \mathbb{R}$ is the subset of arguments on which f is non-vanishing.

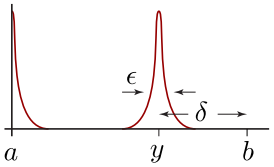


Figure C14: δ-functions defined on finite intervals. Discussion, see text.

of a one-parameter family of functions defined by two conditions, unit normalization, $\int \mathrm{d}x\, \delta^{(\epsilon)}(x) = 1$, and vanishing support in the limit $\epsilon \to 0$. Above we modeled a set of functions obeying these criteria in terms of Gaussian functions. In the next section, we will introduce other realizations of practical relevance. However, before that let us summarize two general points relating to the definition of δ-functions.

▷ It is no problem to **restrict the definition of the δ-function to finite intervals**. For an *open* interval $I \equiv (a, b)$ and $y \in I$ a finite neighborhood surrounding y is contained in I. If the width of that neighborhood is called δ and $\epsilon \ll \delta$ the support of $\delta_y^{(\epsilon)}$, too is almost entirely contained in I (cf. Fig. C14). We then have the asymptotically exact normalization $\int_I \mathrm{d}x\, \delta_y^{(\epsilon)}(x) \simeq 1$. This implies $\int_I \mathrm{d}x\, \delta_y(x) f(x) = 1$, as before.

If one needs to work with a *closed* interval $I = [a, b]$ an exceptional situation arises only at the boundaries $y = a, b$. It is then customary to work with families of functions $\delta_y^{(\epsilon)}$ defined such that $\lim_{\epsilon\to 0} \int_a^b \delta_a^{(\epsilon)} \mathrm{d}x\, f(x) = \int_a^b \delta(x-a) = \frac{1}{2} f(x)$, i.e. one half of the weight of the δ-function lies inside the interval (cf. the figure). The other half is outside and gets lost under integration.

▷ **The δ-function categorically appears under an integral** operation. Properties of integrals containing δ-functions may be understood by temporary substitution of the members of a generating family, $\delta^{(\epsilon)}$, application of standard rules of calculus to them, followed by an eventual limit $\epsilon \to 0$. For example, consider the frequently occurring expression $\int \mathrm{d}x\, \delta'(x) f(x)$. At first sight, this does not make sense, a function as singular as the δ-function certainly is not differentiable. However, one may make sense of this integral by integration by parts of the differentiable members of a family $\delta^{(\epsilon)}$:

$$\int \mathrm{d}x\, \delta'(x) f(x) = \lim_{\epsilon\to 0} \int \mathrm{d}x\, \delta^{(\epsilon)\prime}(x) f(x) = -\lim_{\epsilon\to 0} \int \mathrm{d}x\, \delta^{(\epsilon)}(x) f'(x) = -f'(0),$$

which leads to the identification

$$\int \mathrm{d}x\, \delta'(x) f(x) = -\int \mathrm{d}x\, \delta(x) f'(x) = -f'(0). \tag{C108}$$

Paul Adrien Maurice Dirac (1902-84)

An english physicist who is considered one of the founding fathers of quantum mechanics, and of quantum field theory. His most striking single achievement was the formulation of the Dirac equation, an extension of the Schrödinger equation of quantum mechanics into the realm of relativistic dynamics. The Dirac equation led to a variety of striking predictions including that of the existence of anti-matter. It also necessitated the introduction of quantum fields, a concept of immense importance in modern physics.

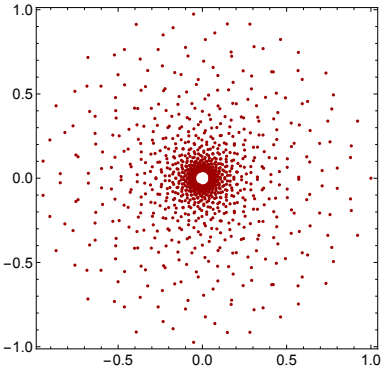
The δ-function plays an important role in applications both in mathematics and physics. It was originally introduced by the *physicist* P.A.M. Dirac as a tool for the description of point charges. (A point charge at y is an object whose charge density is zero everywhere, except for the point y where it diverges, i.e. its charge profile is described by δ_y as in (C105).) It took several decades to capture the essence of Dirac's idea in precise mathematical terms. The result was an extension of the concept of functions, known as **distributions** (see info section below).

INFO For any nonzero ϵ, $\delta^{(\epsilon)}$ is a regular function, however the limit $\delta = \lim_{\epsilon\to 0}\delta^{(\epsilon)}$ is not. To understand the limit one may note that for $y \in I$, δ_y extracts the *number* $f(y)$ from a function $f : I \to \mathbb{R}$: $f(y) = \int \mathrm{d}x\, \delta_y(x) f(x)$. This suggests that we should interpret δ_y as a map from the space of functions to the real numbers. This map acts on functions as $\delta_y[f] = f(y)$, where we followed the convention of enclosing the function-argument, $[f]$, of a map acting on functions by square brackets. For technical reasons, one has to restrict their consideration to argument functions which are smooth and have compact support, the so-called **test functions**. Maps assigning numbers to test functions are called **distributions**, and δ_y belongs to this class of objects. For this reason, mathematicians prefer to speak of a ***δ*-distribution**. However, we here follow physics parlance and use the more sloppy terminology 'δ-function'.

EXERCISE Use the auxiliary identity $\int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{1+x^2} = \pi$ to show that the family of functions

$$\delta^{(\epsilon)}(x) = \frac{1}{\pi}\frac{\epsilon}{\epsilon^2 + x^2} \tag{C109}$$

converges to the δ-function as $\lim_{\epsilon\to 0}\delta^{(\epsilon)}(x) = \delta(x)$. Eq. (C109) is referred to as the **Lorentzian representation of the δ-function**.



In the next section we will need one more representation, namely the **representation of the δ-function in terms of exponential series**. Consider the family of functions

$$\delta^{(\epsilon)}(x) \equiv \frac{1}{L}\sum_k \exp(\mathrm{i}kx - \epsilon|k|), \tag{C110}$$

where k is summed over all values $k = 2\pi n/L$, $n \in \mathbb{Z}$, and $x \in I \equiv [0, L]$. To heuristically understand why these functions have a chance of converging to $\delta(x)$, note that for fixed x and arbitrary k, the 'phase factor' $\exp(\mathrm{i}kx)$ is a complex number of modulus one and phase kx. The summation over k can be interpreted as an 'average' over lots of exponentials with effectively random phases, $kx = 2\pi\mathrm{i}nx/L$. In the limit of small ϵ, a large number of n-values contribute to the sum[3]. If x does not equal 0 or L, the exponentials are spread across the complex plane with quasi-random phases (i.e. quasi-random angles w.r.t. to the real axis), so that their sum essentially yields zero. [The figure illustrates the situation for $L = 100, \epsilon = 0.01, x = \sqrt{2} + \sqrt{3}$. The red points represent the numbers $\exp\big(2\pi n/L(\mathrm{i}x - \epsilon)\big)$ for $n = 1, \ldots, 500$, in the complex plane. For increasing values of n the presence of the 'damping factor' ϵ brings the exponentials closer to zero and guarantees the convergence of (C110). Summation over all exponentials will yield a value close to zero.] Conversely, for $x = 0$, we are summing over $\exp(-\epsilon|k|)$, and in the limit $\epsilon \to 0$ obtain an infinitely large value. This argument shows that the family of sums (C110) is a good candidate for a δ-function limit.

The sums in (C110) have the form of a geometric series, $\sum_n \big(\exp(C)\big)^n$, and can therefore be computed in closed form. As is detailed in the info section below, application of the master formula Eq. (C83) leads to the result

$$\delta^{(\epsilon)}(x) \simeq \frac{1}{\pi}\frac{\epsilon}{\epsilon^2 + x^2}, \qquad |x|, \epsilon \ll L, \tag{C111}$$

i.e. when the argument, x, is small compared to L, the sum converges to the Lorentzian form of the δ-function, Eq. (C109), confirming the expected behaviour.

INFO The **proof of Eq.** (C111) is an instructive exercise in series manipulation. We define $z = \frac{2\pi}{L}(\mathrm{i}x - \epsilon)$ and organize the sum (C110) as

$$\begin{aligned}\delta^{(\epsilon)}(x) &= \frac{1}{L}\left(\sum_{n=0}^{\infty}\mathrm{e}^{nz} + \sum_{n=-\infty}^{0}\mathrm{e}^{-n\bar{z}} - 1\right) = \frac{1}{L}\sum_{n=0}^{\infty}\left(\mathrm{e}^{nz} + \mathrm{e}^{n\bar{z}}\right) - \frac{1}{L} \\ &= \frac{1}{L}\left(\frac{1}{1-\mathrm{e}^{z}} + \frac{1}{1-\mathrm{e}^{\bar{z}}} - 1\right) = \frac{1}{2L}\left(\frac{1+\mathrm{e}^{z}}{1-\mathrm{e}^{z}} + \frac{1+\mathrm{e}^{\bar{z}}}{1-\mathrm{e}^{\bar{z}}}\right).\end{aligned} \tag{C112}$$

Now observe that for x nonzero and $\epsilon = 0$ we have $\bar{z} = -z$. Using this identity we immediately find $\lim_{\epsilon\to 0}\delta^{(\epsilon)}(x) = \delta(x) = 0$. To see what happens for x close to 0 we note that for $|x|, \epsilon \ll L$

[3] Due to the damping factor $\mathrm{e}^{-\epsilon|k|} = \mathrm{e}^{-\epsilon 2\pi|n|/L}$, values $|n| \gtrsim L/\epsilon$ give only exponentially small contributions.

the argument $|z| \ll 1$ is small, and so the numerators and denominators in (C112) may be Taylor expanded to first order, as $1 + \mathrm{e}^z = 2 + \mathcal{O}(z)$ and $1 - \mathrm{e}^z = -z + \mathcal{O}(z^2)$. This yields

$$\delta^{(\epsilon)}(x) \simeq -\frac{1}{L}\left(\frac{1}{z} + \frac{1}{\bar{z}}\right) = -\frac{1}{2\pi}\left(\frac{1}{\mathrm{i}x - \epsilon} + \frac{1}{-\mathrm{i}x - \epsilon}\right) = \frac{1}{\pi}\frac{\epsilon}{\epsilon^2 + x^2}, \tag{C113}$$

as stated above.

Properties of the δ-function

The definition (C104) implies a number of useful **relations obeyed by the δ-function**, which we summarize here for later reference.

- For any smooth function, we have the **defining property**

$$\int \mathrm{d}x\, \delta(x - y) f(x) = f(y), \tag{C114}$$

  which implies the unit-normalization $\int \mathrm{d}x\, \delta(x) = 1$.

- In applications, we often encounter δ-functions whose arguments differ from the integration variable. As a simple example, consider the integral $\int \mathrm{d}x\, \delta(cx) f(x)$, where c is a constant. This integral may be computed by application of the substitution rule Eq. (C26) to change to a new integration variable $u = cx$. We then obtain $\int \mathrm{d}u |c|^{-1} \delta(u) f(u/c) = |c|^{-1} f(0/c) = |c|^{-1} f(0)$, where the defining property of the δ-function has been applied to compute the u-integral. The result

$$\int \mathrm{d}x\, \delta(cx) f(x) = \frac{1}{|c|} f(0), \tag{C115}$$

  is equivalent to the **scaling relation**

$$\delta(cx) = \frac{1}{|c|}\delta(x). \tag{C116}$$

  Remember: the defining property only applies to combinations $\int \mathrm{d}x\, \delta(x)(\dots)$ where the integration variable itself features as an argument of the δ-function. Specifically, the δ-function is inversely proportional to factors appearing in its arguments.

- Eq. (C116) implies symmetry of the δ-function under changes of sign, $\delta(x) = \delta(-x)$.

- Another frequently occurring expression reads $\int \mathrm{d}x\, \delta\big(g(x)\big)\, f(x)$ where g is a function. Since $\delta(g(x)) = 0$ for $g(x) \neq 0$ this integral receives contributions only from an (infinitesimal) neighborhood of the zeros of g. Assume that x_0 is such a zero, assume differentiability of g there, and expand $g(x) = g(x_0) + g'(x_0)(x - x_0) + \dots = g'(x_0)(x - x_0) + \dots$. We

substitute this expression into the integral, note that for $x \to x_0$ the higher order terms in the expansion can be neglected, and apply Eq. (C115) to obtain

$$\int \mathrm{d}x\, \delta(g(x))\, f(x) = \frac{f(x_0)}{\left|\frac{\mathrm{d}g(x_0)}{\mathrm{d}x}\right|}.$$

In cases where g has more than one zero, $x_0, x_1, \ldots$ the contributions of all these to the integral need to be added together. In this way we arrive at the most general representation for the **change of variables under a δ-function**

$$\boxed{\int \mathrm{d}x\, \delta(g(x))\, f(x) = \sum_i \frac{f(x_i)}{\left|\frac{\mathrm{d}g(x_i)}{\mathrm{d}x}\right|}.} \tag{C117}$$

For completeness we mention that integrals over functions with zeros of higher order, such as $\int \mathrm{d}x\, \delta(x^2)$, are ill-defined.

EXAMPLE Consider the integral $I = \int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x^2 + 3x - 10) \cdot (2x + 1)$. The function $g(x) = x^2 + 3x - 10$ has zeros at $x_0 = 2$ and $x_1 = -5$, and at these points its derivative, $g'(x) = 2x + 3$, gives $g'(x_0) = 7$ and $g'(x_1) = -7$. Eq. (C117) thus yields

$$I = \frac{1}{|7|}\big[2 \cdot 2 + 1\big] + \frac{1}{|-7|}\big[2 \cdot (-5) + 1\big] = -\frac{4}{7}.$$

▷ **Derivatives** acting on the δ-function are are defined by the relation Eq. (C108).

▷ Consider the integral $\int_{-\infty}^{x} \mathrm{d}y\, \delta(y) f(y)$. It yields 0 if $x < 0$ (because the interval does not contain $y = 0$), $f(0)$ if $x > 0$, and $f(0)/2$ in the exceptional case where $x = 0$ coincides with the center of the δ-function (cf. Fig. C14 and its discussion). The frequent occurrence of this expression motivates the definition of the **Heaviside step function**[4]

$$\Theta(x) = \begin{cases} 1 & \text{for } x > 0, \\ \frac{1}{2} & \text{for } x = 0, \\ 0 & \text{for } x < 0. \end{cases} \tag{C118}$$

The above results may now be written as

$$\int_{-\infty}^{x} \mathrm{d}y\, \delta(y) f(y) = \Theta(x) f(x). \tag{C119}$$

[4] In the literature, one often finds a simplified version of the Heaviside function, $\Theta(x) = 1$ for $x \geq 0$ and 0 for $x < 0$, which is not perfectly symmetric relative to the jump point, $x = 0$.

For $f = 1$ we have

$$\int_{-\infty}^{x} \mathrm{d}y\, \delta(y) = \Theta(x),$$

which may be considered as an alternative definition of the Heaviside function. Differentiation of this relation w.r.t x yields

$$\Theta'(x) = \delta(x).$$

This formula states that the Θ-function is constant almost everywhere except at the jump-point $x = 0$, where its derivative is singular. Of course, neither the Θ-function, nor the δ-function are truly differentiable. All the expressions above have to be understood as limits of appropriately defined $\delta^{(\epsilon)}$-sequences.

C6.2 Fourier series

Jean Baptiste Fourier (1768-1830)

A French mathematician and physicist best known for the invention of Fourier calculus. Fourier applied his new concept to the study of physical phenomena such as heat conduction or the physics of vibrations. He is considered the discoverer of the greenhouse effect.

We now turn to the principal theme of this chapter, the 'global characterization of functions'. To motivate the topic, suppose an experimentalist has recorded data such as that shown in Fig. C15. (The plot shows oscillations of individual quantum states of a molecule.) How can the 'essence' of the measured signal be described in concise terms? The data clearly contains both experimental noise and a high level of repetitive redundancy. However, just by looking at it one can also identify 'relevant information', notably the presence of an oscillatory pattern that fluctuates at two time scales, one of order $1\mathrm{ps}$, the other of order $10\mathrm{ps}$. Our goal is to distill such relevant information from a complicated and largely redundant background.

The idea of Fourier calculus

The idea of Fourier calculus is to represent a given function f as a sum over many simple functions. In most cases these are the **harmonic functions** $\exp(\mathrm{i}kx), \cos(kx)$, or $\sin(kx)$.[5]

[5] A function $\psi(x)$ is called harmonic if it obeys the condition $\mathrm{d}_x^2\psi(x) = c \times \psi(x)$, where c is a constant. This states that harmonic functions reproduce themselves (up to multiplication by a constant) upon two-fold differentiation. There exists a generalized definition of harmonic functions (and of Fourier calculus) in which the simple two-fold derivative is replaced by a more complicated so-called Laplace operator. However, this extension is beyond the scope of this text.

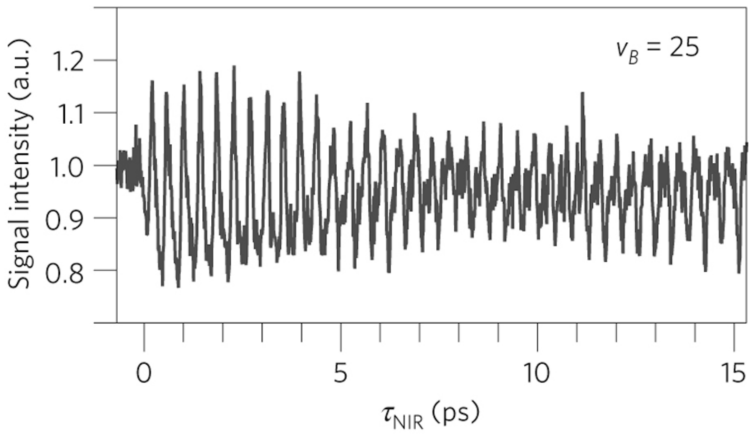


Figure C15: Measurement of collapse and revival phenomena in a single atomic eigenstate. Image taken from H. Goto *et al.*, Nature Physics **7**, 383385 (2011).

Here we focus on the expansion in terms of $\exp$-functions, which play the most important role in physical applications. The straightforward modifications needed for the closely related $\cos$ or $\sin$ series are discussed in problems **??** and **??**, respectively.

Consider a complex valued function $f : I \to \mathbb{C}, x \to f(x)$, defined on a finite interval $I \equiv [0, L]$ and obeying **periodic boundary conditions** $f(0) = f(L)$. Now let us try to 'expand' f in terms of oscillatory exponentials as

$$\boxed{f(x) = \frac{1}{L} \sum_k \tilde{f}_k \, \mathrm{e}^{\mathrm{i}kx},} \tag{C120}$$

where the sum extends over all

$$k = \frac{2\pi n}{L}, \qquad n \in \mathbb{Z}. \tag{C121}$$

These values are chosen such that each of the exponentials in (C120) satisfies $\exp(\mathrm{i}kL) = \exp(0) = 1$. In this way it is guaranteed that the r.h.s. of the equation respects the boundary condition $f(0) = f(L)$ of the l.h.s. Series such as (C120) are called **Fourier series**.

INFO Fourier series are frequently applied to the analysis of **periodic functions**, i.e. functions f which repeat on some interval $[0, L]$, see Fig. C16. All the information about such a function is contained in its restriction to a single-period interval $[0, L]$, where f obeys the periodicity condition $f(0) = f(L)$. This motivates the study of functions restricted to $[0, L]$ and obeying periodic boundary conditions. A function defined on the full real axis may then always be reconstructed by repetition of the restricted function. (For arbitrary $y \in \mathbb{R}$, determine the integer n such that $y = nL + x$, $x \in [0, L]$ and define $f(y) = f(nL + x) = f(x)$ through the restricted function.)

It turns out that for many functions of interest, an expansion as in (C120) fails for a lack of convergence. Since $|\mathrm{e}^{\mathrm{i}kx}| = 1$ the coefficients $\tilde{f}_k$ are required to decay rapidly and this

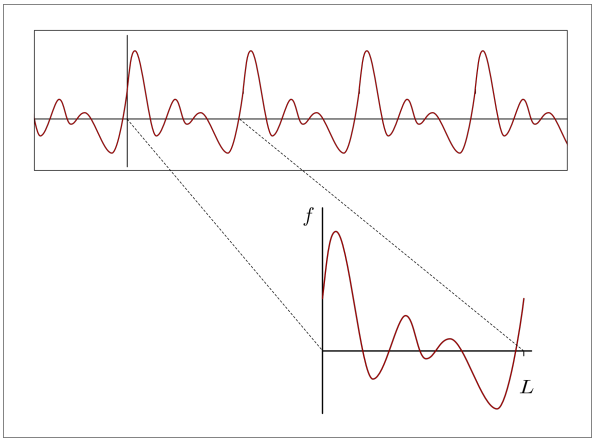


Figure C16: (Real part of a complex) function periodic on the interval $[0, L]$. The full 'information' aboout the function is stored in its restriction to a single-period interval $[0, L]$.

condition limits the option of a series representation to only a narrow class of functions. However, an efficient way to improve on the situation is to redefine the series as

$$f(x) = \frac{1}{L} \lim_{\epsilon \searrow 0} \sum_k \tilde{f}_k \, \mathrm{e}^{\mathrm{i}kx - |k|\epsilon}, \tag{C122}$$

where the notation $\epsilon \searrow 0$ means that ϵ is sent to zero coming from *positive* values. For any finite ϵ the series now converges, unless the coefficients $\tilde{f}_k$ increase exponentially in k. The parameter ϵ is called a **convergence generating factor**. It is customary to not write this factor explicitly even if its presence is required to render a series convergent. However, if seemingly ill-defined series such as $\sum_k \mathrm{e}^{\mathrm{i}kx}$ (coefficients $\tilde{f}_k = 1$) are encountered in the literature, one may safely assume that the presence of a convergence generator is implicit.

Fourier modes

Eq. (C120) contains the functions $\exp(\mathrm{i}kx)$, which in the present context are called **Fourier modes**. They will play an important role throughout and it is worthwhile to summarize their essential features: for each value of k, $\exp(\mathrm{i}kx)$ is an oscillatory functions (cf. Fig. C17) where the oscillation period, $\Delta x = 2\pi/k = L/n$, decreases with n. In physical applications, Fourier modes often appear in the context of with wave-like phenomena and the index k is called the **wave number** of a wave with **wave length** $\lambda = 2\pi/k$. A Fourier mode of index n then contains n oscillation periods in the interval $[0, L]$.

Fourier modes obey a so called **orthogonality relation**

$$\frac{1}{L} \int_I \mathrm{d}x \, \mathrm{e}^{\mathrm{i}(k-k')x} = \delta_{kk'}, \tag{C123}$$

i.e. the integral of the product, $\exp(\mathrm{i}(k - k')x)$, of a Fourier mode, $\exp(\mathrm{i}kx)$, and of its complex conjugate $\exp(-\mathrm{i}k'x)$ vanishes unless their wave numbers are equal.

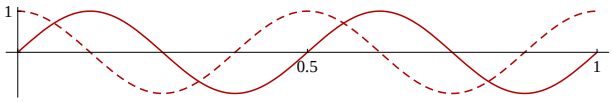


Figure C17: Real part $\cos(kx)$ (solid) and imaginary part ($\sin(kx)$) (dashed) part of the Fourier mode $\exp(\mathrm{i}kx)$, for $k = 2 \times 2\pi/L$ and $L = 1$.

This relation, which we will see is of central importance, can be proven as follows: if $k \neq k'$ we have

$$\frac{1}{L}\int_I \mathrm{d}x\, \mathrm{e}^{\mathrm{i}(k-k')x} = \frac{1}{\mathrm{i}L(k-k')}\, \mathrm{e}^{\mathrm{i}(k-k')x}\Big|_0^L = 0,$$

due to the periodic boundary conditions, $\exp(\mathrm{i}kL) = \exp(\mathrm{i}k0) = 1$ (and the same for k'). However, for $k = k'$, $\exp(\mathrm{i}(k-k')x) = 1$, and the integral trivially yields unity.

INFO In physics and engineering the notation of (C120) is often used when x is a space-like argument. However, just as often Fourier calculus is applied to describe functions $f(t)$, where t is time-like. (For example, Fig. C15 shows a time-like signal.) In that case the alternative notation

$$f(t) = \frac{1}{T}\sum_\omega \tilde{f}_\omega\, \mathrm{e}^{-\mathrm{i}\omega t} \tag{C124}$$

is more frequently used. Here, $f(t)$ is defined on an interval $[0, T]$ and $\omega = 2\pi n/T$ is called the **frequency** of the Fourier mode. Also notice the sign change relative to Eq. (C120) in the exponent of the mode. The details of the definition of Fourier modes are matters of convention and differ from one scientific community to another. In texts involving Fourier calculus it is therefore common practice to open with a remark such as: 'In this text, we will define Fourier series as $f(x) = \ldots$'.

Fourier series construction

In view of the periodic structure of the Fourier modes it may seem surprising that most functions which occur in practice, including aperiodic functions, afford Fourier series representations.

To understand the criteria for Fourier representability let us *assume* that the series exists and ask what conditions for the function f ensue. If f has a series representation then the Fourier coefficients $\tilde{f}_k$ can be easily obtained as follows: multiply $f(x)$ by $\exp(-\mathrm{i}kx)$ and integrate over I:

$$\int_I \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x) = \int_I \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx}\Big(\frac{1}{L}\sum_{k'} \tilde{f}_{k'}\, \mathrm{e}^{\mathrm{i}k'x}\Big) = \sum_{k'} \tilde{f}_{k'}\, \frac{1}{L}\int_I \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}(k-k')x} \overset{(C123)}{=} \tilde{f}_k,$$

where in the last step the orthogonality relation of Fourier modes was used. We thus have the identification

$$\boxed{\tilde{f}_k = \int_I \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x).} \tag{C125}$$

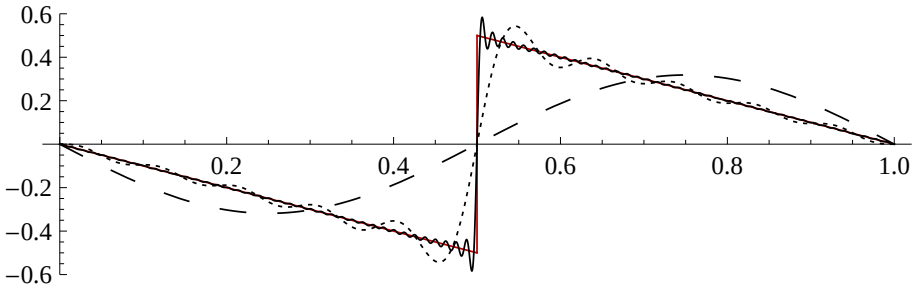


Figure C18: Fourier representation of the function (C127) in terms of a finite series with maximum index $n_{\max} = 1$ (long dashed), 10 (dashed) and 80 (solid).

Notice that even for real functions, $f(x) \in \mathbb{R}$, the coefficients $\tilde{f}_k$ are generally complex. However, we have the symmetry relation,

$$\overline{\tilde{f}_k} = \int_I \mathrm{d}x\, \mathrm{e}^{+\mathrm{i}kx} f(x) = \tilde{f}_{-k}. \tag{C126}$$

EXAMPLE Consider the function (cf. Fig. C18)

$$f(x) = \begin{cases} -x, & x \in \left(0, \frac{1}{2}\right) \\ 1-x, & x \in \left(\frac{1}{2}, 1\right) \end{cases}. \tag{C127}$$

The Fourier coefficients describing f are readily computed: for $k = 0$ we have $\tilde{f}_0 = 0$, and for $k \neq 0$ we obtain

$$k \neq 0: \quad \tilde{f}_k = \int_0^{1/2} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx}(-x) + \int_{1/2}^{1} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx}(1-x) = \frac{\mathrm{e}^{-\mathrm{i}k/2}}{\mathrm{i}k}, \tag{C128}$$

where partial integration was used to integrate $x\mathrm{e}^{-\mathrm{i}kx}$.

The above procedure yields the coefficients $\tilde{f}_k$ *provided* the Fourier expansion exists. To understand under which conditions this is true, we substitute Eq. (C125) into (C120), assume that the order of the summation over k and the integration over x can be exchanged, and obtain

$$\begin{aligned} f(y) &\overset{!}{=} \frac{1}{L} \sum_k \left(\int_I \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x) \right) \mathrm{e}^{\mathrm{i}ky} = \int_I \mathrm{d}x \left(\frac{1}{L} \sum_k \mathrm{e}^{\mathrm{i}k(y-x)} \right) f(x) \\ &\overset{(\text{C110})}{=} \int \mathrm{d}x\, \delta(x-y) f(x), \end{aligned} \tag{C129}$$

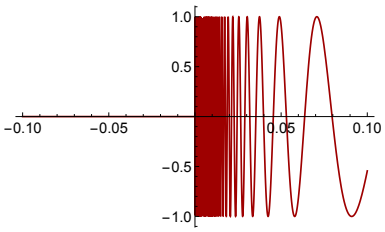
Where in the crucial third equality we noted that the expression in brackets is the δ-function.[6] The final integral yields $f(y)$, so the ansatz of f as a sum over Fourier modes faithfully

[6] Do remember that there is a hidden convergence generating factor, i.e. the expression in brackets should be read as $\lim_{\epsilon\to 0} \frac{1}{L} \sum_k \mathrm{e}^{\mathrm{i}k(y-x)-\epsilon|k|}$, which is Eq. (C110)$_{\epsilon\to 0} = \delta(x)$.

reproduces f as required. However, in deriving this relation, we tacitly assumed that the Fourier coefficients, $\tilde{f}_k$, are finite and that the sum over them exists. For functions obeying the rather mild so-called Dirichlet conditions (see info section below) this is the case, and Fourier expandability is granted.

INFO The three **Dirichlet conditions** sufficient for the Fourier expandability of a function read:

- ▷ The integral of (the modulus) of the function must exist: $\int_I |f(x)|\mathrm{d}x < \infty$.
- ▷ The number of local extrema of f in I must be finite.
- ▷ f must contain only finitely many discontinuities in I.



An example of a function failing this test is given by

$$f(x) = \begin{cases} 0, & x \in [-\pi, 0], \\ \sin(1/x), & x \in (0, \pi]. \end{cases}$$

The infinitely many extrema accumulating in the vicinity of $x = 0$ spoil its Fourier-expandability.

EXAMPLE In the previous example we obtained Eq. (C128) for the Fourier coefficients of the 'sawtooth function'. Using this result, we obtain the series representation

$$f(x) = \sum_{k\neq 0} \mathrm{e}^{\mathrm{i}kx} \frac{\mathrm{e}^{-\mathrm{i}k/2}}{\mathrm{i}k} = \frac{1}{\pi} \sum_{n\in\mathbb{Z}\setminus\{0\}} \frac{\mathrm{e}^{\mathrm{i}2\pi nx}}{2\mathrm{i}} \frac{\mathrm{e}^{-\mathrm{i}\pi n}}{n} = \frac{1}{\pi} \sum_{n>0} \sin(2\pi nx) \frac{(-1)^n}{n}.$$

Fig. C18 illustrates how the series models the function in terms of oscillatory $(\sin)$ contributions. The long-dashed, dashed, and solid curves, respectively, represent finite summations truncated at the index $n_{\max} = 1, 10, 80$, respectively. It is evident that the ensuing approximations are efficient in regions where the function is smooth. However, problems arise in the neighborhood of sharp corners where a large number of terms is required to obtain satisfactory agreement.

INFO Notice that even for an elaborate representation of $f(x)$ in terms of 80 Fourier contributions the series visualized in Fig. C18 'overshoots' at the corners of the function. It can be shown that the excess peak does not diminish upon inclusion of more terms in series; it remains at a level of $\mathcal{O}(10\%)$ of the function value. Only the width of the excess regions shrinks at higher levels of summation accuracy.

This phenomenon is known as **ringing**. Ringing is notorious in audio and video compression algorithms such as MP3 or AAC, or JPEG, which all rely on Fourier signal encoding. The term 'ringing' alludes to the fact that in compressed acoustic data, such overshooting becomes audible as a sharp 'ringing' noise, accompanying the reproduction of dynamical sound sources (such as drums). The JPEG compressed reproduction of a star shown in the figure illustrates how the same effect spoils the accurate reproduction of sharp edges in visual data.

The example above illustrates an important **general feature of Fourier representations**: the series (C120) encodes the information carried by the function $f(x)$. For large k the exponential functions on the r.h.s. oscillate rapidly, i.e. functions with large k carry the information about the 'fine structure' of $f(x)$, or structures at small scales in x. Conversely, the information on large scale structure in x is carried by slowly oscillating contributions with small k. The appearance of k and x in the product $k \cdot x$ in the Fourier modes shows that scales of characteristic length Δx are described in terms of Fourier modes with index $k \sim \Delta x^{-1}$. This fact is known as **Fourier reciprocity** and should be remembered as follows:

Fourier modes of large/small value k describe structures at small/large scales, $x \sim k^{-1}$.

EXAMPLE For functions devoid of sharp singularities, the inclusion of a few Fourier modes can suffice to obtain excellent approximations. Consider, for example, the function

$$f(x) = \mathrm{Re}\,\frac{1}{2+e^{\mathrm{i}x}} = \frac{2+\cos x}{5+4\cos x} \tag{C130}$$

on the interval $x \in [0, 2\pi]$ (Fig. C19). The Fourier coefficients of this function are best computed by geometric series expansion (cf. Eq. C83),

$$f(x) = \frac{1}{2}\mathrm{Re}\frac{1}{1+\frac{1}{2}\mathrm{e}^{\mathrm{i}x}} = \frac{1}{2}\mathrm{Re}\sum_{l=0}^{\infty}\left(-\frac{1}{2}\mathrm{e}^{\mathrm{i}x}\right)^{l}. \tag{C131}$$

Substituting this expression into Eq. (C125) and using Eq. (C123), we obtain $\tilde{f}_k = (-1)^k/2^{k+2}$. The graphics shown in the figure illustrate how the approximation of the function in terms of a sum over only a few Fourier modes yields excellent results.

Conceptual meaning of Fourier series representations

Eq. (C120) has the form 'function$= \sum_k$ (coefficient)$_k \times$ (function)$_k$', where the function on the l.h.s. is $f(x)$, $\tilde{f}_k \equiv$(coefficient)$_k$ are the coefficients, and $\exp(\mathrm{i}kx) \equiv$(function)$_k$ are k-dependent functions of x. If we think of f as an element of a vector space of periodic functions, then this formula has the status of representing the 'vector' f in terms of a linear combination of other vectors, viz. the exponential functions indexed by k. Since every function can be expanded in this way, the set of all exponentials $\{\exp(ikx)\}$ can be viewed as a **basis of function space**, indexed by k. This suggests that

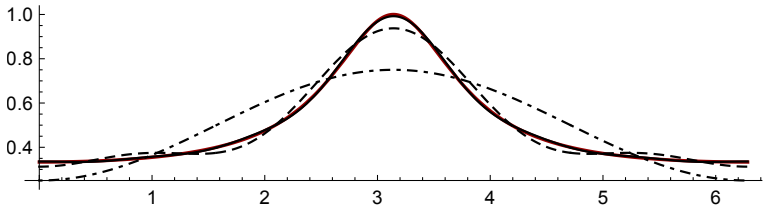


Figure C19: The red curve shows the function (C130) and the dashed, dash-doted, and solid black lines are approximations by 1, 3, and 6 Fourier modes.

A Fourier series representation corresponds to a change of basis in function space.

This interpretation of Fourier representations is rather useful both conceptually and from an applied perspective. Many of the formulae derived in this section have a background in linear algebra and this connection is helpful for understanding and remembering their structure. The observation that functions can be expanded in terms of $\exp$-functions suggests that it might be possible to construct further sets of useful function bases. Indeed there exist several other expansion schemes relevant to physical disciplines such as electrodynamics or quantum mechanics, and the vector space interpretation allows them to be understood in a unified fashion. For a comprehensive discussion of these connections we refer to chapter L10.

C6.3 Fourier transform

Next we explore what happens as we extend the width of our support interval I indefinitely. To this end, we choose an interval $I \equiv [-\frac{L}{2}, \frac{L}{2}]$, and send $L \to \infty$. In the limit, the function f is defined on the entire real axis, $f : \mathbb{R} \to \mathbb{C}$.

Definition of the Fourier transform

For $L \to \infty$ the spacing $\delta k = \frac{2\pi}{L}$ between successive Fourier series wave numbers $k = n2\pi/L$ tends to zero. The Fourier sum then assumes the form of a Riemann sum $\frac{1}{L}\sum_k(\dots) = \frac{1}{2\pi}\delta k \sum_{n\delta k}(\dots) \to \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k(\dots)$. Introducing the shorthand notation $\int \frac{\mathrm{d}k}{2\pi} = \frac{1}{2\pi}\int \mathrm{d}k$ and writing $\tilde{f}_k \to \tilde{f}(k)$ for the infinite-space Fourier coefficients we apply this replacement to the series (C120) to obtain

$$\begin{aligned} \tilde{f}(k) &= \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x), \\ f(x) &= \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{\mathrm{i}kx} \tilde{f}(k). \end{aligned} \tag{C132}$$

The first of Eqs. (C132) defines the **Fourier transform** $\tilde{f}$ of the function f and the second equation is the inverse Fourier transform.

As with the Fourier series Eq. (C120) the definition (C132) has problematic convergence properties: only a few functions can be integrated with an exponential function over an infinite interval. To overcome this problem we introduce a **convergence generating factor** similar to that introduced in Eq. (C122): we generalize the exponentials appearing in the definition as

$$\begin{aligned}\exp(\mathrm{i}kx) &\to \exp(\mathrm{i}kx - \epsilon|k|),\\ \exp(-\mathrm{i}kx) &\to \exp(-\mathrm{i}kx - \epsilon|x|)\end{aligned}$$

where ϵ is positive and sent to zero, $\epsilon \searrow 0$, after all integrals have been done. At any finite ϵ, functions $f(x)$ and $\tilde{f}(k)$ with less than exponential increase at $|x| \to \infty$ and $|k| \to \infty$ can now safely be integrated. The generalized transformation identities are given by

$$\begin{aligned}\tilde{f}(k) &= \lim_{\epsilon\searrow 0}\int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx-\epsilon|x|} f(x),\\ f(x) &= \lim_{\epsilon\searrow 0}\int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{\mathrm{i}kx-\epsilon|k|} \tilde{f}(k),\end{aligned} \tag{C133}$$

Again, it is customary to suppress this factor in the notation in cases where it is not absolutely required.

EXAMPLE Consider the function

$$f(x) = \Theta(x)\mathrm{e}^{-\gamma x+\mathrm{i}qx},$$

where $q \in \mathbb{R}$ and $\gamma \in \mathbb{R}^+$, and Θ is the Heaviside step function (C118). Its Fourier transform is given by

$$\tilde{f}(k) = \int_0^\infty \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx}\mathrm{e}^{-\gamma x+\mathrm{i}qx} = \frac{1}{\gamma + \mathrm{i}(k-q)}.$$

The inverse Fourier transform then reads

$$f(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \frac{\mathrm{e}^{\mathrm{i}kx}}{\gamma + \mathrm{i}(k-q)}.$$

Could you compute the integral defining the inverse transform by elementary means? (Do not try too hard, it is not straightforward.)

Let us demonstrate that Eqs. (C133) define an integral *transform*, i.e. that it is possible to reconstruct the function $f(x)$ from its Fourier transform $\tilde{f}(k)$. To this end, we substitute the first integral without the convergence generating factor (it will not be needed) into the second integral (where the factor does play a role), exchange the order of integrations and obtain

$$f(x) \overset{!}{=} \lim_{\epsilon\searrow 0}\int \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{\mathrm{i}kx-\epsilon|k|} \int \mathrm{d}x'\, \mathrm{e}^{-\mathrm{i}kx'} f(x') = \int \mathrm{d}x' \left(\lim_{\epsilon\searrow 0}\int \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{\mathrm{i}k(x-x')-\epsilon|k|}\right) f(x').$$

We thus require that

$$\lim_{\epsilon\searrow 0}\int\frac{\mathrm{d}k}{2\pi}\,\mathrm{e}^{\mathrm{i}k(x-x')-\epsilon|k|}=\delta(x-x'), \tag{C134}$$

This integral owes its existence to the presence of the convergence generating factor (why?) and can be computed as

$$\begin{aligned}\lim_{\epsilon\searrow 0}\int\frac{\mathrm{d}k}{2\pi}\,\mathrm{e}^{\mathrm{i}k(x-x')-\epsilon|k|}&=\lim_{\epsilon\searrow 0}\left(\int_0^\infty\frac{\mathrm{d}k}{2\pi}\,\mathrm{e}^{\mathrm{i}k(x-x')-\epsilon k}+\int_{-\infty}^0\frac{\mathrm{d}k}{2\pi}\,\mathrm{e}^{\mathrm{i}k(x-x')+\epsilon k}\right)=\\&=\lim_{\epsilon\searrow 0}\frac{1}{2\pi}\left(-\frac{1}{\mathrm{i}(x-x')-\epsilon}+\frac{1}{\mathrm{i}(x-x')+\epsilon}\right)=\\&=\lim_{\epsilon\searrow 0}\frac{1}{\pi}\frac{\epsilon}{(x-x')^2+\epsilon^2}\overset{\text{(C113)}}{=}\delta(x-x').\end{aligned}$$

We thus confirm Eq. (C134) and the Fourier transform identity relying on it. However, notice that the proof relied an exchange of integrals $\int\mathrm{d}k\int\mathrm{d}x(\dots)\to\int\mathrm{d}x\int\mathrm{d}k(\dots)$. Much as with the previous case of Fourier series this exchange operation — an application of Fubini's theorem discussed in C4.1 — relies on the existence of the integrals involved. While generic criteria for the **existence of Fourier integrals** are difficult to state, the rule of thumb is that functions that can be integrated in the presence of a convergence generating factor can be transformed. This includes functions which grow no faster than power laws (for the growth of any power x^n will be compensated by a factor of $\exp(-\epsilon|x|)$, no matter how small ϵ) but excludes functions with exponential growth. There exist modified versions of the Fourier transform, for example, the so-called **Laplace transform** that can be applied to deal with such cases. However, we will not discuss these extensions here.

INFO The relation,

$$\boxed{\int\frac{\mathrm{d}k}{2\pi}\,\mathrm{e}^{\mathrm{i}kx}=\delta(x),} \tag{C135}$$

plays an important role in various contexts beyond the Fourier transform. It is known as the **exponential representation of the δ-function**. Comparing this integral to the series representation of the δ-function, (C110), we notice a subtle difference: Eq. (C110) was defined for arguments $x\in[0,L]$. However, if we consider (C110) for general $x\in\mathbb{R}$ then we obtain a result *periodic* in x with a period L. Since k is summed over values $k=n2\pi/L$, we have $\exp(ik(x+mL))=\exp(ikx+2\pi nm)=\exp(ikx), m\in\mathbb{Z}$. The sum therefore produces a 'comb' of δ-peaks at positions mL. This is consistent with the fact that Fourier series were designed to describe L-periodic functions. In the limit $L\to\infty$ the sum becomes an integral, the period spacing goes to infinity, and the two definitions match.

EXERCISE Occasionally, it may be necessary or just more convenient to generate convergence by a so-called **Gaussian convergence generating factor**,

$$\exp(\mathrm{i}kx)\to\exp(\mathrm{i}kx-\epsilon k^2), \tag{C136}$$

i.e. a generalization which is even better at convergence at large values of k. Use the general formula for Gaussian integrals

$$\int_{-\infty}^{\infty} \mathrm{d}s\, \mathrm{e}^{-as^2+bs} = \sqrt{\frac{\pi}{a}} \mathrm{e}^{-\frac{b^2}{4a}}, \tag{C137}$$

to verify that

$$\lim_{\epsilon \searrow 0} \int \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{\mathrm{i}k(x-x')-\epsilon k^2}$$

produces a Gaussian representation of the δ-function [cf. Eq. (C29)].

Generalized definitions of Fourier integrals

In practice, one often needs to Fourier transform higher-dimensional functions $f : \mathbb{R}^n \to \mathbb{C}, \mathbf{x} \mapsto f(\mathbf{x})$. This is achieved by separate Fourier transformation in each of the variables contained in $\mathbf{x} = (x^1, \ldots, x^n)$. Defining

$$\tilde{f}(k_1, \ldots, k_n) \equiv \int \mathrm{d}x^1\, \mathrm{e}^{-\mathrm{i}x^1 k_1} \ldots \int \mathrm{d}x^n\, \mathrm{e}^{-\mathrm{i}x^n k_n} f(x^1, \ldots, x^n),$$

and combining the products of exponentials to a single exponential we obtain the **Fourier transform of multi-dimensional functions**

$$\boxed{\begin{aligned} \tilde{f}(\mathbf{k}) &= \int \mathrm{d}x^1 \ldots \mathrm{d}x^n\, \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}), \\ f(\mathbf{x}) &= \int \frac{\mathrm{d}k_1}{2\pi} \ldots \frac{\mathrm{d}k_n}{2\pi}\, \mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}} \tilde{f}(\mathbf{k}), \end{aligned}} \tag{C138}$$

where $\mathbf{k}\cdot\mathbf{x} = \sum_i k_i x^i$, $\mathbf{k} = (k_1, \ldots, k_n)^T$,[7] and the second line contains the inverse transform.

The **Fourier transform of functions $f(t)$ depending on time-like arguments** is defined as

$$\boxed{\begin{aligned} \tilde{f}(\omega) &= \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} f(t), \\ f(t) &= \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{-\mathrm{i}\omega t} \tilde{f}(\omega), \end{aligned}} \tag{C139}$$

where ω is a frequency-like variable. As with the definition of the Fourier series (C124), the signs in the exponents are exchanged relative to the 'space–like' Fourier transform. The rationale behind this convention becomes evident once Fourier transforms of functions $f(x,t)$ depending on space– and time–like arguments are considered. This point is usually discussed in texts on classical electrodynamics.

[7] Here we use a fact discussed in analytical mechanics (cf. V.I.Arnonld, *Mathematical Methods of Classical Mechanics*, Springer Verlag 1978), viz. that $\mathbf{k} = (k_1, \ldots, k_n)^T$ is a covariant object whose components should be labeled by subscripts. For the purposes of the present text it is sufficient to consider this as a notational convention.

Properties of the Fourier transform

The following is a list of the most important properties of the Fourier transform:

▷ **The Fourier transform converts derivatives into multiplicative factors**. To see what is meant by this statement, consider the derivative of a function, $\mathrm{d}_x f(x)$. The Fourier transform, $\widetilde{\mathrm{d}_x f}(k)$, of this derivative is obtained as

$$\boxed{\widetilde{\mathrm{d}_x f}(k) = \mathrm{i}k\tilde{f}(k),} \tag{C140}$$

where $\tilde{f}(k)$ is the transform of $f(x)$. This is seen by partial integration as[8]

$$\widetilde{\mathrm{d}_x f}(k) = \int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx}\mathrm{d}_x f(x) = -\int \mathrm{d}x\, (\mathrm{d}_x \mathrm{e}^{-\mathrm{i}kx}) f(x) = \mathrm{i}k \int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x) = \mathrm{i}k\tilde{f}(k),$$

In the same way one verifies the inverse property: a Fourier transform given by $\mathrm{d}_k \tilde{f}(k)$ has inverse Fourier transform $-\mathrm{i}x f(x)$, or

$$\boxed{\mathrm{d}_k \tilde{f}(k) = -\mathrm{i}(\widetilde{xf})(k)\ .} \tag{C141}$$

The key observation here is that

> Derivatives 'simplify' under Fourier transformation. They get converted into multiplicative factors.

In problems involving lots of derivatives it is often convenient to pass to a Fourier representation, work for a while there, and only later transform back to the original representation. We will discuss such strategies in the next chapter when we solve differential equations.

▷ Consider two functions, $f, g : \mathbb{R} \to \mathbb{C}$. What is the Fourier transform of the product fg? To answer this question we define the **convolution** (Faltung) of two functions f, g as

$$(f * g)(x) \equiv \int \mathrm{d}x' f(x - x') g(x'). \tag{C142}$$

This definition applies regardless of where the functions are defined. For example, the convolution of two functions $\tilde{f}, \tilde{g}$ depending on the variable k is given by

$$(\tilde{f} * \tilde{g})(k) \equiv \int \mathrm{d}k' \tilde{f}(k - k')\tilde{g}(k').$$

[8] Keep the presence of convergence generating factors $\exp(-|x|\epsilon)$ in mind. They eliminate the boundary terms $\mathrm{e}^{-\mathrm{i}kx}\mathrm{e}^{-\epsilon|x|} f(x)|_{-\infty}^{\infty}$ generated by the partial integration.

The **Fourier convolution theorem** now states that the Fourier transform of the product of two functions $(fg)(x) = f(x)g(x)$ is given by the convolution of the respective Fourier transforms:

$$\boxed{\widetilde{fg}(k) = \frac{1}{2\pi}(\tilde{f} * \tilde{g})(k).} \tag{C143}$$

Equivalently, the Fourier transform of a convolution is given by the product of the Fourier transforms,

$$\boxed{\widetilde{(f * g)}(k) = \tilde{f}(k)\tilde{g}(k),} \tag{C144}$$

Eq. (C143) is proven by direct calculation:

$$\begin{aligned}
\widetilde{(fg)}(k) &= \int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x)g(x) \\
&= \int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} \int \frac{\mathrm{d}k''}{2\pi}\, \mathrm{e}^{\mathrm{i}k''x} \tilde{f}(k'') \int \frac{\mathrm{d}k'}{2\pi}\, \mathrm{e}^{\mathrm{i}k'x} \tilde{g}(k') \\
&= \int \frac{\mathrm{d}k'}{2\pi} \int \mathrm{d}k''\, \underbrace{\frac{1}{2\pi} \int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}(k-k''-k')x}}_{\delta(k-k''-k')} \tilde{f}(k'')\tilde{g}(k') = \\
&= \int \frac{\mathrm{d}k'}{2\pi}\, \tilde{f}(k-k')\tilde{g}(k').
\end{aligned} \tag{C145}$$

The inverse relation is shown in the same way. Observe that

> Upon Fourier transformation a convolution (complicated) becomes a product (simple), and vice versa.

Convolutions appear in many different contexts. For example, in applied mathematics and engineering they are often applied to smoothen ragged signal structures (see the exercise below).

▷ The **Fourier transform of the exponential function** is a δ-function, and vice versa

$$\widetilde{\mathrm{e}^{\mathrm{i}qx}} = \delta(k-q), \qquad \widetilde{\delta(x-y)} = \mathrm{e}^{\mathrm{i}ky}. \tag{C146}$$

An important special case is $q = 0$, $y = 0$, i.e.

$$\widetilde{1} = \delta(k), \qquad \widetilde{\delta(x)} = 1. \tag{C147}$$

All these relations are straightforward consequences of the definition of the transform.

▷ Another useful relation connects $\tilde{f}(0)$ to the integral of $f(x)$, and $f(0)$ to the integral of $\tilde{f}(k)$

$$\tilde{f}(0) = \int \mathrm{d}x f(x),$$
$$f(0) = \int \frac{\mathrm{d}k}{2\pi} \tilde{f}(k). \tag{C148}$$

These relations are trivial consequences of the definition of the Fourier transform.

For later reference, we state two more properties of the Fourier transform. However, they may be skipped at first and consulted when necessary.

▷ The Fourier transform **preserves the scalar product** on $L^2(\mathbb{R}, \mathbb{C})$, i.e.

$$\int \mathrm{d}x \, \overline{f(x)} g(x) = \int \frac{\mathrm{d}k}{2\pi} \, \overline{\tilde{f}(k)} \tilde{g}(k). \tag{C149}$$

The finite-interval version of this relation is:

$$\int_I \mathrm{d}x \, \overline{f(x)} g(x) = \sum_k \overline{\tilde{f}(k)} \tilde{g}(k), \tag{C150}$$

Eqs. (C149) and (C150) are proven by straightforward calculation. When applied to the case $f = g$ Eq. (C149) assumes the form

$$\int \mathrm{d}x \, |f(x)|^2 = \frac{1}{2\pi} \int \mathrm{d}k \, |\tilde{f}(k)|^2. \tag{C151}$$

This equation goes by the name of the **Plancherel theorem**.

▷ Under **complex conjugation** the Fourier transform behaves as

$$\overline{\tilde{f}(k)} = \widetilde{\overline{f}}(-k), \tag{C152}$$

where $\widetilde{\overline{f}}$ is the Fourier transform of the complex conjugate function $\overline{f}$. For real valued functions the relation simplifies to $\overline{\tilde{f}(k)} = \tilde{f}(-k)$.

INFO Before leaving the formal discussion of the Fourier transform it is worthwhile mentioning that there exists various other integral transforms of similar flavor. A prominent example is the the **Laplace transform**,

$$\tilde{f}(s) \equiv \int_0^\infty \mathrm{d}t \, f(t) e^{-st}. \tag{C153}$$

Here, $f(t)$ is a 'time-dependent' function, and the complex parameter s is a 'frequency-like' variable. (Imaginary parts in frequency-like variables can be interpreted as finite damping rates, see later

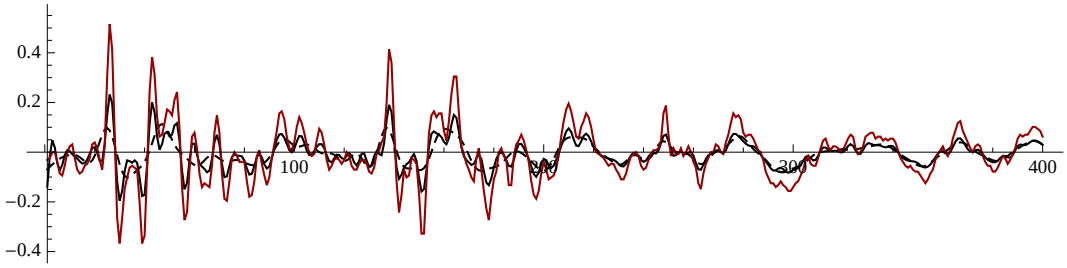


Figure C20: Decomposition of a sound signal of 0.1 sec duration in terms of 500 (dashed) or 1000 (solid) Fourier modes. The latter reduces the raw data (5000 data points) by a factor 5 and already gives a decent approximation to the full signal.

discussion in section C7.3). The required existence of the integral is an implicit part of the definition, i.e. the Laplace transform $\tilde{f}(s)$ is defined only if the integral on the right hand side exists. For example (verify) the Laplace transform of the δ-function $\tilde{\delta}(s) = 1$ exists for all s, and that of the exponential function e^{-t}, $(s+1)^{-1}$ for all arguments $\mathrm{Re}(s) > -1$.

The Laplace transform shares many essential properties with the Fourier transform. For example, it is manifestly linear ($\widetilde{f+g} = \tilde{f} + \tilde{g}$) and satisfies relations such as (verify) $\widetilde{tf(t)} = -\tilde{f}'(s)$, or $\tilde{f}'(s) = -s\tilde{f}(s) - f(0)$. An important difference is that the *inverse*, $f(t)$, of a Laplace represented function $\tilde{f}(s)$ is not as easily obtained as in the Fourier case. Rather, the inverse transformation relies on complex functions integral techniques (of the sort introduced in section C223 below.) For further discussion of the Laplace transform and the occasional applications in differential equation solving where it outperforms the Fourier transform we refer to the literature.

C6.4 Fourier transform applications

REMARK This section illustrates the utility of the Fourier transform on concrete examples. It can be skipped at first reading.

The Fourier transform is a powerful tool in science and engineering. Prominent areas of applications include:

- ▷ The transformation of derivatives into multiplicative factors (cf. Eq. (C140)) makes the Fourier transform an aid in the solution of **differential equations**. We will return to this point in the next chapter.
- ▷ Fourier transformation is used to **analyse, or manipulate measurement data**. Consider, for example, the data shown in Fig. C15. The signal visibly contains two superimposed oscillations, one with period $\sim 0.5\,\mathrm{ps}$ and a slower one with period $\sim 7\,\mathrm{ps}$. Temporal Fourier transformation would make this observation quantitative in terms of pronounced peaks in

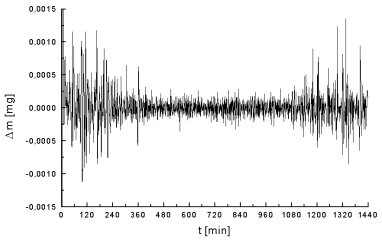
the transform at frequencies corresponding to the two dominant oscillation frequencies.

▷ Fourier transformation plays an important role in the **compression of acoustic or visual data**. The basic idea is to decompose data into Fourier modes and to dispose of modes with wave numbers or frequencies exceeding a certain threshold (cf. Fig. C20). Actual compression algorithms are refined implementations of this approach.

▷ Fourier transformation plays a key role in **imaging** algorithms (cf. the second example below).

In the following, we illustrate the utility of the Fourier transform on two examples.

Noise reduction



In experimental physics and engineering one often records data in which a 'signal' is masked by noise. For example, the figure shows the readout of a measurement device susceptible to the mechanical vibrations caused by human traffic next to the apparatus. (Notice how at nighttimes – the center regions of the plot – the noise is reduced.)

To explore how noisy signals can be processed by Fourier transformation, consider a function $f(x) = f_s(x) + f_n(x)$, where $f_s(x)$ represents a slowly varying 'signal' and $f_n(x)$ is a 'noise' function fluctuating rapidly on scales $\sim \delta$. The noise contribution can be reduced by convolution of f with a suitably chosen smoothing function. Consider, for example, the **box function**

$$g(x) = \frac{1}{\epsilon} \begin{cases} 1, & |x| < \epsilon/2, \\ 0, & \text{else} \end{cases} \tag{C154}$$

where $\epsilon > \delta$ is large compared to the noise fluctuation rate but small compared to the variation scales of the signal and the prefactor is chosen to obtain unit normalization $\int \mathrm{d}x g(x) = 1$. A convolution

$$f(x) \to (f * g)(x) = \int \mathrm{d}y g(y) f(x-y) = \frac{1}{\epsilon} \int_{-\epsilon/2}^{\epsilon/2} \mathrm{d}y f(x-y),$$

effectively 'averages' f an interval of width ϵ around x and hence smoothens the function. It damps out the noise but leaves the signal essentially unaffected if ϵ is not chosen too large. The effect of the convolution becomes even more transparent in the Fourier language. To illustrate the principle, consider the example of the function

$$f_s(x) = \mathrm{e}^{-x/\ell}\Theta(x), \qquad f_n(x) = \eta \cos(Kx), \tag{C155}$$

shown in Fig. C21. Here, f_s represents a 'signal' decaying exponentially on the scale ℓ and f_n simulates 'noise' fluctuating on the scale $2\pi/K \ll \ell$.

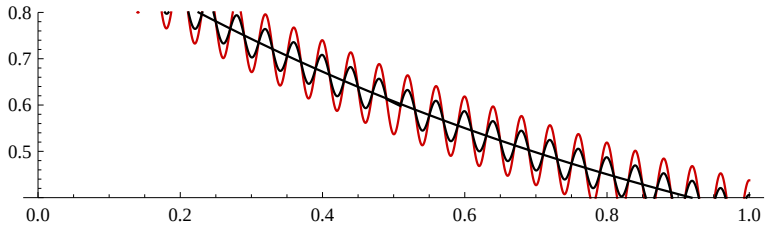


Figure C21: Plot of the function (C155) for $\ell = 1$, $\eta = 0.07, K = 50\pi$). The damped solid and flat curve are the convolution of f against the Gaussian weight (C154) for $\epsilon = 0.01$ and 0.1, respectively.

The Fourier transforms of these two contributions and that of the averaging 'weight function' are readily computed to be [9]

$$\begin{aligned}\tilde{f}_s(k) &= \frac{1}{1/\ell + \mathrm{i}k},\\ \tilde{f}_n(k) &= \pi\eta(\delta(k+K) + (k-K)),\\ \tilde{g}(k) &= \frac{2}{\epsilon k}\sin(\epsilon k/2).\end{aligned}$$

Notice that $\tilde{g}(0) = 1$ which reflects the normalization $\int \mathrm{d}x g(x) = 1$. In Fourier language, the convolution $\widetilde{f * g}(k) = \tilde{f}(k)\tilde{g}(k)$ becomes a simple multiplication,

$$\begin{aligned}\tilde{f}_s(k)\tilde{g}(k) &\overset{k\sim\ell^{-1}}{\simeq} f_s(k),\\ \tilde{f}_n(k)\tilde{g}(k) &\simeq \mathcal{O}(1/\epsilon K).\end{aligned}$$

In the first line we noted that for k values $\sim \ell^{-1}$ relevant to the variation of the signal multiplication with $\tilde{g}(k)$ has little effect, short range averaging does not alter the signal. The second line states that for $k \sim K$ the weight function leads to a strong suppression of rapid fluctuations.

EXERCISE Consider the **Gaussian weight function**,

$$g(x) = \frac{1}{\sqrt{\pi}\epsilon}\mathrm{e}^{-x^2/\epsilon^2}, \tag{C156}$$

and cofirm that

$$\begin{aligned}(f_n * g)(x) &= \mathrm{e}^{-\left(\frac{K\epsilon}{2}\right)^2}\cos(Kx),\\ (f_s * g)(x) &\simeq \mathrm{e}^{-x/\ell + (\epsilon/\ell)^2/4} \qquad (\text{for } x \gg \epsilon)\ .\end{aligned}$$

Compute the Fourier transform

$$\tilde{g}(k) = \mathrm{e}^{-\left(\frac{k\epsilon}{2}\right)^2}.$$

Discuss in what sense convolution with g has little/strong effect on signal/noise.

[9] The Fourier transforms of experimentally recorded data would have to be computed by numerical methods.

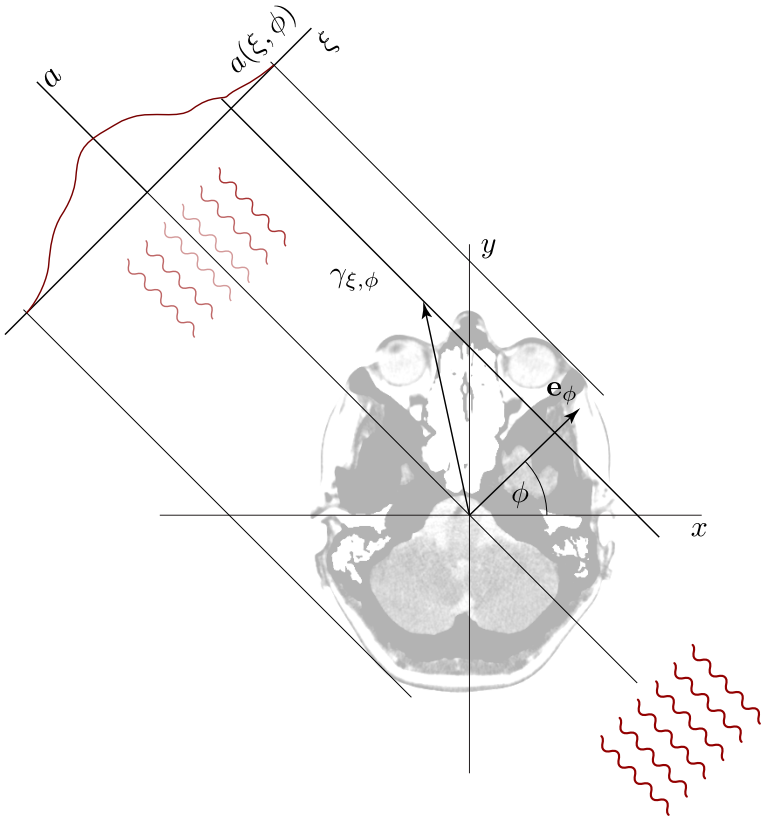


Figure C22: The idea behind tomographic imaging. Discussion, see text.

Tomographic imaging

Tomographic imaging is an important tool for visualization in medicine and technology. Conceptually, it relies on a variant of the Fourier transform known as the Radon transform. To understand the idea, consider a thin slice of some substance, for example a section of a human skull shown in Fig. C22. We choose a fixed xy-coordinate system and assume the object to be described by a yet unknown density profile $f(\mathbf{r})$, with $\mathbf{r} = (x, y)$. The goal is to obtain information on $f(\mathbf{r})$ by X-ray imaging techniques.

To this end, the object is exposed to spatially directed radiation. We define an angle ϕ such that the polar unit vector $\mathbf{e}_\phi = (\cos\phi, \sin\phi)$ is perpendicular to the direction of incidence, and thereby parallel to the radiation wave fronts (cf. Fig. C22). At a detector oriented parallel to $\mathbf{e}_\phi$ the radiation absorbed by the substance is recorded in a spatially resolved manner. This defines an absorption function, $a(\xi, \phi)$, where ξ is the distance from the central axis of the radiation beam (see the figure). It is evident that the profile of the function $a(\xi, \phi)$ depends on the density distribution $f(\mathbf{r})$. However, we still need to understand out how to *quantitatively* reconstruct f from the knowledge of a.

Let us assume that all radiation arriving at a point specified by the coordinates (ϕ, ξ) has traversed along the straight-line path $\gamma_{\xi,\phi}$ indicated in the figure. Points, $\mathbf{r} \equiv (x, y)^T \in \gamma_{\xi,\phi}$, on this path are distinguished by the constancy of the scalar product, $\mathbf{r}\cdot\mathbf{e}_\phi = x\cos(\phi) + y\sin(\phi) =$

ξ. We also assume that the radiation loss incurred locally along the path is proportional to the local density of tissue, $f(\mathbf{r})$. The total loss along the path can be expressed as an integral

$$a(\xi,\phi) = c\int \mathrm{d}x\,\mathrm{d}y\, f(\mathbf{r})\delta(x\cos\phi + y\sin\phi - \xi), \tag{C157}$$

where the δ-function restricts the integration variables to the line $\gamma_{\xi,\phi}$ and c is a constant of proportionality.

Eq. (C157) defines the so-called **Radon transform** of the function f. In a tomographic scan it is obtained by recording the absorption profiles, $a(\xi,\phi_i)$, for a discrete set of incidence angles, ϕ_i. (Changes in the angular direction are responsible for the infamous clicking noise audible during a computer tomography.)

The desired density profile, $f(\mathbf{r})$, is obtained from the measured signal, $a(\xi,\phi)$, in a process of two steps, both involving Fourier transforms. One first transforms $a(\xi,\phi)$ at fixed ϕ in the variable ξ as

$$\begin{aligned}\tilde{a}(k,\phi) &\equiv \int d\xi\, \mathrm{e}^{-\mathrm{i}\xi k} a(\xi,\phi) = c\int \mathrm{d}x\,\mathrm{d}y\, \mathrm{e}^{-\mathrm{i}(k\cos\phi\, x + k\sin\phi\, y)} f(\mathbf{r}) \\ &\equiv c\int \mathrm{d}x\,\mathrm{d}y\, \mathrm{e}^{-\mathrm{i}(k_x x + k_y y)} f(\mathbf{r}) = c\tilde{f}(\mathbf{k}),\end{aligned} \tag{C158}$$

where in the second equality we substituted Eq. (C157) and did the integral over the δ-function. In the third equality we identify $(k\cos\phi, k\sin\phi) \equiv (k_x, k_y)$ with the polar coordinate representation of a two-dimensional Fourier vector $\mathbf{k} = (k_x, k_y)^T$. This is appropriate because the final equality shows that $\tilde{a}(k,\phi) = c\tilde{f}(\mathbf{k})$ is just the x-Fourier transform, $f(\mathbf{k}) = f(k_x, k_y)$, of the density function.

The second step now is the inverse Fourier transform to obtain $f(\mathbf{r})$ from $\tilde{f}(\mathbf{k})$:

$$cf(\mathbf{r}) \overset{(C138)}{=} \int \frac{\mathrm{d}k_x \mathrm{d}k_y}{(2\pi)^2} \mathrm{e}^{\mathrm{i}(k_x x + k_y y)} c\tilde{f}(\mathbf{k}) \overset{(C158)}{=} \frac{1}{(2\pi)^2}\int_0^\infty \mathrm{d}k\, k \int_0^{2\pi} \mathrm{d}\phi\, \tilde{a}(k,\phi)\mathrm{e}^{\mathrm{i}k\cos\phi x + \mathrm{i}k\sin\phi y}\,.$$

Where in the second equality we changed from Cartesian coordinates to an integration in polar coordinates, $\int \mathrm{d}k_x\,\mathrm{d}k_y = \int k\,\mathrm{d}k \int \mathrm{d}\phi$.

To summarize, the two-dimensional density profile $f(\mathbf{r})$ can be obtained from the absorption signal $a(\xi,\phi)$ by computing the one-dimensional Fourier transform $\tilde{a}(k,\phi)$, and from there $f(\mathbf{r})$ by a double inverse transform. In essence, this is the algorithm underlying tomographic image analysis. Our discussion was an oversimplification in that it ignored the fact that in reality $a(\xi,\phi)$ is known only for a discrete set of angles ϕ_i. However, a slightly modified transform known as the **discrete Fourier transform** can be applied to obtain approximate representations of $f(\mathbf{r})$ from discrete data. Of course, the quality of the result will depend on the number of discretization steps.

C7 Differential equations

C7.1 What are they and why do we need them?

A differential equation (DEQ) is an equation involving both a function and its derivatives. A solution is a function for which the conditions defined by the DEQ are satisfied. This means that if the solution and its derivatives are substituted into the DEQ, an equality results. For example,

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = cf(x), \qquad c \in \mathbb{R} \tag{C159}$$

is a differential equation — an equation involving both f and f'. It is solved by all functions of the form $f(x) = \mu \exp(cx), \mu \in \mathbb{R}$. Each value of μ defines a different solution, i.e. we observe that the solution of a differential equation need not be unique.

The set of all solutions of a differential equation is called its **general solution**. To specify a unique solution, additional conditions need to be imposed. For example, one might require that the solution of Eq. (C159) obey a so-called **boundary condition** such as $f(0) = 1$. This would fix a **particular solution** with $\mu = 1$.

However, before turning to a more substantial discussion of the mathematics, let us argue why **differential equations are important to physics**. Physics is about making quantitative predictions for observable phenomena. For example, in celestial mechanics one might aim to predict the position of a planet at a specified time in the future. Such predictions are obtained on the basis of fundamental laws which categorically are formulated in 'differential form': they state how a physical quantity X will *change* if physical quantity Y acts over a small span of time or space. For example, Newton's second law, $m\mathrm{d}_t\mathbf{v} = \mathbf{F}$, can be written as $\mathbf{v}(t + \Delta t) - \mathbf{v}(t) \simeq \mathbf{F}(t)\Delta t$. In this form it states how the velocity $X = \mathbf{v}$ of a body of mass m changes if a force $Y = \mathbf{F}$ is applied over a small time Δt. Similar equations encode the laws of electrodynamics, quantum mechanics, relativity, and other fields. Predictions about physical processes extending over finite intervals of time are obtained by solving such equations, where the uniqueness of the solution requires specifying the boundary data. For example, Newton's equations for the motion of a planet has a unique solution specified in terms of the planet's initial position and velocity. This exemplifies the tight connection between physical prediction making and the solution of differential equations, summarized in general terms in Fig. C23.

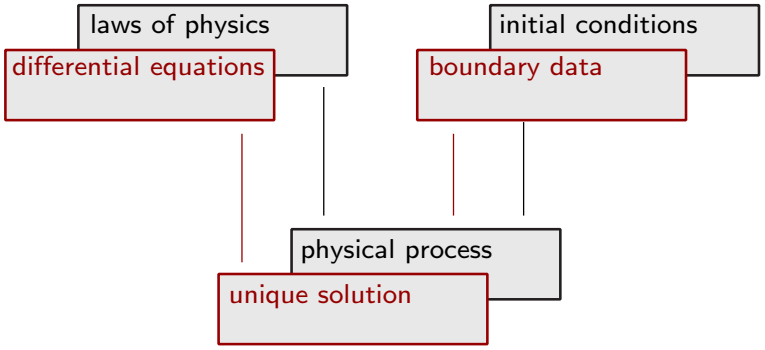


Figure C23: The role of differential equations in physics. Discussion, see text.

C7.2 Typology of differential equations

There exist many **different types of differential equations**: a DEQ can involve the first derivative of a function, f', or higher-order derivatives, $f^{(n)}$, it may be an equation for a one dimensional function, $f(x)$, or for a higher-dimensional function, $f(\mathbf{x})$, it may be an equation for more than one function $f_i, i = 1, \ldots$, it may depend linearly on the function (as in our example), or it may depend on f in complicated ways, etc. Different types of differential equations call for distinct solution strategies and in many cases the solutions are unknown.

For all these reasons, the theory of differential equations is a field difficult to make an overview of. It is therefore all the more important to know the most important criteria for distinguishing between different types of differential equations and their mathematical complexity:

▷ There exist two major families, ordinary and partial DEQs. **Ordinary differential equations** contain derivatives, d_x, with respect to only one variable x. **Partial differential equations** involve several variables, $x^1, x^2, \ldots$ and their derivatives, $\partial_{x^1}, \partial_{x^2}, \ldots$

Examples:

$$\begin{aligned} \mathrm{d}_x f(x) &= g(x), && \text{ordinary} \\ (\partial_x - \partial_t) f(x,t) &= 0, && \text{partial.} \end{aligned}$$

▷ A differential equation of n**-th order** (Ordnung n) contains derivatives of nth and lower order. The majority of differential equations relevant to physics are of order 2 or less.

Examples:

$$\begin{aligned} f'(t) &= g(t, f(t)), && \text{1st order,} \\ \mathrm{d}_t^2 f(t) + \mathrm{d}_t f(t) &= g(t, f(t)), && \text{2nd order} \end{aligned}$$

▷ A **system of differential equations** is a set of $m1$ coupled differential equations.

Example:

$$\begin{aligned} \mathrm{d}_t x(t) &= v(t), \\ \mathrm{d}_t v(t) &= f(x(t)). \end{aligned}$$

▷ A **linear differential equation** contains the function in question only to linear order. **Nonlinear differential equations** depend on the solution in more complicated ways.

Examples:

$\partial_x^2 \phi(x) = -\rho(x)$	linear, ordinary, 2nd order (one-dimensional Poisson equation)
$\mathrm{d}_t^2 x(t) = c \sin(x(t))$	nonlinear, ordinary, 2nd order (eq. of mathematical pendulum).

In the following, we discuss the above classes separately and introduce different types of solution strategies. The focus will be on ordinary DEQs which are much easier to solve than partial DEQs. A few comments on the latter are included at the end of the chapter.

C7.3 Linear first-order equations

The simplest differential equations are linear in the solution function and of first order in derivatives. An equation of this type can always be represented as (why?)

$$\boxed{\mathrm{d}_t f(t) = g(t) f(t) + h(t),} \tag{C160}$$

where g and h are given functions, and f needs to be found. Equations of this form play an important role in the theory of electric circuits and in signal processing. (In these applications, f, g, h are functions of time and this is why the variable is denoted by t.)

The unique solution of a first order (not necessarily linear) DEQ requires the specification of a single additional equation such as $f(t_0) = f_0$ where t_0 and f_0 are constants. In line with the time-like interpretation of t, such conditions are called **initial conditions**. In section C7.6 we will explain why the equation needs precisely one initial condition to be uniquely solvable. For notational convenience we set $t_0 = 0$ throughout.

We first consider the so-called **homogeneous equation** defined by the absence of the f-independent term, $h = 0$. This equation can be solved by a method known as 'separation of variables' (see info section below) and the result reads

$$f(t) = f_0 \exp\left(\int_0^t \mathrm{d}s \, g(s) \right). \tag{C161}$$

That this is a solution is easily verified by computing $f'(t) = f_0 \exp(\int_0^t \mathrm{d}s' g(s)) \, \mathrm{d}_t \int_0^t \mathrm{d}s \, g(s) = f(t)g(t)$. For $t = 0$, the integral vanishes and we obtain $f(0) = f_0$ as required.

INFO The solution (C161) is derived by a method known as **separation of variables**. This scheme is applicable to all differential equations of the form

$$\mathrm{d}_t f(t) = g(t)h(f(t)), \tag{C162}$$

where g and h are arbitrary functions. For $h(f(t)) = f(t)$ this reduces to the linear equation Eq. (C160). To understand the terminology 'separation of variables' we define $y \equiv f(t)$ and rewrite the equation as

$$\frac{\mathrm{d}y}{\mathrm{d}t} = g(t)h(y).$$

Let us now temporarily replace the derivative by a quotient of differences, i.e. think of $\mathrm{d}y$ and $\mathrm{d}t$ as finite quantities defined in such a way that $\lim_{\mathrm{d}t\to 0} \mathrm{d}y/\mathrm{d}t = y'$. We may then rearrange the equation as

$$\frac{\mathrm{d}y}{h(y)} = g(t)\mathrm{d}t.$$

In this representation, variables have been 'separated' in that all y/t-dependence is on the left/right side of the equation. In the final step, we 'sum' over the increments appearing on the two sides of the equation between corresponding bounds, i.e. values between y_0 and y_1 on the l.h.s. and corresponding time arguments t_0 and t_1 on the l.h.s. Using the symbol '$\int$' to represent a sum in the limiting case of infinitely small increments this leads to

$$\int_{y_0}^{y_1} \frac{\mathrm{d}y}{h(y)} = \int_{t_0}^{t_1} g(t)\mathrm{d}t.$$

In the jargon of differential equations theory this is known as a solution up to **quadrature**. Here, 'quadrature' is historical terminology for integration, and what the term means is that the problem is solved up to an integral over functions $(1/h,\, g)$ which are given.

For example, in the case of a linear differential equation, $h(y) = y$, the l.h.s. integrates to $\ln(y/y_0)$. We may then exponentiate $\exp(\ln(y_1/y_0)) = \exp(\int_0^t g\mathrm{d}t)$ to obtain $y_1 = y_0 \exp(\int_{t_0}^{t_1} \mathrm{d}t)$. A final relabelling of variables $t \to s$, $t_0 = 0$, $t_1 = t$, $y_0 = f_0$, $y_1 = f(t)$ leads to the solution (C161).

In section **??** we will show how the above cavalier treatment of the increments, $\mathrm{d}t, \mathrm{d}y$, can be made precise. However, we also note that what counts in differential equation theory is to find solutions. *How* these solutions are found is of secondary importance. One frequently has situations where no clear solution strategy is known and 'experimentation' becomes necessary. Even if these steps involve manipulations of dubious mathematical legitimacy, solutions may always be checked by substitution into the DEQ.

We turn to the **inhomogeneous differential equation** (C160) with non-vanishing h. The strategy to solve the general problem was introduced by Euler and is called **variation of constants**. Euler's proposal was to 'vary the constant' f_0 of the homogeneous solution and to replace it by a function $\tilde{f}(t)$,

$$f(t) = \tilde{f}(t)\, \mathrm{e}^{\Phi(t)}, \tag{C163}$$

where we defined the abbreviation $\Phi(t) = \int_0^t \mathrm{d}s\, g(s)$. The question now is how to find a function $\tilde{f}$ such that the DEQ is solved. To this end, we substitute the ansatz (C164) into the equation and bring all f-dependence to the l.h.s. to obtain

$$(\mathrm{d}_t - g(t))\left(\tilde{f}(t)\mathrm{e}^{\Phi(t)}\right) = (\tilde{f}'(t) + \tilde{f}\Phi'(t) - \tilde{f}g(t))\mathrm{e}^{\Phi(t)} = \tilde{f}'(t)\mathrm{e}^{\Phi(t)} \stackrel{!}{=} h(t),$$

where in the last step we used that $\Phi'(t) = g(t)$. This shows that $\tilde{f}$ is determined by the condition $\tilde{f}' = \mathrm{e}^{-\Phi}h$, i.e. $\tilde{f}$ is the principal function of $\mathrm{e}^{-\Phi}h$: $\tilde{f}(t) = \int_0^t \mathrm{d}s\, h(s)\mathrm{e}^{-\Phi(s)} + c$, where the constant c is determined by substitution of $t = 0$ into the equation, $c = \tilde{f}(0)$. We have thus obtained $\tilde{f}(t) = \tilde{f}(0) + \int_0^t \mathrm{d}s\, h(s)\mathrm{e}^{-\Phi(s)}$ and substitution of this result into (C163) yields

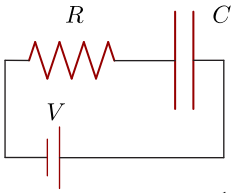
$$f(t) = \tilde{f}(0)\mathrm{e}^{\Phi(t)} + \mathrm{e}^{\Phi(t)} \int_0^t \mathrm{d}s\, h(s)\, \mathrm{e}^{-\Phi(s)}.$$

At $t = 0$ the integral vanishes, $\Phi(0) = 0$, and so the as yet undetermined value $\tilde{f}(0) = f(0) \stackrel{!}{=} f_0$ is fixed by the boundary condition. This leads to the final result

$$\boxed{f(t) = f_0\, \mathrm{e}^{\int_0^t \mathrm{d}s\, g(s)} + \int_0^t \mathrm{d}s\, h(s)\, \mathrm{e}^{\int_s^t \mathrm{d}r\, g(r)}.} \qquad \text{(C164)}$$

(Verify that this result solves Eq. (C160).)

EXAMPLE Linear differential equations play an important role in applications. As an example, consider a so-called RC-circuit containing a resistor of resistance R, a capacitor of capacitance C, and a time dependent voltage source, $V(t)$, in series.



We want to compute the time-dependent current flow, $I(t)$, through the circuit. According to Kirchhoff's voltage law, the sum of the voltage drops across each of the three circuit elements equals zero. The voltage drop at the source is $V(t)$, at the resistor it is RI (Ohm's law), and at the capacitor it is $C^{-1}Q$, where $Q = Q(t)$ is the time-dependent charge on the capacitor. We thus have $C^{-1}Q(t) + RI(t) = V(t)$. We also know that the rate of change of the charge on the capacitor is equal to the current, $\mathrm{d}_t Q(t) = I(t)$. This leads to the inhomogeneous linear differential equation

$$\mathrm{d}_t Q + \frac{1}{RC}Q = \frac{V(t)}{R},$$

for the function $Q(t)$. Comparing to Eq. (C160) we have the identification $g = -1/RC$ and $h = V(t)/R$. The integration over the constant function g yields $\int \mathrm{d}s\, g = -s/RC$ and so the general solution (C164) assumes the form

$$Q(t) = Q_0\mathrm{e}^{-t/RC} + \frac{1}{R}\int_0^t \mathrm{d}s\, V(s)\, \mathrm{e}^{-(t-s)/RC}.$$

Differentiation w.r.t. time, t, yields

$$I(t) = -\frac{Q_0}{RC}\mathrm{e}^{-t/RC} - \frac{1}{R^2C}\int_0^t \mathrm{d}s\, V(s)\,\mathrm{e}^{-(t-s)/RC} + \frac{V(t)}{R},$$

where the first two terms come from the differentiation of the exponential functions and the third from the differentiation w.r.t. the upper limit of the integration boundary.The exponential factors in the solution show that the system possesses an intrinsic **RC-time**, $t_0 = RC$. This time scale sets the rate at which the circuit responds to changes in the external voltage changes. Also note that for constant voltage, $V = \mathrm{const.}$, the current vanishes for time scales $t > t_0$ (try proving it): the presence of the capacitor forbids a static current flow along the loop.

C7.4 Systems of first order linear differential equations

A system of first order linear differential equations is a set of first order DEQ's for n unknown functions $(f^1, \ldots, f^n)$ which is linear in all f^i. Using a 'time-like' notation, $f^i = f^i(t)$, this constrains the system to the form

$$\begin{aligned}
\dot{f}^1(t) &= a^1{}_1(t)f^1(t) + a^1{}_2(t)f^2(t) + \ldots a^1{}_n(t)f^n(t) + g^1(t),\\
&\vdots \qquad \vdots\\
\dot{f}^n(t) &= a^n{}_1(t)f^1(t) + a^n{}_2(t)f^2(t) + \ldots a^n{}_n(t)f^n(t) + g^n(t),
\end{aligned}$$

where the coefficient's $a^i{}_j(t)$ and $g^i(t)$ may be functions of t. Defining a matrix $A = \{a^i{}_j\}$ and combining the functions f^i into a vector, $\mathbf{f} = (f^1, \ldots, f^n)^T$, and likewise, $\mathbf{g} = (g^1, \ldots, g^n)^T$, this assumes the compact form

$$\boxed{\dot{\mathbf{f}}(t) = A(t)\mathbf{f}(t) + \mathbf{g}(t).} \tag{C165}$$

General systems of this form can be difficult to solve. The problem becomes much easier in cases where $A(t) = A$ and $\mathbf{g}(t) = \mathbf{g}$ are constant in time. This defines the so-called **system of first order linear differential equations with constant coefficients**,

$$\dot{\mathbf{f}}(t) = A\mathbf{f}(t) + \mathbf{g}. \tag{C166}$$

The problem becomes even simpler if $\mathbf{g} = \mathbf{0}$ and we have the **homogeneous equation**,

$$\boxed{\dot{\mathbf{f}}(t) = A\mathbf{f}(t).} \tag{C167}$$

We next discuss how the system (C167) can be solved in closed form.

EXERCISE Consider the case $n = 1$, i.e. $\dot{f} = af + g$. Solve this DEQ with the initial condition $f(0) = f_0$.

Solution of the homogeneous linear equation Eq. (C167)

The appearance of a matrix A in the system (C197) suggests considering its eigenvectors, $\mathbf{v}_i$ and eigenvalues, λ_i. Specifically, for an initial condition $\mathbf{f}_0 \equiv c\mathbf{v}_i$, $c \in \mathbb{C}$, proportional to one of the eigenvectors, the system is solved as

$$\mathbf{f}(t) = c\mathrm{e}^{\lambda_i t}\mathbf{v}_i.$$

This is readily checked by substitution, $\mathrm{d}_t\mathbf{f} = \lambda_i\mathbf{f} = \lambda_i c\mathbf{v}_i\mathrm{e}^{\lambda_i t} = cA\mathbf{v}_i\mathrm{e}^{\lambda_i t} = A\mathbf{f}$. Assuming that A is diagonalizable, i.e. that the set $\{\mathbf{v}_i\}$ defines a basis of $\mathbb{C}^n$, we may generalize this result to a full solution of the problem:

1. Expand an arbitrary initial condition in terms of the eigenvectors,

$$\mathbf{f}_0 \equiv \sum_i c^i\mathbf{v}_i, \tag{C168}$$

2. to obtain the solution

$$\mathbf{f}(t) = \sum_i c^i\mathrm{e}^{\lambda_i t}\mathbf{v}_i. \tag{C169}$$

(Substitute Eq. (C169) into the differential equation to check that that it solves the equation and is consistent with the initial conditions.)

INFO (*Requires section L7.5.*) Systems of linear equations play an important role in physics, for example in classical (see the next section) and quantum mechanics. In these fields it is often preferable to work with **'invariant' solutions of the system** (C197), that is solutions not making explicit reference to the eigenvectors of the matrix A. The structural similarity of the system (C197), d_t(solution) = (constant)×(solution) to the single linear equation (C159) indeed suggests that there is an analogous solution, (solution)=exp((constant)×t), where the role of the constant must however be taken by the matrix. Indeed, we may apply the methods of section L7.5 to define

$$\boxed{\mathbf{f}(t) = \mathrm{e}^{At}\,\mathbf{f}(0),} \tag{C170}$$

where the exponential $\exp(At) \equiv \sum_n \frac{1}{n!}(At)^n$ acts as a matrix on the vector of initial conditions. That this is a solution can be checked by direct computation; let us compute

$$\begin{aligned}\mathrm{d}_t\mathbf{f} = \mathrm{d}_t\mathrm{e}^{At}\mathbf{f}(0) &= \mathrm{d}_t\sum_{n=0}^{\infty}\frac{t^n}{n!}A^n\mathbf{f}(0)\\ &= \sum_{n=1}^{\infty}\frac{t^{n-1}}{(n-1)!}A^{n-1+1}\mathbf{f}(0) = A\sum_{n=0}^{\infty}\frac{t^n}{n!}A^n\mathbf{f}(0) = A\,\mathrm{e}^{At}\mathbf{f}(0) = A\mathbf{f}(t),\end{aligned}$$

where in the fifth equality we relabeled the summation index, $(n-1) \to n$.

Eq. (C170) does not assume the matrix A to be diagonalizable. However, if it is, $A = TDT^{-1}$, we may use (L196), to reformulate the result as

$$\mathbf{f}(t) = (T\,\mathrm{e}^{Dt}\,T^{-1})\mathbf{f}(0) = T\,\mathrm{e}^{Dt}(T^{-1}\mathbf{f}(0)).$$

This equation establishes the relationship with the previous solution (C169). To see this, recall (cf. section **??**) that $T = (\mathbf{v}_1, \ldots, \mathbf{v}_n)$ contains the eigenvectors of A as columns, $T\mathbf{e}_i = \mathbf{v}_i$. We may then write the expansion of the initial condition in eigenvectors as $\mathbf{f}(0) = \sum_i c^i(T\mathbf{e}_i)$ which shows that $T^{-1}\mathbf{f}(0) = \sum_i c^i\mathbf{e}_i$. Substitution of this representation into the previous equation leads to

$$\mathbf{f}(t) = T\mathrm{e}^{Dt}\sum_i \mathbf{e}_i c^i = T\sum_i \mathrm{e}^{\lambda_i t}\mathbf{e}_i c^i = \sum_i \mathrm{e}^{\lambda_i t}\mathbf{v}_i c^i,$$

where in the second equality we used that the diagonal matrix, D, acts as $D\mathbf{e}_i = \lambda_i\mathbf{e}_i$.

The solution of the *inhomogeneous* system of linear first order differential equations with constant coefficients (C166) is left as an answered exercise.

Behavior of the solution

The behavior of the solution (C169) crucially depends on the eigenvalues λ_i. In the exceptional case where all eigenvalues are imaginary, $\lambda_i \in \mathrm{i}\mathbb{R}$, the vector $\mathbf{f}(t)$ is a superposition of n oscillatory contributions with frequencies λ_i^{-1}, i.e. all factors $\exp(\lambda_i t) = \exp(\mathrm{i}|\lambda_i|t)$ are purely oscillatory in this case. More generally, if the eigenvalues are complex, the value λ_i with the largest real part $\mathrm{Re}\,\lambda_i$ dominates the solution at large times. The reason is that $|\exp(\lambda_i t)| = \exp((\mathrm{Re}\,\lambda_i)t)$ is exponentially larger than all $|\exp(\lambda_j t)| = \exp((\mathrm{Re}\,\lambda_j)t), j \neq i$ in this case. Without loss of generality, we assume that λ_1 has the largest real part. (For $\mathrm{Re}\,\lambda_{j>1} < 0$ this includes the possibilities of negative or vanishing real part of λ_1.) In this case we may approximate

$$\mathbf{f}(t) \sim c\,\mathrm{e}^{\lambda t}\mathbf{v}$$

for sufficiently large times where the superscript '1' has been omitted for brevity. We now have to discriminate between several different profiles of long-time solutions:

- For $\lambda > 0$ **real and positive** the solution grows exponentially, and
- For $\lambda < 0$ **real and negative** it shrinks to zero.
- For $\lambda = \mathrm{i}\,\omega$ **purely imaginary** the solution is oscillatory in time with frequency ω.
- For $\lambda = c + \mathrm{i}\,\omega$, $c > 0$ **complex with positive real part** the norm of the solution vector grows exponentially and the vector itself performs oscillatory motion, while
- For $\lambda = c + \mathrm{i}\,\omega$, $c < 0$ **complex with negative real part** the vector oscillates and shrinks.

In the next section we illustrate these different types of solutions with a concrete example.

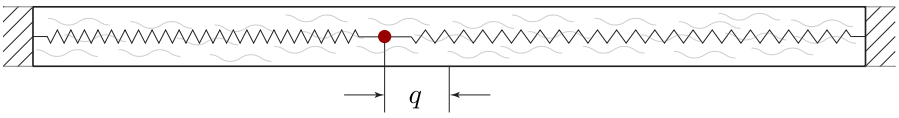


Figure C24: A massive particle acted upon by two springs, all in a tank filled by some viscous liquid. If the deviation, q, of the particle away from the force balance point is small, then the force acting on the particle will be approximately linear in q. The viscous medium acts on the particle by frictional forces.

Application: Damped Oscillator

Phenomena described by linear differential equations include oscillations, damping by frictional motion, or instabilities of mechanical systems. As an example, we consider **a particle of mass m attached to two springs**, see Fig. C24. At the particle coordinate $q = 0$ the net force $F(q)$ exerted by the springs vanishes, $F(0) = 0$. We aim to describe what happens at moderate deviations away from $q = 0$. For small deviations, the force acting to restore equilibrium is linear in q, i.e. $F = -m\omega_0^2 q$, where $\omega_0 > 0$ is a constant. To make the problem more realistic we assume the presence of a **friction** (Reibungskraft) force $F_{\text{fr}} = -2m\tau^{-1}\dot{q}$ where τ^{-1} is a constant and the proportionality of the force to the ~~inverse~~ velocity means that friction slows fast motion.[1] The differential equations describing the motion of the particle then read

$$\begin{aligned} \mathrm{d}_t q &= v, \\ \mathrm{d}_t v &= -2\tau^{-1} v - \omega_0^2 q, \end{aligned} \tag{C171}$$

where the first equation defines the velocity in terms of the particle coordinate and the second is Newton's law, $F = ma = m\mathrm{d}_t v$. The equations have to be solved with an initial condition $(q(0), p(0)) = (q_0, v_0)$. In matrix notation the problem assumes the form

$$\mathrm{d}_t \begin{pmatrix} q \\ v \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\omega_0^2 & -2\tau^{-1} \end{pmatrix} \begin{pmatrix} q \\ v \end{pmatrix},$$

where the 2×2 matrix now assumes the role of the matrix A of the previous section. Its eigenvalues

$$\lambda_\pm = -\tau^{-1} \pm \mathrm{i}\sqrt{\omega_0^2 - \frac{1}{\tau^2}}. \tag{C172}$$

are straightforwardly obtained by solution of a quadratic equation and the corresponding eigenvectors are given by $\mathbf{v}_\pm = (1, \lambda_\pm)^T$. The **general solution of the oscillator equation** then assumes the form

$$\mathbf{y}(t) = \begin{pmatrix} q(t) \\ v(t) \end{pmatrix} = c_+ \begin{pmatrix} 1 \\ \lambda_+ \end{pmatrix} \mathrm{e}^{\lambda_+ t} + c_- \begin{pmatrix} 1 \\ \lambda_- \end{pmatrix} \mathrm{e}^{\lambda_- t}, \tag{C173}$$

[1] The microscopic origin of this force is molecules of the liquid colliding with the particle and thus impeding its motion.

where $c_\pm$ are constants determined by the initial conditions. For definiteness, let us consider a situation where at time $t = 0$ the particle is released at coordinate $q(0) = q_0$ and zero velocity, $v(0) = 0$. We then have $\mathbf{y}_0 = (q_0, 0)^T$ and the expansion of this starting vector in the eigenvectors of the problem yields $\mathbf{y}_0 = \frac{q_0}{\lambda_- - \lambda_+}(\lambda_- \mathbf{v}_+ - \lambda_+ \mathbf{v}_-)$. Substitution of this representation into the general solution yields the specific solution

$$\mathbf{y}(t) = \frac{q_0}{\lambda_- - \lambda_+} \left(\lambda_- \mathbf{v}_+ \mathrm{e}^{\lambda_+ t} - \lambda_+ \mathbf{v}_- \mathrm{e}^{\lambda_- t}\right).$$

It is instructive to discuss the behavior of this solution in a number of physically distinct cases:

- In the **frictionless case**, $\tau^{-1} = 0$, the eigenvalues $\lambda_\pm = \pm \mathrm{i}\omega_0$ are purely imaginary. We then find

  $$\mathbf{y}(t) = q_0 \begin{pmatrix} \cos(\omega_0 t) \\ -\omega_0 \sin(\omega_0 t) \end{pmatrix},$$

  i.e. the particle performs **oscillatory motion** at a frequency set by ω_0. The trajectory $\mathbf{y}(t)$ is shown in the bottom left panel of Fig. C25 and the corresponding q-coordinate in the upper panel.

- For **finite friction**, $0 < \tau^{-1} < \omega_0$, the eigenvalues contain a negative real part. If the friction coefficient is weak, $\tau^{-1} \ll \omega_0$, we may approximate $\lambda_\pm \simeq -\tau^{-1} \pm \mathrm{i}\omega_0$, and this yields,

  $$\mathbf{y}(t) \simeq q_0 \begin{pmatrix} \cos(\omega_0 t) \\ -m\omega_0 \sin(\omega_0 t) \end{pmatrix} \mathrm{e}^{-\frac{t}{\tau}} + \mathcal{O}(1/\tau\omega_0).$$

  The particle performs **damped oscillations**.

- Finally, for $\tau^{-1} > \omega_0$, we are in the so-called **over-damped regime**. The eigenvalues are now real. Considering the case $\tau^{-1} \gg \omega_0$ for simplicity, a first-order Taylor expansion of the square root in (C172) yields $(\tau^{-2} - \omega_0^2)^{1/2} \simeq \tau^{-1} - \tau\omega_0^2/2$ implying $\lambda_+ \simeq -\tau\omega_0^2/2$ and $\lambda_- \simeq -\tau^{-1}$ so that $|\lambda_+| \ll |\lambda_-|$. The large negative value of λ_- makes contributions proportional to $\exp(\lambda_- t)$ damp down rapidly. We thus retain only the longer-lived terms proportional to $\exp(\lambda_+ t)$, yielding

  $$\mathbf{y}(t) \simeq q_0 \begin{pmatrix} 1 \\ -\omega_0 \end{pmatrix} \mathrm{e}^{-\frac{\tau\omega_0^2}{2} t}.$$

  The damping is so strong that the particle no longer performs oscillatory motion. Instead, it slowly 'creeps' from its point of origin back to the equilibrium position at $q = 0$.

C7.5 General nth order linear differential equation

A **general ordinary linear differential equation** can be written as

$$\hat{L}(t) f(t) = g(t),$$

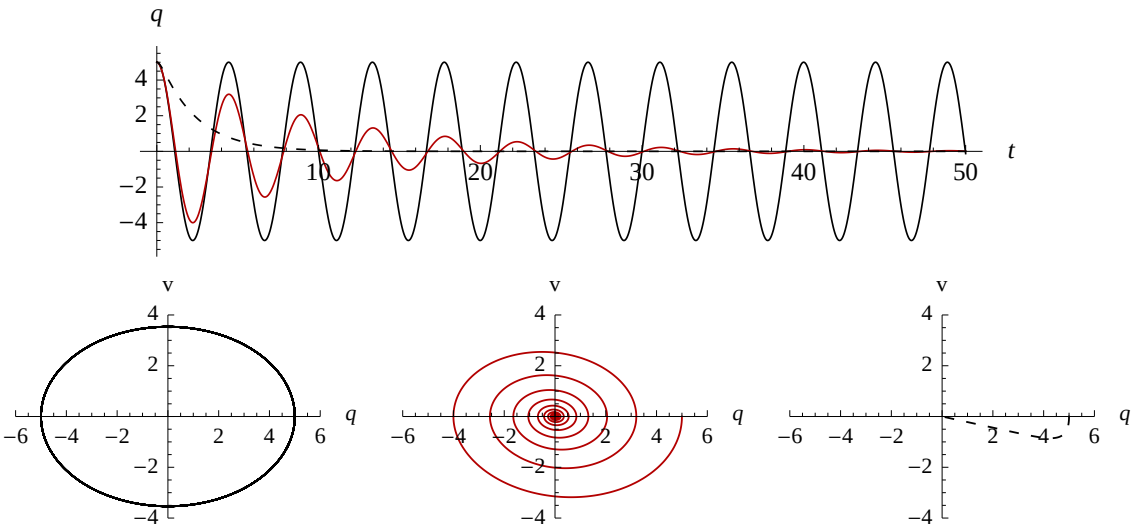


Figure C25: Upper panel: coordinate $q(t)$ of the particle shown in Fig. C24 in the case of no damping (black, solid), finite damping (red, solid), and overdamping (black, dashed). Bottom: the trajectories $\mathbf{y}(t) = (q(t), p(t))^T$ of the particle.

$$\hat{L}(t) = h^{(0)}(t) + h^{(1)}(t)\frac{\mathrm{d}}{\mathrm{d}t} + h^{(2)}(t)\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \ldots, \tag{C174}$$

where $h^{(n)}(t)$ are functions, and the ellipses represent terms containing higher order derivatives. A few comments on this equation: (i) the formal expression $\hat{L}(t)$ is called a **linear differential operator**. It is an 'operator' in the sense that

$$\hat{L}(t)f(t) = h^{(0)}(t)f(t) + h^{(1)}(t)f'(t) + h^{(2)}(t)f''(t) + \ldots \tag{C175}$$

operates on a function to produce a new function. The operator is linear because $\hat{L}(c_1 f_1 + c_2 f_2) = c_1\hat{L}f_1 + c_2\hat{L}f_2$, where we omitted the argument 't' and $c_{1,2}$ are constants. (ii) In practice linear differential **equations of higher than second order** occur rarely. Most equations of relevance to physics are of first or second order. (iii) The unique solution of an nth oder linear differential equation requires the specification of n '**boundary conditions**'. For example, the solution of a second order equation can be made unique by fixing two values, $f(t_i) = f_i$, $i = 1, 2$, or by requiring $f(t_0) = f_0$, $f'(t_1) = d_0$, etc. (iv) Linear differential equations play a highly important **role in physics**. Key physical theories such as electrodynamics of quantum mechanics are linear in the sense that their fundamental laws — the Maxwell equations and the Schrödinger equation, respectively —[2] assume the form of linear differential equations. The fundamental equations of other theories can be *approximated* by linear differential equations in physically important limits. For example, the Einstein equations of general relativity afford a 'linearization' and in this limit describe phenomena such as gravitational waves.

[2] Both the Maxwell equations and the Schrödinger equation are *partial* linear equations, i.e. they contain derivatives with respect to multiple variables. However, most of our below discussion relating to the linearity of DEQs carries over to these cases.

Even complicated-looking linear differential equations can often be solved. The weak spot of these equations is, in fact, their linearity. To appreciate its implications, let f_1 and f_2 be solutions to Eq. (C174) with inhomogeneity g_1 and g_2, respectively. The linearity of the equation then implies that $c_1 f_1 + c_2 f_2$ is a solution to the equation with inhomogeneity $c_1 g_1 + c_2 g_2$. Of course the linear superposition of not just two but arbitrarily many inhomogeneities is given by the corresponding superposition of the partial solutions. This feature, which is sometimes called the **superposition principle**, suggests representing 'complicated' inhomogeneities as sums of simpler ones, and first try to solve the equation for these. This solution strategy goes by the name 'Green function method' and plays an important role, both in physics and mathematics.

INFO The superposition principle has important **physical ramifications**. As an example, consider Maxwell's equations (to be discussed in section V7) whose solutions are electromagnetic fields generated in response to charges and currents, which assume the role of inhomogeneities. If two such sources generate two electromagnetic fields, then the combined action of the sources will be the sum or *superposition* of the fields. This physical superposition principle is responsible for phenomena such as wave interference, i.e. the formation of superimposed wave patterns resulting from the addition of individual waves.

Green function methods

Next to the vanishing function, $g = 0$, δ-functions arguably are the simplest of inhomogeneities. The function $g(t) = \delta(t-u)$ vanishes everywhere except for the point $t = u$, i.e. it has minimal mathematical structure. For historical reasons, the solution of Eq. (C174) with a δ-inhomogeneity

$$\hat{L}G(t,u) = \delta(t-u), \tag{C176}$$

is called a **Green function**. Of course, the Green function depends on the position of the singularity of the δ-inhomogeneity (i.e. for each u we have a different function) and its second argument keeps track of this dependence.

George Green 1793–1841
He owned and worked a Nottingham windmill. His only schooling consisted of four terms in 1801/1802, and where he learned his mathematical skills remains a mystery. Green published only ten mathematical works, the first and most important at his own expense in 1828, "An essay on the application of mathematical analysis to the theories of electricity and magnetism." He left his mill, became an undergraduate at Cambridge in 1833 at the age of 40, then a Fellow of Gonville and Caius College in 1839.

Assume we had managed to compute the Green functions for all values of u. The differential equation for general g is then essentially under control. To understand why, notice that any function $g(t)$ may be represented as a superposition of δ-functions as

$$g(t) = \int \mathrm{d}u\, \delta(t-u) g(u). \tag{C177}$$

In this formula, the function g is represented by a 'sum' (an integral, in fact) over all values of u. The constant, t-independent coefficients in this sum are the values $g(u)$, and

the functions entering the superposition are the δ-functions, $\delta(t-u)$.

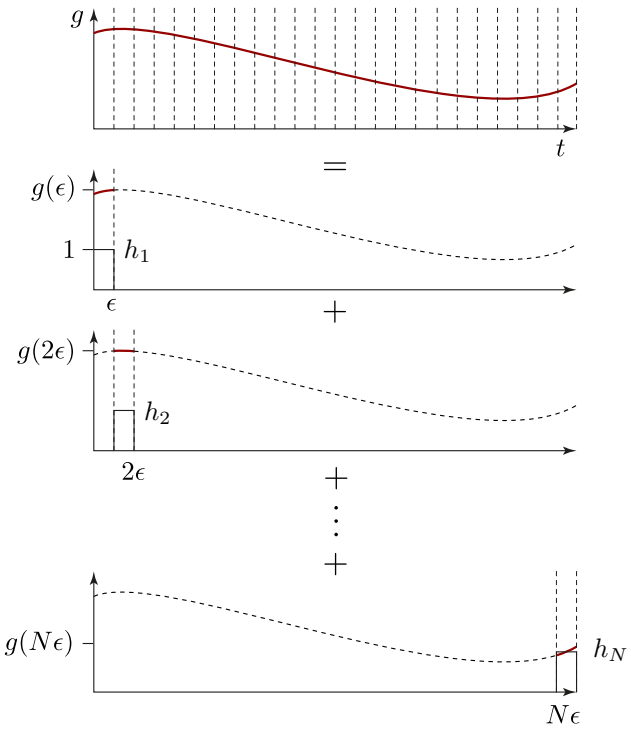


Figure C26: A function, g, can be approximately represented as a sum over unit height functions, h_i, of narrow width ϵ around the coordinates $t = i\epsilon$. In the limit of a large number of discretization steps, the sum $g(t) \simeq \sum_i h_i(t) g(i\epsilon)$ is a good approximation of the continuous function $g(t)$. In the limit $\epsilon \to 0$, the scaled functions $\epsilon^{-1} h_i$ turn into functions $\delta(t-u)$, and the scaled sum $\epsilon \sum_i \to \int du$ becomes an integral. This illustrates how the formal expression (C177) can be understood as a 'sum' over functions $\delta(t-u)$ with 'weights' $g(u)$.

EXERCISE Formally, Eq. (C177) ~~identity~~ is proven by doing the integral over u and using the defining property of the δ-function. However, in the present context, it is more useful to think of it in the spirit of the discrete representation shown in the figure **??**. Before reading the caption of that figure discuss in what sense it shows a discrete representation of the continuum Eq. (C177).

The representation of the inhomogeneity, g, as a sum over δ-functions with 'coefficients', $g(u)$, implies that the solution of the differential equation, too, assumes the form of a sum,

$$f(t) = \int \mathrm{d}u\, G(t,u)\, g(u), \tag{C178}$$

with the same coefficients, $g(u)$. That this is a solution can be verified by direct computation. Using that the differential operator, $\hat{L}(t)$, acts on functions of t, and is linear we obtain

$$\hat{L}(t) f(t) = \int \mathrm{d}u\, (\hat{L}(t) G(t,u))\, g(u) \overset{(C176)}{=} \int \mathrm{d}u\, \delta(t-u) g(u) = g(t).$$

However, as mentioned above, this solution is not unique unless boundary conditions are provided. To an arbitrary solution, f, a solution f_0 of the *homogeneous* differential equation, $\hat{L}(t)f_0(t) = 0$, may be added to obtain another solution $f(t) + f_0(t)$ of the inhomogeneous equation ($\hat{L}(f + f_0) = \hat{L}f + \hat{L}f_0 = g + 0 = g$.) Conversely, two solutions $f_{1,2}$ of the inhomogeneous equation[3] differ by a solution of the homogeneous equation ($\hat{L}(f_1 - f_2) = g - g = 0$). This means that the **general solution of the inhomogeneous equation** can be written as $f + f_0$, where f is a fixed but arbitrary solution of the inhomogeneous equation, and f_0 runs through all solutions of the homogeneous problem. For a differential operator of nth degree, the specification of n boundary conditions then selects a uniquely defined specific solution.[4]

Of course, the solution (C178) remains a formal expression as long as the Green functions $G(t, u)$ are not known. In the theory of inhomogeneous linear differential equations, the computation of the Green functions is more or less equivalent to the solution of the problem. Accordingly, sophisticated machinery for the computation of Green functions, both exactly and approximately, have been developed, and their teaching is a standard subject of theoretical physics courses. In the next section, we will discuss how Green functions of certain classes of linear DEQs can be computed on a simple yet important example.

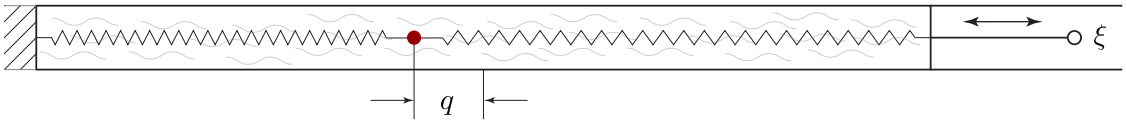


Figure C27: An oscillating particle subject to friction and external driving. Discussion, see text.

Application: Driven damped oscillator

REMARK Requires familiarity with chapter C6 on Fourier calculus.

Consider the damped oscillator problem described by Eq. (C171) extended to the presence of an external driving force, $\xi(t)$, cf. Fig. (C27). The external driving adds to the balance of forces which means that the second of Eqs. (C171) generalizes to $\mathrm{d}_t v = -2\tau^{-1} - \omega_0^2 q + \xi$. We substitute the first equation, $\mathrm{d}_t q = v$ into the second to obtain the second order linear

[3] Eq. (C178) does not specify a unique solution because prior to the fixation of boundary conditions the Green function is not uniquely defined either. The addition of an arbitrary solution of the homogeneous equation to the Green function then defines another valid Green function.

[4] For a detailed discussion of why n conditions are required we refer to the specialized literature. Heuristically, the statement follows from the fact that an nth order linear differential equation, can be transformed to a system of n first order equations (cf. section C7.7 below for a general discussion of this statement). In section (C7.6) we will show that a single first order equation requires the specification of one boundary condition. A system of n equations, equivalent to a single equation of nth order therefore need n conditions.

equation

$$\left(\mathrm{d}_t^2 + \frac{2}{\tau}\mathrm{d}_t + \omega_0^2\right) q(t) = \xi(t). \tag{C179}$$

Comparison with Eq. (C174) shows that the differential operator governing this equation, $\hat{L} = \mathrm{d}_t^2 + 2\tau^{-1}\mathrm{d}_t + \omega_0^2$ is of second order. Its weight functions, $h^{(0)} = \omega_0^2$, $h^{(1)} = 2\tau^{-1}$, $h^{(2)} = 1$ are *coefficients*, i.e. they do not depend on time, t, and this facilitates the solution of the problem .

INFO The equation Eq. (C179) finds many **applications in the natural sciences.** Depending on the context, it describes mechanical, electrical, chemical, or biological systems in which a quantity of interest (q) is subject to effective forces restoring equilibrium (ω_0^2), friction (τ^{-1}), and external influence (ξ). In the mechanical context, this situation is realized for the majority of 'realistic' systems performing oscillatory motion. As an example of an electrical system described by these equations, we mention a resonator, where the role of q is played by a time dependent voltage, oscillatory motion is caused by the interplay of a capacitor (Kondensator) and a coil (Spule), friction by a resistor (Widerstand), and the external forcing is due to an external voltage. For the discussion of this and other applications we refer to specialized courses.

The Green function of the oscillator problem obeys the equation

$$\left(\mathrm{d}_t^2 + \frac{2}{\tau}\mathrm{d}_t + \omega_0^2\right) G(t-u) = \delta(t-u).$$

Its heuristic meaning is that of a solution of the problem in the presence of a δ-function force acting only at time $t = u$. Due to the absence of time dependent coefficients we anticipate the existence of a solution $G(t,u) = G(t-u)$ depending only on the *difference* between the time t at which the solution is evaluated and the time u at which the force acts (think about this point). From this function, the desired $q(t)$ is obtained as

$$q(t) = \int \mathrm{d}u\, G(t-u)\xi(u). \tag{C180}$$

The key to the computation of the Green function lies in the **Fourier transform** identity (C138). Applied to a time dependent function it states that $\widetilde{\mathrm{d}_t F(t)} = -\mathrm{i}\omega\tilde{F}(\omega)$. (The relative minus sign is due to the fact that the Fourier transform of a time dependent function (C139) is defined with an exponent $+\mathrm{i}\omega t$ rather than the $-\mathrm{i}kx$ of the spatial transform.) Repeated application of this identity leads to $\widetilde{\mathrm{d}_t^n F(t)} = (-\mathrm{i}\omega)^n \tilde{F}(\omega)$, i.e. under the Fourier transform derivatives d_t can be converted to algebraic factors $-\mathrm{i}\omega$. To make use of this feature, we substitute $t \to t+u$ into the equation for the Green function to rewrite it as $(\mathrm{d}_t^2 + 2\tau^{-1}\mathrm{d}_t + \omega_0^2)G(t) = \delta(t)$. In a second step we Fourier transform both the left and the right hand side to obtain

$$\left(-\omega^2 - \frac{2\mathrm{i}\omega}{\tau} + \omega_0^2\right) \tilde{G}(\omega) = 1,$$

where we noted that the Fourier transform of a δ-function equals unity, Eq. (C147). The expression in parenthesis now has become an algebraic factor. We divide by it to obtain the result

$$\tilde{G}(\omega) = \frac{1}{-\omega^2 - \frac{2\mathrm{i}\omega}{\tau} + \omega_0^2}. \tag{C181}$$

This has been the most important step in the solution of the equation. We now know the Fourier transform of the Green function, and this reduces the solution of the problem to the computation of integrals. Depending on the type of the driving force, however, these integrals may be non-trivial and one of three different strategies may be favorable:

- ▷ One may first compute the **inverse Fourier transform of the Green function** to obtain (cf. Eq. (C139))

$$G(t) = \int \frac{\mathrm{d}\omega}{2\pi} e^{-\mathrm{i}\omega t} G(\omega). \tag{C182}$$

  The solution is then obtained by substitution of the result into Eq. (C180). For completeness, we discuss the behavior of the function $G(t)$ in the info section below.

- ▷ Alternatively one may observe that the solution of the problem has the form of a **convolution** $q(t) = \int \mathrm{d}u G(t-u)\xi(u) = (G * \xi)(t)$ of the Green function and the driving force. Eq. (C144) then implies that $\tilde{q}(\omega) = G(\omega)\xi(\omega)$: the Fourier transform of the solution is obtained as the *product* of the Green function (C181) and the Fourier transform, $\tilde{\xi}(\omega)$ of the driving force (which needs to be computed from the given $\xi(t)$). In a final step, one computes $q(t)$ from $\tilde{q}(\omega)$.

- ▷ For driving forces with simple time dependence it may be preferable to compute the result by **direct substitution** of the formal representation Eq. (C182) into Eq. (**??**). We give an example of this strategy in the second info section below.

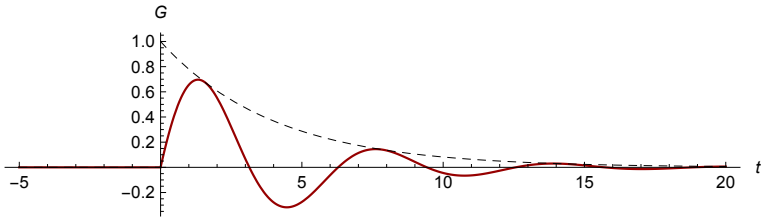


Figure C28: Green function of the harmonic oscillator for the underdamped configuration, $\omega/\tau = 1/4$.

INFO Let us discuss the **temporal behavior of the harmonic oscillator Green function**. The inverse Fourier integral Eq. (C182) leading from $\tilde{G}(\omega)$ to $G(t)$ actually is hard to do, unless one

computes it by the complex function techniques introduces in chapter C9. As shown in the example on p. 336, the result in the underdamped regime, $|\omega_0| > \tau^{-1}$ is given by

$$G(t-u) = \frac{1}{\tilde{\omega}} \sin(\tilde{\omega}(t-u)) \exp\left(-\frac{t}{\tau}\right) \Theta(t-u) + G_0(t-u), \qquad \tilde{\omega} \equiv (\omega^2 - \tau^{-1})^{1/2}, \quad \text{(C183)}$$

where $\Theta(t)$ is the Heaviside step function (C118), and $G_0(t)$ is an arbitrary solution of the homogeneous equation. In Eq. (**??**) these have been identified as the q-component of the general homogeneous solution Eq. (C173), which in the presently used notation assumes the form

$$G_0(t) = \exp\left(-\frac{t}{\tau}\right) (c_+ \mathrm{e}^{\mathrm{i}\tilde{\omega}t} + c_- \mathrm{e}^{-\mathrm{i}\tilde{\omega}t}).$$

The two undetermined constants of the general solution, $c_\pm$, are sitting in the homogeneous solution. Notice that, regardless of the choice of these constants, it decays exponentially in time. A very natural choice of boundary conditions would be $G(t \to \pm\infty) = 0$, i.e. the vanishing of the oscillatory motion at both negative infinity, prior to the action of the δ-function, and at positive infinity when the damped oscillation has fully relaxed. This requires the choice $c_\pm = 0$, and consequently $G_0 = 0$. In this case, the Green function is given by the first term in Eq. (C183), and affords an intuitive interpretation: prior to the action of the δ-function force at $t = u$ the oscillator is at rest, $G(t-u) = 0$. At $t = u$ it starts to perform oscillatory motion, attenuated by the damping rate τ.

INFO As an example of the third solution strategy mentioned above, let us consider an **harmonic oscillator subject to periodic driving** $\xi(t) = \xi_0 \cos(\omega_\mathrm{d} t)$. We use the Euler formula Eq. (C92), substitute Eq. (C182) into Eq. (C180) and obtain

$$\begin{aligned} q(t) &= \frac{\xi_0}{2} \int \mathrm{d}u \int \frac{\mathrm{d}\omega}{2\pi} \frac{(\mathrm{e}^{-\mathrm{i}\omega_\mathrm{d} u} + \mathrm{e}^{\mathrm{i}\omega_\mathrm{d} u}) \mathrm{e}^{-\mathrm{i}\omega(t-u)}}{-\omega^2 - \frac{2\mathrm{i}\omega}{\tau} + \omega_0^2} = \\ &= \frac{\xi_0}{2} \int \frac{\mathrm{d}\omega}{2\pi} \frac{(\delta(\omega-\omega_\mathrm{d}) + \delta(\omega+\omega_\mathrm{d})) \mathrm{e}^{-\mathrm{i}\omega t}}{-\omega^2 - \frac{2\mathrm{i}\omega}{\tau} + \omega_0^2} = \\ &= -\mathrm{Re} \frac{\xi_0 \, \mathrm{e}^{-\mathrm{i}\omega_\mathrm{d} t}}{\omega_\mathrm{d}^2 + \frac{2\mathrm{i}\omega_\mathrm{d}}{\tau} - \omega_0^2} = -\frac{\xi_0}{(\omega_0^2 - \omega_\mathrm{d}^2)^2 + \frac{\omega_\mathrm{d}^2}{(2\tau)^2}} \left((\omega_0^2 - \omega_\mathrm{d}^2) \cos(\omega_\mathrm{d} t) + \frac{2\omega_d}{\tau} \sin(\omega_\mathrm{d} t) \right) \end{aligned}$$

where in the second line Eq. (C134) was used in its frequency/time incarnation, $\int \mathrm{d}u \, \exp(i\epsilon u) = 2\pi\delta(\epsilon)$. The subsequent integral of the δ-function over the frequency argument leads to the stated result.

For an in-depth discussion of this result we refer to lecture courses in mechanics. Notice, however, that time dependence of the forced oscillations is periodic ($\sin$ / $\cos$) in the driving frequency, and that the amplitude becomes largest when the driving frequency $\omega_\mathrm{d} = \omega_0$ equals the intrinsic frequency of the oscillator. This observation is at the root of all **resonance phenomena**. In the limit of small damping, $\omega \to 0$, the response may actually diverge at the resonance frequency. Resonance phenomena may occur in the presence of even moderate forcing (the strength of the prefactor, ξ_0) if only the damping is weak enough. As an example, we mention the evacuation of TechnoMart, a 37 story high rise in Seoul, in 2011, which became necessary due to a resonance building up when a group of only 17 aerobic enthusiasts performed a rhythmic exercise.

Linear algebraic interpretation of the Green function

REMARK Requires chapter L10

Although the construction of the Green function solution scheme follows a well motivated logic, it may look somewhat alien to first time readers. It turns out, however, that the formalism becomes rather transparent when interpreted from the perspective of *linear algebra*. To this end, let us consider the functions f and g in (C174) as infinite dimensional limits of finite dimensional vectors $\mathbf{f}$ and $\mathbf{g}$. The linear operator, $\hat{L}$, then acts as finite dimensional linear map, L, and the linear DEQ assumes the form of a matrix equation $L\mathbf{f} = \mathbf{g}$. When written in this form, it is evident how to solve the equation: multiply from the left by the *inverse* of the linear map (assuming that it exists), to obtain $\mathbf{f} = L^{-1}\mathbf{g}$, or $f^i = (L^{-1})^i{}_j g^j$. In the infinite dimensional limit, vector components become function values, $f^i \to f(t)$, and sums become integrals. The solution equation will therefore assume the form

$$f(t) = \int \mathrm{d}u\, (\hat{L}^{-1})(t,u) g(u).$$

Comparison with Eq. (C178) shows that

$$G(t,u) = (\hat{L}^{-1})(t,u), \tag{C184}$$

The Green function is the inverse of the operator defining a linear differential equation.

To connect this general view with the concrete formulae used to compute the Green function above, recall that the inverse of a matrix is defined as $L^i{}_j G^j{}_k = \delta^i{}_k$. In the limit, $\delta^i{}_k \to \delta(t-u)$ becomes a δ-function, and so the equation should assume the form $\int \mathrm{d}v\, \hat{L}(t,v) G(v,u) = \delta(t-u)$. This looks almost, but not quite like Eq. (C176), the seeming discrepancy being that the latter does not contain an integral over the running variable, v. The reason for this is that $\hat{L}$ is not a totally generic linear operator in function space but one that is 'almost diagonal' (see info block below). Much like the application of a diagonal matrix, $D^i{}_j = d^i \delta^i{}_j$ to a generic matrix, $(DA)^i{}_j = d^i A^i{}_j$ does not contain an index summation, $(\hat{L}f)(t) = \hat{L}(t) f(t)$ does not contain an integral over a running variable. Likewise, the defining equation for the continuum inverse assumes the form, $\hat{L}(t) G(t,u) = \delta(t,u)$, and this completes the identification of the Green function as an operator inverse.

There remains one unexplained subtlety, though. In our discussion above we talked a lot about '**homogeneous solutions**' of the equation, $\hat{L}f = 0$. In the finite dimensional context this becomes $L\mathbf{f} = 0$, i.e. the existence of a non-vanishing homogeneous solution would be equivalent to the existence of a zero eigenvalue, in conflict with the assumed invertibility of the operator. There is, however, no reason for concern: prior to fixing the boundary conditions the operator $\hat{L}$ is indeed not invertible. In our discussion above this showed in the absence of a uniquely defined Green function. After fixing boundary conditions, invertibility is granted

and G is uniquely specified.[5]

INFO Let us try to understand in what sense a differential operator corresponds to an **almost diagonal matrix**. A derivative acts on a function as $\mathrm{d}_t f(t) = \lim_{\delta\to 0}(f(t+\delta) - f(t))$. In a representation discretized as $t = i\delta$ this corresponds to the 'discrete derivative' $(\mathrm{d}f)^i \equiv f^{i+1} - f^i$. The matrix representing d is given contains 1 on the main diagonal and -1 on its neighboring diagonal: $\mathrm{d}^i{}_j = \delta^{i+1}{}_j - \delta^i{}_j$. Upon multiplying this matrix with a function, $(\mathrm{d}f)^i = \mathrm{d}^i{}_j f^j = f^{i+1} - f^i$, the j-index summation collapses to just two terms. Likewise, the continuum representation $(\mathrm{d}f)(t) = \int \mathrm{d}u\, \mathrm{d}(t,u) f(u) = \mathrm{d}_t f(t)$ does not contain an integral over an intermediate variable. If we multiply matrices to represent higher derivatives, $\mathrm{d}^n \leftrightarrow \mathrm{d}_t^n$, the diagonals 'shift', for example, $(\mathrm{d}^2 f)_i = f_{i+2} - 2f_{i+1} + f_i$, however the fact remains that in the limit of very large dimensions, the ~~representing~~ matrices look almost diagonal. The multiplication of derivatives with time dependent functions, $h(t)\mathrm{d}_t \leftrightarrow h_i(\delta^{i+1}{}_j - \delta^i{}_j)$ does not change this structure, either. This explains the absence of integrals in the product $\hat{L}G$.

Importantly, however, the *inverse* of an almost diagonal matrix need not be almost diagonal at all. This is exemplified by the fact that G, the inverse of the almost diagonal $\hat{L}$, has non-vanishing 'matrix elements', $G(t,u)$ even for large separations $|t-u|$. As an instructive exercise, try to compute the inverse of $\mathrm{d}^i{}_j$ for low matrix dimensions (or even general matrix dimension, if you are feeling ambitious) to explore this point.

C7.6 General first-order differential equation

Consider the first-order differential equation

$$\boxed{\mathrm{d}_t f(t) = g(f(t), t),} \tag{C185}$$

where $g = g(x,t)$ may be a general function. If that function does not depend on the argument, t, i.e. if $g = g(x)$ the DEQ

$$\mathrm{d}_t f(t) = g(f(t)) \tag{C186}$$

is called an **autonomous differential equation**.

[5] In this argument we tacitly assume that the assumed boundary conditions define a function *space*. For example, the conditions $f(\pm\infty) = 0$ satisfy this criterion: the linear combination of two functions vanishing at infinity again vanishes at infinity. However, the $f(t_1) = f(t_2) = 1$ is an example of boundary conditions not defining a function space. For the rigorous algebraic interpretation of this situation we refer to specialized courses on differential equations.

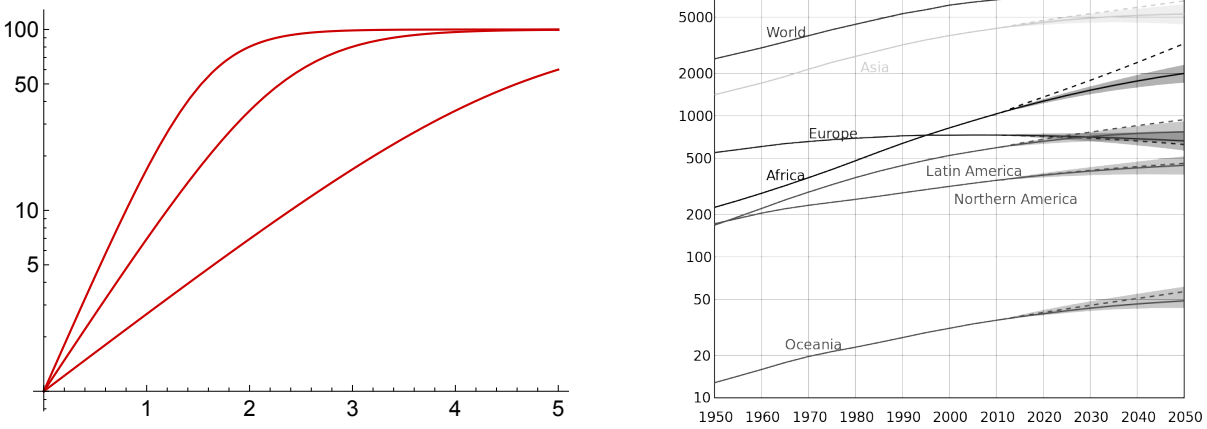


Figure C29: Left: Logistic growth for system parameters $\Gamma = 100$, $f_0 = 1$, and $c = 0.01, 0.02, 0.03$, where the largest value of c corresponds to the steepest growth. Notice that the vertical axis is in logarithmic units. Right: Demographic predictions of world population growth.

Solution of the autonomous equation

The autonomous equation can be solved by separation of variables (cf. info section on p. 287):

$$\frac{\mathrm{d}f}{\mathrm{d}t} = g(f) \Rightarrow \frac{\mathrm{d}f}{g(f)} = \mathrm{d}t \Rightarrow \int_{f_0}^{f(t)} \frac{\mathrm{d}f}{g(f)} = \int_0^t \mathrm{d}t = t. \tag{C187}$$

The integral defines a solution of Eq. (C186) with initial condition $f(0) = f_0$. That it is a solution may be checked by differentiating the left and the right hand side w.r.t. t. Application of the chain rule gives $\mathrm{d}_t \int_{f_0}^{f(t)} \frac{\mathrm{d}f}{g(f)} = \left(\mathrm{d}_f \int_{f_0}^{f} \frac{\mathrm{d}f'}{g(f')}\right)\Big|_{f=f(t)} \mathrm{d}_t f(t) = \frac{1}{g(f(t))} \mathrm{d}_t f$ which should be equal to $\mathrm{d}_t t = 1$. Equating the two results, we get back to the differential equation. To obtain $f(t)$ in more explicit terms, the integral in Eq. (C187) needs to be done. Denoting the result by $F(f) \equiv \int \mathrm{d}f \frac{1}{g(f)}$ one then obtains the algebraic equation [6] $F(f(t)) - F(0) = t$. The solution of this equation for $f(t)$ finally leads to **the solution of Eq.** (C186)

$$f(t) = F^{-1}(t + F(f_0)), \qquad F(f) = \int \frac{\mathrm{d}f}{g(f)}, \tag{C188}$$

where F^{-1} is the inverse function of F.[7]

EXAMPLE Consider the so-called **logistic differential equation**

$$\mathrm{d}_t f = cf(\Gamma - f),$$

[6] An algebraic equation contains no derivatives.

[7] The existence of an inverse of F is equivalent to the solvability of the differential equation.

where c and Γ are positive constants. This equation is often employed to model **population growth**. The rationale is that a small population of individuals will initially grow at a constant rate. Denoting the population size by f and the growth rate by $c\Gamma$ this is described by the linear equation $\mathrm{d}_t f = c\Gamma f$. This equation predicts exponential growth, $f(t) = f_0 \exp(c\Gamma)$. The logistic equation takes into account that at some point the host medium will reach its load capacity and the exponential growth must come to an end. In the equation this is described by a diminishing of the growth rate $\mathrm{d}_t f$ as $f \nearrow \Gamma$. Applying the procedure outlined above, we compute

$$F(f) = \int \frac{\mathrm{d}f}{cf(\Gamma - f)} = \frac{1}{c\Gamma} \ln\left(\frac{f}{\Gamma - f}\right).$$

The function $f(t)$ is then obtained by solution of $F(f(t)) - F(f_0) = t$ which readily leads to

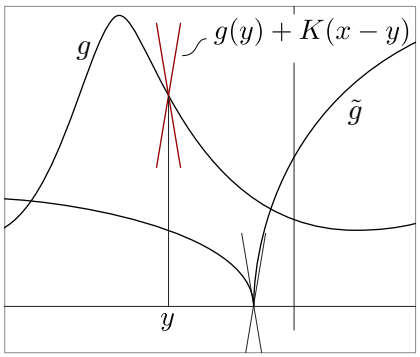
$$f(t) = \frac{\Gamma f_0}{(\Gamma - f_0)\mathrm{e}^{-c\Gamma t} + f_0}.$$

A plot of f for different growth rates, c, is shown in the left panel of Fig. C29. The right panel shows predictions for the population growth on various continents. Can we interpret these as logistic growth profiles?

For the solution theory of the non-autonomous first order DEQ we refer to the specialized literature.

Existence of solution

The general first order equation is important in its own right, but also features as a building block in the solution of more complex equations. An important question to ask, therefore, is whether the DEQ (C185) always possesses a solution and if yes whether its solutions are unique. In the following, we explore this question for the autonomous equation. (The construction for its non-autonomous generalization is similiar.)



The answer is that Eq. (C185) does possess a unique solution provided that an initial condition $f(0) = f_0$ at the 'left end' of the interval $I = [0, L]$ is specified and $g(f, t)$ does not vary too rapidly as a function of f. To formulate the latter condition in more precise terms we need to introduce the notion of Lipschitz continuity.

A function $g : I \to \mathbb{R}$ is called **Lipschitz continuous**, if

$$\exists K \in \mathbb{R}^+ : \quad \forall x, y \in I : \quad |g(x) - g(y)| \leq K|x - y|.$$

The visual interpretation of this statement is shown in the figure: the graph, $\{(y, g(y))|y \in I\}$, of a Lipschitz continuous function, g, with **Lipschitz constant**, K, is such that for all points $(y, g(y))$ it lies outside a cone bounded by two lines with slope K and $-K$, respectively,

intersecting at that point. The function g in the figure satisfies this criterion whereas $\tilde{g}$ does not. In essence, the condition states that nowhere does the derivative of g become infinitely large. For example, the function $\sqrt{|x|}$ is not Lipschitz continuous at $x = 0$, where $\lim_{x\searrow 0} \sqrt{x}' = \frac{1}{2\sqrt{x}}$ diverges.

Lipschitz continuity is required for the existence and uniqueness of solutions of DEQs. The idea of the existence proof is that the differential equation (C186) becomes equivalent to the $\Delta t \to 0$ limit of the discrete equations

$$f(t + \Delta t) \simeq f(t) + \Delta t\, g(f(\tilde{t})).$$

provided the function g does not fluctuate too wildly. Under this condition $\tilde{t} \in [t, t + \Delta t]$ may be chosen arbitrarily and in the limit $\Delta t \to 0$ the discrete expression converges to the differential equation. The degree of continuity required to grant the existence of the limit is expressed by the Lipschitz condition. To see this, we define $\tilde{t} = t + \epsilon$ and write $g(f(\tilde{t})) \simeq g(f(t) + \epsilon f'(t)) = g(f(t)) + X$ where $|X| \leq K\epsilon|f'(t)| \leq K|f'(t)|\Delta t$, and K is a Lipschitz constant for g. The error X introduced by the ambiguity in choosing the evaluation point $\tilde{t}$ is of $\mathcal{O}(\Delta t)$, so we have

$$f(t + \Delta t) = f(t) + \Delta t g(f(t)) + \mathcal{O}(\Delta t^2),$$

where the abbreviated notation $g(f) = g(f, t)$ has been used. We conclude that $f(t + \Delta t)$ may be obtained from $f(t)$ up to an error vanishing in the limit $\Delta t \to 0$, provided g is Lipschitz continuous. Under this condition the full solution may be constructed iteratively, starting from $t = 0$:

$$\begin{aligned}
f(0) &= f_0, \\
f(\Delta t) &= f_0 + \Delta t\, g(f_0), \\
f(2\Delta t) &= f(\Delta t) + \Delta t\, g(f(\Delta t)) = f_0 + \Delta t\, g(f_0) + \Delta t\, g(f(\Delta t)) \\
f(3\Delta t) &= f(2\Delta t) + \Delta t g(f(2\Delta t) = f_0 + \Delta t\, g(f_0) + \Delta t\, g(f(\Delta t)) + \Delta t\, g(f(2\Delta t)) \\
&\vdots \qquad\qquad \vdots
\end{aligned}$$

Notice that in the limit $\Delta t \to 0$ this expression converges to the integral equation $f(t) = f_0 + \int_0^t \mathrm{d}t\, g(f(t))$. Differentiation of the left and the right hand side makes the equivalence of the integral equation to the DEQ (C186) explicit. However, the main point of the discussion is that for Lipschitz continuous g a unique solution is constructible by iteration. The mathematically precise formulation of these statements is made by the **Picard-Lindelöf theorem** discussed in mathematics courses on differential equations.

C7.7 nth-order differential equation

We next consider DEQs of higher order in the number of derivatives. For example, the Newton equation $\ddot{q} = \frac{1}{m}F(q)$ is an equation relating second derivatives of the coordinate

function q to a force $F(q)$. The generalization to a generic ***n*th-order differential equation** is often expressed in the form

$$G(f^{(n)}(t), f^{(n-1)}(t), f^{(n-2)}(t), \dots, f^{(0)}(t), t) = 0, \tag{C189}$$

with an arbitrary function $G(y_1, \dots, y_{n+1}, t)$.[8] (The Newton equation fits into this scheme as $\ddot{q} - \frac{1}{m}F(q) = 0$, i.e. $G(y^1, y^2) = y^1 - \frac{1}{m}F(y^2)$.) It is often convenient to transform this equation into an equivalent system of first order equations. To this end, a set of n functions $x^1(t) \equiv f(t), x^2(t) \equiv f^{(1)}(t) = \mathrm{d}_t x^1(t), \dots, x^n(t) \equiv f^{(n-1)}(t) = \mathrm{d}_t x^{n-1}(t)$ is defined. The differential equation (C189) then becomes equivalent to the **system of *n* first-order differential equations**,

$$\begin{aligned} \mathrm{d}_t x^1 &= x^2, \\ \mathrm{d}_t x^2 &= x^3, \\ &\vdots \quad \vdots \\ \mathrm{d}_t x^{n-1} &= x^n, \\ G(\mathrm{d}_t x^n, x^n, x^{n-1}, \dots, x^1, t) &= 0, \end{aligned} \tag{C190}$$

for the vector of functions $\mathbf{x} = (x^1, \dots, x^n)^T$. Once $\mathbf{x}(t)$ is found, the function of interest, $f = x^1$, is given by the first component of the solution vector. Although the system of n first order equations amounts to just a rewriting of the original problem this change of representation is often advantageous. Specifically, we will see in the next section that systems of first order differential equations can be handled using powerful geometric methods.

EXAMPLE Turning back to the one-dimensional **Newton equation**,

$$\ddot{q} = \frac{1}{m}F(q),$$

we define the vector $\mathbf{x}^T \equiv (q, p)$ comprising the particle's coordinate, $x^1 = q$, and the particle's momentum, $x^2 = p = mv = m\mathrm{d}_t q$.[9] The Newton equation can now be equivalently expressed as

$$\begin{aligned} \mathrm{d}_t q &= \frac{1}{m}p, \\ \mathrm{d}_t p &= F(q). \end{aligned}$$

This representation appeared before in section **??**. In an analogous manner, Newton's equation in d-dimensional space, $\ddot{\mathbf{q}} = \frac{1}{m}\mathbf{F}(\mathbf{q})$, assumes the form

$$\begin{aligned} \mathrm{d}_t \mathbf{q} &= \frac{1}{m}\mathbf{p}, \\ \mathrm{d}_t \mathbf{p} &= \mathbf{F}(\mathbf{q}), \end{aligned}$$

[8] The first equation discussed in the previous section is a special case of this structure, i.e. $f'(t) = g(f(t), t) \Leftrightarrow G(f'(t), f(t), t) = 0$ where $G(y^1, y^2, y^3) = y^1 - g(y^2, y^3)$.

[9] Slightly deviating from the general scheme, a constant, m, is included in the definition of $x^2 = m d_t x^1$.

which is a first-order equation for the $2d$-component vector $\mathbf{x} \equiv \binom{\mathbf{q}}{\mathbf{p}}$. The $2d$-dimensional space hosting the vectors $\mathbf{x}$ is called the **phase space** (Phasenraum) of a mechanical system. It plays an important role in the modern theory of mechanical systems.

Systems of first-order equations

In the previous section we have seen how an nth-order differential equation can be transformed to a particular system of first-order equations (C190). The general **system of coupled first-order differential equations** is defined by [10]

$$\begin{aligned} \mathrm{d}_t x^1 &= f_1(x^1, x^2, \ldots, x^n, t), \\ \mathrm{d}_t x^2 &= f_2(x^1, x^2, \ldots, x^n, t), \\ &\vdots \qquad \vdots \\ \mathrm{d}_t x^n &= f_n(x^1, x^2, \ldots, x^n, t), \end{aligned} \tag{C191}$$

where $x^i = x^i(t)$ are the desired solutions. We introduce a compact vector notation $\mathbf{x} \equiv (x^1, \ldots, x^n)^T$, $\mathbf{f} = (f^1, \ldots, f^n)^T$, to represent the system as

$$\boxed{\mathrm{d}_t \mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t), t).} \tag{C192}$$

This notation suggests an interpretation of $\mathbf{x}(t)$ as a curve. The curve is *defined* by the condition that at every instant of time, t, its velocity, $d_t\mathbf{x}(t)$, equals the given vector function $\mathbf{f}(\mathbf{x}(t))$. If the function $\mathbf{f}$ does not carry explicit time dependence, $\mathbf{f}(\mathbf{x}, t) = \mathbf{f}(\mathbf{x})$, the system is called **autonomous**.

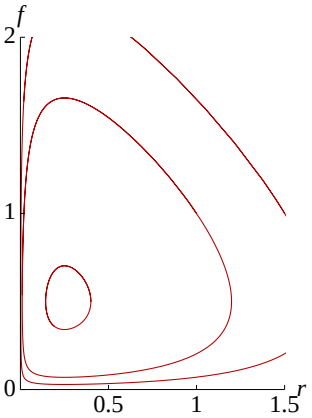
Systems of first-order differential equations play an important role not only in physics but also in biology, chemistry, engineering, and the social sciences. They are used to describe the time evolution of multi-component quantities (the coordinates and momenta of a mechanical system, the concentrations of chemical compounds, the population numbers describing a multi-species habitat, the stock market value of a system of companies, etc.) in response to 'forces' driving that evolution (generalized forces, chemical reactions, environmental changes, economic market forces, etc.). The connection between cause and effect is then represented in terms of a system of differential equations where the coupling between the equations expresses the interaction between the agents of the systems.

EXAMPLE Let us illustrate the application of coupled first order DEQs with a toy model for ecological inter-dependence, the **Lotka-Volterra (LV) system**.[11] The LV system describes a population of f predators (foxes) r prey (rabbits), $\mathbf{x} = (r, f)^T$. It is assumed that the number of rabbits proliferates at a constant rate, α, and diminishes at a rate βf due to the presence of the f foxes.

[10] Eq. (C191) fits into this scheme by defining $f^i(x^1, \ldots, x^n, t) = x^{i+1}$, $i = 1, \ldots, n-1$ and solving the algebraic equation $G(\mathrm{d}_t x^n, x^n, \ldots, x^1, t) = 0$ for $\mathrm{d}_t x^n$ as $\mathrm{d}_t x^n \equiv f^n(x^1, \ldots, x^n, t)$.

[11] A.J. Lotka, *Elements of Physical Biology*, Williams and Wilkins, (1925); V. Volterra, *Variazioni e fluttuazioni del numero dindividui in specie animali conviventi*, Mem. Acad. Lincei Roma **2**, 31 (1926).

Conversely, the population of the foxes is controlled by a mortality rate, γ, and a proliferation rate, δr, proportional to the available food ressources, i.e. the rabbit population. Cast in the form of a system of two differential equations, this model assumes the form

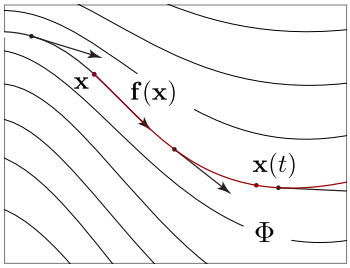


$$\begin{aligned} \mathrm{d}_t r &= (\alpha - \beta f) r, \\ \mathrm{d}_t f &= (-\gamma + \delta r) f. \end{aligned} \tag{C193}$$

The analytic solution of this system of equations is possible but complicated. The plot of numerically computed solutions shows a periodic pattern in the population balance: an abundance of rabbits causes a flourishing of the fox population which leads to a decimation of the rabbits. This in turn suppresses the fox population, and the cycle starts again.

Observe that the system possesses a so-called **fixed point**, where the populations remain stationary: for $f = f^* \equiv \alpha/\beta, r = r^* \equiv \gamma/\delta$ the right hand side of the system vanishes, which means that $\mathrm{d}_t r = \mathrm{d}_t f = 0$. Consequently the populations remain stationary. Fixed points are important characteristics of systems of DEQs in general. Methods of finding them and exploring what happens in their vicinity will be introduced in the next section.

Although the LV system is based on oversimplifying assumptions it describes important aspects of population fluctuations. More complicated models of ecological systems are often constructed by generalization of LV-type differential equations. Generally speaking, finite systems of equations can never faithfully describe 'reality'. The goal of modeling nature or society in terms of systems of differential equations is to reduce real world processes down to a manageable level of complexity which is still sufficiently 'realistic' to have predictive power.



Only in exceptional cases can systems of DEQs be solved in closed form and this motivates the development of **qualitative methods** for their description. One frequently employs a language in which t is considered as a time-like variable, and the system (C191) interpreted as a '**dynamical system**'. For a given $\mathbf{x}$, the curve $\mathbf{x}(t)$ solving the system with initial condition $\mathbf{x}(0) = \mathbf{x}$ is called a **trajectory of the DEQ**. The full information on all trajectories is carried by the **flow of the DEQ**. Mathematically, the flow is a map

$$\begin{aligned} \mathbf{\Phi} &: I \times M \to M, \\ &(t, \mathbf{x}) \mapsto \mathbf{\Phi}_t(\mathbf{x}), \end{aligned} \tag{C194}$$

where I a time interval and M, the domain of definition of the functions $\mathbf{x}$, is often called the **phase space** of the system.[12] The flow map obeys the condition $\mathbf{\Phi}_0(\mathbf{x}) = \mathbf{x}$. For finite t, the

[12] The phase space defined by the time dependent coordinates and momenta $(\mathbf{q}, \mathbf{p})^T$ of a mechanical system is an important example of this notion. In fact, physicists tend to reserve the term 'phase space' for this particular realization.

flow $\mathbf{\Phi}_t(\mathbf{x}) = \mathbf{x}(t)$ is defined by the trajectory through $\mathbf{x}$. As such it obeys the composition rule,

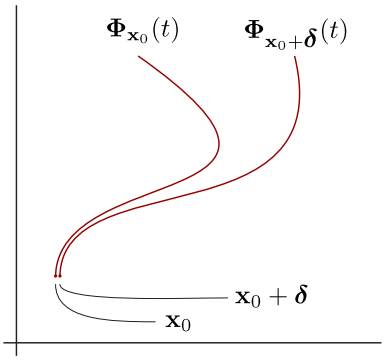
$$\mathbf{\Phi}_{t+s}(\mathbf{x}) = \mathbf{x}(t+s) = \mathbf{\Phi}_t(\mathbf{\Phi}_s(\mathbf{x})),$$

i.e. the trajectory point $\mathbf{x}(t+s)$ can be understood as the endpoint of a trajectory of duration t starting at $\mathbf{x}(s) = \mathbf{\Phi}_s(\mathbf{x})$. This composition rule can be used to extend the definition of flow to negative times: $\mathbf{x} = \mathbf{\Phi}_0(\mathbf{x}) = \mathbf{\Phi}_{t+(-t)}(\mathbf{x}) = \mathbf{\Phi}_{-t}(\mathbf{\Phi}_t(\mathbf{x}))$. Also notice that

$$\mathrm{d}_t\mathbf{\Phi}_t(\mathbf{x}) = \mathrm{d}_t\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t)) = \mathbf{f}(\mathbf{\Phi}_t(\mathbf{x})),$$

i.e. considered as a function of t the flow is a solution of the DEQ. Plotting the flow lines $\mathbf{\Phi}_t(\mathbf{x})$ for a set of initial points $\mathbf{x}$ gives the trajectories starting at these points. In the exceptional case of a stationary flow, $\mathbf{\Phi}_t(\mathbf{x}^*) = \mathbf{x}^*$, we call the point $\mathbf{x}^*$ a stationary point, or a **fixed point** of the system. The fixed-point property is equivalent to the condition $\mathrm{d}_t\mathbf{x}^* = \mathbf{f}(\mathbf{x}^*) = 0$. Finding the fixed points is, thus, equivalent to finding the zeros of $\mathbf{f}$, and this is usually the first step in the analysis of a system of DEQs. In a second step, one then analyses the behavior of the system in the vicinity of its stationary points.

Deterministic chaos: introduction in a nutshell



Before turning to the discussion of near-fixed-point dynamics, let us stay for a moment at the global level. In the previous section we argued that a DEQ possesses a unique solution provided the defining function g is sufficiently well-behaved. That existence criterion can be generalized to systems of DEQs: we are granted unique solutions if initial conditions have been specified and $\mathbf{f}$ obeys a generalized Lipschitz criterion.

Often, however, the formal existence criterion is of only limited practical usefulness. The reason is that the flows of many systems of DEQs exhibit the phenomenon of **deterministic chaos**. A defining feature of chaotic flows is their exponential sensitivity to initial conditions: consider two initial configurations $\mathbf{x}_0$ and $\mathbf{x}_0 + \delta\mathbf{x}$ where $|\delta\mathbf{x}|$ is 'infinitesimally' small. If the flow is chaotic the trajectories $\mathbf{\Phi}_{\mathbf{x}_0}(t)$ and $\mathbf{\Phi}_{\mathbf{x}_0+\delta\mathbf{x}}(t)$ starting from these configurations will deviate strongly from each other no matter how small the initial displacement $|\delta\mathbf{x}|$. The deviation grows exponentially in time, i.e. there exists a so-called **Lyapunov exponent**, λ, such that

$$|\mathbf{\Phi}_{\mathbf{x}+\delta\mathbf{x}}(t) - \mathbf{\Phi}_{\mathbf{x}}(t)| \sim |\delta\mathbf{x}| \exp(\lambda t). \tag{C195}$$

This means that for times $t \gg \lambda^{-1}$ even tiny changes in the initial conditions take a drastic effect on the course of the trajectory. The mathematician and meteorologist Edward Lorenz described this phenomenon by saying that the flap of a butterfly's wings in Brazil could set off a tornado in Texas.

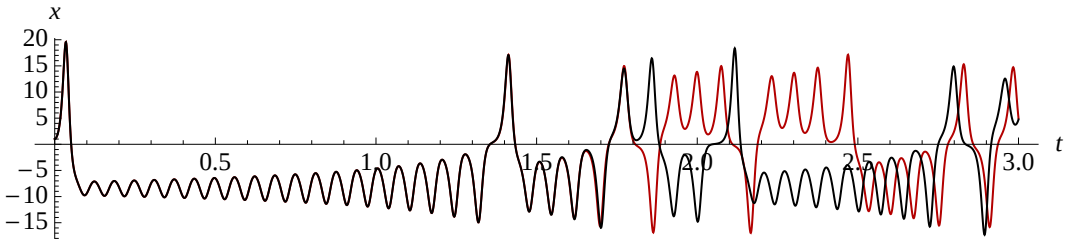


Figure C30: A single component (x) of two trajectories (black and red) of the Lorenz system (C196). Both trajectories are computed for the parameters $\sigma = 10, \rho = 28, \beta = 8/3$, but are started using slightly different initial conditions $\mathbf{x}_0 = (x_0, y_0, z_0) = (1, 1, 1)$ and $(1.01, 1, 1)$, respectively. While for short times the trajectories are visually indistinguishable, the uncontrolled growth of the relative deviation becomes apparent at times $t \sim 2$ (arbitrary units).

EXAMPLE **The phenomenon of chaos** occurs even in very simple systems. For example, the $n = 3$ system

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} &= \sigma(y - x), \\ \frac{\mathrm{d}y}{\mathrm{d}t} &= x(\rho - z) - y, \\ \frac{\mathrm{d}z}{\mathrm{d}t} &= xy - \beta z, \end{aligned} \tag{C196}$$

with constants σ, ρ, β was proposed by Lorenz[13] as a model of atmospheric convection phenomena. In spite of its relatively simple form – three functions f^i of quadratic order in the variables (x, y, z) – it cannot be solved analytically. However, a numerical solution reveals its sensitivity to variations in the boundary conditions, as shown in Fig. C30.

The structure of a typical trajectory in the three dimensional space of variables is illustrated in Fig. C31. The panels of the figure show the curve $\mathbf{\Phi}_{\mathbf{x}_0}(t)$ at times $t = 0.1, 0.3, 1.5, 5$. These values correspond to different dynamical stages of the dynamics, also visible in Fig. C30: an initial sweep from the starting point to a center region $t \lesssim 0.1$, followed by a spiraling motion ($t \lesssim 1.5$). At larger times, the trajectory traces out a two-winged structure known as the **Lorenz attractor**. This is an example of a **strange attractor**, a region in space which binds trajectories to it. The attribute 'strange' is well deserved. Trajectories captured by the Lorenz attractor perform perpetual motion about it and their flow traces an infinitely filigree pattern of 'fractal geometry'. This defines an object that looks almost, but not quite, like a 'surface' in space. In mathematics, these structures are characterized in terms of a **fractal dimension** ($d \simeq 2.05$ for the Lorenz attractor). The fascinating physics and mathematics of chaotic dynamics is explored in fields including **chaos theory**, **nonlinear dynamics**, and **turbulence** and for further discussion we refer to texts introducing these disciplines.

[13] E.N. Lorenz, *Deterministic non-periodic flow*. Journal of the Atmospheric Sciences **20**, 130 (1963).

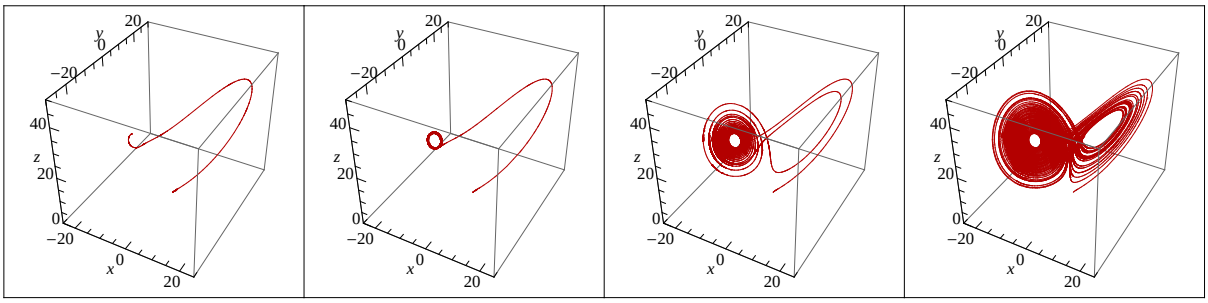


Figure C31: A trajectory of the Lorenz system with boundary condition $(1, 1, 1)$, as in Fig. C30. The inset figures illustrate different stages of the dynamics, as discussed in the text.

C7.8 Linearizing differential equations

Consider a set of differential equations for a solution vector $\mathbf{x} = (x^1, \ldots, x^n)$. It may be expedient to think of $\mathbf{x}$ as the vector of coordinates specifying a complex mechanical system, or that of populations in a biological context. Let us assume that the system is initially at rest. In mathematical terms, this means that it is initialized at a stationary point $\mathbf{x}^*$ of a differential equation $d_t\mathbf{x} = \mathbf{f}(\mathbf{x})$ where $\mathbf{f}$ is the vector of generalized forces describing the evolution. A 'perturbation' of the system will cause a deviations away from the stationary point, $\mathbf{x}^* \to \mathbf{x}^* + \mathbf{y}$. Since $\mathbf{x} + \mathbf{y}$ no longer is a stationary point, $\mathbf{y}(t)$ now becomes a function of time. For example, it may perform a damped oscillatory motion describing the vibrational relaxation, $\mathbf{y}(t) \searrow 0$, of an elastic mechanical system. However, the perturbation may also cause more dramatic effects. For example, the small perturbation of a spherical body initially at rest on the top a hill may cause accelerated motion *away* from the initial configuration.

Even if the full equation, $\mathrm{d}_t\mathbf{x} = \mathbf{f}(\mathbf{x})$, describing the system is complicated, motion in the vicinity of fixed points can generally be described analytically. To understand how, we substitute $\mathbf{x} = \mathbf{x}^* + \mathbf{y}$ into the equation and obtain

$$\mathrm{d}_t(\mathbf{x}^* + \mathbf{y}) = \mathrm{d}_t\mathbf{y} = \mathbf{f}(\mathbf{x}^* + \mathbf{y}),$$

where $\mathrm{d}_t\mathbf{x}^* = \mathbf{f}(\mathbf{x}^*) = 0$ was used. For sufficiently small $\mathbf{y}$ we may Taylor expand the r.h.s. to first order in the small increment $\mathbf{y}$. Eq. (C103) then tells us that

$$f^i(\mathbf{x}^* + \mathbf{y}) \simeq f^i(\mathbf{x}^*) + \mathbf{y} \cdot \nabla f^i(\mathbf{x}^*) = \sum_j \frac{\partial f^i(\mathbf{x}^*)}{\partial x^j}\, y^j$$

where the fixed-point condition $f^i(\mathbf{x}^*) = 0$ was used again. From these equations we obtain the **system of linear differential equations with constant coefficients**

$$\mathrm{d}_t y^i = \sum_{j=1}^{n} A^i{}_j\, y^j, \qquad A^i{}_j = \frac{\partial f^i(\mathbf{x}^*)}{\partial x^j},$$

for the deviations y^i. The constancy (i.e. independence of time) of the coefficient matrix A follows from its definition as a fixed point property. Formulated in vector/matrix notation, the equation assumes the compact form

$$\boxed{\mathrm{d}_t \mathbf{y} = A\,\mathbf{y}.} \tag{C197}$$

We may now relate back to our discussion of section C7.4 to predict the different types of dynamics in the vicinity of fixed points. The structure of the general solution (C169) implies that everything depends on the structure of A's eigenvalues, λ_i. These eigenvalues are generally complex and depending on their value one may observe either:

- ▷ **Oscillatory motion** around the fixed point: all eigenvalues purely imaginary, $\mathrm{Re}(\lambda_i) = 0$,
- ▷ **Damped oscillatory motion**: eigenvalues have finite negative real part, $\mathrm{Re}(\lambda_i) < 0$,
- ▷ **Attenuated motion back to the fixed point**: eigenvalues real and negative, $\mathrm{Re}(\lambda_i) < 0$, $\mathrm{Im}(\lambda_i) = 0$,
- ▷ **Instability**: the exist eigenvalues with positive real part, $\mathrm{Re}(\lambda_i) > 0$, for at least one i.

In the latter case the system is unstable, and will diverge from its fixed point. In such cases, the condition that the deviation $\mathbf{y}$ is small holds only for short timescales and different solution methods must be applied to describe the dynamics at longer timescales.

C7.9 Partial differential equations

Partial differential equations are differential equations involving derivatives w.r.t. several variables. A simple example is the **wave equation in one dimension**,

$$(v^2\partial_t^2 - \partial_x^2)u(x,t) = 0, \tag{C198}$$

where x and t are a spatial and temporal coordinate, respectively, v is a constant and $u(x,t)$ is a function representing the medium undergoing wave-like motion (the pressure of a gas, the height of a water wave, etc.).

From a physical perspective, the two most important facts about differential equations are:

- ▷ They are of profound importance to all disciplines of physics. This follows from our reasoning in section C7.1: the laws of physics are naturally expressed in terms of differential equations and most involve more than one variable.
- ▷ Their solution theory is *much* more complex than that of ordinary differential equations.

Partial differential equations take center stage in the physics curriculum, examples include the Hamilton equations (mechanics), the Maxwell equations (electrodynamics), the Schrödinger equation (quantum mechanics), or the Einstein equations (general relativity). Due to the

mathematical complexity of these equations, lecture courses generally invest a lot of effort into discussing solution schemes for the families of DEQs relevant to them.

The **typology of partial DEQs**, too, is much richer than that of ordinary DEQs. Again, we have to discriminate between linear and non-linear equations, or equations of different order. On top of that, however, there exist other criteria classifying different types of partial DEQs whose discussion is beyond the scope of this text. Also, the question of existence and uniqueness of solutions becomes more complicated. For example, it is straightforward to verify that for arbitrary one-dimensional functions f and g, $u_1(x,t) \equiv f(x-vt)$ and $u_2(x,t) \equiv g(x+vt)$ solve equation (C198). This illustrates that it is not enough to specify an 'initial condition': for $f = g$, the two solutions obey the same initial condition $u_1(x,0) = u_2(x,0) = f(x)$, but for finite times they are clearly distinct. In the case of the wave equation, different information is required to fix a solution.[14]

How do we know that 'all' general solutions of a partial DEQ have been found? How much additional information is required to uniquely specify a unique solution and in what 'form' can this information be provided? These are questions of considerable depth which are addressed in mathematics lecture courses on partial DEQs and, from a more applied perspective, in all lecture courses of theoretical physics.

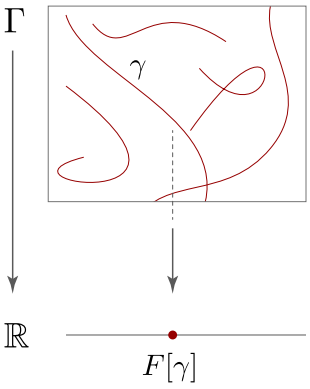
[14] In the case of the wave equation, unique solutions may be fixed by providing 'initial conditions' in the form $u(x,0) = g(x)$ and $\partial_t u(x,t) = h(x)$, or 'boundary data' such as $u(0,t) = u(L,t) = 0$. For a discussion of these statements we refer to lecture courses in mechanics and electrodynamics.

C8 Functional calculus

In standard calculus, one deals with functions $F(\mathbf{v})$ that take vectors $\mathbf{v} \in \mathbb{R}^n$ as arguments. Functional calculus generalizes standard calculus, in that one considers 'functions' $F[f]$ taking functions as arguments. Now, 'function of a function' does not sound nice, and for this reason F is called a **functional**. Likewise, it is customary to indicate the argument of a functional in square brackets. To understand why functionals have a lot in common with ordinary functions, recall that their argument functions can always be discretized as $f \to \{f^i | i = 1, \ldots, N\}$, i.e. they may be interpreted as $N \to \infty$ limits of N-dimensional vectors. This indicates that one may work with functionals much like one would with ordinary functions. In particular, we anticipate that standard operations of calculus must have a generalization to functionals.

EXAMPLE (a) Consider the set of functions $\{f : [0,1] \to \mathbb{R}\}$ mapping the interval $[0,1]$ into the reals. For $0 \leq a \leq 1$, we may define a functional $\delta_a[f] \equiv f(a)$, i.e. we simply read out the value of the argument function at a fixed argument to produce a number. (b) We may also define $\mathrm{Av}[f] \equiv \int_0^1 f(x)\mathrm{d}x$, i.e. a functional yielding the average value of f over the domain of definition. (c) Consider the set of curves $\Gamma \equiv \{\gamma : \text{curve in three-dimensional space}\}$. Curves are a particular class of functions, so a map assigning function values to individual curves will be a functional. For example, we may define the functional $L[\gamma]$=(Length of γ) to be discussed in some detail below.

C8.1 Definitions



For the sake of concreteness, we will focus on functionals taking curves as arguments throughout. (This choice is motivated by the fact that functionals of curves are the first encountered in the physics curriculum. Most concepts relevant to generic functionals are already realized with this subclass.) Let Γ be the set of all smooth curves γ in $\mathbb{R}^d$. A real valued functional on Γ is then a smooth map

$$\begin{aligned} F : \Gamma &\longrightarrow \mathbb{R}, \\ \gamma &\longmapsto F[\Gamma], \end{aligned} \tag{C199}$$

assigning to individual curves a real number. (Of course, we may imagine functionals mapping

into target spaces different from the reals ...) In many applications, the value a functional takes on a curve is encoded in local properties of that curve, its curve velocity, local curvature, etc. If we parameterize the curve as $\gamma : I \to \mathbb{R}^{\mathrm{d}}, t \mapsto \mathbf{r}(t)$, its local properties at $\mathbf{r}(t)$ are encoded in the instantaneous derivatives, $\mathrm{d}_t\mathbf{r}(t)$, $\mathrm{d}_t^2\mathbf{r}(t), \dots$ This observation motivates the definition of a **local functional** as one whose value is described by an integral,

$$F[\gamma] = \int \mathrm{d}t\, L(\mathbf{r}(t), \mathrm{d}_t\mathbf{r}(t), \mathrm{d}_t^2\mathbf{r}(t), \dots), \tag{C200}$$

where $L : \mathbb{R}^d \oplus \mathbb{R}^d \oplus \cdots \to \mathbb{R}, (\mathbf{x}, \mathbf{y}, \dots) \mapsto L(\mathbf{x}, \mathbf{y}, \dots)$ is a function.[1] By contrast, an example of a **non-local functional** would be

$$X[\gamma] = \int \mathrm{d}t\, \mathrm{d}s\, r^i(t) K_{ij}(t,s)\, r^j(s), \tag{C201}$$

where $K_{ij}(t,s)$ is some function depending on t and s in some manner.

Notice one important point: to define a local functional, we need an explicit coordinate representation $\mathbf{r}(t)$ of our curves. (How else would we compute derivatives?) However, the functional as such is an object assigning to the curve γ, i.e. an object existing independently of concrete coordinate representations, a number. This entails the **coordinate invariance** of local functionals: parameterizing the same curve γ in terms of two different coordinate representations $\mathbf{r}(t)$ and $\mathbf{n}(s)$, the value of $F[\gamma]$ must not change, although the form of the corresponding functions $L(\mathbf{r}(t), \dots)$ and $K(\mathbf{n}(s), \dots)$ will in general be different. All these features are illustrated by the curve-length example discussed below.

EXAMPLE The **length of a curve** $\gamma : I \to \mathbb{R}^d, t \mapsto \mathbf{r}(t)$ is defined as

$$L[\gamma] \equiv \int_{t_0}^{t_1} dt\, L(\dot{\mathbf{r}}(t)), \qquad L(\dot{\mathbf{r}}) = \left(\dot{r}^i \dot{r}^i\right)^{1/2} \equiv |\dot{\mathbf{r}}|, \tag{C202}$$

The functional $L[\gamma]$ (not to be confused with its representing function $L(\dot{\mathbf{r}})$) assigns to each curve its euclidean length.

It is instructive to check that the functional does not change under reparameterization. For example, we may parameterize the curve in terms of a different parameter $s(t)$. Assuming a Cartesian coordinate system for notational simplicity, we then have $L(\mathrm{d}_s\mathbf{r}) = |\mathrm{d}_s\mathbf{r}(t(s))| = |\mathrm{d}_s t(s)\, \mathrm{d}_t\mathbf{r}(t)| = |\mathrm{d}_s t(s)| L(\mathrm{d}_t\mathbf{r})$. Changing variables in the integral, we then obtain

$$L[\gamma] = \int \mathrm{d}s\, L(\mathrm{d}_s\mathbf{r}) = \int \mathrm{d}t\, \underbrace{|\mathrm{d}_t s(t)|\, |\mathrm{d}_s t(s)|}_{1}\, L(\mathrm{d}_t\mathbf{r}) = \int \mathrm{d}t\, L(\mathrm{d}_t\mathbf{r}). \tag{C203}$$

[1] More generally, $L(\mathbf{r}(t), \mathrm{d}_t\mathbf{r}(t), \mathrm{d}_t^2\mathbf{r}(t), \dots, t)$ may explicitly depend on the curve parameter, t. However, to keep the notation simple, we do not discuss this complication here. As an exercise you may ask yourself what changes (not much) if such an explicit dependence is present.

C8.2 Functional derivative

Much like ordinary functions, functionals are characterized by their local extrema. Formulated in the language of the curve functional, the first question we will ask is on what curve(s) $\gamma \in \Gamma$ does $F[\gamma]$ assume extremal values. Judging from the analogy with functions, we expect the extremal condition to be equivalent to the vanishing of some kind of 'functional derivative'. These considerations motivate the following definitions:

Consider two curves $\gamma, \gamma' \in \Gamma$ that lie 'close' to each other. For example, we may require that $|\mathbf{r}(t) - \mathbf{r}'(t)| < \epsilon$ for all t and some positive ϵ. We are interested in the increment $F[\gamma] - F[\gamma']$. Defining $\gamma' = \gamma + h$, the **functional is called differentiable** *iff*

$$F[\gamma + h] - F[\gamma] = \mathrm{d}F\big|_\gamma[h] + \mathcal{O}(h^2), \tag{C204}$$

where $\mathrm{d}F\big|_\gamma[h]$ is a *linear* functional of h, i.e. a functional obeying $\mathrm{d}F\big|_\gamma[c_1 h_1 + c_2 h_2] = c_1 \mathrm{d}F\big|_\gamma[h_1] + c_2 \mathrm{d}F\big|_\gamma[h_2]$ for $c_1, c_2 \in \mathbb{R}$ and $h_{1,2} \in \Gamma$. In (C204), $\mathcal{O}(h^2)$ indicates residual contributions of order h^2. For example, if $|h(t)| < \epsilon$ for all t, these terms would be of $\mathcal{O}(\epsilon^2)$.

The functional $\mathrm{d}F|_\gamma$ is called the **differential** of the functional F at γ. Notice that $\mathrm{d}F|_\gamma$ need not depend linearly on γ. Comparison with Eq. (C2) shows that the differential generalizes the notion of a derivative to functionals (for a more comprehensive discussion of differentials, see section **??**). Alternatively, we may think of $F[\gamma + h] = F[\gamma] + \mathrm{d}F|_\gamma[h] + \mathcal{O}(h^2)$ as a generalized Taylor expansion. The linear functional $F|_\gamma$ describes the behavior of F in the vicinity of the reference curve γ. A curve γ is called an **extremal curve** of F if $F|_\gamma = 0$.

EXAMPLE Consider the length functional $L[\gamma]$ restricted to all curves $\mathbf{r}(t_0) = \mathbf{r}_0$, $\mathbf{r}(t_1) = \mathbf{r}_1$ beginning and ending at fixed initial and final points $\mathbf{r}_0$ and $\mathbf{r}_1$. To obtain the differential of that functional, we denote the parameterization of $\gamma(t)$ and $\gamma + h$ by $\mathbf{r}(t)$ and $\mathbf{r}(t) + \mathbf{y}(t)$, and consider the variation

$$\begin{aligned} L[\gamma + h] - L[\gamma] &= \int_{t_0}^{t_1} \mathrm{d}t\, (|\dot{\mathbf{r}} + \dot{\mathbf{y}}| - |\dot{\mathbf{r}}|) = \int_{t_0}^{t_1} dt\, \left(\frac{\dot{r}^i \dot{y}^i}{|\mathbf{r}|} + \mathcal{O}(y^2) \right) = \\ &= \int_{t_0}^{t_1} dt\, \left(\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\dot{r}^i}{|\mathbf{r}|} \right) y^i + \mathcal{O}(y^2) \right), \end{aligned} \tag{C205}$$

where in the second line we integrated by parts. (Why does the integration by parts not generate boundary terms?) This identifies the differential of the length functional as

$$\mathrm{d}F|_\gamma[h] = \int_{t_0}^{t_1} dt\, \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\dot{r}^i}{|\dot{\mathbf{r}}|} \right) y^i. \tag{C206}$$

The differential vanishes at γ, if for all smooth 'test curves' curves h, $F|_\gamma[h] = 0$. Inspection of the integral representation shows that this is equivalent to the condition

$$\forall t: \qquad \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{\dot{r}^i}{|\dot{\mathbf{r}}|} \right) = 0, \qquad i = 1, \ldots, n. \tag{C207}$$

For example, let us consider Cartesian coordinates, $g_{ij} = \delta_{ij}$ in which a straight connection between the initial and final point reads

$$\mathbf{r}(t) = \frac{1}{t_1 - t_0} \left[-\mathbf{r}_0(t - t_1) + \mathbf{r}_1(t - t_0) \right]. \tag{C208}$$

We then have $\dot{r}^i = \text{const.}$, so that the above stationarity condition is trivially fulfilled. The straight connection has extremal (shortest) length. More generally, we may consider a straight connection of the two points,

$$\mathbf{r}'(t) = \mathbf{r}_0 + f(t)(\mathbf{r}_1 - \mathbf{r}_0), \tag{C209}$$

where $f : [t_0, t_1] \to \mathbb{R}$ is a function with boundary condition $f(t_0) = 0$ and $f(t_1) = 1$. We may think of this as a reparameterization of the straight curve, or as the same curve traversed at inhomogeneous velocity $\dot{f}(t)(\mathbf{r}_1 - \mathbf{r}_0)$. (A car performing accelerated motion along a straight line still moves along the shortest possible track.) Substitute this form into the extremal condition to verify that the latter is still satisfied – the reparameterization invariance of functional extrema conditions.

EXERCISE Re-familiarize yourself with the definition of the derivative $f'(x)$ of higher dimensional functions $f : \mathbb{R}^k \to \mathbb{R}$. Interpret the functional $F[\gamma]$ as the limit of a function $F : \mathbb{R}^N \to R, \{\gamma^i\} \to F(\{\gamma^i\})$ where the vector $\{\gamma^i | i = 1, \ldots, N\}$ is a discrete approximation of the curve γ. Think how the definition (C204) generalizes the notion of differentiability and how $F|_\gamma \leftrightarrow f'(x)$ generalizes the definition of a derivative.

C8.3 Euler-Lagrange equations

Calculating extrema of local functionals by explicit manipulation of the corresponding integrals is always an option, but can be tedious in practice. It is therefore good to know that there exist ways to derive extremal conditions which hold regardless of the specific form of the functional. To illustrate the principle, consider the the set of smooth curves

$$\Gamma_{\mathbf{r}_0 \to \mathbf{r}_1} = \{\gamma : [t_0, t_1] \to \mathbb{R}^d, t \mapsto \mathbf{r}(t) | \mathbf{r}(t_0) = \mathbf{r}_0, \mathbf{r}(t_1) = \mathbf{r}_1\}, \tag{C210}$$

Joseph–Louis Lagrange 1736–1813

A mathematician who excelled in all fields of analysis, number theory, and celestial mechanics. In 1788 he published *Mécanique Analytique*, which formulated Newtonian mechanics in the then modern language of differential equations.

connecting two fixed points $\mathbf{r}_0$ and $\mathbf{r}_1$. On this set, we define the class of functionals

$$S[\gamma] = \int_{t_0}^{t_1} dt\, L(\mathbf{r}(t), \dot{\mathbf{r}}(t)), \qquad \text{(C211)}$$

where $L : \mathbb{R}^n \oplus \mathbb{R}^n \to \mathbb{R}$ is a function. These are local functionals depending only on the instantaneous positions of the curves, and on their velocities. We adopt notation standard in physics, where S is called an **action (functional)** and L is called a **Lagrangian function**.

We can now prove that the local functional $S[\gamma]$ is differentiable and that its derivative is given by[2]

$$\mathrm{d}F\big|_\gamma[h] = \int_{t_0}^{t_1} dt\, \left(\partial_{r^i} L - d_t \partial_{\dot{r}^i} L\right) y^i, \qquad \text{(C212)}$$

where we use coordinate vectors $\mathbf{r}$ and $\mathbf{y}$ to parameterize the curves γ and h, respectively. Eq. (C212) is verified by straightforward Taylor series expansion:

$$\begin{aligned} S[\gamma + h] - S[\gamma] &= \int_{t_0}^{t_1} dt\, \left(L(\mathbf{r} + \mathbf{y}, \dot{\mathbf{r}} + \dot{\mathbf{y}}, t) - L(\mathbf{r}, \dot{\mathbf{r}}, t)\right) = \\ &= \int_{t_0}^{t_1} dt\, \left[\partial_{\mathbf{r}} L \cdot \mathbf{y} + \partial_{\dot{\mathbf{r}}} L \cdot \dot{h}\right] + \mathcal{O}(y^2) = \\ &= \int_{t_0}^{t_1} dt\, \left[\partial_{\mathbf{r}} L - d_t(\partial_{\dot{\mathbf{r}}} L)\right] \cdot \mathbf{y} + \partial_{\dot{\mathbf{r}}} L \cdot \mathbf{y}\big|_{t_0}^{t_1} + \mathcal{O}(y^2), \end{aligned}$$

where in the last step, we have integrated by parts. The boundary term vanishes due the condition that all curves begin and end at the same point. Applied to the original curve, $\mathbf{r}(t)$, and the shifted one, $\mathbf{r}(t) + \mathbf{y}(t)$, this means $\mathbf{r}(t_i) = (\mathbf{r} + \mathbf{y})(t_i) = \mathbf{r}_i, i = 0, 1$, which enforces $\mathbf{y}(t_0) = \mathbf{y}(t_1) = 0$. Comparison with the definition (C204) leads to the identification (C212).

Eq. (C212) may now be read as follows: the local functional S is extremal on all curves obeying the so-called **Euler-Lagrange equations**

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{r}^i} - \frac{\partial L}{\partial r^i} = 0, \quad i = 1, \ldots, d.} \qquad \text{(C213)}$$

The reason is that if and only if these d conditions hold, will the linear functional (C212) vanish on arbitrary curves h.

[2] Do not be confused by the notation $\partial_{\dot{r}^i} L$. It simply means the partial derivative of the function L w.r.t. its second set of arguments: $\partial_{\dot{r}^i} L = \partial_{y^i} L(\mathbf{x}, \mathbf{y})|_{\mathbf{y}=\dot{\mathbf{r}}}$.

EXERCISE Compute the Euler-Lagrange equations of the length functional (C202) to re-establish the results discussed above.

EXERCISE Above we have argued that the extremal condition is an intrinsic property of a curve, and not tied to a specific coordinate representation. This means that if we parameterize a given curve γ in two different coordinate representations $\mathbf{r}(t)$ and $\mathbf{q}(t)$, the Euler-Lagrange equations must hold for both sets of coordinates, r^i and q^i, i.e.

$$\begin{aligned} &\gamma \text{ extremal} \Rightarrow, \\ &\qquad \left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial \dot{r}^i} - \frac{\partial}{\partial r^i}\right) L(\mathbf{r}, \dot{\mathbf{r}}) = 0, \\ &\qquad \left(\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial}{\partial \dot{q}^i} - \frac{\partial}{\partial q^i}\right) L(\mathbf{q}, \dot{\mathbf{q}}) = 0, \end{aligned} \tag{C214}$$

Where $L(\mathbf{q}, \dot{\mathbf{q}}) = L(\mathbf{r}(\mathbf{q}), \dot{\mathbf{r}}(\mathbf{q}))$ is the $\mathbf{r}$-Lagrange function expressed in $\mathbf{q}$-coordinates. To show the **coordinate invariance of the Euler-Lagrange equations**, i.e. that the second line above follows from the first, use the chain rule, i.e. $\partial_{\dot{q}^i} L = \sum_j \partial_{\dot{r}^j} L \frac{\partial \dot{r}^j}{\partial \dot{q}^i}$. To compute the partial derivative on the right use that $\dot{r}^i(\mathbf{q}) = \mathrm{d}_t r^i = \sum_j \frac{\partial r^i}{\partial q^j} \mathrm{d}_t q^j$, and the resulting equation $\frac{\partial \dot{r}^i}{\partial \dot{q}^j} = \frac{\partial r^i}{\partial q^j}$.

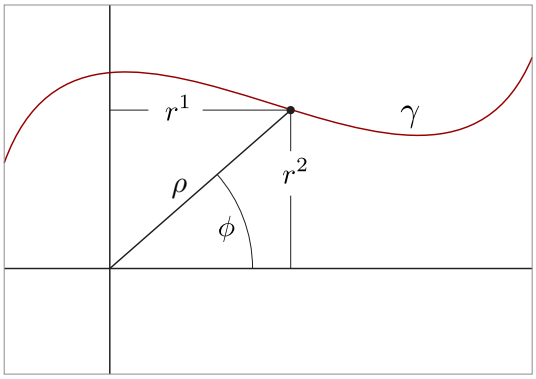


Figure C32: Parameterization of a two-dimensional curve in terms of Cartesian (r^1, r^2) and polar (ρ, ϕ) coordinates.

EXAMPLE Let us illustrate the coordinate invariance of the variational formalism with the example of the length functional C202 in the case $d = 2$, i.e. the functional measuring the length of planar curves. This functional depends only on first order time derivatives, i.e. it is described by the Lagrangian function $L(r^1, r^2, \dot{r}^1, \dot{r}^2) = \left((\dot{r}^1)^2 + (\dot{r}^2)^2\right)^{1/2}$, depending only on the derivatives $\dot{r}^i$, but not on the coordinates r^i themselves. Compute the explicit form of the Euler-Lagrange equations (C213) for this functional to rediscover our earlier extremal condition (C207).

Let us now reparameterize the two dimensional (r^1, r^2)-plane in terms of polar coordinates (for a comprehensive discussion of non-Cartesian coordinates, see chapter V2) $r^1 = \rho\cos(\phi), r^2 = \rho\sin(\phi)$.

Each curve has now two alternative descriptions, $(r^1(t), r^2(t))$ and $(\rho(t), \phi(t))$, see Fig. C32. Substituting $\dot{r}^1 = \dot{\rho}\cos(\phi) - \rho\sin(\phi)\dot{\phi}$ and $\dot{r}^2 = \dot{\rho}\sin(\phi) + \rho\cos(\phi)\dot{\phi}$ into the Euler-Lagrange equation, we obtain the representation

$$L(\rho, \phi, \dot{\rho}, \dot{\phi}) = \left(\dot{\rho}^2 + \rho^2\dot{\phi}^2\right)^{1/2}, \tag{C215}$$

It is now straightforward to compute the Euler-Lagrange equations

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\rho}} - \frac{\partial L}{\partial \rho} = \dot{\phi}(\dots) \stackrel{!}{=} 0,$$
$$\frac{d}{dt}\frac{\partial L}{\partial \dot{\phi}} - \frac{\partial L}{\partial \phi} = \dot{\phi}(\dots) \stackrel{!}{=} 0.$$

Here, the notation $\dot{\phi}(\dots)$ indicates that we are getting a lengthy list of terms which, however, are all multiplied by $\dot{\phi}$. Putting the initial point into the origin, i.e. a point with radial coordinate $\rho(t_0) = 0$ and the final point somewhere into the plane, $(\rho(t_1), \phi(t_1)) = (\rho_1, \phi_1)$, we conclude that curves connecting the origin along a straight line, i.e. one without variation in the angular coordinate, $\phi(t) = \phi_1 = \text{const.}$, are solutions of the Euler-Lagrange equations; they have vanishing derivative $\dot{\phi} = 0$, implying that both equations are satisfied. (It is less straightforward to show that these are the *only* solutions.)

C9 Calculus of complex functions

Although the complex number field $\mathbb{C}$ may be superficially more complicated than the real one we have frequently seen in this text that the 'complex' description of problems can be a lot simpler than a 'real one' – think of Fourier calculus as an example. However, so far we have not really harvested the full potential of complex numbers. We will do so in this chapter where we introduce the complex version of *calculus*, complex differentiation, integration, etc. The ensuing complex calculus will turn out to be much more powerful than real calculus. For example, we will discuss integration theorems so strong that one often chooses to 'complexify' real integrals (in a manner to be discussed) to benefit from them.

At first sight, the above remarks may be surprising: hadn't we said that the complex numbers $z = x + \mathrm{i}y$ can be parameterized in terms of two real coordinates x, y and therefore may be regarded as a two dimensional real vector space, $\mathbb{Z} \simeq \mathbb{R}^2$? Which would then suggest that complex calculus is more or less equivalent to two-dimensional real calculus. What this argument misses is that complex numbers can be multiplied with each other. Staying with the vector space picture this means that we are dealing with a variant of $\mathbb{R}^2$ in which vectors can be multiplied to produce new vectors (which is the defining feature of an *algebra*, cf. p. 71, i.e. the complex numbers are equivalent to a two-dimensional real algebra). It is this added feature which gives complex calculus its strength.

C9.1 Holomorphic functions

Definition

Complex calculus addresses the properties of differentiable complex functions $f : U \to \mathbb{C}, z \mapsto f(x)$, where $U \subset \mathbb{C}$ is an open subset of $\mathbb{C}$. In analogy to Eq. (C1) we call f **complex differentiable** at $z \in U$ if the limit

$$f'(z) \equiv \frac{\mathrm{d}f(z)}{\mathrm{d}z} \equiv \lim_{\Delta z \to 0} \frac{1}{\delta_z}(f(z + \Delta z) - f(z)) \tag{C216}$$

exists. If f is differentiable for all $z \in U$ we call it **holomorphic** in U. Examples of functions for which holomorphy in all of $\mathbb{C}$ can be established by explicit construction of the limit (i.e. as with real functions) include the monomials z^l, $l \in \mathbb{N}$, convergent power series, or the functions $\exp(z), \sin(z), \cos(z)$ (by virtue of their power series representations).

Recall that the two most important rules of real differentiation, the product rule and the chain rule, follow directly from the limit definition Eq. (C1). Since Eq. (C216) has the same structure, complex generalizations of these rules follow in an analogous manner:

$$\begin{aligned} \text{product rule:} \quad & \frac{\mathrm{d}}{\mathrm{d}z}(fg)(z) = f'(z)g(z) + f(z)g'(z), \\ \text{chain rule:} \quad & \frac{\mathrm{d}}{\mathrm{d}z}(f(g(z))) = f'(g(z))g'(z), \end{aligned} \tag{C217}$$

where the existence of all derivatives is assumed.

Cauchy-Riemann differential equations

Is holomorphy equivalent to the condition of real differentiability of the function $f(x, y)$ when $z = x + \mathrm{i}y$ is interpreted as a two-dimensional real variable? No it is not, holomorphy is a much stronger condition and this follows from the above mentioned algebraic structure of the complex numbers. To understand this point let us represent $z = (x, y)^T$ as as a two component vector containing its real and imaginary part. Now consider another complex number $w = r + \mathrm{i}s$ and build the product $z' \equiv x' + \mathrm{i}y' = wz = rx - sy + \mathrm{i}(ry + sx)$. In matrix representation this reads

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} r & -s \\ s & r \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \tag{C218}$$

We split $f = u + \mathrm{i}v$ into real and imaginary part and temporarily interpret it as a real two-dimensional function

$$\begin{aligned} & f : \mathbb{R}^2 \longrightarrow \mathbb{R}^2, \\ & \begin{pmatrix} x \\ y \end{pmatrix} \longmapsto \begin{pmatrix} u \\ v \end{pmatrix}_{(x,y)}, \end{aligned} \tag{C219}$$

where the argument is indicated as a subscript for notational convenience. This function is differentiable in the real sense if all partial derivatives $\partial_x u, \partial_y u, \partial_x v, \partial_y v$ exist and a small increment of the function can be represented as

$$\begin{pmatrix} u \\ v \end{pmatrix}_{(x+\Delta x, y+\Delta y)} = \begin{pmatrix} u \\ v \end{pmatrix}_{(x,y)} + \begin{pmatrix} \partial_x u & \partial_y u \\ \partial_x v & \partial_y v \end{pmatrix}_{(x,y)} \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} + \mathcal{O}(\Delta x^2, \Delta y^2).$$

By contrast, complex differentiability calls for the condition

$$f(z + \Delta z) = f(z) + f'(z)\Delta z + \mathcal{O}(\Delta z^2),$$

where on the r.h.s. we have the multiplication of complex numbers. If we write out this relation in a real two-component representation we understand that (i) $f'(z)$ is to be identified with

Auguistin-Louis Cauchy (1789-1857)

A French mathematician generally considered as one of the fathers of modern analysis and in particular of complex analysis. However, Cauchy also contributed to many other areas of mathematics and physics including algebra, number theory, wave mechanics, and elasticity.

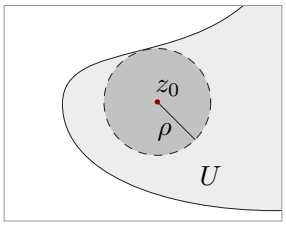
the 2×2 in the real derivative. At the same time, $f'(z)\Delta z$ is the multiplication of two complex numbers and Eq. (C218) requires that

$$\boxed{\partial_x u = \partial_y v, \qquad \partial_y u = -\partial_x v.} \tag{C220}$$

These equations are known as **Cauchy-Riemann differential equations** and they express the condition of complex differentiability in the language of real numbers.

Analyticity

One can show that a function is holomorphic in U iff it can be expanded in a **complex Taylor series** around each $z_0 \in U$, i.e. if there exists a representation



$$\boxed{f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n, \qquad a_n = \frac{f^{(n)}(z_0)}{n!},} \tag{C221}$$

where the identification of the coefficients, $a_n = f^{(n)}(z_0)/n!$ follows from n-fold differentiation of the left and the right hand side of the equation at z_0, as in the case of real Taylor series. The series exists (converges) in a disk with radius ρ around z_0. A *lower* bound for ρ is the radius of the maximal disk centered at z_0 and contained in U (see figure). Functions having this property are called **analytic** in U. The attributes 'analytic in U' and 'holomorphic in U' are synonymous and both in widespread use.

Here are a few examples of functions along with their analyticity properties:

- $\exp(z), \sin(z), \cos(z)$ — power series expandable around any $z \in C$ and therefore globally analytic.
- $\overline{z} = x - \mathrm{i}y$ — not analytic, because it violates Eqs. (C220).
- $|z|$ — also not analytic, for the same reason.
- $\frac{1}{z-w}$ — analytic on $\mathbb{C}\backslash\{w\}$.

A point $z_0 \in \mathbb{C}$ where a function f is not analytic is called the point of a **singularity**. Notice that a singularity need not imply diverging behavior. For example $z = 0$ is a singularity of the function $|z|$, which vanishes at the singular point.

Geometric interpretation of holomorphy

Let us turn back to the $\mathbb{R}^2$-interpretation of complex functions to give the concept of holomorphy a geometric meaning. Consider the map (C219) and in particular the set of curves in the uv-plane generated by keeping one of the coordinates x, y constant, e.g. $(u, v)(x, y_0)$, where $y_0 = \mathrm{const.}$. We may think of this as a map from a perpendicular grid of parameter lines in

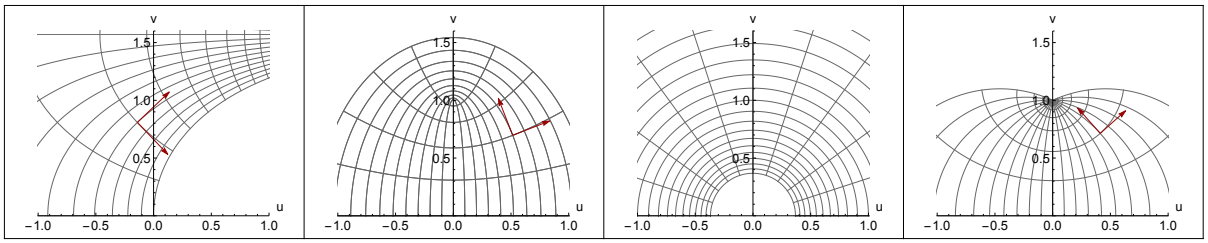


Figure C33: Image curves of the holomorphic functions (left to right) $\log(z), \sinh(z), \exp(z)$ and $\tanh(z)$. For arguments $z = x + \mathrm{i}y$ with $x \in [-1, 1]$ and $y \in [0, 2\pi]$ discretized into an argument grid with 20×20 lines. The arrows are the tangents at arguments $(x_0, y_0) = (0.6, \pi/5)$.

the xy-plane to a distorted grid of image lines in the uv-plane, see. Fig. C34. A key feature of that image-grid is that its lines still cross at 90deg angles, like those of the argument-grid. We say that the map $(x, y)^T \mapsto (u, v)^T$ is **conformal** or **angle preserving**, and this feature is a direct consequence of holomorphy.

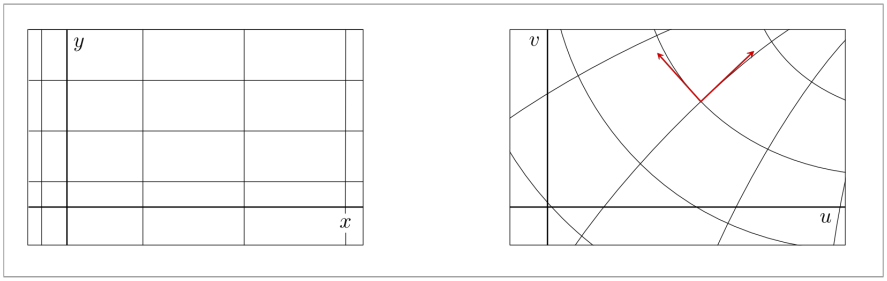


Figure C34: A holomorphic map $f(x+\mathrm{i}y) = (u+\mathrm{i}v)(x+\mathrm{i}y)$ sends a perpendicular grid of coordinate lines in the xy-plane to a distorted but angle-preserving grid in the uv-plane.

To understand this connection, consider a curve $(u, v)^T(x) \equiv (u, v)(x + \mathrm{i}y_0)$ in the uv-plane obtained by keeping y_0 constant. Its tangent vector at the point $x_0 + \mathrm{i}y_0$ is given by $(\partial_x u, \partial_x v)^T_{(x_0+\mathrm{i}y_0)}$. Likewise, the tangent vector of the curve with constant x_0 passing through $x_0 + \mathrm{i}y_0$ reads $(\partial_y u, \partial_y v)^T_{(x_0+\mathrm{i}y_0)}$. The scalar product of these two tangents is given by

$$\partial_x u \partial_y u + \partial_x v \partial_y v \overset{\text{(C220)}}{=} \partial_x u \partial_y u - \partial_y u \partial_x u = 0.$$

The fact that it vanishes means that the parametric curves intersect at a 90deg angle, just like those of the xy-argument grid, i.e. the image grid locally preserves the angular structure of the argument grid. (Think why the local preservation of the angle is not tied to the perpendicularity of the argument grid used in the construction above.) For illustration, Fig. C33 shows image grids for a number of specific conformal maps.

C9.2 Complex integration

REMARK Requires section **??**.

The Cauchy-Riemann differential equations are at the root one side of a coin whose other are strong theorems applying to the integrals of complex functions. These theorems are instrumental in most applications of complex functions in physics, mathematics, and engineering.

Definition of complex integrals

As before with differentiation, we may approach complex integration by interpreting the complex quantities involved as elements in $\mathbb{R}^2$. To this end, consider a curve γ in $\mathbb{R}^2$ beginning and ending at $(x_0, y_0)^T$ and $(x_1, y_1)^T$, respectively. Assume γ to be parameterized as $\gamma : [0,1] \to \mathbb{R}^2, t \mapsto (x(t), y(t))^T$. Let $(u, -v)^T_{(x,y)}$ and $(v, u)^T_{(x,y)}$ be the component representation of two vector fields, where $u_{(x,y)}$ and $v_{(x,y)}$ are real functions. We then know that the line integral of the fields along the curve are given by the integral of the scalar product of the curve-velocity $(\dot{x}, \dot{y})^T$ with the vector fields $(u, -v)^T$ and $(v, u)^T$, respectively, cf. Eq. (V12). In a component representation this leads to the two results

$$\begin{aligned} I &\equiv \int_0^1 \mathrm{d}t\, (\dot{x}(t)u(t) - \dot{y}(t)v(t)), \\ J &\equiv \int_0^1 \mathrm{d}t\, (\dot{x}(t)v(t) + \dot{y}(t)u(t)). \end{aligned} \tag{C222}$$

These formulae can be cast into a convenient complex represenation. To this end we interpret γ as a curve in the complex numbers with representation $z(t) \equiv x(t) + \mathrm{i}y(t)$. In a similar manner we combine the vector field components to define a complex function $f(z) \equiv (u + \mathrm{i}v)(z)$. Now let us define the **complex line integral** along γ as

$$\boxed{\int_\gamma f(z)\mathrm{d}z \equiv \int_0^1 \mathrm{d}t\, \dot{z}(t) f(z(t)).} \tag{C223}$$

As always with line integrals, notations such as $\int_\gamma f \mathrm{d}z$ are symbolic representations for a concrete definition through a time-like parameter integral, here given by the expression on the r.h.s.

Defining the complex number $K \equiv \int_\gamma f \mathrm{d}z$ and using that $\dot{z}f = \dot{x}u - \dot{y}v + \mathrm{i}(\dot{x}v + \dot{y}u)$, we realize that $K = I + \mathrm{i}\, J$, i.e. the real and imaginary parts of our complex definition are just the two real line integrals introduced above. This is an important observation as it connects the complex definition to the two-dimensional geometry of conventional vector field integration. For example, this correspondence tells us that the complex integral does not depend on the choice of the representation $z(t)$ of the complex curve (because the corresponding real vector field integrals don't, still you may want to verify this by explicit computation).

EXAMPLE Let $z_0 = R$, $R \in \mathbb{R}^+$ be a point on the positive real axis and $z_1 = Re^{\mathrm{i}\phi}$ a terminal point at the same distance R from the origin. Consider a circular arc S_ϕ connecting the two points according to the parameterization $z(t) = \exp(\mathrm{i}t\phi), t \in [0,1]$. Let us compute the complex line integral of the function z^n along this curve:

$$\int_{S_\phi} \mathrm{d}z\, z^n = \int_0^1 \mathrm{d}t(\mathrm{i}\phi R\mathrm{e}^{\mathrm{i}\phi t})(R\mathrm{e}^{\mathrm{i}\phi t})^n = \frac{R^{n+1}}{(n+1)}\left(\mathrm{e}^{\mathrm{i}(n+1)\phi} - 1\right).$$

Suppose we close the curve by choosing $\phi = 2\pi$, i.e. we now integrate around a closed curve $S_{2\pi}$ of constant radius R around the origin. In this case, $\exp(\mathrm{i}2\pi(n+1)) = 1$, and the integrals all vanish as long as $n \geq 0$. This is a remarkable result. It tells us that the line integral of any function holomorphic at $z = 0$, i.e. any function that can be represented in terms of a Taylor series $f(z) = \sum_n a^n z^n$ (whose radius of convergence exceeds R) has a vanishing line integral along the circle. In fact, the closed line integral vanishes even for all negative powers $n < 0$, i.e. for functions singular at the origin, *unless* $n = 1$. Only in this case we obtain the finite result $\int_{S_{2\pi}} \mathrm{d}z\, z^{-1} = 2\pi\mathrm{i}$. For later reference, we summarize these findings as

$$\boxed{\int_S \mathrm{d}z(z - z_0)^n = 2\pi i\delta_{n,-1},} \tag{C224}$$

where S is a curve surrounding z_0 at constant radius.

Clearly something is going on here, and in the next section we discuss what it is.

INFO The result above implies a useful representation of the coefficients, c_n, of the complex series, Eq. (C221) of holomorphic functions: let S be a circle of radius smaller than the series of convergence around a z_0 where a function is holomorphic. For any given n consider the line integral of $f(z)/(z - z_0)^{n+1}$ along that circle:

$$\oint_S dz \frac{f(z)}{(z - z_0)^{n+1}} = \sum_m a_m \oint_S dz(z - z_0)^{m-n-1} = 2\pi i a_n,$$

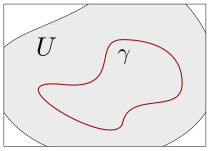
where in the last step Eq. (C224) was used. We thus have the representation

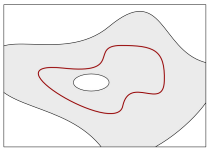
$$a_n = \frac{1}{2\pi i}\oint_S dz \frac{f(z)}{(z - z_0)^{n+1}}. \tag{C225}$$

This representation can be used to obtain non-trivial results, cf. the proof of Liouville's theorem below.

C9.3 Cauchy theorem

Let U be a simply connected domain in the complex plane. We recall (cf. section V3.2) that a domain is called simply connected if it is connected (any two points $z_1, z_2 \in U$ can be connected by a curve in U) and any closed curve in U can be shrunk to a point (see the figure, where the upper domain is simply connected while the lower one is not). Let γ be a closed curve in U and f a function holomorphic in U. **Cauchy's theorem** then states that





$$\boxed{\int_\gamma \mathrm{d}z\, f(z) = 0,} \qquad \text{(C226)}$$

i.e. the line integral of a holomorphic function along a closed curve is zero. Before proving this important fact, we note the equally important consequence that

> The integral of a holomorphic function f along a curve connecting two points $z_{1,2}$ in a simply connected domain does not depend on the choice of the curve.

This follows from the fact[1] that if you have two curves $\gamma_{1,2}$ connecting the two points, you may concatenate them to form a *closed curve* $\gamma_1 \cup \gamma_2$ going from z_1 to z_2 (along γ_1) and back (along γ_2). But then we have $\int_{\gamma_1} f - \int_{\gamma_2} f = \int_{\gamma_1 \cup \gamma_2} f = 0$, where the last equality is due to Cauchy. This feature gives us the freedom to 'deform' integration contours at will. As long as we don't hit any points where the function is non-holomorphic the value of an integral will not change.

To **prove Cauchy's theorem**, we turn back to the real interpretation of the complex line integral. Both, I, J in (C222) are line integrals of vector fields in the two-dimensional xy-plane. We may apply Stoke's theorem (V104) to convert them to integrals of the curl of our fields over the the bounded by the integration curve in the xy-plane. Embedding the integration plane into a three-dimensional space with third coordinate z, the integral I can then be represented as the integral of $(\nabla \times (u, -v, 0)^T)_z = \partial_x(-v) - \partial_y u$. However, this combination of derivatives vanishes because our function is analytic and hence obeys the Cauchy-Riemann equations (C220). By the same token, the curl of the second vector field $(\nabla \times (v, u, 0)^T)_z = \partial_x u - \partial_y v$ vanishes as well. We therefore conclude that both $I = J = 0$ and this means that the complex line integral $K = I + \mathrm{i}J$ vanishes.

The vanishing of the integrals of z^n along the circular contour discussed in the example of the previous section is now understood as a manifestation of Cauchy's theorem. The theorem also tells us that the integration contour might have been deformed to any other one surrounding the origin, and the holomorphy of z^n (outside the origin for $n < 0$) would ensure the invariance of the integral.

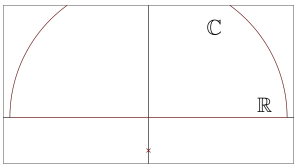
Cauchy's theorem and a a few of its cousins which we are going to discuss are powerful allies in both complex *and* real integration theory. Integrals over real functions can often be

[1] Recall the very similar reasoning employed in section V3.2 to show the path independence of integrals of gradient fields.

processed by interpreting the integral as a complex one, followed by application of a complex integration theorem. In the following example, we apply this strategy to the computation of a real integral over a rational function.

EXAMPLE Suppose we wanted to compute the integral $I \equiv \int_{-\infty}^{\infty} \mathrm{d}x\, r(x)$ over the rational function $r(x) = \frac{x^2-1}{(x^2+1)^2}$. Integrals of this type can generally be computed by elementary yet somewhat laborious variable substitutions (do the above integral in this way). However, one may often proceed in more efficient and certainly more elegant ways by complex integration methods. To illustrate this strategy let us define the function $f(z) \equiv \frac{1}{(z+\mathrm{i})^2}$. Consider the integral of this function along the real axis, i.e. from $-\infty + \mathrm{i}0$ to $+\infty + \mathrm{i}0$. Using the real variable x as an integration parameter, we find

$$\int_{\mathbb{R}} \mathrm{d}z\, f(z) = \int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{(x+\mathrm{i})^2} = \int_{-\infty}^{\infty} \mathrm{d}x \left(\frac{x^2-1}{(x^2+1)^2} - \frac{2\mathrm{i}}{(x^2+1)^2} \right).$$



We observe that the real part of the line integral is just the integral we are interested in. We now compute the complex integral by a commonly played trick: we imagine the integration contour closed by a giant semicircle of radius $\to \infty$ through the upper complex plane (see figure). Does this operation change the result of the integral? The answer is no, and this is because the integrand decays as $\sim z^{-2}$ for $|z| \to \infty$. However, the circumference of the circle grows only as $\sim |z|$. So the contribution from the semicircle to the line integral decays as $\sim |z|^{-1}$. (If you feel uneasy about this argument, inspect the line integral more closely.) We now have transformed our integral to one along a closed contour, and one that runs through a simply connected part of the complex plane. Furthermore, the function f has only one singularity at $z = -\mathrm{i}$ (the cross in the figure), and so it is analytic everywhere inside the contour. Cauchy's theorem then tells us that the integral equals $0 = 0 + \mathrm{i}0$, i.e. $I = 0$ as a consequence of the complex integration theorem.

C9.4 Singularities

Most functions of interest are not holomorphic throughout all of $\mathbb{C}$. For example, one can prove (**Liouville's theorem**) that every function f that is bounded $|f(z)| < M$, for some $M > 0$, and holomorphic in all of $\mathbb{C}$ must necessarily be constant. This means that interesting bounded functions (of which there are many) contain singularities.

INFO The **proof of Liouville's theorem** nicely illustrates the power of series expansions in complex calculus: let $f : C \to C, z \mapsto f(z)$ be holomorphic in all of $\mathbb{C}$ *and* bounded, $|f(z)| < R$ for some $R > 0$. Holomorphy in all of $\mathbb{C}$ implies the existence of a series representation (C221) centered around any point in $\mathbb{C}$, say $z_0 = 0$, and unlimited radius of convergence, $f(z) = \sum_{n=0}^{\infty} a_n z^n$. Consider a circle S of radius R centered around $z = 0$, and represent the coefficients of f's series as

in Eq. (C225). We then obtain the estimate,

$$|a_n| \leq \frac{1}{2\pi} \oint_S dz \left| \frac{f(z)}{z^{n+1}} \right| \leq \frac{1}{2\pi} (2\pi R) \frac{M}{R^{n+1}} = MR^{-n}, \tag{C227}$$

where the factor $2\pi R$ in the numerator comes from the circumference of the integration contour. (If you feel uneasy about this estimate, use a parameterization $z(t) = Re^{i\phi t}$ to formulate an explicit representation of the line integral and count the factors of R then.) This means that $|a_n| \leq MR^{-n}$ for arbitrary R, which in turn implies $a_n = 0$, unless $n = 0$. The series thus collapses to $f(z) = a_0$, showing the constancy of f.

As we will see below, complex singularities are interesting objects which can be potent allies, especially when it comes to the integration of functions. However, before we turn to the discussion of this point we need to classify them according to their severity. We first need to discriminate between isolated singularities and extended singularities. A function has an **isolated singularity** at $z_0 \in U$ if it is holomorphic on $U\backslash\{z_0\}$, where U is some open neighborhood of z_0. For example, the function z^{-1} has an isolated singularity at $z = 0$ because it can be expanded (is analytic) around any point different from zero. The square root function $z^{1/2}$, has a singularity at $z = 0$, too, but it is not an isolated one. As we will discuss in more detail below, one cannot even define a continuous square root function on a punctured neighborhood $U\backslash\{0\}$ of the origin. (As you may have guessed, this is related to the notorious sign ambiguity, e.g. $\sqrt{4} = \pm 2$.)

Turning to the isolated singularities, the 'least singular' of those is a **removable singularity** (hebbare Singularität). This is an isolated singularity at some z_0 where a function $f(z)$ just is not properly defined. However it is 'removable' in the sense that a holomorphic extension covering z_0 is possible. The canonical example in this context is the function $\mathrm{sinc}(z) \equiv \sin(z)/z$ which has a problem at $z_0 = 0$ where it shows a $0/0$ ambiguity. However, we may define $\mathrm{sinc}(0) = 1$ to remove the singularity and obtain a globally holomorphic function. (Discuss the function now is holomorphic and construct a Taylor series representation centered around $z = 0$.)

A **pole** is an example of a more serious singularity. The function $f(z)$ has a pole at z_0 if it is analytic on $U\backslash\{z_0\}$, but not at z_0, and if there exists a holomorphic function $g : U \to \mathbb{C}$ with non-vanishing $g(z_0)$ such that for all $z \neq z_0$

$$f(z) = \frac{g(z)}{(z - z_0)^n.} \tag{C228}$$

The smallest n for which such a representation exists is called the **order of the pole**. A few examples:

- ▷ The function $f(z) = \frac{1}{(z-\mathrm{i})^2}$ has a pole of order 2 at $z = \mathrm{i}$.
- ▷ The function $f(z) = \frac{1}{(z-1)^2(z+1)}$ has a pole of order 2 at $z = 1$ and one of order 1 at $z = -1$.

▷ The function $f(z) = \frac{1}{e^{iz}+1}$ has a pole of order 1 at $z = \pi$. This is best seen by expanding the exponential function in the vicinity of $i\pi$ as $e^{i\pi+z} = -1 - z - z^2/2 - \ldots$. Substitution into $f(z)$ leads to $f(z) \simeq 1/(-z - z^2) = -1/z(z+1)$ which is of the form Eq. (C228) with $g(z) \simeq -1/(1+z)$.

An isolated singularity which is neither removable, nor a pole is called an **essential singularity**. For example, $z = 0$ is an essential singularity of the function $|z|$ (but notice the absence of divergences!) This wording suggests that poles are somehow considered 'non-essential'. But why is this? The answer lies in the analyticity of the function g in (C228) which in turn implies the existence of a Taylor series expansion $g(z) = \sum_{m\geq 0} b_m (z - z_0)^m$. If we substitute this into the pole expression, we obtain the series representation

$$\boxed{f(z) = \sum_{m=-n}^{\infty} a_m (z - z_0)^m,} \tag{C229}$$

where the coefficients $a_m = b_{m+n}$ are determined by the expansion of g. Series of this type, i.e. power series starting at some finite negative exponent $-n$ are called **Laurent series**. The singularity of the function f is now encoded in finitely many *simple* functions $(z - z_0)^{m<0}$, and in this sense is non-essential. Functions that are holomorphic except for finitely many points where they afford Laurent expansions (i.e. contain poles) are called **meromorphic functions**. The terminology (inspired by the Greek word *meros*='part') suggests that they stand halfway between the holomorphic and the truly singular functions. The coefficient $a_{-1} \equiv \mathrm{Res}(f, z_0)$ of the expansion is called the **residue** (Residuum) of f at z_0. We will see in a moment how the residue plays an important role in the complex integration of f.

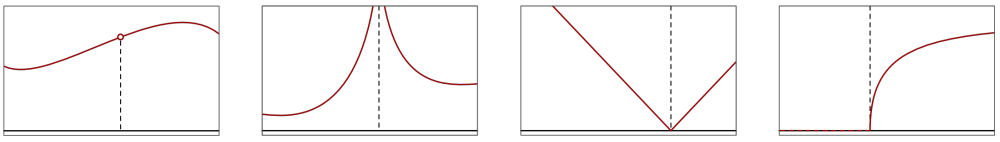


Figure C35: A one-dimensional cartoon of function singularities in ascending order of severity.

For example, the second function in the list above $f(z) = \frac{1}{(z-1)^2(z+1)}$ is meromorphic in $\mathbb{C}$. In the vicinity of its second order pole at $z = 1$, the second factor $(z+1)^{-1}$ may be expanded as

$$\frac{1}{z+1} = \frac{1}{(z-1)+2} = -\sum_{m=0}^{\infty} \left(-\frac{1}{2}\right)^{m+1} (z-1)^m,$$

and from there we obtain the Laurent series representation

$$\frac{1}{(z-1)^2(z+1)} \overset{z\simeq 1}{=} -\sum_{m=-2}^{\infty} \left(-\frac{1}{2}\right)^{m+3} (z-1)^m, \tag{C230}$$

with a residue of $-1/4$. To conclude, we have seen that the severity of singularities can be classified according to the hierarchy removable → essential indicated in Fig. C35.

C9.5 Residue theorem

Deforming integration contours

Suppose we want to integrate a meromorphic function f around a path γ encircling one or more of its poles (cf. Fig. C36, first panel) in mathematically positive, counter-clockwise direction. What can we say in general about the outcome of the integration? Of course, one would suspect not much — should the result of the integration not depend on the choice of the integration curve?

However, it is one of the marvels of complex calculus that the choice of the curve is inessential to the value of the integral, all what matters is how many point-singularities of f it encircles. To see this, consider the composite curve $\gamma' \cup c_l \cup (-S) \cup c_r$ shown in the second panel, where $c_{l,r}$ are parallel stretches from some point of γ to the neighborhood of the singularity and back, γ' is a cut version of γ and $-S$ a small circular curve surrounding the singularity in mathematically negative, clockwise direction. We indicate the sense of orientation by a minus sign in the notation. This new curve surrounds a region in which f is holomorphic and so Cauchy's theorem tells us that

$$\int_{\gamma' \cup c_l \cup (-S) \cup c_r} \mathrm{d}z f = \int_{\gamma'} \mathrm{d}z f + \int_{c_r} \mathrm{d}z f + \int_{-S} \mathrm{d}z f + \int_{c_l} \mathrm{d}z f = 0.$$

The integrals along $c_{l,r}$ mutually cancel out because they are along geometrically identical stretches traversed in opposite direction, $\int_{c_r} + \int_{c_l} = \int_{c_r} + \int_{-c_r} = 0$. We also know that the integral over γ' equals that over γ because cutting a curve at a single point does not change the value of an integral. Finally, $\int_{-S} \mathrm{d}z f = -\int_S \mathrm{d}f$, where S is the positively traversed circle. Combining these observations we arrive at the result

$$\int_\gamma \mathrm{d}z f = \int_S \mathrm{d}z f. \tag{C231}$$

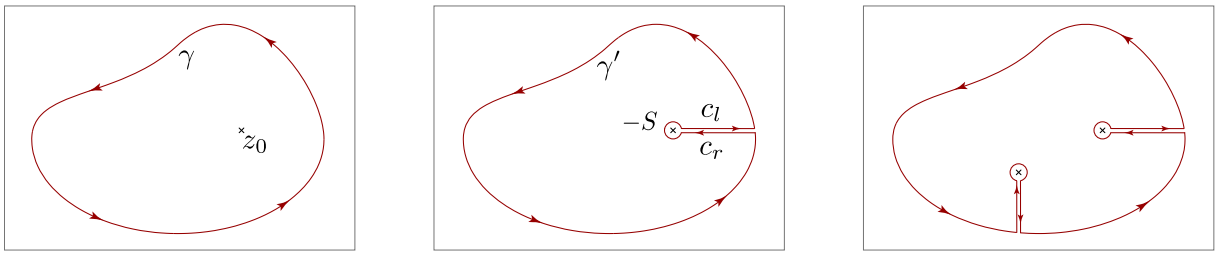
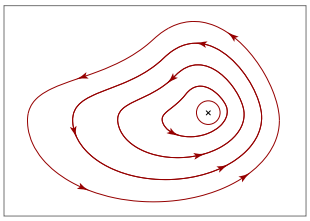


Figure C36: First panel: integration of a meromorphic function along a contour encircling singularities. Second panel: the contour can be deformed (without changing the value of the integral) to one encircling the residues along small circles. Those integrals in turn yield $2\pi\mathrm{i}\times$ the corresponding residues of the function at the singular points. Third panel: the method works for an arbitrary number of singularties inside the contour.

If there are several singularities the construction may be generalized as shown in the right panel of the figure, i.e.

$$\int_\gamma \mathrm{d}z f = \sum_i \int_{S_i} \mathrm{d}z f, \tag{C232}$$

where the sum is over all singular points, and the S_i's are small circles surrounding these points.



A good way to think about the construction is to imagine γ as a **rubber band** and the singularities as nails. Outside the nail's positions the rubber band can be deformed arbitrarily without changing the integral over holomorphic functions. If there is just one nail, the band may be shrunk to an arbitrarily small one encircling its position. Think how to rationalize the multi-singularity generalization (C232) within the rubbery analogy.

The residue theorem

Now imagine a meromorphic f expanded in a Laurent series (C229) around one of its singularities. The formula Eq. (C224) then tells us that the integration along the corresponding circle will yield $2\pi\mathrm{i}$ times the coefficient of order $m = -1$, i.e. the coefficient termed residue of the function at the singularity:

$$\int_{S_i} \mathrm{d}z f(z) = 2\pi\mathrm{i}\,\mathrm{Res}(f, z_i). \tag{C233}$$

Combining this formula with Eq. (C232) we arrive at the **residue theorem**,

$$\boxed{\int_\gamma \mathrm{d}z f(z) = 2\pi\mathrm{i} \sum_i \mathrm{Res}(f, z_i).} \tag{C234}$$

The integral of a meromorphic function along a curve equals $2\pi\mathrm{i}$ times the sum over the residues of all the singular points enclosed by the curve.

INFO As we will see momentarily, the theorem of residues is a powerful aid, both in real and complex integration. This being so it is expedient to know recipes for the efficient **computation of residues of meromorphic functions**. One approach is to start from a representation as in Eq. (C228), followed by Taylor series expansion of the function g. In practice, the function g is often easy to guess and this method works reasonably well. Alternatively, one may compute the derivative

$$\boxed{\mathrm{Res}(f, z_0) = \frac{1}{(n-1)!} \partial_z^{n-1} \left((z - z_0)^n f(z) \right) \Big|_{z=z_0},} \tag{C235}$$

where n is the order of the pole of f at z_0. To understand this formula consider the Laurent series of f and notice that

$$\partial_z^{n-1}((z-z_0)^n f(z)) = \partial_z^{n-1} \sum_{m=-n}^{\infty} a_m (z-z_0)^{n+m} = \sum_{m=-1}^{\infty} \frac{(n+m)!}{m!} a_m (z-z_0)^{m+1},$$

where in the second step we noted that powers of $(z-z_0)$ of order smaller than $n-1$ vanish under the derivative. If we now set $z=z_0$ all contributions to the series except the lowest, $m=-1$ vanish. So we are left with $a_{-1} \times (n-1)!$ and that explains why Eq. (C235) picks out the residue of the function at z_0.

Examples

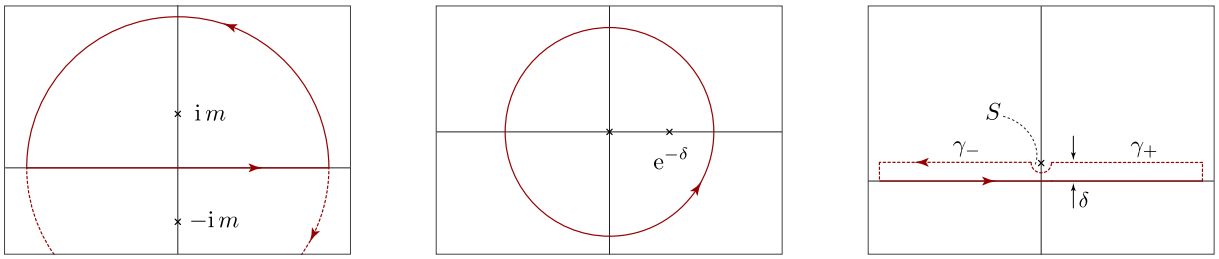


Figure C37: Three examples of contour integration aided by the theorem of residues. Discussion, see text.

Example 1: like Chauchy's theorem the theorem of residues may be applied to the computation of real integrals. Consider, for example, the integral

$$I \equiv \int_{-\infty}^{\infty} \mathrm{d}x \, \frac{1}{x^2+m^2}.$$

We proceed as in the example of p C9.3 and interpret I as an integral of the complex function $1/(z^2+m^2)$ over the real axis. A semicircle closing the contour either in the upper or lower complex plane at distance $\to \infty$ may be added without altering the value of the integral. Now we have a closed contour and the theorem of residues instructs us to inspect the singularities of $\frac{1}{z^2+m^2} = \frac{1}{(z-\mathrm{i}m)(z+\mathrm{i}m)}$, where we assume $m > 0$. There are two poles of order unity at $z_0 = \pm \mathrm{i}m$, with residue $\pm 1/2m$, see left panel of Fig. C37. If we close the contour in the upper complex plane we encircle the pole at $+\mathrm{i}m$ and the theorem of residues immediately gives $I = \frac{\pi}{m}$. Verify this result from the fact that $\arctan'(x) = \frac{1}{x^2+1}$. Check that the closure of the integration contour in the lower complex plane yields the same result. (In doing so keep an eye on the direction of travel, clockwise or anti-clockwise, of contours.)

A generalized variant of the above integral which plays an important role in both electrodynamics and quantum mechanics reads

$$I \equiv \int_{-\infty}^{\infty} \mathrm{d}x \, \frac{e^{\mathrm{i}kx}}{x^2+m^2},$$

where $k > 0$ for concreteness. Calculate the integral by the same method as above to verify

$$I = \frac{\pi}{m} e^{-|k|m}.$$

Discuss why the choice of the upper contour now is required by the sign of k.
Example 2: occasionally, one encounters integrals over complex functions which do not yet have the canonical form of a complex line integral Eq. (C223). As an example, consider the integral (which again plays a role in some areas of quantum mechancis)

$$I \equiv \int_0^{2\pi} \mathrm{d}\phi \frac{1}{1 - \mathrm{e}^{\delta}\mathrm{e}^{\mathrm{i}\phi}},$$

where $\delta > 0$. Defining $z = \mathrm{e}^{\mathrm{i}\phi}$ and noting that $\mathrm{d}_\phi z = \mathrm{i}z$, we realize that the integral can be written as

$$I = \int_\gamma \mathrm{d}z \frac{1}{z(1 - \mathrm{e}^{\delta} z)},$$

where the integral is along a unit circle around the complex origin, and ϕ was used as a curve parameter (cf. Fig. C37), center. This integral has two poles of order unity at $z_0 = 0$ and $z_1 = \mathrm{e}^{-\delta}$ with residues 1 and -1, resp. Application of the theorem of residues thus yields $I = 0$.

An alternative way to obtain this result is to expand the ϕ-representation of the integral in a power series in $\mathrm{e}^{\mathrm{i}\phi}$ and to show that each term in the expansion vanishes (try it!) As an exercise you may explore what happens if $\delta < 0$. Does the integral still vanish? Compute its value by an explicit expansion and by the theorem of residues.
Example 3: as a final example consider the integration

$$I \equiv \int_{-\infty}^{\infty} \mathrm{d}x \frac{f(x)}{x - \mathrm{i}\delta}. \tag{C236}$$

of the product of a function $f(z)$ analytic in a strip around the real axis and the factor $\frac{1}{z-\mathrm{i}\delta}$, where $\delta > 0$ is assumed to be infinitesimally small, along the real axis. As a concrete example we may consider $f(z) = \frac{1}{1+z^2}$ which is analytic for $|\mathrm{Im}(z)| < 1$.

The function $\frac{1}{z-\mathrm{i}\delta}$ has a pole at $z = \mathrm{i}\delta$, see Fig. C37, right panel. This means that if we close our integration contour as shown in the figure, we have a closed loop integral over an analytic function, i.e. an integral that yields a vanishing result. The infinitesimally short pieces connecting the two parallel integration stretches along the real axis $\mathbb{R}$ and the backward contour $\mathbb{R} + \mathrm{i}\delta$ do not contribute to the integral, so we may write

$$0 = \int_{\mathbb{R}} \mathrm{d}z \frac{f(z)}{z - \mathrm{i}\delta} - \int_{\gamma_l \cup S \cup \gamma_r} \mathrm{d}z \frac{f(z)}{z - \mathrm{i}\delta} = I - \int_{\gamma_l \cup S \cup \gamma_r} \mathrm{d}z \frac{f(z)}{z - \mathrm{i}\delta},$$

where $\gamma_l = (-\infty, -\epsilon) + \mathrm{i}\delta$, $\gamma_r = (\epsilon, \infty) + \mathrm{i}\delta$, and S is an semicircle of infinitesimally small radius ϵ around the point $\mathrm{i}\delta$, $0 < \epsilon < \delta$. Parameterizing these contours as $\gamma_l \leftrightarrow (x + \mathrm{i}\delta, x < -\epsilon)$, $\gamma_r \leftrightarrow (x + \mathrm{i}\delta, x > \epsilon)$, and $S \leftrightarrow (\mathrm{i}\delta - \epsilon e^{\mathrm{i}t}, t \in [0, \pi])$, we obtain

$$\int_{\gamma_l} \mathrm{d}z \frac{f(z)}{z - \mathrm{i}\delta} = \int_{-\infty}^{-\epsilon} \mathrm{d}x \frac{f(x + \mathrm{i}\epsilon)}{x} \simeq \int_{-\infty}^{-\epsilon} \mathrm{d}x \frac{f(x)}{x},$$

$$\int_{\gamma_r} \mathrm{d}z \frac{f(z)}{z - \mathrm{i}\delta} = \int_\epsilon^\infty \mathrm{d}x \frac{f(x + \mathrm{i}\epsilon)}{x} \simeq \int_\epsilon^\infty \mathrm{d}x \frac{f(x)}{x},$$

$$\int_S \mathrm{d}z \frac{f(z)}{z - \mathrm{i}\delta} = \int_0^\pi \mathrm{d}t \, (-\mathrm{i}\epsilon \, \mathrm{e}^{\mathrm{i}t}) \frac{f(\mathrm{i}\delta - \epsilon e^{\mathrm{i}t})}{-\epsilon e^{\mathrm{i}t}} \simeq \mathrm{i}\pi f(0),$$

where the last equalities are based on the assumed continuity of f, i.e. the assumption that f does not vary noticeably over scales δ, ϵ. We combine these results to obtain

$$\int_{-\infty}^\infty \mathrm{d}x \frac{f(x)}{x - \mathrm{i}\delta} = \mathrm{P} \int_{-\infty}^\infty \mathrm{d}x \frac{f(x)}{x} + \mathrm{i}\pi f(0), \tag{C237}$$

where we have defined the so-called **principal value integral** (Hauptwertintegral)

$$\mathrm{P} \int_{-\infty}^\infty \mathrm{d}x \, g(x) \equiv \lim_{\epsilon \to 0} \left(\int_{-\infty}^\epsilon \mathrm{d}x + \int_\epsilon^\infty \mathrm{d}x \right) g(x). \tag{C238}$$

The result above is often abbreviated in symbolic notation as

$$\boxed{\frac{1}{x - \mathrm{i}\delta} = \mathrm{P}\frac{1}{x} + \mathrm{i}\pi\delta(x).} \tag{C239}$$

However, this formula makes sense only under an integral, and in the limit $\delta \to 0$. For example, with $f(x) = \frac{1}{1+x^2}$, we have

$$\int_{\mathbb{R}} \mathrm{d}x \frac{1}{1+x^2} \frac{1}{x - \mathrm{i}\delta} = P \int_{-\infty}^\infty \mathrm{d}x \frac{1}{x(1+x^2)} + \mathrm{i}\pi \int_{-\infty}^\infty \mathrm{d}x \, \frac{\delta(x)}{1+x^2} = i\pi,$$

where we used that the principal value integral vanishes due to the evenness of the integrand under $x \leftrightarrow (-x)$.

EXERCISE Compute the imaginary part $\mathrm{Im}(x - \mathrm{i}\delta)^{-1}$ and convince yourself that in the limit $\delta \to 0$ a representation of the δ-function is obtained. This is an alternative way to understand the appearance of $\mathrm{i}\pi\delta(x)$ in Eq(C239).

EXAMPLE As a concrete and final example let us compute the inverse Fourier transform,

$$G(t) = \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{\mathrm{i}t\omega} \tilde{G}(\omega) = -\int \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{e}^{\mathrm{i}t\omega}}{\omega^2 - 2\mathrm{i}\omega\tau^{-1} - \omega_0^2},$$

of the **Green function of the driven oscillator**, Eq. (C181). Inspection of the quadratic denominator shows that for **oscillator frequencies larger than the damping rate**, $\omega_0 > \tau^{-1}$, the integral has poles of first order in the upper complex plane at $\omega_\pm = \mathrm{i}\tau^{-1} \pm \tilde{\omega}$, where we defined the shifted

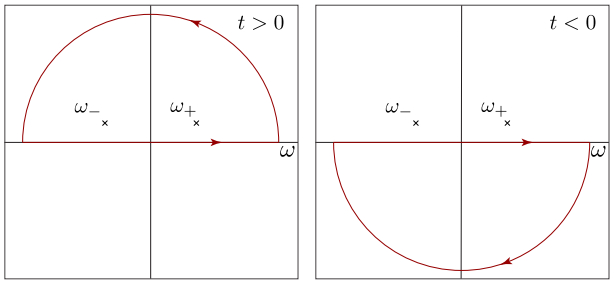


Figure C38: Computation of the Green's function of the oscillator as an residue integral, discussion, see text.

frequency, $\tilde{\omega} = (\omega_0^2 - \tau^{-2})^{1/2}$. *If* the time t is positive, then the numerator of the integrand is exponentially decaying in the upper complex plane, i.e. $\mathrm{Re}(\mathrm{i}\omega t) < 0$ for $\mathrm{Im}\,\omega > 0$. In this case, the integration contour along the real axis may be closed via an infinitely large semicircle as in *Example 1* above (see Fig. (C38), left panel). Application of the theorem then yields

$$G(t) = \frac{1}{\tilde{\omega}} \sin(\tilde{\omega} t) \exp\left(-\frac{t}{\tau}\right), \qquad t \geq 0 \tag{C240}$$

For negative times, $t < 0$, the exponential factor decays in the lower complex plane and the integral may be closed there, Fig. C38, right panel. The integrand now does not enclose any singularities and application of the Cauchy theorem yields a vanishing result, $G(t) = 0$, $t < 0$. Combining the results for the two domains $t \geq 0$ and $t < 0$ in a single formula, we arrive at the first term in Eq. (C183). Discuss the integral in the over-damped regime, $\omega_0 < \tau^{-1}$ and extend the physical discussion of section C7.5 to this case.

C9.6 Essential Singularities

We finally turn to the discussion of complex functions with 'real' singularities, of which the square root function $\sqrt{z}$ is the perhaps the simplest one. The real square root $\sqrt{x}$ appears so frequently that it is easy to forget how strange this 'function' really is. To begin with, it is no function at all: $\sqrt{4} = \pm 2$ has two solutions, i.e. $\sqrt{x}$ is intrinsically multi-valued. It is customary to restrict oneself to one 'branch' of the function, e.g. $\sqrt{4} \equiv 2$, but the fact remains that there is an ambiguity. And of course the domain of definition cannot be extended to the negative real numbers, because $\sqrt{-1}$ does not exist in the reals. This latter limitation disappears once we pass to the complex numbers. However, there is a price to pay, the sign ambiguity now looks even worse! To understand what is going on let us parameterize the complex number $z = r\mathrm{e}^{\mathrm{i}\phi}, r \geq 0$ and define $z^{1/2} = r^{1/2}\mathrm{e}^{\mathrm{i}\phi/2}$, where $r^{1/2} \geq 0$ is the positive branch of the real square root. This function is a valid 'square root', because, $(z^{1/2})^2 = (r^{1/2})^2(\mathrm{e}^{\mathrm{i}\phi/2})^2 = z$.

Consider what happens with the real part $\mathrm{Re}(z^{1/2}) = r^{1/2}\cos(\phi/2)$ of this function as we move from an 'almost real' argument $z = 1 + \mathrm{i}\delta$, $\delta > 0$ infinitesimal, at fixed modulus $|z| = 1$ once around the complex plane to arrive at the 'almost real' argument $z = 1 - \mathrm{i}\delta$. In the

parameterization above, this circular motion is described by $\phi \simeq \delta \to 2\pi - \delta$, at constant $r = 1$. Along it the square root function smoothly changes from $1 \overset{\delta\searrow 0}{=} \sqrt{1 + \mathrm{i}\delta} = \cos(\delta/2)$ to $-1 \overset{\delta\searrow 0}{=} \sqrt{1 - \mathrm{i}\delta} = \cos(\pi - \delta/2)$. At first sight, this looks like an acceptable result: the complex square root function incorporates the two branches of the real square root in such a way that the imaginary part of the argument $\sqrt{1 \pm \mathrm{i}\delta} = \pm 1$ signals which branch to pick. The price to be payed for that 'switch functionality' is a singular jump of hight $1 - (-1) = 2$ as the positive real axis at $r = 1$ is crossed in imaginary direction, see the first panel of Fig. C39 for a visualization.

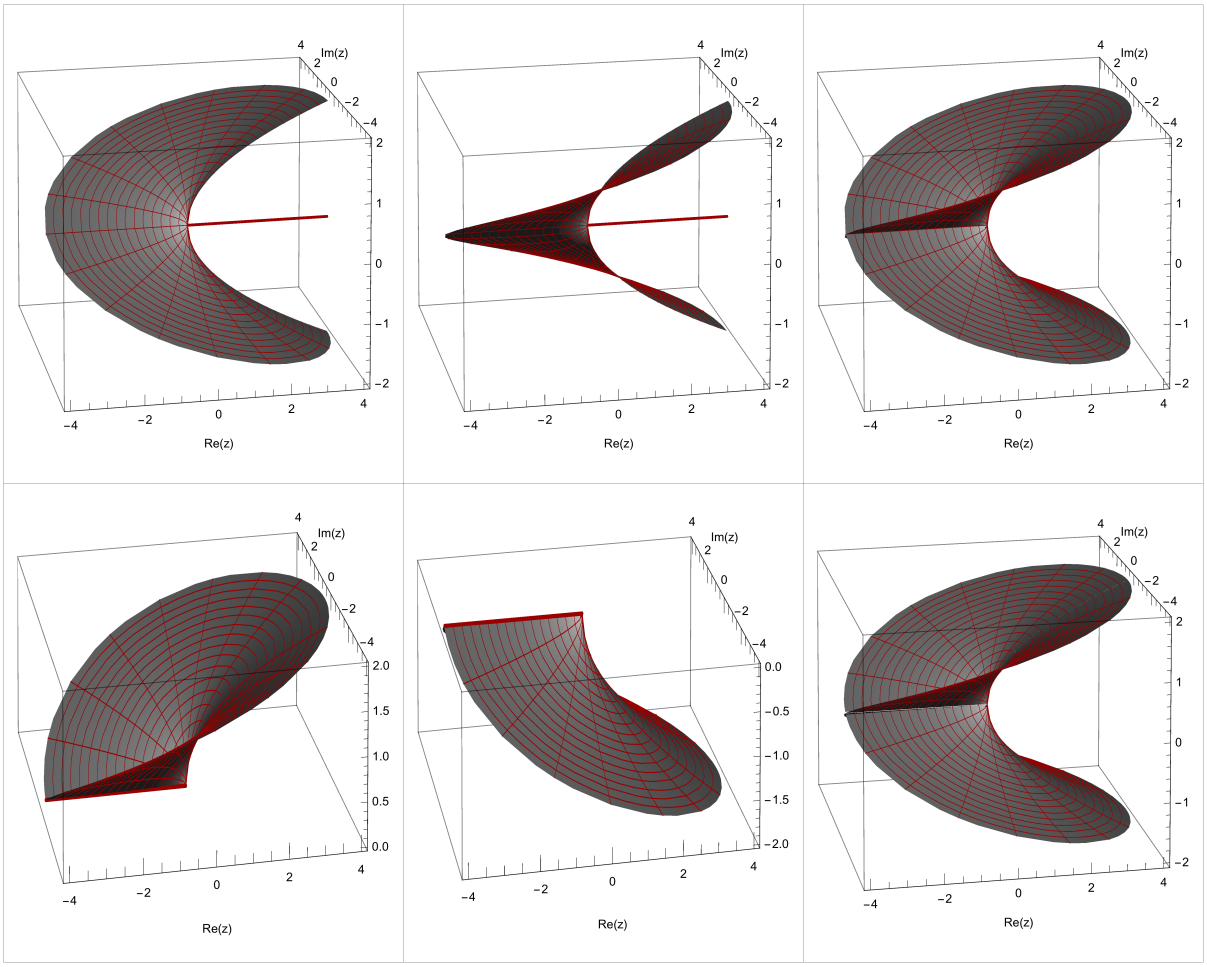
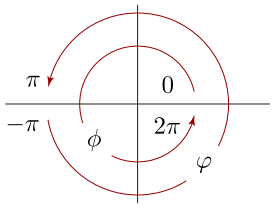


Figure C39: The two branches of the multi-valued function $\sqrt{z}$. Further discussion, see text.

However, on closer inspection it becomes apparent that the construction recipe above remains unacceptably ambiguous. First, even the complex $\sqrt{}$-function has two branches, $\pm z^{1/2} = \pm r^{1/2} \mathrm{e}^{\mathrm{i}\phi/2}$ both square to z and are legitimate options. (The sign inverted branch is shown in the second panel of the top row of Fig. C39). So, the question of which branch to pick is still with us. However, what is



worse is that the construction is 'parameterization dependent' and therefore does not really define a function: we might have decided to parameterize the complex plane in terms of a differently chosen angle $\varphi \in (-\pi, \pi)$ as shown in the figure. If we now define $z = re^{i\varphi}$ we obtain branches $\sqrt{z} = \pm r^{1/2} e^{i\varphi/2}$ very different from the ones before (see the first and second panel in the second row of Fig. C39).

All this indicates that $z^{1/2}$ cannot be an ordinary function. As a first step towards a better understanding of $z^{1/2}$, let us combine the two branches $\pm z^{1/2}$ to a set $S \equiv \{(z^{1/2}, -z^{1/2}) | z \in \mathbb{C}\}$. This set affords different interpretations. We can think of it as the set of solutions, w, of the complex equation $w^2 = z$, i.e. $w = \pm z^{1/2}$. Alternatively, it may be interpreted as the image of a 'bi-valued' function, i.e. a function that takes two values at each z. However, the most expedient view is geometric: S defines a two-sheeted 'surface', where the two vertically superimposed sheets represent the choices $\pm z^{1/2}$. A visualization of real and imaginary part of this surface[2] is shown in the right panels of Fig. C39 where we the sheets are represented in one plot. The most apparent features of this construction are: (i) the ensuing double-sheeted surfaces are globally smooth, they do not contain jumps of any kind, and (ii) the surfaces obtained for the two different parameterizations above are identical. This latter observation is important and indicates that the construction $S = \{(z^{1/2}, -z^{1/2}) | z \in \mathbb{C}\}$ might contain the key to a good understanding of the square root: no matter what specific 'coordinate representation' for $z^{1/2}$ is chosen, e.g. $z^{1/2} = \pm r^{1/2} e^{i\phi}, \pm r^{1/2} e^{i\varphi}, \ldots$, the union of all values leads to the same surface, S.

C9.7 Riemann surfaces

The construction above suggests a new way to think about a whole class of functions: consider a function $w = f(z)$ defined for $z \in U$ whose inverse $z = g(w)$ has several solutions $w_1, \ldots, w_n$ (such as $z = w^2$ has the solutions $w = \pm z^{1/2}$). We may then combine the solutions to define $\{w_1(z), ..., w_n(z) | z \in U\}$. This set is the n-sheeted **Riemann surface** of the function. Fig. C40 shows the real (left) and imaginary (right) part of the Riemann surfaces of the two-sheeted function $z^{1/2}$, the three-sheeted function $z^{1/3}$, and the infinite-sheeted function $\ln(z)$. The individual **Riemann sheets** $w_i(z)$ of the surface are glued together at lines which are called **branch cuts** and which emanate at **branch points**. Branch points are essential singularities — they are the end points of cut lines and therefore fundamentally distinct from isolated singularities — whose positions in the complex plane follow from the definition of the function. However, both the choice of Riemann sheets and that of the branch cuts are not canonical. For example, in our first/second parameterization above, the cut line is along the positive/negative reals (indicated by solid red lines in Fig. C39) and we observed the differences in the Riemann sheets corresponding to the two choices. In either choice, the square root function has one branch point at $z = 0$ and the other at

[2] Calling S a 'surface' is metaphoric inasmuch as its elements are complex numbers. Surfaces in the traditional sense ensue when we consider real and imaginary part of S separately. However, although this is necessary for graphical visualizations, the split way of thinking real/imaginary is not really natural in the present context. It is better to widen ones understanding of surfaces and mentally allow them to be complex.

$|z| = \infty$. For an example of a function with two branch points at finite values of z consider $f(z) = \sqrt{1-z^2} = \sqrt{(1-z)(1+z)}$ which has branch points at $z = \pm 1$ corresponding to the essential singularities of the two square root factors. Depending on how one chooses the branch cuts of those, $f(z)$ has a finite cut $(-1, 1)$ along the real axis connecting the two branch points, or two disconnected segments $(-\infty, -1) \cup (1, \infty)$ connecting ± 1 with $\pm\infty$.

Each Riemann sheet $w_i(z)$ has a discontinuity at the cut lines, i.e. approaching the line from different directions we get different values for w_i.[3] For example, a common choice for the branch cut of the function $\ln(z)$ is the negative real axis $\mathbb{R}^-$. Each sheet of the function then has a discontinuity $\lim_{\delta\to 0}(\ln(-r + \mathrm{i}\delta) - \ln(-r - \mathrm{i}\delta) = 2\pi\mathrm{i}$, where both values correspond to the same value of the inverse $\lim_{\delta\to 0} \mathrm{e}^{-r+\mathrm{i}\delta} = \lim_{\delta\to 0} e^{-r-\mathrm{i}\delta+2\pi\mathrm{i}}$. However as Fig. C40 shows, the Riemann surface of $\ln$ itself is a smooth object. We may interpret the singularity by saying that upon crossing the cut we smoothly pass from one Riemann sheet w_i to the next one w_{i+1} where $\lim_{\delta\to 0} w_i(-r + \mathrm{i}\delta) = \lim_{\delta\to 0} w_{i+1}(-r - \mathrm{i}\delta)$. Riemann surfaces demystify the spurious ambiguities otherwise observed with functions such as $z^q, q \in \mathbb{Q}$. They establish a beautiful connection between complex function theory and the geometry of two-dimensional surfaces. In fact, Riemann surfaces are two-dimensional real manifolds in the sense of our discussion of section V4.1. However, a comprehensive discussion of their rich geometry is beyond the scope of this text and interested readers are referred to courses in complex analysis.

[3] In Fig. C39, the second parameterization of the square root function appears continuous at the cut line. However, this is because only the real part is plotted. The imaginary part is discontinuous (check this).

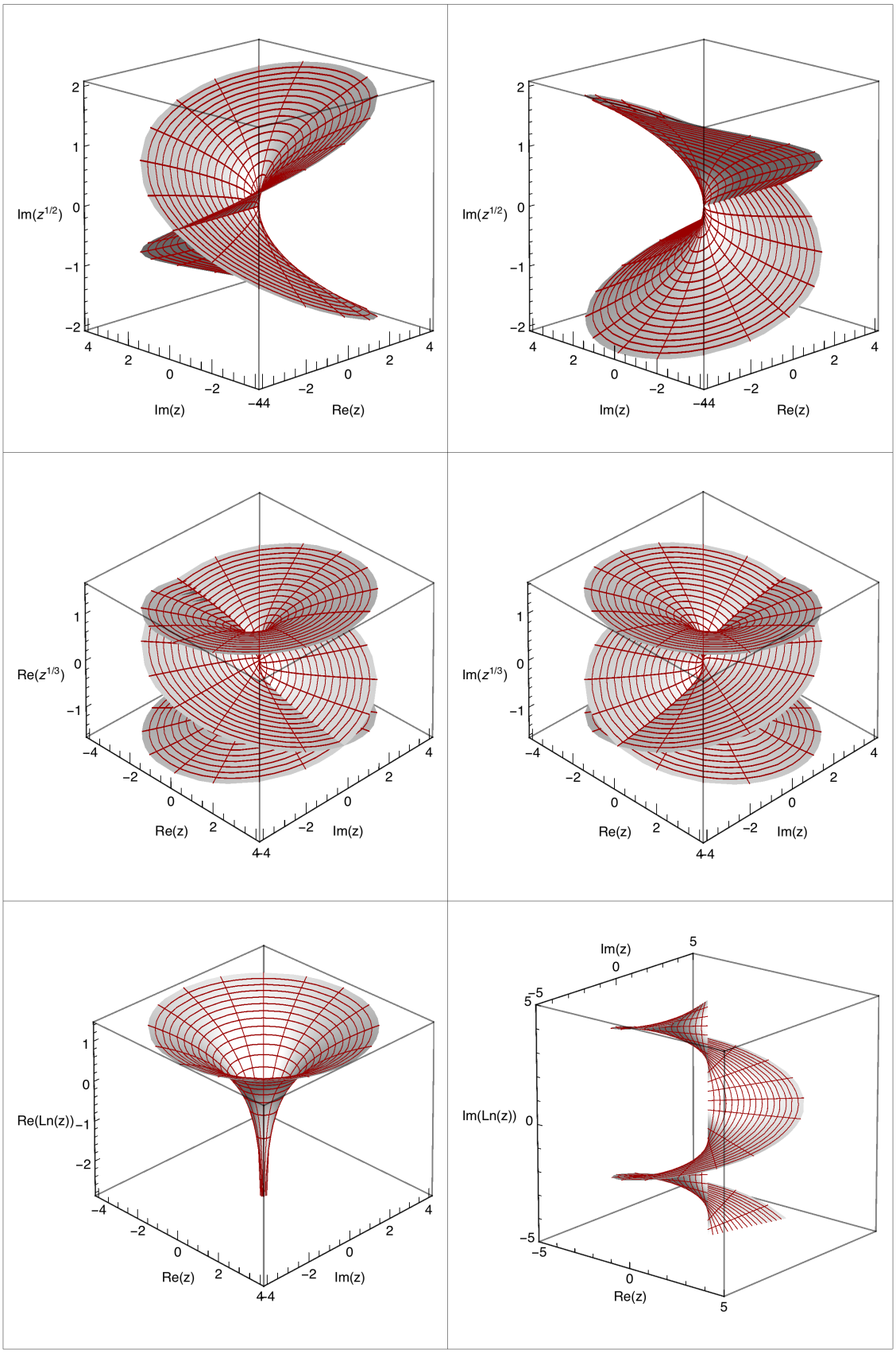


Figure C40: Riemann surfaces of the three functions $z^{1/2}$ (top), $z^{1/3}$ (center), and $\ln(z)$ (bottom). The plots show the real (left) and imaginary (right) parts of the functions over the complex plane. Further discussion, see text.

PC Problems: Calculus

The excerises come in odd–even–numbered pairs, labelled E for 'example' and P for 'practice'. Each example problem prepares the reader for tackling the subsequent practice problem. The solutions to the odd-numbered example problems are given in chapter SC. Lecturers can obtain the solutions to the even-numbered practice problems from the publishers by request.

P.C1 Differentiation of one-dimensional functions

P.C1.3 Derivatives of selected functions

EC1.3.1 Derivatives

Compute the first derivative of the following functions.
[Check your results against those in square brackets, where $[a, b]$ stands for $f'(a) = b$.]

(a) $f(x) = \frac{1}{4}x^3 - 3x^2 + 9x$ $[2, 0]$

(b) $f(x) = -\dfrac{1}{\sqrt{2x}}$ $\left[2, \frac{1}{8}\right]$

(c) $f(x) = \mathrm{e}^x(2x - 3)$ $[1, \mathrm{e}]$

(d) $f(x) = x \sin\left[\pi\left(x + \frac{1}{6}\right)\right]$ $\left[0, \frac{1}{2}\right]$

(e) $f(x) = \sin^2(\pi x)$ $\left[\frac{1}{4}, \pi\right]$

(f) $f(x) = \tan(x) \equiv \dfrac{\sin x}{\cos x}$ $\left[\frac{\pi}{6}, \frac{4}{3}\right]$

(g) $f(x) = x \ln x$ $[1, 1]$

(h) $f(x) = x \ln(9x^2)$ $\left[\frac{1}{3}, 2\right]$

(i) $f(x) = \cosh x \equiv \frac{1}{2}(\mathrm{e}^x + \mathrm{e}^{-x})$ $\left[\ln 3, \frac{4}{3}\right]$

(j) $f(x) = \tanh x \equiv \dfrac{\mathrm{e}^x - \mathrm{e}^{-x}}{\mathrm{e}^x + \mathrm{e}^{-x}}$ $[0, 1]$

PC1.3.2 Derivatives

Compute the first derivative of the following functions.
[Check your results against those in square brackets, where $[a, b]$ stands for $f'(a) = b$.]

(a) $f(x) = (x - 1)(1 + x)(x - 2)$ $[2, 3]$

(b) $f(x) = \sqrt[3]{x^2}$ $\left[8, \frac{1}{3}\right]$

(c) $f(x) = -\mathrm{e}^{(1-x^2)}$ $[1, 2]$

(d) $f(x) = -x^2 \cos(\pi x)$ $[1, 2]$

(e) $f(x) = -\cos^4(3x^2/\pi - x)$ $\left[\frac{\pi}{2}, 2\right]$

(f) $f(x) = \cot(x) \equiv \dfrac{\cos x}{\sin x}$ $\left[\frac{\pi}{2}, -1\right]$

(g) $f(x) = \ln\sqrt{x^2 + 1}$ $\left[1, \frac{1}{2}\right]$

(h) $f(x) = -2\dfrac{\sqrt{\ln x}}{x}$ $\left[\mathrm{e}, \frac{1}{\mathrm{e}^2}\right]$

(i) $f(x) = \sinh x \equiv \frac{1}{2}(\mathrm{e}^{x} - \mathrm{e}^{-x})$ $\quad [0, 1]$ (j) $f(x) = \coth x \equiv \dfrac{\mathrm{e}^{x} + \mathrm{e}^{-x}}{\mathrm{e}^{x} - \mathrm{e}^{-x}}$ $\quad [\ln 2, -\frac{16}{9}]$

EC1.3.3 Derivatives of inverse functions

If a bijective function f is differentiable at the point x, with derivative $f'(x) \neq 0$, then the inverse function f^{-1} is likewise differentiable at the point $y = f(x)$, with

$$\frac{\mathrm{d}f^{-1}(y)}{\mathrm{d}y} = \left(\frac{\mathrm{d}f(x)}{\mathrm{d}x}\Big|_{x=f^{-1}(y)} \right)^{-1} . \tag{1}$$

Use this relation to compute the following derivatives, and specify for each on which y-domain your answer holds. [Check your results: $[a, b]$ stands for $(f^{-1})'(a) = b$.]

(a) $\frac{\mathrm{d}}{\mathrm{d}y} \ln y$, $\quad [2, \frac{1}{2}]$; (b) $\frac{\mathrm{d}}{\mathrm{d}y} \arctan(y)$, $\quad [1, \frac{1}{2}]$; (c) $\frac{\mathrm{d}}{\mathrm{d}y} \arccos(y)$ $\quad [3, -\frac{3}{\sqrt{8}}]$.

Hint: The identity $\sec^2 y = 1 + \tan^2 y$ is useful for (b), and $\sin^2 y + \cos^2 y = 1$ for (c).

PC1.3.4 Derivatives of inverse functions

Use $(f^{-1})'(y) = 1/f'(f^{-1}(y))$ to compute the following derivatives of inverse functions. [Check your results: $[a, b]$ stands for $(f^{-1})'(a) = b$.]

(a) $\frac{\mathrm{d}}{\mathrm{d}y} \operatorname{arcsinh}(y)$, $\quad [2, \frac{1}{\sqrt{5}}]$; (b) $\frac{\mathrm{d}}{\mathrm{d}y} \operatorname{arctanh}(y)$, $\quad [\frac{1}{2}, \frac{4}{3}]$; (c) $\frac{\mathrm{d}}{\mathrm{d}y} \operatorname{arccosh}(y)$ $\quad [2, \frac{1}{\sqrt{3}}]$.

Hint: The identity $\cosh^2 y = 1 + \sinh^2 y$ is useful for (a,c), and $\operatorname{sech}^2 y = 1 - \tanh^2 y$ for (b).

P.C2 Integration of one-dimensional functions

EC2.3.1 Integration by parts

Integrals of the form $I(z) = \int_{z_0}^{z} \mathrm{d}x \; u(x)v'(x)$ can be written as $I(z) = [u(x)v(x)]_{z_0}^{z} - \int_{z_0}^{z} \mathrm{d}x \; u'(x)v(x)$ using integration by parts. This is useful if $u'v$ can be integrated – either directly, after further integrations by parts [see (b)], or after other manipulations [see (e,f)]. When doing such a calculation, we recommend that you clearly indicate the factors u, v', v and u'. Always check that the derivative $I'(z) = \mathrm{d}I/\mathrm{d}z$ of your result reproduces the integrand! If a single integration by parts suffices to calculate $I(z)$, you'll find that its derivative exhibits the cancellation pattern $I' = u'v + uv' - u'v = uv'$ [see (a,c,d)]; otherwise, more involved cancellations occur [see (b,e,f)].
Integrate the following integrals by parts. [Check your results against those in square brackets, where $[a, b]$ stands for $I(a) = b$.]

(a) $I(z) = \displaystyle\int_0^z \mathrm{d}x \; x \, \mathrm{e}^{2x}$ $\quad \left[\frac{1}{2}, \frac{1}{4}\right]$ (b) $I(z) = \displaystyle\int_0^z \mathrm{d}x \; x^2 \, \mathrm{e}^{2x}$ $\quad \left[\frac{1}{2}, \frac{\mathrm{e}}{8} - \frac{1}{4}\right]$

(c) $I(z) = \int_0^z \mathrm{d}x\ \ln x \qquad [1, -1]$ (d) $I(z) = \int_0^z \mathrm{d}x\ \ln x \frac{1}{\sqrt{x}} \qquad [1, -4]$

(e) $I(z) = \int_0^z \mathrm{d}x\ \sin^2 x \qquad [\pi, \frac{\pi}{2}]$ (f) $I(z) = \int_0^z \mathrm{d}x\ \sin^4 x \qquad [\pi, \frac{3\pi}{8}]$

PC2.3.2 Integration by parts

Integrate the following integrals by parts. [Check your results against those in square brackets, where $[a, b]$ stands for $I(a) = b$.]

(a) $I(z) = \int_0^z \mathrm{d}x\ x \sin(2x) \qquad [\frac{\pi}{2}, \frac{\pi}{4}]$ (b) $I(z) = \int_0^z \mathrm{d}x\ x^2 \cos(2x) \qquad [\frac{\pi}{2}, -\frac{\pi}{4}]$

(c) $I(z) = \int_0^z \mathrm{d}x\ (\ln x)\ x \qquad [1, -\frac{1}{4}]$ (d) $I(z) \overset{[n>-1]}{=} \int_0^z \mathrm{d}x\ (\ln x)\ x^n \qquad [1, \frac{-1}{(n+1)^2}]$

(e) $I(z) = \int_0^z \mathrm{d}x\ \cos^2 x \qquad [\pi, \frac{\pi}{2}]$ (f) $I(z) = \int_0^z \mathrm{d}x\ \cos^4 x \qquad [\pi, \frac{3}{8}\pi]$

EC2.3.3 Integration by substitution

Integrals of the form $I(z) = \int_{z_0}^z \mathrm{d}x\ y'(x) f(y(x))$ can be written as $I(z) = \int_{y(z_0)}^{y(z)} \mathrm{d}y f(y)$ by using the substitution $y = y(x)$, $\mathrm{d}y = y'(x)\mathrm{d}x$. When doing such integrals, we recommend that you explicitly write down $y(x)$ and $\mathrm{d}y$, to ensure that you correctly identify the prefactor of $f(y)$. Always check that the derivative $I'(z) = \mathrm{d}I/\mathrm{d}z$ of your result reproduces the integrand! You'll notice that the factor $y'(z)$ emerges via the chain rule for differentiating composite functions.

Calculate the following integrals by substitution. [Check your results against those in square brackets, where $[a, b]$ stands for $I(a) = b$.]

(a) $I(z) = \int_0^z \mathrm{d}x\ x \cos(x^2 + \pi) \qquad [\sqrt{\frac{\pi}{2}}, -\frac{1}{2}]$ (b) $I(z) = \int_0^z \mathrm{d}x\ \sin^3 x \cos x \qquad [\frac{\pi}{4}, \frac{1}{16}]$

(c) $I(z) = \int_0^z \mathrm{d}x\ \frac{\sqrt{1 + \ln(x+1)}}{x+1} \qquad [\mathrm{e}^3 - 1, \frac{14}{3}]$ (d) $I(z) = \int_0^z \mathrm{d}x\ x^3 \mathrm{e}^{-x^4} \qquad [\sqrt[4]{\ln 2}, \frac{1}{8}]$

PC2.3.4 Integration by substitution

Calculate the following integrals by substitution. [Check your results versus those in square brackets, where $[a, b]$ stands for $I(a) = b$.]

(a) $I(z) = \int_0^z \mathrm{d}x\ x^2\ \sqrt{x^3 + 1} \qquad [2, \frac{52}{9}]$ (b) $I(z) = \int_0^z \mathrm{d}x\ \sin x\ \mathrm{e}^{\cos x} \qquad [\frac{\pi}{3}, \mathrm{e} - \sqrt{\mathrm{e}}]$

(c) $I(z) = \int_0^z \mathrm{d}x\ \frac{\sin\sqrt{\pi x}}{\sqrt{x}} \qquad [\frac{\pi}{9}, \frac{1}{\sqrt{\pi}}]$ (d) $I(z) = \int_0^z \mathrm{d}x\ \sqrt{x}\ \mathrm{e}^{\sqrt{x^3}} \qquad [(\ln 4)^{2/3}, 2]$

EC2.3.5 $\sqrt{1-x^2}$ Integrals by trigonometric substitution

The sine and cosine functions satisfy the following identities:

$$\tfrac{\mathrm{d}}{\mathrm{d}y}\sin(y) = \cos(y), \qquad \tfrac{\mathrm{d}}{\mathrm{d}y}\cos(y) = -\sin(y), \qquad \cos^2(y) = 1 - \sin^2(y).$$

The last of these is useful for solving integrals that contain $\sqrt{1-x^2}$ by using the trigonometric substitution $x = \sin(y)$, since $\sqrt{1-x^2} = \cos(y)$.
Calculate the following integrals ($|z| < 1$ for (a), and $|z| < \frac{1}{2}$ for (b)); check your results by calculating $\frac{\mathrm{d}I(z)}{\mathrm{d}z}$.

(a) $I(z) = \displaystyle\int_0^z \mathrm{d}x\, \frac{1}{\sqrt{1-x^2}}.$ [Check your result: $I\left(\frac{1}{\sqrt{2}}\right) = \frac{\pi}{4}.$]

(b) $I(z) = \displaystyle\int_0^z \mathrm{d}x\, \sqrt{1-4x^2}.$ [Check your result: $I\left(\frac{1}{2}\right) = \frac{\pi}{8}.$]

Hint: The $\cos^2 y$ integral that emerges after substitution can be solved by integrating by parts!

PC2.3.6 $\sqrt{1+x^2}$ Integrals by hyberbolic substitution

The 'hyperbolic sine' and 'hyperbolic cosine' functions, defined by

$$\sinh(y) = \tfrac{1}{2}(\mathrm{e}^y - \mathrm{e}^{-y}), \qquad \cosh(y) = \tfrac{1}{2}(\mathrm{e}^y + \mathrm{e}^{-y}),$$

satisfy the following identities:

$$\tfrac{\mathrm{d}}{\mathrm{d}y}\sinh(y) = \cosh(y), \qquad \tfrac{\mathrm{d}}{\mathrm{d}y}\cosh(y) = \sinh(y), \qquad \cosh^2(y) = 1 + \sinh^2(y).$$

The last of these is useful for solving integrals that contain $\sqrt{1+x^2}$ by using the hyperbolic substitution $x = \sinh(y)$, since $\sqrt{1+x^2} = \cosh(y)$.
Calculate the following integrals; check your results by calculating $\frac{\mathrm{d}I(z)}{\mathrm{d}z}$.

(a) $I(z) = \displaystyle\int_0^z \mathrm{d}x\, \frac{1}{\sqrt{1+x^2}}.$ [Check your result: $I\left(\frac{3}{4}\right) = \ln 2.$]

(b) $I(z) = \displaystyle\int_0^z \mathrm{d}x\, \sqrt{1+\tfrac{x^2}{4}}.$ [Check your result: $I\left(\frac{3}{2}\right) = \ln 2 + \frac{15}{16}.$]

Hint: The $\cosh^2 y$ integral that emerges after substitution can be solved by integrating by parts!

EC2.3.7 $1/(1-x^2)$ Integrals by hyperbolic substitution

(a) Show that the functions $\tanh(y)$ ('hyperbolic tangent') and $\operatorname{sech}(y) = \frac{1}{\cosh(y)}$ ('hyperbolic secant') satisfy the following identities:

$$\frac{\mathrm{d}}{\mathrm{d}y}\tanh(y) = \operatorname{sech}^2(y), \qquad 1 - \tanh^2(y) = \operatorname{sech}^2(y).$$

The second of these is useful for solving integrals that contain $1-x^2$ by using the trigonometric substitution $x = \tanh(y)$, with inverse function $y = \operatorname{arctanh}(y)$, since $1 - x^2 = \operatorname{sech}^2(y)$.

Calculate the following integral for $|z| < 1$; check your results by calculating $\frac{\mathrm{d}I(z)}{\mathrm{d}z}$.

(b) $I(z) = \displaystyle\int_0^z \mathrm{d}x\, \frac{1}{1-x^2}.$ [Check your result: $I\big(\frac{3}{5}\big) = \ln 2.$]

PC2.3.8 $1/(1+x^2)$ Integrals by trigonometric substitution

(a) Show that the functions $\tan(y)$ and $\sec(y) = \frac{1}{\cos(y)}$ ('secant') satisfy the following identities:

$$\frac{\mathrm{d}}{\mathrm{d}y}\tan(y) = \sec^2(y), \qquad 1 + \tan^2(y) = \sec^2(y).$$

The second of these is useful for solving integrals that contain $1+x^2$ by using the trigonometric substitution $x = \tan(y)$, with inverse function $y = \arctan(x)$, since $1 + x^2 = \sec^2(y)$.

Calculate the following integrals; check your results by calculating $\frac{\mathrm{d}I(z)}{\mathrm{d}z}$. [In (c), $a \in \mathbb{R}$.]

(b) $I(z) = \displaystyle\int_0^z \mathrm{d}x\, \frac{1}{1+x^2}.$ [Check your result: $I\big(\infty\big) = \frac{\pi}{2}.$]

(c) $I(z) = \displaystyle\int_0^z \mathrm{d}x\, \frac{1}{(1+a^2x^2)^3}.$ [Check your result: for $a = 1$, $I\big(1\big) = \frac{1}{32}(8+3\pi).$]

EC2.3.9 $1/(1+x^2)$ Integral via partial fraction decomposition

A function f is called a 'rational function' if it can be expressed as a ratio $f(x) = P(x)/Q(x)$ of two polynomials P and Q. Integrals of rational functions can be computed using a 'partial fraction decomposition', a procedure that expresses f as the sum of a polynomial (possibly with degree 0) and several ratios of polynomials with simpler denominators. To achieve this, the denominator Q is factorized into a product of polynomials q_j of lower degree, $Q(x) = \prod_j q_j(x)$, and the function f is written as $f(x) = \sum_j p_j(x)/q_j(x)$. The form of the polynomials p_j in the numerators is fixed uniquely by the form of the polynomials P and q_j. (Since a partial fraction decomposition starts with a common denominator and ends with a sum of rational functions, it is in a sense the inverse of the procedure of adding rational functions by finding a common denominator.) If a complete factorization of Q is used, this yields a decomposition

of the integral $\int \mathrm{d}x f(x)$ into a sum of integrals that can be solved by elementary mean. In Problems C2.3.9 to C2.3.12, we illustrate the method using some simple examples; for a systematic treatment, consult textbooks on calculus.

(a) Compute the integral $I(z) = \displaystyle\int_0^z \mathrm{d}x \frac{1}{1+x^2}$ using a partial fraction decomposition. [Check your result: $I(1) = \frac{\pi}{4}$.]

(b) Alternatively, this integral can also be computed using the trigonometric substitution $x = \tan(y)$, resulting in $I(z) = \arctan(z)$ (see Problem C2.3.6). To establish that the latter result agrees with that from (a), solve the equation $x = \tan(y) = \frac{\mathrm{e}^{\mathrm{i}y} - \mathrm{e}^{-\mathrm{i}y}}{\mathrm{i}(\mathrm{e}^{\mathrm{i}y} + \mathrm{e}^{-\mathrm{i}y})}$ explicitly to find y as function of x; the resulting expression is equal to $\arctan(x)$. [The abovementioned expression for $\tan(y)$ in terms of exponentials of $\mathrm{i}y$ is established in Sec. C5.2, see Eq. (C92).]

PC2.3.10 $1/(1-x^2)$ Integral via partial fraction decomposition

(a) Compute the integral $I(z) = \displaystyle\int_0^z \mathrm{d}x \frac{1}{1-x^2}$ using a partial fraction decomposition. [Check your result: $I(\frac{1}{2}) = \frac{1}{2}\ln 3$.]

(b) Alternatively, this integral can also be computed using the hyperbolic substitution $x = \tanh(y)$, resulting in $I(z) = \operatorname{arctanh}(z)$ (see Problem **??**). To establish that the latter result agrees with that from (a), solve the equation $x = \tanh(y) = \frac{\mathrm{e}^{y} - \mathrm{e}^{-y}}{\mathrm{e}^{y} + \mathrm{e}^{-y}}$ explicitly to find y as function of x; the resulting expression is equal to $\operatorname{arctanh}(x)$.

EC2.3.11 Partial fraction decomposition

Use partial fraction decomposition to compute the following integrals, for $z \in \mathbb{R}$, $z > -1$:

(a) $I(z) = \displaystyle\int_0^z \mathrm{d}x \ \frac{3x+3}{(x+1)^2(x-2)}$, (b) $I(z) = \displaystyle\int_0^z \mathrm{d}x \ \frac{3x}{(x+1)^2(x-2)}$.

[Check your results: (a) $I(3) = -\ln 8$, (b) $I(3) = -\ln 4 + \frac{3}{4}$.]

PC2.3.12 Partial fraction decomposition

Use partial fraction decomposition to compute the following integrals, for $z \in \mathbb{R}$, $z < 1$:

(a) $I(z) = \displaystyle\int_0^z \mathrm{d}x \frac{x+2}{x^3 - 3x^2 - x + 3}$, (b) $I(z) = \displaystyle\int_0^z \mathrm{d}x \ \frac{4x-1}{(x+2)(x-1)^2}$.

[Check your results: (a) $I(\frac{1}{2}) = \frac{5}{8}\ln 5 - \frac{1}{2}\ln 3$, (b) $I(\frac{1}{2}) = 1 - \ln\left(\frac{5}{2}\right)$.]

EC2.3.13 Elementary Gaussian integral

(a) Show that the two-dimensional Gaussian integral $I = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mathrm{d}x\mathrm{d}y\, \mathrm{e}^{-(x^2+y^2)}$ has the value $I = \pi$. *Hint:* Use polar coordinates; the radial integral can be solved by substitution.

(b) Now calculate the one-dimensional Gaussian integral $I_0(a) = \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-ax^2}$ (here and below, $a \in \mathbb{R},\ a > 0$). *Hint:* $I = [I_0(1)]^2$. Explain why! [Check your result: $I_0(\pi) = 1$.]

PC2.3.14 Gaussian integral with linear term in exponent

(a) Compute the one-dimensional Gaussian integral with a linear term in the exponent:

$$I_0(a,b) = \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-ax^2+bx} \quad (a,b \in \mathbb{R}, a > 0).$$

Hint: Write the exponent in the form $-ax^2 + bx = -a(x-C)^2 + D$ (called 'completing the square') and then substitute $\tilde{x} = x - C$. You may use $\int_{-\infty}^{\infty} \mathrm{d}x\ \mathrm{e}^{-x^2} = \sqrt{\pi}$.

Compute the following integrals:

(b) $I_1(c) = \int_{-\infty}^{\infty} \mathrm{d}x\ \mathrm{e}^{-\frac{1}{2}\left(x^2+3x+\frac{c}{4}\right)}$ (c) $I_2(c) = \int_{-\infty}^{\infty} \mathrm{d}x\ \mathrm{e}^{-2(x+3)(x-c)}$

[Check your results: $I_0(\pi, \sqrt{\pi}) = \mathrm{e}^{\frac{1}{4}}$, $I_1(1) = \sqrt{2\pi}$, $I_2(-3) = \sqrt{\frac{\pi}{2}}$.]

EC2.3.15 Definite exponential integrals

Calculate the integral $I_n(a) = \int_0^{\infty} \mathrm{d}x\, x^n e^{-ax}$ (with $a \in \mathbb{R},\ a > 0,\ n \in \mathbb{N}$) using two different methods: (a) repeated partial integration, and (b) repeated differentiation:

(a) Calculate I_0, I_1 and I_2 by using partial integration where necessary. Then use partial integration to show that $I_n(a) = \frac{n}{a} I_{n-1}(a)$ for all $n \geq 1$. Use this relation iteratively to determine $I_n(a)$ as a function of a and n.

(b) Show that taking n derivatives of $I_0(a)$ with respect to a yields $I_n(a) = (-1)^n \frac{\mathrm{d}^n I_0(a)}{\mathrm{d}a^n}$. Then calculate these derivatives for a few small values of n. From the emerging pattern, deduce the general formula for $I_n(a)$.

[Check your result: $I_3(2) = \frac{3}{8}$.]

PC2.3.16 General Gaussian integrals

Determine the value of the x^{2n} Gaussian integral, $I_n(a) = \int_{-\infty}^{\infty} \mathrm{d}x\, x^{2n}\, \mathrm{e}^{-ax^2}$ (with $n \in \mathbb{N}$), using two different methods: (a) repeated partial integration, and (b) repeated differentiation:

(a) Starting from the Gaussian integral $I_0(a) = \sqrt{\frac{\pi}{a}}$, compute the integrals I_1 and I_2 by using partial integration where necessary. Then use partial integration to show that $I_n(a) = \frac{2n-1}{2a} I_{n-1}(a)$ holds for all $n \geq 1$. Use this relation iteratively to determine $I_n(a)$ as a function of a and n.

(b) Show that taking n derivatives of $I_0(a)$ with respect to a times yields $I_n(a) = (-1)^n \frac{\mathrm{d}^n I_0(a)}{\mathrm{d}a^n}$. Then calculate these derivatives for a few small values of n. From the emerging pattern, deduce the general formula for $I_n(a)$.

P.C3 Partial differentiation

P.C3.1 Partial derivative

EC3.1.1 Partial derivatives

Compute the partial derivates $\partial_x f(x,y)$ and $\partial_y f(x,y)$ of the following functions:
[Check your results against those in square brackets.]

(a) $f(x,y) = x^2y^3 - 2xy$ $\qquad [\partial_x f(2,1) = 2, \quad \partial_y f(1,2) = 10]$

(b) $f(x,y) = \sin\left[x\mathrm{e}^{2y}\right]$ $\qquad \left[\partial_x f(0,\tfrac{1}{2}) = \mathrm{e}, \quad \partial_y f(\pi,0) = -2\pi\right]$

PC3.1.2 Partial derivatives

Compute the partial derivates $\partial_x f(x,y)$ and $\partial_y f(x,y)$ of the following functions:
[Check your results against those in square brackets.]

(a) $f(x,y) = \dfrac{x^2}{y^3} + \dfrac{4y}{x}$ $\qquad [\partial_x f(2,1) = 3, \quad \partial_y f(3,3) = 1]$

(b) $f(x,y) = \ln\left(x^2 \sin(y)\right)$ $\qquad \left[\partial_x f(2,1) = 1, \quad \partial_y f(1,\tfrac{\pi}{4}) = 1\right]$

(c) $f(x,y) = \mathrm{e}^{-x^2\cos(y)}$ $\qquad \left[\partial_x f(1,\pi) = 2\mathrm{e}, \quad \partial_y f(1,\tfrac{\pi}{2}) = 1\right]$

(d) $f(x,y) = \sinh\left(\frac{x}{y}\right)$ $\qquad \left[\partial_x f(\ln 2,1) = \tfrac{5}{4}, \quad \partial_y f(\ln 2,1) = -\tfrac{5}{4}\ln 2\right]$

P.C3.2 Multiple partial derivatives

EC3.2.1 Partial derivates of first and second order

Consider the function $f : \mathbb{R}^2\backslash(0,0)^T \to \mathbb{R}$, $\mathbf{r} = (x,y)^T \mapsto f(\mathbf{r}) = \frac{x}{r} + 1$, with $r = \sqrt{x^2+y^2}$. Calculate all possible partial derivatives of first and second order.

PC3.2.2 Partial derivates of first and second order

Consider the function $f : \mathbb{R}^3 \to \mathbb{R}$, $\mathbf{r} = (x, y, z)^T \mapsto f(\mathbf{r}) = z^2 \mathrm{e}^{xy}$. Calculate all possible partial derivatives of first and second order.

P.C3.3 Chain rule for functions of several variables

EC3.3.1 Chain rule for functions of two variables

This problem aims to illustrate the inner life of the chain rule for a function of several variables. Consider the function $f : \mathbb{R}^2 \to \mathbb{R}$, $\mathbf{y} = (y^1, y^2)^T \mapsto f(\mathbf{y}) = \|\mathbf{y}\|^2$ and the vector field $\mathbf{g} : \mathbb{R}^2_+ \to \mathbb{R}^2$, $\mathbf{x} = (x^1, x^2)^T \mapsto \mathbf{g}(\mathbf{x}) = (\ln x^2, 3 \ln x^1)^T$, then $f(\mathbf{g}(\mathbf{x}))$ gives the norm of $\mathbf{g}$ as a function of $\mathbf{x}$. Find the partial derivatives $\partial_{x^1} f(\mathbf{g}(\mathbf{x}))$ and $\partial_{x^2} f(\mathbf{g}(\mathbf{x}))$ as functions of x^1 and x^2 in two ways,

(a) by first computing $f(\mathbf{x}) = f(\mathbf{g}(\mathbf{x}))$ as function of $\mathbf{x}$ and then taking partial derivatives;

(b) by using the chain rule $\partial_{x^k} f(\mathbf{g}(\mathbf{x})) = \sum_j \partial_{g^j} f(\mathbf{g}(\mathbf{x}))\, \partial_{x^k} g^j(\mathbf{x})$.

Why do both routes yield the same answer? Identify the similarities in both computations!
[Check your results: if $x^1 = 9$, $x^2 = 2$, then $\partial_{x^1} f = 4 \ln 3$, $\partial_{x^2} = \ln 2$.]

PC3.3.2 Chain rule for functions of two variables

Consider the function $f : \mathbb{R}^2 \to \mathbb{R}$, $\mathbf{y} = (y^1, y^2)^T \mapsto f(\mathbf{y}) = \mathbf{y} \cdot \mathbf{a}$, where $\mathbf{a} = (a^1, a^2)^T \in \mathbb{R}^2$, and the vector field $\mathbf{x} = (x^1, x^2)^T \mapsto \mathbf{g} : \mathbb{R}^2 \to \mathbb{R}^2$, $\mathbf{g}(\mathbf{x}) = \mathbf{x}(\mathbf{x} \cdot \mathbf{b})$, where $\mathbf{b} = (b^1, b^2)^T \in \mathbb{R}^2$. Compute the partial derivatives $\partial_{x^k} f(\mathbf{g}(\mathbf{x}))$ (with $k = 1, 2$) as functions of $\mathbf{x}$,

(a) by first computing $f(\mathbf{g}(\mathbf{x}))$ explicitly and then taking partial derivatives;

(b) by using the chain rule $\partial_{x^k} f(\mathbf{g}(\mathbf{x})) = \sum_j \partial_{g^j} f(\mathbf{g}(\mathbf{x})) \partial_{x^k} g^j(\mathbf{x})$.

[Check your result: if $\mathbf{a} = (0, 1)^T$, $\mathbf{b} = (1, 0)^T$, then $\partial_1 f(\mathbf{g}(\mathbf{x})) = x^2$, $\partial_2 f(\mathbf{g}(\mathbf{x})) = x^1$.]
Hint: If compact notation is used, such as $\mathbf{a} \cdot \mathbf{x} = a_l x^l$ and $\partial_{x^k} x^l = \delta^l{}_k$, the computations are quite short.

P.C4 Multi-dimensional integration

P.C4.1 Cartesian area and volume integrals

EC4.1.1 Two-dimensional integration (Cartesian coordinates)

Calculate the surface integral $I(a) = \int_{G_a} \mathrm{d}x\, \mathrm{d}y\, f(x, y)$ of the function $f(x, y) = xy$, over the area $G = \{(x, y) \in \mathbb{R}^2;\ 0 \le y \le 1;\ 1 \le x \le a - y\}$, with $2 \le a \in \mathbb{R}$. [Check your result: $I(2) = \frac{5}{24}$].

PC4.1.2 Two-dimensional integration (Cartesian coordinates)

Calculate the surface integral $I(a) = \int_G \mathrm{d}x\,\mathrm{d}y\, f(x,y)$ of the function $f(x,y) = y^2 + x^2$ over the surface $G = \{(x,y) \in \mathbb{R}^2;\ 0 \le x \le 1;\ 0 \le y \le \mathrm{e}^{ax}\}$, with $a \in \mathbb{R}$. *Hint:* for $\int \mathrm{d}x\, x^2 \mathrm{e}^{ax}$, use partial integration twice! [Check your result: $I(1) = \mathrm{e} + (\mathrm{e}^3 - 19)/9$.]

EC4.1.3 Area enclosed by curves (Cartesian coordinates)

Consider the curve $\gamma_1 : \mathbb{R} \to \mathbb{R}^2, t \mapsto (t, b(1 - t/a))^T$ and the closed curve $\gamma_2 : (0, 2\pi) \subset \mathbb{R} \to \mathbb{R}^2, t \mapsto (a\cos t, b \sin t)^T$ in Cartesian coordinates, with $0 < a, b \in \mathbb{R}$.

(a) Sketch the curves γ_1 and γ_2.

(b) Compute the area $S(a,b)$ enclosed by γ_2. [Check your result: $S(1,1) = \pi$.]

(c) γ_1 divides the area enclosed by γ_2 into two parts. Find the area $A(a,b)$ of the smaller part by computing an area integral. Check your result using elementary geometrical considerations.

PC4.1.4 Area enclosed by curves (Cartesian coordinates)

Consider the curves $\gamma_1 : \mathbb{R} \to \mathbb{R}^2, t \mapsto ((t-2a)^2 + 2a^2, t)^T$ and $\gamma_2 : \mathbb{R} \to \mathbb{R}^2, t \mapsto (2(t-a)^2, t)^T$ in Cartesian coordinates, with $0 < a \in \mathbb{R}$.

(a) Sketch the curves γ_1 and γ_2.

(b) Compute the finite area $S(a)$ enclosed between these curves. [Check your result: $S(\frac{1}{2}) = \frac{4}{3}$.]

EC4.1.5 Area integral for volume of a pyramid (Cartesian coordinates)

Consider the pyramid bounded by the xy plane, the yz plane, the xz plane and the plane $E = \{(x,y,z) \in \mathbb{R}^3, z = c(1 - x/a - y/b\}$, with $0 < a, b, c \in \mathbb{R}$.

(a) Make a qualitative sketch of the pyramid. Find its volume $V(a,b,c)$ using geometric arguments [Check your result: $V(1,1,1) = \frac{1}{6}$.]

(b) Compute $V(a,b,c)$ by integrating the height $h(x,y)$ of the pyramid over its base area in the xy plane.

PC4.1.6 Area integral for volume of ellipsoidal tent (Cartesian coordinates)

A tent has a flat, ellipsoidal base, given by the equation $(x/a)^2 + (y/b)^2 \le 1$. The shape of the tent's roof is given by the height function $h(x,y) = c\big[1 - (x/a)^2 - (y/b)^2\big]$.

(a) Give a qualitative sketch of the shape of the tent, for $a = 2$, $b = 1$ and $c = 2$.

(b) Calculate the volume V of the tent via a surface integral of the height function . [Check your result: if $a = b = c = 1$, then $V = \pi/2$.]
Hint: Show by a suitable trigonometric substitution that $\int_0^1 \mathrm{d}x\,(1-x^2)^{3/2} = \frac{3}{16}\pi$.

P.C4.2 Curvilinear area integrals

EC4.2.1 Area of an ellipse (elliptical polar coordinates)

(a) Let $f : \mathbb{R}^2 \to \mathbb{R}$ be a function of the coordinates x and y that depends only on the combined variable $(x/a)^2 + (y/b)^2$. Show that a two-dimensional area integral of f over $\mathbb{R}^2$ can be written as

$$I = \int_{\mathbb{R}^2} \mathrm{d}x\mathrm{d}y\, f\left((x/a)^2 + (y/b)^2\right) = 2\pi ab \int_0^\infty \mathrm{d}\mu\, \mu\, f(\mu^2)\ ,$$

by transforming from Cartesian coordinates to elliptical polar coordinates, defined as follows:

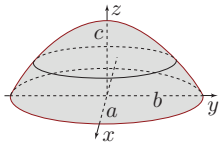
$$\begin{aligned} x &= \mu a \cos\phi, & y &= \mu b \sin\phi\ , \\ \mu^2 &= (x/a)^2 + (y/b)^2, & \phi &= \arctan(ay/bx)\ . \end{aligned}$$

Hint: For $a = b = 1$, they correspond to polar coordinates. For $a \neq b$, the local basis is *not* orthogonal!

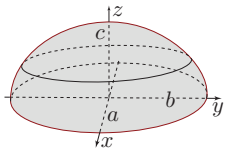
(b) Using a suitable function f, calculate the area of an ellipse with semi-axes a and b, with a and b defined by $(x/a)^2 + (y/b)^2 \leq 1$.

PC4.2.2 Area integral for volume (elliptical polar coordinates)

In the following, use elliptical coordinates in two dimensions, defined as $x = \mu a \cos\phi$, $y = \mu b \sin\phi$, with $a, b \in \mathbb{R}$, $a > b > 0$. Calculate the volume $V(a,b,c)$ of the following objects T, E and C, as a function of the length parameters a, b and c.



(a) T is a tent with an elliptical base with semi-axes a and b. The height of its roof is described by the height function $h_T(x,y) = c\big[1 - (x/a)^2 - (y/b)^2\big]$.



(b) E is an ellipsoid with semi-axes a, b and c, defined by $(x/a)^2 + (y/b)^2 + (z/c)^2 \leq 1$.

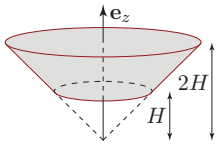
(c) C is a cone with height c and an elliptical base with semi-axes a and b. All cross sections parallel to the base are elliptical, too. *Hint:* Augment the elliptical coordinates by another coordinate, z (in analogy to passing from polar to cylindrical coordinates).

[Check your answers: if $a = 1/\pi$, $b = 2$, $c = 3$, then (a) $V_T = 3$, (b) $V_E = 8$, (c) $V_C = 2$.]

P.C4.3 Curvilinear volume integrals

EC4.3.1 Volume and moment of inertia (cylindrical coordinates)

The moment of inertia of a rigid body with respect to a given axis of rotation is defined as $I = \int_V \mathrm{d}V\, \rho_0(\mathbf{r}) d_\perp^2(\mathbf{r})$, where $\rho_0(\mathbf{r})$ is the density at the point $\mathbf{r}$, and $d_\perp(\mathbf{r})$ the perpendicular distance from $\mathbf{r}$ to the rotation axis.



Let $F = \{\mathbf{r} \in \mathbb{R}^3 \,|\, H \le z \le 2H, \sqrt{x^2+y^2} \le az\}$ be a homogeneous conical frustum (cone with tip removed) centered on the z-axis. Calculate, using cylindrical coordinates,

(a) its volume $V_F(a)$, and

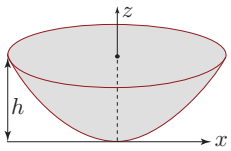
(b) its moment of inertia $I_F(a)$ with respect to the z axis,

as functions of the dimensionless, positive scale factor a, the length parameter H, and the mass m of the frustum. [Check your results: $V_F(3) = 21\pi H^3$, $I_F(1) = \frac{93\pi}{70} M H^2$.]

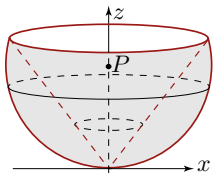
PC4.3.2 Volume and moment of inertia (cylindrical coordinates)

Consider the homogeneous rigid bodies C, P and B specified below, each with density ρ_0. For each body, use cylindrical coordinates to compute its volume $V(a)$ and moment of inertia $I(a) = \rho_0 \int_V \mathrm{d}V\, d_\perp^2$ with respect to the axis of symmetry, as functions of the dimensionless, positive scale factor a, the length parameter R, and the mass of the body, M.

(a) C is a hollow cylinder with inner radius R, outer radius aR, and height $2R$. [Check your results: $V_C(2) = 6\pi R^3$, $I_C(2) = \frac{15}{6} M R^2$.]



(b) P is a paraboloid with height $h = aR$ and curvature $1/R$, defined by $P = \{\mathbf{r} \in \mathbb{R}^3 \,|\, 0 \le z \le h, (x^2+y^2)/R \le z\}$ [Check your results: $V_P(2) = 2\pi R^3$, $I_P(2) = \frac{2}{3} M R^2$.]

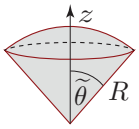


(c) B is the bowl obtained by taking a sphere, $S = \{\mathbf{r} \in \mathbb{R}^3 | \, x^2+y^2+(z-aR)^2 \le a^2R^2\}$, with radius aR, centered on the point P: $(0,0,aR)^T$, and cutting a cone from it, $C = \{\mathbf{r} \in \mathbb{R}^3 | \, (x^2+y^2) \le (a-1)z^2, a \ge 1\}$, which is symmetric about the z axis, with apex at the origin. [Check your results: $V_B\left(\frac{4}{3}\right) = \frac{16}{9}\pi R^3$, $I_B\left(\frac{4}{3}\right) = \frac{14}{15} M R^2$. What do you get for $a = 1$? Why?]

Hint: First, for a given z, find the radial integration boundaries, $\rho_1(z) \le \rho \le \rho_2(z)$, then the z integration boundaries, $0 \le z \le z_m$. What do you find for z_m, the maximal value of z?

EC4.3.3 Volume of a buoy (spherical coordinates)

Consider a buoy, with its tip at the origin, bounded from above by a sphere centered on the origin, with $x^2+y^2+z^2 \le R^2$, and from below by a cone with tip at the origin, with $z \ge a\sqrt{(x^2+y^2)}$.



(a) Show that the half angle at the tip of the cone is given by $\widetilde{\theta} = \arctan(1/a)$.

(b) Use spherical coordinates to calculate the volume $V(R, a)$ of the buoy as a function of R and a. [Check your results: $V(2, \sqrt{3}) = (16\pi/3)(1 - \sqrt{3}/2)$.]

PC4.3.4 Volume integral over quarter sphere (spherical coordinates)

Use spherical coordinates to calculate the volume integral $F(R) = \int_Q \mathrm{d}V f(\mathbf{r})$ of the function $f(\mathbf{r}) = xy$ on the quadrant Q, defined by $x^2 + y^2 + z^2 \leq R^2$ and $x, y \geq 0$. Sketch Q. [Check your result: $F(2) = \frac{64}{15}$.]

EC4.3.5 Wave functions of two-dimensional harmonic oscillator (polar coordinates)

The quantum mechanical treatment of a two-dimensional harmonic oscillator leads to so-called 'wave functions',

$$\Psi_{nm} : \mathbb{R}^2 \to \mathbb{C}, \mathbf{r} \mapsto \Psi_{nm}(\mathbf{r}), \quad \text{with} \quad n \in \mathbb{N}_0, \quad m \in \mathbb{Z}, \quad m = -n, -n+2, \ldots, n-2, n,$$

which have a factorized form when written in terms of polar coordinates, $\Psi_{nm}(\mathbf{r}) = R_{n|m|}(\rho) Z_m(\phi)$, with $Z_m(\phi) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}m\phi}$. The wave functions satisfy the following 'orthogonality relation':

$$O_{nn'}^{mm'} \equiv \int_{\mathbb{R}^2} \mathrm{d}S \, \overline{\Psi}_{nm}(\mathbf{r}) \Psi_{n'm'}(\mathbf{r}) = \delta_{nn'} \delta_{mm'} \, .$$

Verify these for $n = 0$, 1 and 2, where the radial wave functions have the form:

$$R_{00}(\rho) = \sqrt{2}\mathrm{e}^{-\rho^2/2}, \quad R_{11}(\rho) = \sqrt{2}\rho\mathrm{e}^{-\rho^2/2}, \quad R_{22}(\rho) = \rho^2 \, \mathrm{e}^{-\rho^2/2}, \quad R_{20}(\rho) = \sqrt{2}[\rho^2 - 1]\mathrm{e}^{-\rho^2/2}.$$

Proceed as follows. Due to the product form of the wave function Ψ, each area integral separates into two factors that can be calculated separately, $O_{nn'}^{mm'} = P_{nn'}^{|m||m'|} \widetilde{P}^{mm'}$, where P is a radial integral and $\widetilde{P}$ an angular integral.

(a) Find general expressions for P and $\widetilde{P}$ as integrals over R or Z functions, respectively.

(b) Compute the angular integral $\widetilde{P}^{mm'}$ for arbitrary values of m and m'.

(c) Now compute those radial integrals that arise in combination with $\widetilde{P} \neq 0$, namely P_{00}^{00}, P_{11}^{11}, P_{22}^{22}, P_{22}^{00} and P_{20}^{00}.

Hint: The Euler identity, $\mathrm{e}^{\mathrm{i}2\pi k} = 1$ if $k \in \mathbb{Z}$, is useful for evaluating the angular integral, and $\int_0^\infty \mathrm{d}x \, x^n \mathrm{e}^{-x} = n!$ for the radial integrals.

Background information: The functions $\Psi_{nm}(\mathbf{r})$ are the 'eigenfunctions' of a quantum mechanical particle in a two-dimensional harmonic potential, $V(\mathbf{r}) \propto \mathbf{r}^2$, where n and m are 'quantum numbers' that specify a particular 'eigenstate'. A particle in this state is found with probability $|\Psi_{nm}(\mathbf{r})|^2 \mathrm{d}S$ within the area element $\mathrm{d}S$ at position $\mathbf{r}$. The total probability of being found anywhere in $\mathbb{R}^2$ equals 1, hence the normalization integral yields $O_{nn}^{mm} = 1$ for *every* eigenfunction $\Psi_{nm}(\mathbf{r})$. The fact that the area integral of two eigenfunctions vanishes if their quantum numbers are not equal, reflects the fact that the eigenfunctions form an orthonormal basis in the space of square-integrable complex functions on $\mathbb{R}^2$.

PC4.3.6 Wave functions of the hydrogen atom (spherical coordinates)

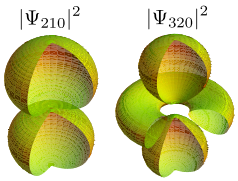
Show that the volume integral $P_{nlm} = \int_{\mathbb{R}^3} \mathrm{d}V |\Psi_{nlm}(\mathbf{r})|^2$ for the following functions $\Psi_{nlm}(\mathbf{r}) = R_{nl}(r) Y_l^m(\theta,\phi)$, with spherical coordinates $\mathbf{r} = \mathbf{r}(r,\theta,\phi)$, yields $P_{nlm} = 1$:

(a) $\Psi_{210}(\mathbf{r}) = R_{21}(r) Y_1^0(\theta,\phi)$, $\quad R_{21}(r) = \dfrac{r\mathrm{e}^{-r/2}}{\sqrt{24}}$, $\quad Y_1^0(\theta,\phi) = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$

(b) $\Psi_{320}(\mathbf{r}) = R_{32}(r) Y_2^0(\theta,\phi)$, $\quad R_{32}(r) = \dfrac{4\,r^2\mathrm{e}^{-r/3}}{81\sqrt{30}}$, $\quad Y_2^0(\theta,\phi) = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$

(c) Show that the so-called 'overlap integral' $O = \int_{\mathbb{R}^3} \mathrm{d}V\, \overline{\Psi}_{320}(\mathbf{r}) \Psi_{210}(\mathbf{r})$ yields zero.

Hint: $I_n = \int_0^\infty \mathrm{d}x\, x^n\, \mathrm{e}^{-x} = n!$.



Background information: The $\Psi_{nlm}(\mathbf{r})$ are quantum mechanical 'eigenfunctions' of the hydrogen atom, where n, l and m are 'quantum numbers' which specify the quantum state of the system. A particle in this state is found with probability $|\Psi_{nm}(\mathbf{r})|^2 \mathrm{d}V$ within the volume element $\mathrm{d}V$ at position $\mathbf{r}$. The total probability for being found anywhere in $\mathbb{R}^3$ equals 1, hence $P_{nlm} = 1$ holds for *every* eigenfunction $\Psi_{nm}(\mathbf{r})$.
The figures each show a surface on which $|\Psi_{nlm}|^2$ has a constant value. The eigenfunctions form an orthonormal basis in the space of square-integrable complex functions on $\mathbb{R}^3$, hence the volume integral of two eigenfunctions vanishes if their quantum numbers are not equal.

P.C4.4 Curvilinear integration in arbitrary dimensions

EC4.4.1 Surface integral: area of a sphere

Consider a sphere S with radius R. Compute its area, A_S, using (a) Cartesian coordinates, and (b) spherical coordinates, by proceeding as follows.

(a) Choose Cartesian coordinates, with the origin at the center of the spere. Its area is twice that of the half-sphere S_+ lying above the xy-plane. S_+ can be parametrized as

$$\mathbf{r} : D \to S_+, \qquad (x,y)^T \mapsto \mathbf{r}(x,y) = (x, y, \sqrt{R^2 - x^2 - y^2})^T,$$

where $D = \{(x,y)^T \in \mathbb{R}^2 | x^2 + y^2 < R^2\}$ is a disk of radius R. Use this parametrization to compute the area of the sphere as $A_S = 2\int_D \mathrm{d}x\mathrm{d}y\, \|\partial_x \mathbf{r} \times \partial_y \mathbf{r}\|$.

(b) Now choose spherical coordinates and parametrize the sphere as

$$\mathbf{r} : U \to S, \qquad (\theta,\phi)^T \mapsto \mathbf{r}(\theta,\phi) = R(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)^T,$$

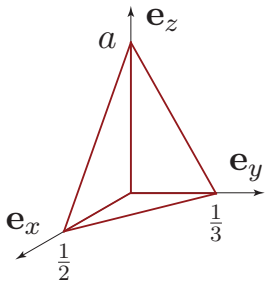
with $U = (0,\pi) \times (0, 2\pi)$. Compute the area of the sphere as $A_S = \int_U \mathrm{d}\theta\mathrm{d}\phi\, \|\partial_\theta \mathbf{r} \times \partial_\phi \mathbf{r}\|$.

PC4.4.2 Surface integral: area of slanted face of rectangular pyramid

Consider the pyramid shown in the sketch. Find a parametrization of its slanted face, F_{slant}, of the form

$$\mathbf{r} : U \subset \mathbb{R}^2 \to F_{\text{slant}} \subset \mathbb{R}^3, \quad (x, y)^T \mapsto \mathbf{r}(x, y),$$

i.e. specify the domain U and the Cartesian vector $\mathbf{r}(x, y)$. Then compute the area of the slanted face as $A_{\text{slant}} = \int_U \mathrm{d}x\mathrm{d}y \, \|\partial_x \mathbf{r} \times \partial_y \mathbf{r}\|$. [Check your result: if $a = 2$, then $A_{\text{slant}} = \frac{\sqrt{53}}{12}$.]



EC4.4.3 Volume and surface integral: parabolic solid of revolution

Let the solid of revolution K be the volume bounded from above by the plane $z = z_{\max}$, and from below by the surface of revolution P, which is defined via the rotation of the parabola $z(x) = x^2$ about the z-axis.

(a) Calculate the volume V of the body K.

(b) Calculate the surface area A of the curved part of the surface of K.

[Check your results: For $z_{\max} = \frac{3}{4}$ we have $V = \frac{9\pi}{32}$ and $A = \frac{7\pi}{6}$.]

PC4.4.4 Surface integral: hyperbolic solid of revolution (Gabriel's horn)

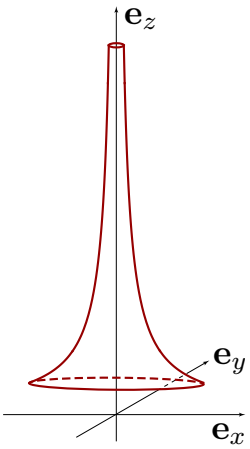
Let K be the solid body generated by rotating the function $\rho(z) = 1/z$ with $1 \le z \le a$ about the z-axis. This shape is known as Gabriel's horn or Torticelli's trumpet.

(a) Compute the volume, $V(a)$, of the body K. [Check your result: $V(2) = \frac{\pi}{2}$.]

(b) Write down the integral for the surface area of this solid, $A(a)$, and calculate its derivative $A'(a) = \frac{\mathrm{d}}{\mathrm{d}a}A(a)$. [Check your result: $A'(1) = 2\sqrt{2}\pi$.]

(c) Find a lower bound for the value of the integral $A(a)$ by using the inequality $\sqrt{z^{-4} + 1} \ge 1$.

(d) How large are the volume and (the lower bound for) the area in the limit as $a \to \infty$?



EC4.4.5 Surface area of a circular cone

Consider a circular cone C of radius R and height h. Compute the area, $A_C(R, h)$, of its (slanted) conical surface S_C as a function of R and h. [Check your result: $A_C(3, 4) = 15\pi$.]

PC4.4.6 Surface area of an elliptical cone

Consider an elliptical cone C with semi-axes a and b and height h. Use generalized polar coordinates to show that the area, A_C, of its (slanted) conical surface S_C is given by an integral of the form,

$$A_C = \int_{S_C} \mathrm{d}S = P \int_0^{2\pi} \mathrm{d}\phi \, \sqrt{1 + Q \sin^2 \phi}\,,$$

and find $P(a,b,h)$ and $Q(a,b,h)$ as functions of a, b and h. *Remark*: This integral belongs to the class of so-called **elliptical integrals**, which cannot be solved in closed form.
[Check your results: if $a = 3$, $b = 2$ and $h = 4$, then $C = 5$ and $D = \frac{32}{25}$.]

P.C4.5 Changes of variables in higher-dimensional integration

EC4.5.1 Jacobian determinant for cylindrical coordinates

Calculate the Jacobian determinant $\left|\frac{\partial(x^1,x^2,x^3)}{\partial(\rho,\phi,z)}\right|$ for the transformation from Cartesian to cylindrical coordinates.

PC4.5.2 Jacobian determinant for spherical coordinates

Calculate the Jacobian determinant $\left|\frac{\partial(x^1,x^2,x^3)}{\partial(r,\theta,\phi)}\right|$ for the transformation from Cartesian to spherical coordinates.

EC4.5.3 Three-dimensional Gaussian integral via linear transformation

Calculate the following three-dimensional Gaussian integral (with $a,b,c > 0$, $a,b,c \in \mathbb{R}$):

$$I = \int_{\mathbb{R}^3} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\, \mathrm{e}^{-\left[a^2(x+y)^2 + b^2(z-y)^2 + c^2(x-z)^2\right]}$$

Hint: Use the substitution $u = a(x+y)$, $v = b(z-y)$, $w = c(x-z)$ and calculate the Jacobian determinant, using $J = \left|\frac{\partial(u,v,w)}{\partial(x,y,z)}\right|^{-1}$. You may use $\int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-x^2} = \sqrt{\pi}$. [Check your result: if $a = b = c = \sqrt{\pi}$, then $I = \frac{1}{2}$.]

PC4.5.4 Three-dimensional Lorentzian integral via linear transformation

Calculate the following triple Lorentz integral (with $a,b,c,d > 0$, $a,b,c,d \in \mathbb{R}$):

$$I = \int_{\mathbb{R}^3} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\, \frac{1}{[(xd+y)^2 + a^2]} \cdot \frac{1}{[(y+z-x)^2 + b^2]} \cdot \frac{1}{[(y-z)^2 + c^2]}$$

Hint: Use the change of variables $u = (xd+y)/a$, $v = (y+z-x)/b$, $w = (y-z)/c$ and calculate the Jacobian determinant using $J = \left|\frac{\partial(u,v,w)}{\partial(x,y,z)}\right|^{-1}$. You may use $\int_{-\infty}^{\infty} \mathrm{d}x (x^2+1)^{-1} = \pi$. [Check your result: if $a = b = c = \pi$, $d = 2$, then $I = \frac{1}{5}$.]

EC4.5.5 General Gaussian integrals

[This problem and the next presume that you know how to diagonalize a symmetric matrix, see Sec. **??**.]
Multiple Gaussian integrals are integrals of the form

$$I = \int_{\mathbb{R}^n} \mathrm{d}x^1 \dots \mathrm{d}x^n \, \mathrm{e}^{-\mathbf{r}^T A \mathbf{r}} ,$$

where $\mathbf{r} = (x^1, \dots, x^n)^T$ and the matrix A is symmetric and positive definite (i.e. all eigenvalues of A are > 0). The characteristic property of this class of integrals is that the exponent is a 'quadratic form', i.e. a *quadratic* function of all integration variables. In general this function contains mixed terms, but these can be removed by a basis transformation: Let S be the similarity transformation that diagonalizes A, so that $D = S^T A S$ is diagonal, with eigenvalues $\lambda_1, \dots, \lambda_n$. Since A is symmetric, S is orthogonal, with $S^{-1} = S^T$ and $\det S = 1$. Now define $\tilde{\mathbf{r}} = (\tilde{x}^1, \dots, \tilde{x}^n)^T$ by $\tilde{\mathbf{r}} \equiv S^T \mathbf{r}$, then we have

$$\mathbf{r}^T A \mathbf{r} = \mathbf{r}^T S D S^T \mathbf{r} = \tilde{\mathbf{r}}^T D \, \tilde{\mathbf{r}} = \sum_i \lambda_i (\tilde{x}^i)^2 . \tag{1}$$

When expressed through the new variables $\tilde{\mathbf{r}}$, the exponent thus no longer contains any mixed terms, so that the Gaussian integral can be solved by the variable substitution $\mathbf{r} = S\tilde{\mathbf{r}}$:

$$I = \int_{\mathbb{R}^n} \mathrm{d}x^1 \dots \mathrm{d}x^n \, \mathrm{e}^{-\mathbf{r}^T A \mathbf{r}} = \int_{\mathbb{R}^n} \mathrm{d}\tilde{x}^1 \dots \mathrm{d}\tilde{x}^n \, J \, \mathrm{e}^{-\sum_i^n \lambda_n (\tilde{x}^i)^2} = \sqrt{\tfrac{\pi}{\lambda_1}} \cdots \sqrt{\tfrac{\pi}{\lambda_n}} = \sqrt{\tfrac{\pi^n}{\det A}} .$$

We have here exploited two facts: (i) Since $\partial x^i / \partial \tilde{x}^j = S^i{}_j$, the Jacobian determinant of the variable substitution equals the determinant of S and thus equal to 1:

$$J = \left| \frac{\partial(x^1, \dots, x^n)}{\partial(\tilde{x}^1, \dots, \tilde{x}^n)} \right| = \left| \det \begin{pmatrix} \frac{\partial x^1}{\partial \tilde{x}^1} & \cdots & \frac{\partial x^1}{\partial \tilde{x}^n} \\ \vdots & & \vdots \\ \frac{\partial x^n}{\partial \tilde{x}^1} & \cdots & \frac{\partial x^n}{\partial \tilde{x}^n} \end{pmatrix} \right| = \left| \det \begin{pmatrix} S^1{}_1 & \cdots & S^1{}_n \\ \vdots & & \vdots \\ S^n{}_1 & \cdots & S^n{}_n \end{pmatrix} \right| = |\det S| = 1 .$$

(ii) The product of the eigenvalues of a matrix equals its determinant, $\prod_i^n \lambda_i = \det A$.

Now use the above strategy to compute the following integral ($a > 0$):

$$I(a) = \int_{\mathbb{R}^2} \mathrm{d}x \, \mathrm{d}y \, \mathrm{e}^{-\left[(a+3)x^2 + 2(a-3)xy + (a+3)y^2\right]}$$

Execute all steps of the above argumentation explicitly:

(a) Bring the exponent into the form $-\mathbf{r}^T A \mathbf{r}$, with $\mathbf{r} = (x, y)^T$ and A symmetric. Identify and diagonalize the matrix A. In particular, explicitly write out equation (1) for the present case.

(b) Find S. Calculate the Jacobian determinant explicitly.

(c) What is the value of the Gaussian integral? [Check your result: $I(1) = \frac{\pi}{2\sqrt{3}}$.]

PC4.5.6 General Gaussian integrals

Compute the following three-dimensional Gaussian integral ($a > 0$):

$$I(a) = \int_{\mathbb{R}^3} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{e}^{-\left[(a+2)x^2+(a+2)y^2+(a+2)z^2+2(a-1)xy+2(a-1)yz+2(a-1)xz\right]}$$

(a) Bring the exponent into the form $-\mathbf{r}^T A\mathbf{r}$, with $\mathbf{r} = (x, y, z)^T$ and A symmetric.

(b) Diagonalize the matrix A. You do not need to compute the corresponding similarity transformation explicitly.

(c) Compute $I(a)$ by expressing it as a product of three one-dimensional Gaussian integrals. [Check your result: $I(3) = \frac{1}{9}\sqrt{\pi^3}$.]

P.C5 Taylor series

P.C5.1 Approximating functions by polynomials

P.C5.2 Taylor expansion

EC5.2.1 Addition theorems for sine and cosine

Prove the addition theorems for sine and cosine:

(a) $\cos(a+b) = \cos a \cos b - \sin a \sin b$,

(b) $\sin(a+b) = \cos a \sin b + \sin a \cos b$.

Hint: Use the Euler-de Moivre identity on both sides of $\mathrm{e}^{\mathrm{i}(a+b)} = \mathrm{e}^{\mathrm{i}a}\mathrm{e}^{\mathrm{i}b}$.

PC5.2.2 Powers of Sine and Cosine

Use the Euler-de Moivre identity to prove the following identities:

(a) $\cos^2 a = \frac{1}{2} + \frac{1}{2}\cos(2a)\,,$ $\qquad \sin^2 a = \frac{1}{2} - \frac{1}{2}\cos(2a)\,.$

(b) $\cos^3 a = \frac{3}{4}\cos a + \frac{1}{4}\cos(3a)\,,$ $\qquad \sin^3 a = \frac{3}{4}\sin a - \frac{1}{4}\sin(3a)\,.$

P.C5.3 Finite-order expansion

EC5.3.1 Taylor series

Taylor expand the following functions. You may choose to either calculate the coefficients of the Taylor series by taking the corresponding derivatives, or to use the known Taylor expansions of $\sin(x)$, $\cos(x)$, $\frac{1}{1-x}$ and $\ln(1+x)$.

(a) $f(x) = \frac{1}{1-\sin(x)}$ around $x = 0$, up to and including fourth order.

(b) $g(x) = \sin(\ln(x))$ around $x = 1$, up to and including second order.

(c) $h(x) = \mathrm{e}^{\cos x}$ around $x = 0$, up to and including second order.

[Check your results: the highest-order term requested in each case is: (a) $\frac{2}{3}x^4$, (b) $-\frac{1}{2}(x-1)^2$, (c) $-\mathrm{e}\frac{1}{2}x^2$.]

PC5.3.2 Taylor series

Taylor expand the following functions. You may choose to either calculate the coefficients of the Taylor series by taking the corresponding derivatives, or to use the known Taylor expansions of $\sin(x)$, $\cos(x)$, $\frac{1}{1-x}$ and $\ln(1+x)$.

(a) $f(x) = \frac{\cos(x)}{1-x}$ around $x = 0$. Keep all terms up to and including third order.

(b) $g(x) = \mathrm{e}^{\cos(x^2+x)}$ about $x = 0$, up to and including third order.

(c) $h(x) = \mathrm{e}^{-x}\ln(x)$ around $x = 1$, up to and including third order.

[Check your results: the highest-order term requested in each case is: (a) $\frac{1}{2}x^3$, (b) $-\mathrm{e}\,x^3$, (c) $\frac{4}{3}\mathrm{e}^{-1}(x-1)^3$.]

P.C5.4 Solving equations by Taylor expansion

EC5.4.1 Series expansion for iteratively solving an equation

(a) Solve the quadratic equation $y^2 - 1 = 2\varepsilon y$ up to and including $\mathcal{O}(\varepsilon^2)$ for small ε, i.e. express y in the form $y = y_0 + y_1\varepsilon + \frac{1}{2!}y_2\varepsilon^2 + \mathcal{O}(\varepsilon^3)$. *Hint:* Note that the equation can have more than one solution. [Check your results: $y_2 = \pm 1$.]

(b) Next, find the exact solutions of this equation, and calculate the first three terms of their Taylor series. Check that these expansions match those obtained from the iterative solution.

PC5.4.2 Series expansion for iteratively solving an equation

A real and analytic function $f(x)$ satisfies the following equation, for $|x| \ll 1$:

$$\ln\left[(x+1)^2\right] + \mathrm{e}^{y(x)} = 1 - y(x)\ .$$

Determine $y(x)$ iteratively up to order $\mathcal{O}(x^2)$, using a series expansion of the form $y(x) = y_0 + y_1 x + \frac{1}{2!}y_2 x^2 + \mathcal{O}(x^3)$. *Hint:* Start by showing that the solution has the property $y(0) = 0$. [Check your results: $y_2 = \frac{1}{2}$.]

EC5.4.3 Taylor series for inverse function

Learning objective: Calculate the series expansion of an inverse function by iteratively solving an equation.
The inverse $g(x)$ of the function $f(x)$ fulfills the defining equation $f(g(x)) = x$. The series expansion of the inverse function around the point x_0, of the form $g(x_0 + x) \equiv y(x) \equiv \sum_{n=0}^{\infty} \frac{1}{n!} y^{(n)}(0) x^n$, can be determined by iteratively solving the equation $f(y(x)) = x_0 + x$ for $y(x)$. In this manner, calculate the series expansion of the following functions around $x = 0$, up to and including second order in x:

(a) $\ln(1 + x)$, (b) 2^x.

[Check your results: the highest-order term requested in each case is: (a) $-\frac{1}{2}x^2$, (b) $\frac{1}{2}\ln^2(2)x^2$.]

PC5.4.4 Taylor series for inverse function

Calculate the series expansion of $\arcsin(x)$ around $x = 0$, up to and including order three, using the following two alternative methods:

(a) Find $\arcsin(x) \equiv y(x)$ by iteratively solving the equation $\sin[y(x)] = x$.

(b) Starting from the identity $\arcsin(\sin(y)) = y$, use the known series expansion for $\sin(y)$ as well as the ansatz $\arcsin(x) = c_1 x^1 + c_3 x^3 + \mathcal{O}(x^5)$, and determine c_1 and c_3 by a comparison of coefficients. [Why are there only odd powers of x?]

Learning objective: realizing that some approaches may be easier than others!
[Check your results: $c_3 = \frac{1}{6}$.]

P.C5.5 Higher-dimensional Taylor expansion

EC5.5.1 Taylor expansions in two dimensions

Find the Taylor expansion of the function $g(x, y) = \mathrm{e}^x \cos(x + 2y)$ in x and y, around the point $(x, y) = (0, 0)$. Calculate explicitly all terms up to and including second order,

(a) by multiplying out the series expansions for the exponential and cosine functions;

(b) by using the formula for the Taylor series of a function of two variables.

[Check your results: the mixed second-order term in each case is: (a) $-2xy$, (b) $-2xy$.]

PC5.5.2 Taylor expansion in two dimensions

For the following functions, calculate the Taylor expansion in x and y around the point $(x, y) = (0, 0)$, up to and including second order:

(a) $f(x, y) = e^{-(x+y)^2}$, (b) $g(x, y) = \dfrac{1 + x}{\sqrt{1 + xy}}$.

[Check your results: the mixed second-order term in each case is: (a) $-2xy$, (b) $-\frac{1}{2}xy$.]

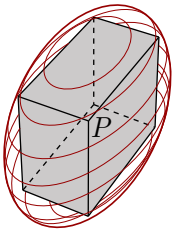
EC5.5.3 Lagrange multipliers

Find the extremum of the function $j(\mathbf{r}) = x^2+y^2+z^2$ subject to the constraints $x+y+z=1$ and $x-y+2z=2$.

PC5.5.4 Lagrange multipliers

(a) A manufacturer would like to pack his product in a rectangular box using as little material as possible, by minimizing the box' surface area A for a given volume V. Find the side lenghts x, y and z and the minimal surface area $A_{\min}$ of the box in terms of V, by solving an appropriate extremization problem. [Check your result: if $V = \frac{1}{8}\text{m}^3$ then $A = \frac{3}{2}\text{m}^2$.]

(b) Consider the ellipsoid defined by $\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$. Also consider a rectangular box whose corners lie on the surface of the ellipsoid and whose edges are parallel to the elipsoid's symmetry axes. Let $P = (x_p,\, y_p,\, z_p)^T$ denote that corner of the box that lies in the positive quadrant ($x_p > 0,\, y_p > 0,\, z_p > 0$). How should this corner by chosen to maximize the volume of the box? What is the value of the maximal volume?



Hint: Maximize the volume $V(x,y,z) = 8\,xyz$ of a box having a corner at $(x,y,z)^T$, under the constraint that this point lies on the ellipsoid.
[Check your result: if $a = \frac{1}{2}$, $b = 3$, $c = \sqrt{3}$, then $V_{\max} = 4$.]

P.C6 Fourier calculus

P.C6.1 δ-Function

EC6.1.1 Integrals with δ function

Calculate the following integrals (with $a \in \mathbb{R}$):

(a) $I_1(a) = \displaystyle\int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x-\pi)\sin(ax)$

(b) $I_2(a) = \displaystyle\int_{\mathbb{R}^3} \mathrm{d}^3x\, \delta(\mathbf{x}-\mathbf{y})\,\mathbf{x}^2\,, \quad \text{with} \quad \mathbf{y} = (a,1,2)^T$

(c) $I_3(a) = \displaystyle\int_0^a \mathrm{d}x\, \delta(x-\pi)\frac{1}{a+\cos^2(x/2)}$

(d) $I_4(a) = \displaystyle\int_0^3 \mathrm{d}x\, \delta(x^2-6x+8)\sqrt{\mathrm{e}^{ax}}$

[Check your results: $I_1(\frac{1}{2}) = 1$, $I_2(1) = 6$, $I_3(\pi) = \frac{1}{2\pi}$, $I_4(\ln 2) = 1$.]

PC6.1.2 Integrals with δ function

Calculate the following integrals (with $a \in \mathbb{R}$, $n \in \mathbb{N}$):

(a) $I_1(a) = \int_1^4 \mathrm{d}x\, \delta(x-2)\,(a^x+3)$

(b) $I_2(a) = \int_{\mathbb{R}^2} \mathrm{d}^2x\, \delta(\mathbf{x}-\mathbf{y})\,(x_1+x_2)^2\, \mathrm{e}^{3-x_1}\,, \quad \text{with} \quad \mathbf{y} = (3,a)^T$

(c) $I_3(a) = \int_{-1}^1 \mathrm{d}x\, \sqrt{2+2x}\; \delta(ax-2)\,, \quad \text{with} \quad a \neq 0$

(d) $I_4(a) = \int_{-\infty}^{\infty} \mathrm{d}x\, \delta(3^{-x}-9)(1-x^a)$

(e) $I_5(n) = \int_{-\pi/2}^{9\pi/2} \mathrm{d}x\; \cos(nx)\; \delta\,(\sin x)$

[Check your results: $I_1(3) = 12$, $I_2(-5) = 4$, $I_3(2) = \frac{1}{2}$, $I_4(3) = \frac{1}{\ln 3}$, $I_5(7) = 1$.]

EC6.1.3 Lorentz representation of the Dirac delta function

Show that in the limit $\epsilon \to 0^+$, the Lorentz peak function $\delta^{[\epsilon]}(x)$ given below is a representation of the Dirac delta function $\delta(x)$. To this end, calculate (i) the height, (ii) the width x_b (defined by $\delta^{[\epsilon]}(x_\mathrm{b}) = \frac{1}{2}\delta^{[\epsilon]}(0)$, $x_\mathrm{b} > 0$) and (iii) the area of the peak. Furthermore, calculate the functions $\theta^{[\epsilon]}(x) = \int_{-\infty}^{x} \mathrm{d}x' \delta^{[\epsilon]}(x')$ and $\delta'^{[\epsilon]}(x) = \frac{\mathrm{d}}{\mathrm{d}x}\delta^{[\epsilon]}(x)$. Sketch all three functions $\theta^{[\epsilon]}$, $\delta^{[\epsilon]}$, $\delta'^{[\epsilon]}$ in separate scetches (one beneath the other, with aligned y-axes and the same scaling for the x-axes).

Lorentz-Peak: $\delta^{[\epsilon]}(x) = \dfrac{\epsilon/\pi}{x^2+\epsilon^2}\,.$

Hint: When calculating the peak weight, use the substitution $x = \epsilon \tan y$.
Remark: Lorentzian functions are common in physics. Example: the energy of a discrete quantum state, which is weakly coupled to the environment, has the form of a Lorentzian function, the width of which is determined by the strength of the coupling to the environment. As the coupling strength approaches zero, we obtain a δ peak.

PC6.1.4 Representations of the Dirac delta function

Show that in the limit $\epsilon \to 0^+$, each of the three peak-shaped functions $\delta^{[\epsilon]}(x)$ given below is a representation of the Dirac delta function $\delta(x)$. To this end, calculate (i) the height, (ii) the width x_b (defined by $\delta^{[\epsilon]}(x_\mathrm{b}) = \frac{1}{2}\delta^{[\epsilon]}(0)$, $x_\mathrm{b} > 0$) and (iii) the area of each peak. Furthermore, calculate the functions $\theta^{[\epsilon]}(x) = \int_{-\infty}^{x} \mathrm{d}x' \delta^{[\epsilon]}(x')$ and $\delta'^{[\epsilon]}(x) = \frac{\mathrm{d}}{\mathrm{d}x}\delta^{[\epsilon]}(x)$. For

each peak shape, sketch all three functions $\theta^{[\epsilon]}$, $\delta^{[\epsilon]}$, $\delta'^{[\epsilon]}$ in separate scetches (one beneath the other, with aligned y-axes and the same scaling for the x-axes).

(a) Gaussian peak: $\delta^{[\epsilon]}(x) = \dfrac{1}{\epsilon\sqrt{\pi}} \mathrm{e}^{-(x/\epsilon)^2}$.

Hint: The function $\theta^{[\epsilon]}(x)$ cannot be calculated in terms of elementary functions; instead write it in terms of the 'error function', $\mathrm{Erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \mathrm{d}y\, \mathrm{e}^{-y^2}$, with $\mathrm{Erf}(\infty) = 1$.
Remark: Gaussians appear very often in physics. Example: A quantum mechanical harmonic oscillator with spring constant k and potential energy $\frac{1}{2}kx^2$ has a Gaussian wavefunction for its ground state, with width $\sim 1/\sqrt{k}$.

(b) Derivative of the Fermi function: $\delta^{[\epsilon]}(x) = \dfrac{1}{4\epsilon} \dfrac{1}{\cosh^2[x/(2\epsilon)]}$.

Hint: When calculating the peak weight, use the substitution $y = \tanh[x/(2\epsilon)]$.
Remark: In condensed matter physics and nuclear physics the function $\delta^{[\epsilon]}(x)$ plays an important role: it arises as the derivative of the so-called 'Fermi function', $f(E) = \frac{1}{\mathrm{e}^{E/k_\mathrm{B}T}+1} = \theta^{[k_\mathrm{B}T]}(-E)$, with $-\frac{\mathrm{d}}{\mathrm{d}E} f(E) = \delta^{[k_\mathrm{B}T]}(E)$, where $f(E)$ is the occupation probability of a fermionic single-particle state with energy E as function of the system's temperature T (k_B is the so-called Boltzmann constant). In the limit of zero temperature, $T \to 0$, the derivative of the Fermi function reduces to a Dirac δ function.

(c) Second derivative of the absolute value function: $\delta^{[\epsilon]}(x) = \dfrac{1}{2} \dfrac{\varepsilon^2}{(x^2+\varepsilon^2)^{3/2}}$.

Hint: When calculating the peak weight, use the substitution $x = \epsilon \tan y$.
Remark: This peak form can be written as $\delta^{[\epsilon]}(x) = \frac{\mathrm{d}^2}{\mathrm{d}x^2} \frac{1}{2} |x|_\epsilon$, where $|x|_\epsilon = (\epsilon^2 + x^2)^{1/2}$ represents a 'smeared' version of the absolute value function, with $\lim_{\epsilon\to 0} |x|_\epsilon = |x|$. [Using $\epsilon \neq 0$ 'smears out' the sharp 'kink' in $|x|$ at $x = 0$.] The first and second derivatives of $\frac{1}{2}|x|_\epsilon$ yield 'smeared' versions of the step function $\theta(x)$ and the Dirac delta function $\delta(x)$, respectively. To illustrate this, include a scetch of the function $|x|_\epsilon$ above your scetch of $\theta^{[\epsilon]}$.

ᴇC6.1.5 Series representation of the coth function

Show that the series $\sum_{n\in\mathbb{Z}} \mathrm{e}^{-y|n|}$, with $0 < y \in \mathbb{R}$, converges to the coth function.

ᴘC6.1.6 Series representation of the periodic δ function

Show that the function $\delta^{[\epsilon]}(x)$, defined by

$$\delta^{[\epsilon]}(x) = \frac{1}{L} \sum_k \mathrm{e}^{\mathrm{i}kx - \epsilon|k|}\,, \quad k = 2\pi n/L, \quad n \in \mathbb{Z}\,, \quad x, \epsilon, L \in \mathbb{R}\,, \quad 0 < \epsilon \ll L\,, \tag{1}$$

has the following properties:

(a) $\delta^{[\epsilon]}(x) = \delta^{[\epsilon]}(x+L)$. (2)

(b) $\displaystyle\int_{-L/2}^{L/2} \mathrm{d}x\, \delta^{[\epsilon]}(x) = 1$. *Hint:* Treat $k=0$ and $k\neq 0$ separately in $\displaystyle\sum_k$. (3)

(c) $\displaystyle\delta^{[\epsilon]}(x) = \frac{1}{2L}\left[\frac{1+w}{1-w} + \frac{1+\overline{w}}{1-\overline{w}}\right] = \frac{1}{L}\frac{1-\mathrm{e}^{-4\pi\epsilon/L}}{1+\mathrm{e}^{-4\pi\epsilon/L}-2\mathrm{e}^{-2\pi\epsilon/L}\cos(2\pi x/L)}$, (4)

where $w = \mathrm{e}^{2\pi(\mathrm{i}x-\epsilon)/L}$ and $\overline{w} = \mathrm{e}^{2\pi(-\mathrm{i}x-\epsilon)/L}$.
Hint: Write out the sum in Eq. (1) as a geometric series in powers of w and $\overline{w}$.

(d) $\displaystyle\lim_{\epsilon\to 0}\delta^{[\epsilon]}(x) = 0$ for $x \neq mL$, with $m\in\mathbb{Z}$. *Hint:* Start from Eq. (4). (5)

(e) $\displaystyle\delta^{[\epsilon]}(x) \simeq \frac{\epsilon/\pi}{\epsilon^2+x^2}$ for $|x|/L \ll 1$ and $\epsilon/L \ll 1$. (6)

Hint: Taylor expand the numerator in Eq. (4) up to first order in $\tilde{\epsilon} = 2\pi\epsilon/L$, and the denominator up to second order in $\tilde{\epsilon}$ and $\tilde{x} = 2\pi x/L$.

(f) Sketch the function $\delta^{[\epsilon]}(x)$ qualitatively for $\epsilon/L \ll 1$ and $x\in[-\frac{7}{2}L, \frac{7}{2}L]$.
(g) Deduce that in the limit of $\epsilon\to 0$, $\delta^{[\epsilon]}(x)$ represents a periodic δ function, with

$$\delta^{[0]}(x) = \frac{1}{L}\sum_k \mathrm{e}^{\mathrm{i}kx} = \sum_{m\in\mathbb{Z}} \delta(x-mL)\ . \tag{7}$$

P.C6.2 Fourier series

EC6.2.1 Fourier series of the sawtooth function

Let $f(x)$ be a sawtooth function, defined by $f(x) = x$ for $-\pi < x < \pi$, $f(\pm\pi) = 0$ and $f(x+2\pi) = f(x)$. Calculate the Fourier coefficients $\tilde{f}_n$ in the representation $f(x) = \frac{1}{L}\sum_n \mathrm{e}^{\mathrm{i}k_n x}\tilde{f}_n$. How should k_n and L be chosen? Sketch the function $f(x)$, as well as the sum of the $n=1$ and $n=-1$ terms of the Fourier series (i.e. the first term of the corresponding sine series). [Check your result: $\tilde{f}_6 = \frac{1}{3}\mathrm{i}\pi$.]

PC6.2.2 Fourier series

Determine the Fourier series for the following periodic functions, i.e. calculate the Fourier coefficients $\tilde{f}_n$ in the representation $f(x) = \frac{1}{L}\sum_n \mathrm{e}^{\mathrm{i}k_n x}\tilde{f}_n$. How should k_n and L be chosen in each case? Sketch the functions first.

(a) $f(x) = |\sin x|$, (b) $f(x) = \begin{cases} 4x & \text{for } -\pi \le x < 0\,, \\ 2x & \text{for } 0 \le x < \pi\,, \end{cases}$ and $f(x+2\pi) = f(x)$.

[Check your results: (a) $\tilde{f}_3 = -\frac{2}{35}$, (b) $\tilde{f}_3 = \frac{2}{9}(2-9\mathrm{i}\pi)$.]

EC6.2.3 Cosine Series

For the function $f : I \to \mathbb{C}$, $x \mapsto f(x)$, with $I = [-L/2, L/2]$, consider the Fourier series representation $f(x) = \frac{1}{L}\sum_k \mathrm{e}^{\mathrm{i}kx}\tilde{f}_k$, with $k = \frac{2\pi n}{L}$ and $n \in \mathbb{Z}$.

(a) Show that the Fourier coefficients are given by $\tilde{f}_k = \int_{-L/2}^{L/2} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x)$.

(b) Now let f be an even function, i.e. $f(x) = f(-x)$. Show that then the Fourier coefficients are given by $\tilde{f}_k = 2\int_0^{L/2} \mathrm{d}x\, \cos(kx) f(x)$, and furthermore, that $f(x)$ can be represented by a cosine series of the form $f(x) = \frac{1}{2}a_0 + \sum_{k>0} a_k \cos(kx)$, with $k = \frac{2\pi n}{L}$ and $n \in \mathbb{N}_0$. Find a_k, expressed via $\tilde{f}_k$.

(c) Now consider the following function: $f(x) = 1$ for $|x| < L/4$, $f(x) = -1$ for $L/4 < |x| < L/2$. Scetch it, and compute the coefficients $\tilde{f}_k$ and a_k of the corresponding Fourier and cosine series. [Check your result: for $k = \frac{2\pi}{L}$, $a_k = \frac{4}{\pi}$ and $\tilde{f}_k = \frac{2L}{\pi}$.]

PC6.2.4 Sine Series

For the function $f : I \to \mathbb{C}$, $x \mapsto f(x)$, with $I = [-L/2, L/2]$, consider the Fourier series representation $f(x) = \frac{1}{L}\sum_k \mathrm{e}^{\mathrm{i}kx}\tilde{f}_k$, with $k = \frac{2\pi n}{L}$ and $n \in \mathbb{Z}$, with Fourier coefficients $\tilde{f}_k = \int_{-L/2}^{L/2} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x)$.

(a) Let f be an odd function, i.e. $f(x) = -f(-x)$. Show that then the Fourier coefficients are given by $\tilde{f}_k = -\mathrm{i}2\int_0^{L/2} \mathrm{d}x\, \sin(kx) f(x)$, and furthermore, that $f(x)$ can be represented by a sine series of the form $f(x) = \sum_{k>0} b_k \sin(kx)$ with $k = \frac{2\pi n}{L}$ und $n \in \mathbb{N}_0$. What does b_k look like when expressed via $\tilde{f}_k$?

(b) Now consider the following function: $f(x) = 1$ for $0 < x < L/2$, $f(x) = -1$ for $-L/2 < x < 0$. Sketch it, and compute the coefficients $\tilde{f}_k$ and b_k of the corresponding Fourier and sine series. [Check your result: for $k = \frac{2\pi}{L}$, $b_k = \frac{4}{\pi}$ and $\tilde{f}_k = \frac{2L}{\mathrm{i}\pi}$.]

EC6.2.5 Parseval's identity and convolution

Let $f(x)$ be a sawtooth function, defined by $f(x) = x$ for $-\pi < x < \pi$, $f(\pm\pi) = 0$ and $f(x+2\pi) = f(x)$. In the Fourier representation $f(x) = \frac{1}{2\pi}\sum_{n\in\mathbb{Z}} \mathrm{e}^{\mathrm{i}nx}\tilde{f}_n$ its Fourier coefficients are $\tilde{f}_n = 2\pi\mathrm{i}(-1)^n/n$ []. Let $g(x) = \sin x$.

(a) Using this concrete example, check that Parseval's identity holds, by computing both the integral $\int_{-\pi}^{\pi} \mathrm{d}x \overline{f}(x) g(x)$ and the sum $(1/2\pi)\sum_n \overline{\tilde{f}}_n \tilde{g}_n$ explicitly.

(b) Prove the famous identity $\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$, by computing the integral $\int_{-\pi}^{\pi} \mathrm{d}x f^2(x)$ in two ways: first, by direct integration, and second, by expressing it as a sum over Fourier modes using Parseval's identity.

(c) Calculate the convolution $(f * g)(x)$ both by directly computing the convolution integral and by using the convolution theorem and a summation of Fourier coefficients.

PC6.2.6 Performing an infinite series using the convolution theorem

Learning objective: This problem illustrates how a complicated sum may be calculated explicitly using the convolution theorem.
Consider the function $f_\gamma(t) = f_\gamma(0)\mathrm{e}^{\gamma t}$ for $t \in [0,\tau)$ and $f(t+\tau) = f(t)$ with $f_\gamma(0) = 1/(\mathrm{e}^{\gamma\tau}-1)$.

(a) Consider a Fourier series representation of $f_\gamma(t)$ of the following form:

$$f_\gamma(t) = \frac{1}{\tau}\sum_{\omega_n} \mathrm{e}^{-\mathrm{i}\omega_n t}\tilde{f}_{\gamma,n}, \qquad \tilde{f}_{\gamma,n} = \int_0^\tau dt \mathrm{e}^{\mathrm{i}\omega_n t} f_\gamma(t), \quad \text{with} \quad \omega_n = 2\pi n/\tau, \quad n \in \mathbb{Z}.$$

Show that the Fourier coefficients are given by $\tilde{f}_{\gamma,n} = 1/(\mathrm{i}\omega_n + \gamma)$.

(b) Use this result and the convolution theorem to express the following series as a convolution of f_γ and $f_{-\gamma}$:

$$S(t) = \sum_{n=-\infty}^{\infty} \frac{\mathrm{e}^{-\mathrm{i}\omega_n t}}{\omega_n^2+\gamma^2} = -\tau \int_0^\tau dt' f_\gamma\left(t-t'\right) f_{-\gamma}\left(t'\right) . \tag{1}$$

(c) Sketch the functions $f_\gamma(t-t')$ and $f_{-\gamma}(t')$ occurring in the convolution theorem as functions of t', for $t' \in [-\tau, 2\tau]$. Assume $0 \le t \le \tau$ and show that the convolution integral (1) is given by the following expression:

$$S(t) = \frac{\tau\left[\sinh\left(\gamma\left(t-\tau\right)\right) - \sinh\left(\gamma t\right)\right]}{2\gamma\left[1-\cosh\left(\gamma\tau\right)\right]} .$$

Hint: The integral $\int_0^\tau \mathrm{d}t'$ involves an interval of t' values for which $t-t'$ lies outside of $[0,\tau)$. It is therefore advisable to split the integral into two parts, with $\int_0^t \mathrm{d}t'$ and $\int_t^\tau \mathrm{d}t'$.

P.C6.3 Fourier transform

EC6.3.1 Properties of Fourier transformations

Demonstrate the following properties of the Fourier transformation, where a is an arbitrary real constant.

(a) The Fourier transform of $f(x-a)$ is $e^{-ika}\tilde{f}_k$.

(b) The Fourier transform of $f(ax)$ is $\tilde{f}_{k/a}/|a|$, where $a \neq 0$.

PC6.3.2 Properties of Fourier transformations

Prove that the following properties of the Fourier transform hold in 2 dimensions, where $\mathbf{a} \in \mathbb{R}^2$, $\alpha \in \mathbb{R} \setminus \{0\}$ and R is a rotation matrix.

(a) The Fourier transform of $f(\mathbf{x} - \mathbf{a})$ is $\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{a}}\tilde{f}_{\mathbf{k}}$.

(b) The Fourier transform of $f(\alpha\mathbf{x})$ is $\frac{1}{|\alpha|^2}\tilde{f}_{\mathbf{k}/\alpha}$.

(c) The Fourier transform of $f(R\mathbf{x})$ is $\tilde{f}_{R\mathbf{k}}$.

EC6.3.3 Fourier transformation of a Gauss peak

Show that the Fourier transform of a normalized Gaussian distribution with width σ, $g^{[\sigma]}(x) = \frac{1}{\sqrt{2\pi}\sigma}\mathrm{e}^{-x^2/2\sigma^2}$, with $\int_{-\infty}^{\infty} \mathrm{d}x\, g^{[\sigma]}(x) = 1$, is given by $\tilde{g}_k^{[\sigma]} = \mathrm{e}^{-\sigma^2 k^2/2}$. *Hint*: The Fourier integral can be calculated by completing the square in the exponent.

PC6.3.4 Convolution of Gauss peaks

Learning objective: To illustrate the following statement: 'The fine structure of a function (i.e. noise in a test signal) can be smoothed out via convolution with a peaked function of suitable width.'

A normalized Gaussian function with width σ has the form $g^{[\sigma]}(x) = \frac{1}{\sqrt{2\pi}\sigma}\mathrm{e}^{-x^2/2\sigma^2}$. Show that the convolution of two normalized Gaussians with widths σ_1 and σ_2 is again a normalized Gaussian with width $\sigma = \sqrt{\sigma_1^2 + \sigma_2^2}$, i.e. show that $\left(g^{[\sigma_1]} * g^{[\sigma_2]}\right)(x) = g^{[\sigma]}(x)$. Do this via two different methods, (a) and (b):

(a) Calculate the convolution integral by completing the square in the exponent.

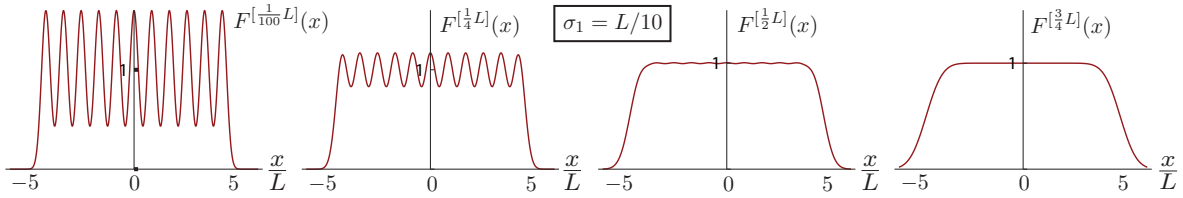
(b) Use the following property of convolution $\widetilde{\left(g^{[\sigma_1]} * g^{[\sigma_2]}\right)}(k) = \tilde{g}^{[\sigma_1]}(k)\tilde{g}^{[\sigma_2]}(k)$, and the known form of the Fourier transform of a Gaussian, $\tilde{g}^{[\sigma_j]}(k)$.

(c) Draw two qualitative sketches, the first of $g^{[\sigma_1]}(x)$, $g^{[\sigma_2]}(x)$ and $g^{[\sigma]}(x)$, the second of their respective Fourier spectra $\tilde{g}^{[\sigma_1]}(k)$, $\tilde{g}^{[\sigma_2]}(k)$ and $\widetilde{\left(g^{[\sigma_1]} * g^{[\sigma_2]}\right)}(k)$. Explain using the sketch why the convolution of a function (here $g^{[\sigma_1]}$) with a peaked function (here $g^{[\sigma_2]}$) leads to a widened version of the first function.

Let $f^{[\sigma_1]}(x) = \sum_{n=-5}^{5} g_n^{[\sigma_1]}(x)$, with $g_n^{[\sigma_1]}(x) = g^{[\sigma_1]}(x - nL)$, be a 'comb' of 11 identical, normalized Gaussians of width σ_1, with peak-to-peak distance L, and let $F^{[\sigma_2]}(x) = \left(f * g^{[\sigma_2]}\right)(x)$ be the convolution of this crest with a normalized Gaussian of width σ_2.

(d) Find a formula for $F^{[\sigma_2]}(x)$, expressed as a sum over the normalized Gaussians. What is the width of this peak?

(e) The sketch shows $F^{[\sigma_2]}(x)$ for $\sigma_1/L = \frac{1}{4}$ and four values of σ_2/L: $\frac{1}{100}$, $\frac{1}{4}$, $\frac{1}{2}$ and $\frac{3}{4}$. Explain the observed behaviour based on your formula from part (c) of the exercise. Why does the fine structure vanish in $F^{[\sigma_2]}(x)$ for $\sigma_2 \gtrsim \frac{1}{2}L$?



(f) Regarding the statement about the smoothing of the noise in the signal: Explain in general how the width of the peaked function should be chosen to smooth out the noise in the signal.

EC6.3.5 Poisson summation formulas

(a) Show that every function $f(x)$, for which a Fourier-integral representation of the form $f(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi}\, \mathrm{e}^{\mathrm{i}kx} \tilde{f}(k)$ exists, fulfills the following remarkable relationship:

'Poisson summation formula': $\displaystyle\sum_{m\in\mathbb{Z}} f(m) = \sum_{n\in\mathbb{Z}} \tilde{f}(2\pi n)\,.$

The sum of the function values $f(m)$ over all the integers is exactly the same as the sum over all the Fourier coefficients $\tilde{f}(2\pi n)$!

Hint: multiply the completeness relation for discrete Fourier modes, namely $\frac{1}{L}\sum_{n\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}2\pi n y/L} = \sum_{m\in\mathbb{Z}} \delta(y - Lm)$, with $f(y/L)$ then integrate over $x = y/L$.

Using the Poisson summation formula and the following functions $f(x)$, prove the following identities (with $0 < a \in \mathbb{R}$):

(b) $f(x) = \mathrm{e}^{-a|x|}$: $\displaystyle\sum_{n\in\mathbb{Z}} \frac{2a}{(2\pi n)^2 + a^2} = \coth(a/2)\,.$

(c) $f(x) = \mathrm{e}^{-(ax^2+bx+c)}$: $\displaystyle\sum_{m\in\mathbb{Z}} \mathrm{e}^{-(am^2+bm+c)} = \sqrt{\frac{\pi}{a}}\mathrm{e}^{\left(\frac{b^2}{4a}-c\right)} \sum_{n\in\mathbb{Z}} \mathrm{e}^{-\frac{1}{a}\left(\pi^2 n^2 + \mathrm{i}\pi n b\right)}\,.$

The identity (c) is the so-called 'Poisson resummation formula' for infinite sums over discrete Gaussian functions. Note that this is an example of Fourier reciprocity: the width of the discrete Gaussian functions on the left and right hand sides of the equation are proportional to $1/a$ and a/π^2 respectively.

P.C6.4 Fourier transform applications

P.C7 Differential equations

P.C7.3 Linear first-order equations

EC7.3.1 Separation of variables

A first order differential equation is called 'autonomous' if it has the form $\dot{x} = f(x)$, i.e. the right hand side is time independent [non-autonomous equations have $\dot{x} = f(x,t)$]. Such an equation can the solved by separation of variables.

a) Solve the autonomous differential equation $\dot{x} = x^2$ for two different initial conditions: (i) $x(0) = 1$ and (ii) $x(2) = -1$. [Check your results: (i) $x(-2) = \frac{1}{3}$, and (ii) $x(2) = -1$.]

b) Sketch the obtained solutions qualitatively. Convince yourself that your scetches for the function $x(t)$ and its derivative $\dot{x}(t)$ satisfy the relation specified by the differential equation.

PC7.3.2 Separation of variables

(a) Solve the differential equation $y' = -x^2/y^3$ for the function $y : \mathbb{R} \to \mathbb{R}$, $x \mapsto y(x)$ by separation of variables, for two different initial conditions: (i) $y(0) = 1$, and (ii) $y(0) = -1$. [Check your result: (i) $y(-1) = \left(\frac{7}{3}\right)^{1/4}$, (ii) $y(-1) = -\left(\frac{7}{3}\right)^{1/4}$.]

(b) Sketch the obtained solution qualitatively. Convince yourself that your scetches for the function $y(x)$ and its derivative $y'(x)$ satisfy the relation specified by the differential equation.

EC7.3.3 Separation of variables: barometric formula

The standard barometric formula for atmospheric pressure $p(x)$ as a function of x is given by: $\frac{\mathrm{d}p(x)}{\mathrm{d}x} = -\alpha \frac{p(x)}{T(x)}$. Solve this equation with initial value $p(x_0) = p_0$ for the case of a linear temperature gradient, $T(x) = T_0 - b(x - x_0)$. *Hint:* Separation of variables!
[Check your result: if $\alpha, b, T_0, x_0, p_0 = 1$, then $p(1) = 1$.]

PC7.3.4 Separation of variables: bacterial culture with toxin

A bacterial culture is exposed to the effects of a toxin. The death rate induced by the toxin is proportional to the number $n(t)$ of bacteria still alive in the culture at a time t and the amount of toxin $T(t)$ remaining in the system, which is given by $\tau n(t) T(t)$, where τ is a positive constant. On the other hand, the natural growth rate of the bacteria in the culture is exponential, i.e. it grows with a rate $\gamma n(t)$, with $\gamma > 0$. In total, the number of bacteria in the culture is given by the differential equation

$$\dot{n} = \gamma n - \tau n T(t), \quad \text{for } t \geq 0.$$

(a) Find the general solution to the given linear differential equation with $n(0) = n_0$.

(b) Assume now that the toxin is injected into the system at a constant rate $T(t) = at$, where $a > 0$. Show, using a qualitative analysis of the differential equation (i.e. without solving it explicitly), that the bacterial population grows up to a time $t = \gamma/(a\tau)$, and decreases thereafter. Furthermore, show that as $t \to \infty$, $n(t) \to 0$, i.e. the bacterial culture is practically wiped out.

(c) Now find the explicit solution $n(t)$ to the differential equation and sketch $n(t)$ qualitatively as a function of t. Convince yourself that the sketch fulfils the relation between $n(t)$, $\dot{n}(t)$ and t that is specified by the differential equation. [Check your result: if $\tau = 1$, $a = 1$, $n_0 = 1$ and $\gamma = \sqrt{\ln 2}$, then $n(\sqrt{\ln 2}) = \sqrt{2}$.]

(d) Find the time t_h at which the number of bacteria in the culture drops to half the initial value. [Check your result: if $\tau = 4$, $a = 2/\ln 2$ and $\gamma = 3$, then $t_h = \ln 2$.]

EC7.3.5 Substitution and separation of variables

(a) Show that the differential equation $y' = f(y/x)$ for the function $y(x)$ can be converted by the substitution $y = ux$ into a differential equation for the function $u(x)$, which is solvable using separation of variables.

(b) Use this method to solve the equation $xy' = 2y + x$ with the initial condition $y(1) = 0$. [Check your result: $y(2) = 2$.]

PC7.3.6 Substitution and separation of variables

Often differential equations can be solved by convenient substitution. Here we examine differential equations of the type

$$y'(x) = f(ax + by(x) + c)\,. \tag{1}$$

(a) Substitute $u(x) = ax + by(x) + c$ and find a differential equation for $u(x)$.

(b) Find an implicit expression for the solution $u(x)$ of the new differential equation using an integral that contains the function f. *Hint:* Separation of variables!

(c) Use the substitution strategy of (a,b) to solve the differential equation $y'(x) = \mathrm{e}^{x+3y(x)+5}$, with initial condition $y(0) = 1$.
[Check your result: $y(\ln(e^{-8} + 3) - 2\ln 2) = \frac{1}{3}(2\ln 2 - \ln(e^{-8} + 3) - 5)$.]

(d) Check: Solve the differential equation given in (c) directly (without substitution) using separation of variables. Is the result in agreement with the result from (c)?

(e) Solve the differential equation $y'(x) = [a(x + y) + c]^2$ with initial condition $y(x_0) = y_0$ using the substitution given in (a).
[Check your result: if $x_0 = y_0 = 0$ and $a = c = 1$, then $y(0) = 0$.]

EC7.3.7 Inhomogeneous linear differential equation: variation of constant

Solve the inhomogeneous differential equation $\dot{x} + 2x = t$ with $x(0) = 0$, as follows:

(a) Determine the general solution of the homogeneous equation.

(b) Then find a special (particular) solution to the inhomogeneous problem by means of variation of constants. [Check your result: $x(-\ln 2) = \frac{3}{4} - \frac{1}{2}\ln 2$.]

PC7.3.8 Inhomogeneous linear differential equation, variation of constants

The function $x(t)$ satisfies the inhomogeneous differential equation

$$\dot{x}(t) + tx(t) = \mathrm{e}^{-\frac{t^2}{2}}, \qquad \text{with initial condition} \quad x(0) = x_0. \tag{1}$$

(a) Find the solution $x_h(t)$ of the corresponding homogeneous equation with $x_h(0) = x_0$.

(b) Find the particular solution $x_p(t)$ of the inhomogeneous equation (1), with $x_p(0) = 0$ using variation of constants, $x_p(t) = c(t)x_h(t)$. What is the general solution?
[Check your result: if $x_0 = 0$, then $x(1) = e^{-1/2}$.]

(c) For a differential equation of the form $\dot{x}(t) + a(t)x(t) = b(t)$ (ordinary, first order, linear and inhomogeneous), the sum of the homogeneous and inhomogeneous solutions has the form:

$$x(t) = x_h(t) + x_p(t) = x_h(t) + c(t)x_h(t) = (1 + c(t))x_h(t) = \tilde{c}(t)x_h(t)\,.$$

The initial condition $x(0) = x_0$ can therefore also be satisfied by imposing on $x_h(t)$ and $\tilde{c}(t)$ the initial conditions $x_h(0) = 1$ and $\tilde{c}(0) = x_0$. Use this approach to construct a solution to the differential equation (1) of the form $x(t) = \tilde{c}(t)x_h(t)$. Does the result agree with the result as obtained in (b)? (*Learning objective of (c):* Realize that the same initial condition can be implemented in more than one way.)

P.C7.4 Systems of first order linear differential equations

EC7.4.1 System of linear differential equations with non-diagonizable matrix

We consider a procedure to solve the differential equation

$$\dot{\mathbf{x}} = A \cdot \mathbf{x} \tag{1}$$

for the case of a matrix $A \in \mathrm{Mat}(\mathbb{R}, n, n)$ that has $n-1$ distinct eigenvalues λ_j and associated eigenvectors $\mathbf{v}_j$, with $j = 1, \ldots, n-1$, where the eigenvalue λ_{n-1} is a two-fold zero of the

characteristic polynomial. Since λ_{n-1} has only *one* eigenvector, this matrix not diagonalizable. However, it can be brought into the so-called Jordan normal form:

$$S^{-1}AS = J, \qquad J = \begin{pmatrix} \lambda_1 & 0 & \cdots & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ 0 & 0 & \ddots & \cdots & 0 \\ \vdots & \cdots & \cdots & \lambda_{n-1} & 1 \\ 0 & \cdots & \cdots & 0 & \lambda_{n-1} \end{pmatrix}, \qquad S = (\mathbf{v}_1, \cdots, \mathbf{v}_{n-1}, \mathbf{v}_n)\,. \tag{2}$$

Using $A = SJS^{-1}$, as well as $\mathbf{v}_j = S\mathbf{e}_j$ and $J\mathbf{e}_j = \lambda_j \mathbf{e}_j + \delta_{jn}\mathbf{e}_{j-1}$, one finds that this is equivalent to

$$A \cdot \mathbf{v}_j = \lambda_j \mathbf{v}_j + \mathbf{v}_{j-1}\delta_{jn}, \quad \forall j = 1, \ldots, n. \tag{3}$$

For $j = 1, \ldots, n-1$ this corresponds to the usual eigenvalue equation, and $\mathbf{v}_j$ to the usual eigenvectors. $\mathbf{v}_n$, however, is not an eigenvector, but is rather determined by the following equation:

$$(A - \mathbb{1}\lambda_n)\mathbf{v}_n = \mathbf{v}_{n-1}. \tag{4}$$

Since $(A - \mathbb{1}\lambda_n)$ is not invertible, this equation does not uniquely fix the vector $\mathbf{v}_n$. Different choices of $\mathbf{v}_n$ lead [via (2)] to different similarity transformation matrices S, but they all yield the same form for the Jordan-Matrix J.
The λ_j and $\mathbf{v}_j$ thus obtained can be used to find a solution for the DE (1), using an exponential ansatz together with 'variation of the constants':

$$\mathbf{x}(t) = \sum_{j=1}^{n} \mathbf{v}_j e^{\lambda_j t} c^j(t), \qquad \text{with} \quad \lambda_n \equiv \lambda_{n-1}. \tag{5}$$

The coefficients $c^j(t)$ can be determined by inserting this ansatz into (1):

$$0 = \left(\tfrac{\mathrm{d}}{\mathrm{d}t} - A\right)\mathbf{x}(t) = \sum_{j=1}^{n} \mathbf{v}_j e^{\lambda_j t}\left[\lambda_j c^j(t) + \dot{c}^j(t) - \lambda_j c^j(t)\right] - \mathbf{v}_{n-1} e^{\lambda_n t} c^n(t). \tag{6}$$

Comparing coefficients of $\mathbf{v}_j$ we obtain:

$$\mathbf{v}_{j\neq n-1}: \qquad \dot{c}^j(t) = 0 \qquad \Rightarrow \qquad c^j(t) = c^j(0) = \text{const.}\,, \tag{7}$$

$$\mathbf{v}_{n-1}: \qquad \dot{c}^{n-1}(t) = c^n(t) \qquad \Rightarrow \qquad c^{n-1}(t) = c^{n-1}(0) + t\,c^n(0)\,. \tag{8}$$

The values of $c^j(0)$ are fixed by the initial conditions $\mathbf{x}(0)$:

$$\mathbf{x}(0) = \sum_j \mathbf{v}_j c^j(0) = S\mathbf{c}(0)\,, \quad \Rightarrow \quad \mathbf{c}(0) = S^{-1}\mathbf{x}(0)\,. \tag{9}$$

Now use this method to find the solution of the DE

$$\dot{\mathbf{x}} = A\mathbf{x}, \quad \text{with} \quad A = \frac{1}{3}\begin{pmatrix} 7 & 2 & 0 \\ 0 & 4 & -1 \\ 2 & 0 & 4 \end{pmatrix} \quad \text{and} \quad \mathbf{x}(0) = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}. \tag{10}$$

(a) Show that the characteristic polynomial for A has a simple zero, say λ_1, and a two-fold zero, say $\lambda_2 = \lambda_3$.

(b) Show that the eigenspaces associated with λ_1 and λ_2 are both one-dimensional (which implies that A is not diagonalizable), and find the corresponding normalized eigenvectors $\mathbf{v}_1$ and $\mathbf{v}_2$.

(c) Use Eq. (4) to find a third, normalized vector $\mathbf{v}_3$, having the property that A is brought into a Jordan normal form using $S = (\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$. While doing so, exploit the freedom of choice that is available for $\mathbf{v}_3$ to choose the latter orthonormal to $\mathbf{v}_1$ and $\mathbf{v}_2$. [*Remark:* For the present example orthonormality is achievable (and useful, since then $S^{-1} = S^T$ holds), but this is not generally the case.]

(d) Now use an ansatz of the form (5) to find the solution $\mathbf{x}(t)$ to the DE (10). [Check your result: $\mathbf{x}(\ln 2) = (2, 4, 0)^T + \frac{4}{3}(1 + \ln 2)(2, -1, 2)^T$.]

(e) Check your result explicitly by verifying that it satisfies the DE.

PC7.4.2 System of linear differential equations with non-diagonizable matrix: critically damped harmonic oscillator

Find the general solution for the damped, homogeneous, harmonic oscillator,

$$\ddot{x} + 2\gamma\dot{x} + \Omega^2 x = 0\,,$$

for the critically damped case $\gamma = \Omega$, by finding a first order matrix differential equation and solving the corresponding eigenvalue problem.

(a) In this case, both the eigenvalues are degenerate and there is only one corresponding eigenvector. Find the corresponding solution $x_1(t)$.

(b) Find a second solution via variation of constants by inserting the ansatz $x_2(t) = c(t)x_1(t)$ into the DE for x. Find a differential equation for $c(t)$ and solve this equation.

(c) Find the solution $x(t)$ that satisfies the initial conditions $x(0) = 1$, $\dot{x}(1) = 1$.
[Check your result: if $\gamma = 2$, then $x(\ln 2) = \frac{1}{4}\,(1 - \ln 2(2 + e^2))$.]

(d) The critically damped harmonic oscillator can be thought of as the limit $\lambda \to \Omega$ of both the over-damped and under-damped harmonic oscillator. Perform a Taylor expansion of the general solution of both the over-damped and under-damped cases for small values of ϵt, with $\epsilon \equiv \sqrt{|\gamma^2 - \Omega^2|}$, and show that the result in both cases can be written as a linear combination of the solutions to the critically damped harmonic oscillator found in (a) and (b).

P.C7.5 General nth order linear differential equation

EC7.5.1 Inhomogeneous linear differential equation of order 2: driven overdamped harmonic oscillator

Consider the following driven, over-damped harmonic oscillator with $\gamma > \Omega$:

Differential equation: $$\ddot{x} + 2\gamma\dot{x} + \Omega^2 x = f_{\mathrm{A}}(t). \tag{1}$$

Initial value: $$x(0) = 0, \quad \dot{x}(0) = 1\ , \tag{2}$$

Driving function: $$f_{\mathrm{A}}(t) = \begin{cases} f_{\mathrm{A}} & \text{for} \quad t \geq 0, \\ 0 & \text{for} \quad t < 0. \end{cases}$$

For $t > 0$, find a solution to this equation of the form $x(t) = x_{\mathrm{h}}(t) + x_{\mathrm{p}}(t)$, where $x_{\mathrm{h}}(t)$ and $x_{\mathrm{p}}(t)$ are the homogeneous and particular solutions to the homogeneous and inhomogeneous differential equation that have the initial values (2) or $x_{\mathrm{p}}(0) = \dot{x}_{\mathrm{p}}(0) = 0$, respectively. Proceed as follows:

(a) Rewrite as matrix equation: Write the DE (1) in the matrix form

$$\dot{\mathbf{x}} = A \cdot \mathbf{x} + \mathbf{b}(t), \quad \text{with} \quad \mathbf{x} \equiv (x, \dot{x})^T \equiv (x^1, x^2)^T\ . \tag{3}$$

Find the matrix A, the driving force vector $\mathbf{b}(t)$, and the initial value $\mathbf{x}_0 = \mathbf{x}(0)$.

(b) Homogeneous solution: Find the solution $\mathbf{x}_{\mathrm{h}}(t)$ of the homogeneous DEQ (3)$|_{\mathbf{b}(t)=0}$ that has the initial value $\mathbf{x}_{\mathrm{h}}(0) = \mathbf{x}_0$. Use the ansatz $\mathbf{x}_{\mathrm{h}}(t) = \sum_j c_{\mathrm{h}}^j \mathbf{x}_j(t)$, with $\mathbf{x}_j(t) = \mathbf{v}_j e^{\lambda_j t}$, where λ_j and $\mathbf{v}_j$ $(j = 1, 2)$ are the eigenvalues and the eigenvectors of A. What does the corresponding solution $x_{\mathrm{h}}(t) = x^1{}_{\mathrm{h}}(t)$ of the homogeneous differential equation (1)$|_{f_{\mathrm{A}}(t)=0}$ look like? [Check your result: if $\gamma = \sqrt{2}\ln 2$ and $\Omega = \ln 2$, then $x_h(1) = \frac{3}{4}\frac{2^{-\sqrt{2}}}{\ln 2}$.]

(c) Particular solution: Using the ansatz $\mathbf{x}_{\mathrm{p}}(t) = \sum_j c_{\mathrm{p}}^j(t)\mathbf{x}_j(t)$ (variation of constants), find the particular solution for the inhomogeneous differential equation (3) that has the initial value $\mathbf{x}_{\mathrm{p}}(0) = \mathbf{0}$. What is the corresponding solution $x_{\mathrm{p}}(t) = x^1{}_{\mathrm{p}}(t)$ of the inhomogeneous DE (1)? [Check your result: if $\gamma = 3\ln 2$, $\Omega = \sqrt{5}\ln 2$ and $f_A = 1$, then $x_p(1) = \frac{49}{640}\frac{1}{(\ln 2)^2}$.]

(d) Qualitative discussion: The desired solution of the inhomogeneous DE (1) is given by $x(t) = x_{\mathrm{h}}(t) + x_{\mathrm{p}}(t)$. Sketch your result for this function qualitatively for the case $f_{\mathrm{A}} < 0$, and explain the behavior as $t \to 0$ and $t \to \infty$.

PC7.5.2 Inhomogeneous linear differential equation of order 3

Consider the following third order inhomogeneous linear differential equation:

Differential equation: $$\dddot{x} - 6\ddot{x} + 11\dot{x} - 6x = f_{\mathrm{A}}(t), \tag{1}$$

Initial value: $$x(0) = 1, \quad \dot{x}(0) = 0, \quad \ddot{x}(0) = a\ , \qquad \text{with} \quad a \in \mathbb{R}. \tag{2}$$

Driving: $$f_{\rm A}(t) = \begin{cases} \mathrm{e}^{-bt} & \text{for} \quad t \geq 0\,, \\ 0 & \text{for} \quad t < 0\,, \end{cases} \qquad \text{with} \quad 0 < b \in \mathbb{R}. \tag{3}$$

For $t > 0$, find a general solution to this equation of the form $x(t) = x_{\rm h}(t) + x_{\rm p}(t)$, where $x_{\rm h}(t)$ and $x_{\rm p}(t)$ are the homogeneous and particular solutions to the homogeneous and inhomogeneous differential equation that have the initial values (2) or $x_{\rm p}(0) = \dot{x}_{\rm p}(0) = \ddot{x}_{\rm p}(0) = 0$ respectively. Proceed as follows:

(a) Write the differential equation (1) in the matrix form

$$\dot{\mathbf{x}} = A \cdot \mathbf{x} + \mathbf{b}(t), \quad \text{with} \quad \mathbf{x} \equiv (x, \dot{x}, \ddot{x})^T \equiv (x^1, x^2, x^3)^T, \quad \mathbf{x}_0 = (x(0), \dot{x}(0), \ddot{x}(0))^T\,. \tag{4}$$

(b) Find the homogeneous solution $\mathbf{x}_{\rm h}(t)$ of $(4)|_{\mathbf{b}(t)=0}$ with $\mathbf{x}_{\rm h}(0) = \mathbf{x}_0$; then $x_{\rm h}(t) = x^1{}_{\rm h}(t)$.

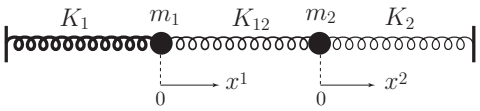
(c) Find the inhomogeneous solution $\mathbf{x}_{\rm p}(t)$ of (4), with $\mathbf{x}_{\rm p}(0) = \mathbf{0}$; then $x_{\rm p}(t) = x^1{}_{\rm p}(t)$.

Hint: The eigenvalues λ_1, λ_2, λ_3 of A are integers, with $\lambda_1 = 1$.

ᴇC7.5.3 Coupled oscillations of two point masses

Consider a system of two point masses, with masses m_1 and m_2, which are connected to two fixed walls and to each other by means of three springs (spring constants K_1, K_{12} and K_2) (see sketch). The equations of motion for both masses are

$$\begin{aligned} m_1\ddot{x}^1 &= -K_1 x^1 - K_{12}(x^1 - x^2), \\ m_2\ddot{x}^2 &= -K_2 x^2 - K_{12}(x^2 - x^1). \end{aligned}$$



(a) Bring the system of equations into the form $\ddot{\mathbf{x}}(t) = -A \cdot \mathbf{x}(t)$, with $\mathbf{x} = (x^1, x^2)^T$. What is the form of matrix A? [Check your result: $\det A = [K_1K_2 + (K_1 + K_2)K_{12}]/(m_1m_2)$.]

(b) Using the ansatz $\mathbf{x}(t) = \mathbf{v}\cos(\omega t)$, this system of differential equations can be converted to an algebraic eigenvalue problem. What does it look like?

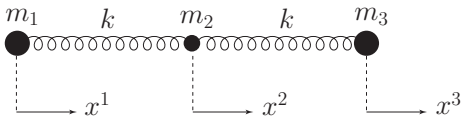
(c) Set $m_1 = m_2$, $K_2 = m_1\Omega^2$, $K_1 = 4K_2$ and $K_{12} = 2K_2$ (note that Ω has the dimension of frequency.). Find the eigenvalues λ_j and the eigenvectors $\mathbf{v}_j$ of the matrix $\frac{1}{\Omega^2}A$, and therefore the corresponding 'eigenfrequencies' ω_j and 'eigenmodes' $\mathbf{x}_j(t)$ of the coupled masses (with $\mathbf{x}_j(0) = \mathbf{v}_j$). [Check your result: $\lambda_1 + \lambda_2 = 9$.]

(d) Make a sketch of both eigenmodes $\mathbf{x}_j(t)$ which shows both the $j = 1$ and 2 cases on the same set of axes. Comment on the physical behaviour that you observe!

PC7.5.4 Coupled oscillations of three point masses

Consider a system consisting of three masses, m_1, m_2 and m_3, coupled through two identical springs, each with spring constant k (see sketch). The equations of motion for the three masses read:

$$\begin{aligned} m_1\ddot{x}^1 &= -k(x^1 - x^2), \\ m_2\ddot{x}^2 &= -k\left([x^2 - x^1] - [x^3 - x^2]\right), \\ m_3\ddot{x}^3 &= -k(x^3 - x^2), \end{aligned}$$



(a) Bring this system of equations into the form $\ddot{\mathbf{x}}(t) = -A \cdot \mathbf{x}(t)$, with $\mathbf{x} = (x^1, x^2, x^3)^T$. What is the matrix A?

(b) By making the ansatz $\mathbf{x}(t) = \mathbf{v}\cos(\omega t)$, this system of equations can be reduced to an algebraic eigenvalue problem. Find this eigenvalue equation. [Check your result: $\det A = 0$.]

(c) From now on, set $m_1 = m_3 = m$, $m_2 = \frac{2}{3}m$, and $k = m\Omega^2$. (Ω has the dimension of a frequency.) Find the eigenvalues λ_j and normalized eigenvectors $\mathbf{v}_j$ of the matrix $\frac{1}{\Omega^2}A$, and thus the corresponding 'Eigenfrequencies' ω_j and 'Eigenmodes' $\mathbf{x}_j(t)$ of the coupled masses (with $\mathbf{x}_j(0) = \mathbf{v}_j$). [Check your result: $\lambda_1 + \lambda_2 + \lambda_3 = 5$.]

(d) Sketch the three Eigenmodes $\mathbf{x}_j(t)$ as functions of time: for each $j = 1$, 2 and 3, make a separate sketch that displays the three components $x_j^1(t)$, $x_j^2(t)$ and $x_j^3(t)$ on the same axis. Comment on the physical behaviour that you observe!

EC7.5.5 Green's function of $(\mathrm{d}_t + a)$

Let $D(\mathrm{d}_t) = (\mathrm{d}_t + a)$ be a first order differential operator, and a be a positive, real constant. The corresponding Green's function is defined by the differential equation:

$$D(\mathrm{d}_t)G(t) = \delta(t)\ . \tag{1}$$

(a) Show that the ansatz

$$G(t) = \theta(t)x_\mathrm{h}(t) \qquad \text{with } \theta(t) = \begin{cases} 1 & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases}, \tag{2}$$

satisfies the defining equation (1), provided that $x_\mathrm{h}(t)$ is a solution to the homogeneous equation $D(\mathrm{d}_t)x_\mathrm{h}(t) = 0$ with initial condition $x_\mathrm{h}(0) = 1$. [Hint: The initial condition guarantees that $\delta(t)x_\mathrm{h}(t) = \delta(t)$.]

(b) Determine $G(t)$ explicitly by solving the homogeneous equation for $x_\mathrm{h}(t)$. [Check your result: $G(\frac{1}{a}\ln 2) = \frac{1}{2}$.]

(c) Calculate the Fourier integral $\tilde{\mathcal{G}}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}G(t)$. [Check your result: for $a = 1$, $|\tilde{\mathcal{G}}(a)| = \frac{1}{\sqrt{2}}$.]

(d) Consistency check: Alternatively, determine $\tilde{\mathcal{G}}(\omega)$ via a Fourier transformation of the defining equation (1). Is the result in agreement with the result from part (c) of the exercise?

(e) Find a solution to the inhomogeneous differential equation $(\mathrm{d}_t + a)x(t) = \mathrm{e}^{2at}$ by convolving the function $G(t)$ with the inhomogeneity. Verify the obtained solution explicitly by inserting it into the differential equation.

PC7.5.6 Green's function of critically damped harmonic oscillator

A driven, critically damped harmonic oscillator with frequency $\Omega > 0$ and damping rate $\gamma = \Omega$ satisfies the equation $D(\mathrm{d}_t)x(t) = f(t)$, with $D(\mathrm{d}_t) = (\mathrm{d}_t^2 + 2\Omega\mathrm{d}_t + \Omega^2)$. The corresponding Green's function is defined by the differential equation

$$D(\mathrm{d}_t)G(t) = \delta(t)\,. \tag{1}$$

(a) Show that the Ansatz

$$G(t) = \theta(t)x_\mathrm{h}(t)\,, \qquad \text{with} \qquad \theta(t) = \begin{cases} 1 & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases}\,, \tag{2}$$

satisfies the defining equation (1) if $x_\mathrm{h}(t)$ is a solution of the homogeneous equation $D(\mathrm{d}_t)x_\mathrm{h}(t) = 0$, with initial values $x_\mathrm{h}(0) = 0$ and $\mathrm{d}_t x_\mathrm{h}(0) = 1$. [Hint: the initial values ensure that $\delta(t)x_\mathrm{h}(t) = 0$ and $\delta(t)\mathrm{d}_t x_\mathrm{h}(t) = \delta(t)$.]

(b) Determine $G(t)$ explicitly by solving the homogeneous equation for $x_\mathrm{h}(t)$. [Check your result: for $\Omega = 1$, $G(1) = 1/\mathrm{e}$.]

(c) Compute the Fourier integral $\tilde{\mathcal{G}}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G(t)$. [Check your result: for $\Omega = 1$, $|\tilde{\mathcal{G}}(\Omega)| = \frac{1}{2}$.]

(d) Consistency check: find $\tilde{\mathcal{G}}(\omega)$ in an alternative way by Fourier transforming the defining equation (1). Does the result agree with that of subproblem (c)?

(e) Find a solution of the inhomogeneous differential equation $D(\mathrm{d}_t)x(t) = q\sin(\omega_0 t)$ by convolving $G(t)$ with the inhomogeneity. Check explicitly that your result satisfies this equation. [Hint: it is advisable to represent the sine function by $\mathrm{Im}\left[\mathrm{e}^{\mathrm{i}\omega_0 t}\right]$ and use $\mathrm{e}^{\mathrm{i}\omega_0 t}$ as inhomogeneity, and to take the imaginary part only at the very end of the calculation.]

P.C7.6 General first-order differential equation

EC7.6.1 Field lines in two dimensions

Consider the vector field $\mathbf{F} = (-ay,\, x)^T$ in the xy-plane, with $a > 0$. Calculate and sketch the corresponding field lines by solving the appropriate differential equation (set $a = 1/2$ for the purposes of the sketch).

PC7.6.2 Field lines of electric quadrupole field in two dimensions

Consider the field $\mathbf{E} = F \begin{pmatrix} x \\ -3z \end{pmatrix}$ in the xz plane, generated by an electric quadrupole. The constant F governs the field strength. Compute and sketch the shape of the field lines by solving the corresponding differential equation. [Check your result: for all points on a field line, $x^3 z = \text{const.}$]

P.C7.7 nth-order differential equation

P.C7.8 Linearizing differential equations

EC7.8.1 Fixed points of a differential equation in one dimension

Consider the autonomous differential equation $\dot{x} = f_\lambda(x) = (x^2 - \lambda)^2 - \lambda^2$ for the real function $x(t)$, with $\lambda \in \mathbb{R}$.

(a) Find the fixed points of this differential equation as a function of λ for (i) $\lambda \leq 0$, and (ii) $\lambda > 0$. [Check your results: for $\lambda = 2$, the fixed points lie at 0, 2, and -2.]

(b) Make two separate sketches of $f(x)$ as a function of x for the following fixed values of λ: (i) $\lambda = -1$ and (ii) $\lambda = +1$, and mark on your sketches the fixed points found in (a).

(c) Determine the stability of each of these fixed points via a graphical analysis of the function, and show the flow of $x(t)$ in the neighbourhood of these fixed points on the sketch from (b).

PC7.8.2 Fixed points of a differential equation in one dimension

Consider the differential equation $\dot{x} = f(x) = \tanh[5(x-3)] \tanh[5(x+1)] \sin(\pi x)$ for the real-valued function $x(t)$.

(a) Find the fixed points of this differential equation. [Hint: there are infinitely many!]

(b) Sketch $f(x)$ as a function of x with $x \in [-4, 5]$, and mark on it the fixed points that you found in (a).

(c) From an analysis of your sketch, determine the stability of each of these fixed points, and show the flow of $x(t)$ near the fixed points in the sketch from (b).

EC7.8.3 Stability analysis in two dimensions

The function $\mathbf{x} : \mathbb{R} \to \mathbb{R}^2$, $t \mapsto \mathbf{x}(t)$ satisfies the following differential equation, with $0 < c \in \mathbb{R}$:

$$\dot{\mathbf{x}} = \begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \mathbf{f}(\mathbf{x}) = \begin{pmatrix} 2x^2 - xy \\ c(1-x) \end{pmatrix}.$$

(a) Find the fixed point $\mathbf{x}^*$ of the differential equation.

(b) For a small displacement $\boldsymbol{\eta} = \mathbf{x} - \mathbf{x}^*$ from the fixed point, linearize the differential equation and bring it into the form $\dot{\boldsymbol{\eta}} = A\boldsymbol{\eta}$. What is the matrix A?

(c) Check that the matrix elements of A are given by $a^i{}_j = \left(\frac{\partial f^i}{\partial x^j}\right)|_{\mathbf{x}=\mathbf{x}^*}$.

(d) Find the eigenvalues and eigenvectors of A.

(e) Analyze the stability of the fixed point: For displacements relative to the fixed point, in which directions do these displacements grow or shrink the fastest? On which timescales?

[Check your results, for $c = 3$: (a) $\|\mathbf{x}^*\| = \sqrt{5}$. (b) $\det A = -3$. (d) eigenvalues: $\lambda_+ = 3$, $\lambda_- = -1$; eigenvectors: $\mathbf{v}_+ = (1, -1)^T$ and $\mathbf{v}_- = (1, 3)^T$.]

ᵖC7.8.4 Stability analysis in three dimensions

Consider the following autonomous differential equation:

$$\dot{\mathbf{x}} = \begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} x^{10} - y^{24} \\ 1 - x \\ -3z - 3 \end{pmatrix}.$$

(a) Find the fixed points of this equation. [Check your result: for all fixed points, $\|\mathbf{x}^*\| = \sqrt{3}$.]

(b) Show that the fixed points are in general unstable, however are stable to deviations in certain directions. Determine the linear approximation to this equation for small deviations about the fixed point, and calculate the eigenvalues and eigenvectors of the corresponding matrix, A. [Check your results: for all fixed points, $|\det A| = 72$. Some of the eigenvalues for these fixed points are 6, 4, 12, -2.]

(c) Identify the stable directions, and the respective characteristic timescales for each deviation from the fixed point to decay to zero.

P.C7.9 Partial differential equations

P.C8 Functional calculus

P.C8.1 Definitions

P.C8.2 Functional derivative

P.C8.3 Euler-Lagrange equations

P.C9 Calculus of complex functions

P.C9.1 Holomorphic functions

EC9.1.1 Cauchy-Riemann equations

Write the following functions of $z = x+\mathrm{i}y$ and $\bar{z} = x-\mathrm{i}$ in the form $f(x,y) = u(x,y)+\mathrm{i}v(x,y)$ and explicitly check if the Cauchy-Riemann equations are satisfied. Which of these functions are analytic in z?

(a) $f(z) = \mathrm{e}^z$, (b) $f(z) = \bar{z}^2$.

PC9.1.2 Cauchy-Riemann equations

Investigate, using the Cauchy-Riemann equations, which of the following functions are analytic in $z = x + \mathrm{i}y$, and if so, in which domain in $\mathbb{C}$. Check your conclusions by attempting to express each function in terms of z and $\bar{z}$.

(a) $f(x,y) = (x^3 - 3xy^2) + \mathrm{i}(3x^2y - y^3)$.

(b) $f(x,y) = xy + \mathrm{i}\frac{1}{2}y^2$.

(c) $f(x,y) = \dfrac{x - \mathrm{i}y}{x^2 + y^2}$.

(d) $\left.\begin{matrix} f_+(x,y) \\ f_-(x,y) \end{matrix}\right\} = \mathrm{e}^x\big[x\cos y \pm y\sin y\big] + \mathrm{i}\mathrm{e}^x\big[x\sin y \mp y\cos y\big]$.

P.C9.2 Complex integration

EC9.2.1 Cauchy's theorem

The function $f(z) = \mathrm{e}^z$ for $z \in \mathbb{C}$ is analytic. Cauchy's theorem then states that (a) closed path integrals over simply connected domains are zero, and (b) path integrals between two points are independent of the chosen path. Check these claims explicitly by calculating the following complex path integrals:

(a) $I_{\gamma_R} = \oint_{\gamma_R} \mathrm{d}z\, f(z)$, along the circle γ_R with radius R about the origin $z = 0$.

(b) $I_{\gamma_i} = \int_{\gamma_i} \mathrm{d}z\, f(z)$, between the points $z_0 = 0$ and $z_1 = 1 - \mathrm{i}$, along (i) the straight line $\gamma_1(t) = (1-\mathrm{i})t$ and (ii) the curve $\gamma_2(t) = t^3 - \mathrm{i}t$, with $t \in [0,1]$. Calculate explicitly the difference $F(z_1) - F(z_0)$, where $F(z)$ is the antiderivative of $f(z)$.

PC9.2.2 Cauchy's theorem

Calculate the complex path integral $I_{\gamma_i} = \int_{\gamma_i} \mathrm{d}z\,(z-\mathrm{i})^2$ along the following curves γ_i, and explain your answers with reference to Cauchy's theorem.

(a) γ_1 is the straight line from $z_0 = 0$ to $z_1 = 1$, γ_2 is the line from $z_1 = 1$ to $z_2 = \mathrm{i}$, and γ_3 is the line from $z_2 = \mathrm{i}$ to $z_0 = 0$. What is $I_{\gamma_1} + I_{\gamma_2} + I_{\gamma_3}$? Explain your answer.

(b) γ_4 is the quarter-circle with radius 1 from z_1 to z_2. Is there a connection between I_{γ_4} and the integrals from (a)?

P.C9.3 Singularities

EC9.3.1 Laurent series, residues

Let $p(z)$ be a polynomial of order $k \geq 0$ on $\mathbb{C}$, then $f_m(z) = \frac{p(z)}{(z-z_0)^m}$ (with $m \geq 1$) is an analytic function on $\mathbb{C}\backslash z_0$, with a pole of order m at z_0.

(a) Show, using a Taylor series of $p(z)$ about z_0, that the Laurent series of $f_m(z)$ has the following form:

$$f_m(z) = \sum_{n=-m}^{k-m} \frac{p^{(n+m)}(z_0)}{(n+m)!}(z-z_0)^n\,, \quad \text{with} \quad p^{(n)}(z_0) = \frac{\mathrm{d}^n}{\mathrm{d}z^n} p(z)\bigg|_{z=z_0}\,.$$

(b) Find, for $f_m(z) = \frac{z^3}{(z-2)^m}$, the Laurent series about the pole at $z_0 = 2$.

(c) Find for $m = 1$, 2, 3, 4 and 5 the residues of $f_m(z) = \frac{z^3}{(z-2)^m}$ about the pole $z_0 = 2$, using the formula $\mathrm{Res}(f, z_0) = \lim_{z\to z_0} \frac{1}{(m-1)!} \frac{\mathrm{d}^{m-1}}{\mathrm{d}z^{m-1}} [(z-z_0)^m f(z)]$.
[Check your results: are the residues from (c) consistent with the Laurent series of (b)?]

PC9.3.2 Laurent series, residues

For each of the following functions, determine their poles, as well as the residues using the residue formula. Then find the Laurent series about each pole using an appropriately chosen Taylor series.

(a) $\dfrac{2z^3 - 3z^2}{(z-2)^3}\,,$ (b) $\dfrac{1}{(z-1)(z-3)}\,,$ (c) $\dfrac{\ln z}{(z-5)^2}\,,$ (d) $\dfrac{\mathrm{e}^{\pi z}}{(z-\mathrm{i})^m}$ with $m \geq 1\,.$

Hint: The Laurent series of a function of the form $f(z) = g(z)/(z-z_0)^m$, with $g(z)$ analytic in some neighbourhood of z_0, follows from the Taylor series of $g(z)$ about z_0.
[Check your results: The constant terms [coefficient of $(z-z_0)^0$] in the Laurent series are for (a) 2, (b) $-\frac{1}{4}$ for the poles at $z_0 = 1$ and 3, (c) $-\frac{1}{25}$, (d) $-\pi^m/m!$. Further check: Do the residues match the coefficients of $(z-z_0)^{-1}$ for each Laurent series?]

P.C9.4 Residue theorem

EC9.4.1 Circular contours, residue theorem

(a) Calculate the integrals $I_+^{(k)} = \oint_{k \text{ mal: } |z|=R} \frac{\mathrm{d}z}{z}$ and $I_-^{(k)} = \oint_{k \text{ mal: } |z|=R} \frac{\mathrm{d}z}{z}$,

where $I_+^{(k)}$ (resp. $I_-^{(k)}$) is a circular path with radius R which winds around the origin k times in the mathematically positive (negative) direction, i.e. anticlockwise (clockwise). Do not use the residue theorem; rather calculate the integral directly using the parametrization $z(\phi) = R\,\mathrm{e}^{\mathrm{i}\phi}$ and a suitable choice of integration interval for ϕ.

Calculate the following closed contour integrals in the complex plane, for $0 < a \in \mathbb{R}$:

(b) $I_1(a) = \oint_{|z|=\frac{1}{2}} \mathrm{d}z\, g(z)\,, \qquad I_2(a) = \oint_{2 \text{ times: } |z|=2} \mathrm{d}z\, g(z)\,, \quad \text{with} \quad g(z) = \dfrac{\mathrm{e}^{\mathrm{i}az}}{z^2+1}\,.$

(c) $I_3(a) = \oint_{|z|=4} \mathrm{d}z\, f(z)\,, \qquad \text{with} \quad f(z) = \dfrac{z}{z^3 + (a\mathrm{i}-6)z^2 + (9-6a\mathrm{i})z + 9a\mathrm{i}}\,.$

Hint: One of the poles of $f(z)$ is at $z_1 = -a\mathrm{i}$.

[Check your results: (b) $I_2(\ln 2) = 3\pi$, (c) $I_3(1) = 0$, $I_3(6) = \frac{4\pi}{25}(1 + \frac{4}{3}\mathrm{i})$.]

PC9.4.2 Circular contours, residue theorem

Consider the function $f(z) = \dfrac{4z}{(z-a)(z+1)^2}$, with $1 < a \in \mathbb{R}$.

(a) Determine the residues of the function f at each of its poles.

Calculate the integral $I_{\gamma_i}(a) = \int_{\gamma_i} \mathrm{d}z\, f(z)$ for the following integration contours:

(b) γ_1: a circle with radius $R = 1$ about $z = a$, traversed in the anticlockwise direction.

(c) γ_2: a circle with radius $R = 1$ about $z = -1$, traversed in the clockwise direction.

(d) γ_3: a circle with radius $R = 2a$ about the origin, traversed in the anticlockwise direction.

[Check your results: (b) $I_{\gamma_1}(2) = \frac{16}{9}\pi\mathrm{i}$, (c) $I_{\gamma_2}(3) = \frac{3}{2}\pi\mathrm{i}$].

EC9.4.3 Integrating by closing contour and using residue theorem

Calculate the following integral, with $a, b \in \mathbb{R}$, by closing the contour along a suitably chosen half-circle with radius $\to \infty$:

$$I(a,b) = \int_{-\infty}^{\infty} \mathrm{d}x\, \frac{1}{x^2 - 2xa + a^2 + b^2}\,. \qquad \text{[Check your results: } I(-1,-2) = \tfrac{\pi}{2}\text{.]}$$

PC9.4.4 Integrating by closing contour and using residue theorem

Calculate the following integrals (with $a, b \in \mathbb{R}$ and $a > 0$) by closing the contour with a semicircle of radius $\to \infty$ in the upper or lower complex half-planes (show that both choices give the same result!):

(a) $I(a,b) = \displaystyle\int_{-\infty}^{\infty} \mathrm{d}x \frac{x}{(x^2+b^2)(x-\mathrm{i}a)}$, (b) $I(a,b) = \displaystyle\int_{-\infty}^{\infty} \mathrm{d}x \frac{x}{(x+\mathrm{i}b)^2(x-\mathrm{i}a)}$.

[Check your results: (a) $I(3,-2) = \frac{\pi}{5}$, (b) $I(3,2) = \frac{6\pi}{25}$.]

EC9.4.5 Various integration paths, residue theorem

Consider the function $f(z) = \dfrac{z^2}{(z^2+4)(z^2+a^2)}$, with $a \in \mathbb{R}$, $3 \le a < 4$.

(a) Determine the residues of f at each of its poles.

Calculate the integral $I_{\gamma_i}(a) = \int_{\gamma_i} \mathrm{d}z\, f(z)$ for the following integration contours:

(b) γ_1: a circle with radius $R = 1$ about the origin, traversed in the anticlockwise direction.

(c) γ_2: a circle with radius $R = \frac{1}{2}$ about $z = 2\mathrm{i}$, traversed in the anticlockwise direction.

(d) γ_3: a circle with radius $R = 2$ about $z = 2\mathrm{i}$, traversed in the clockwise direction.

(e) γ_4: the real axis, traversed in the positive direction.

[Check your results: (c) $I_{\gamma_2}(3) = -\frac{2\pi}{5}$, (d) $I_{\gamma_3}(\frac{10}{3}) = -\frac{3\pi}{16}$, (e) $I_{\gamma_4}(\frac{7}{2}) = \frac{2\pi}{11}$.]

PC9.4.6 Various integration paths, residue theorem

Consider the function $f(z) = \dfrac{1}{[z^2 - 2az + a^2 + \frac{1}{4}]^2\,(4z^2+1)}$, with $1 < a \in \mathbb{R}$.

(a) Determine the residues of the function f at each of its poles.

Calculate the integrals $I_{\gamma_i}(a) = \int_{\gamma_i} \mathrm{d}z\, f(z)$ for the following integration contours:

(b) γ_1: a circle with radius $R = 1$ about $z_1 = 0$, traversed in the anticlockwise direction.

(c) γ_2: a circle with radius $R = \frac{1}{\sqrt{2}}a$ about $z_2 = \frac{1}{2}a(1-\mathrm{i})$, traversed in the clockwise direction.

(d) γ_3: a circle with radius $R = a + \frac{1}{2}$ about $z_3 = \frac{1}{2}a$, traversed in the anticlockwise direction.

(e) γ_4: the line $z = x$, with $x \in [-\infty, \infty]$, traversed in the positive x-direction.

(f) γ_5: the line $z = \frac{1}{3}a + \mathrm{i}y$, with $y \in [-\infty, \infty]$, traversed in the positive y-direction.

[Check your results: (b) $I_{\gamma_1}(2) = \frac{\pi\mathrm{i}}{25}$, (c) $I_{\gamma_2}(2) = \frac{7\pi}{25}$, (e) $I_{\gamma_4}(3) = \frac{3\pi}{25}$, (f) $I_{\gamma_5}(3) = \frac{\pi\mathrm{i}}{150}$.]

EC9.4.7 Inverse Fourier transform via contour closure

(a) The Green's function defined by the equation $(\mathrm{d}_t + a)G(t) = \delta(t)$ (with $0 < a \in \mathbb{R}$) has corresponding Fourier transform given by $\tilde{\mathcal{G}}(\omega) = (a - \mathrm{i}\omega)^{-1}$. Show that the corresponding inverse Fourier transform yields the following result:

$$G(t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}\omega t}}{a - \mathrm{i}\omega} = \theta(t)\,\mathrm{e}^{-at}\,, \quad \text{with} \quad \theta(t) = \begin{cases} 1 & \text{for } t > 0\,, \\ 0 & \text{for } t < 0\,. \end{cases}$$

(b) The Fourier transform of the exponential function, $\tilde{L}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{-a|t|} = \frac{2a}{\omega^2 + a^2}$ (with $0 < a \in \mathbb{R}$), is a Lorentz curve. Find the inverse Fourier transform $L(t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-\mathrm{i}\omega t} \tilde{L}(\omega)$, by explicitly calculating the integral.

Hint: Calculate the integral for $t \neq 0$ as a complex path integral, by closing the contour with a suitably chosen semicircle with radius $\to \infty$.

PC9.4.8 Inverse Fourier transform via contour closure: Green's function of damped harmonic oscillator

The Green's function of the damped harmonic oscillator is defined by the differential equation $(\mathrm{d}_t^2 + 2\gamma \mathrm{d}_t + \Omega^2)G(t) = \delta(t)$ (with $0 < \Omega, \gamma \in \mathbb{R}$). Its Fourier transform, defined by $G(t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-\mathrm{i}\omega t} \tilde{\mathcal{G}}(\omega)$, is given by $\tilde{\mathcal{G}}(\omega) = (\Omega^2 - \omega^2 - 2\gamma \mathrm{i}\omega)^{-1}$. Express the Green's function in the form $G(t) = \int_{-\infty}^{\infty} \mathrm{d}z\, f(z)$, and calculate the integral by closing the contour in the complex plane. You should proceed as follows:

(a) Find the residues of $f(z)$. Distinguish between the following cases:
(i) $\Omega > \gamma$ (underdamped), (ii) $\Omega = \gamma$ (critically damped) und (iii) $\Omega < \gamma$ (overdamped).
Hint: (i) and (iii) each have two poles of first order; (ii) has only a single pole, but of second order.

(b) Calculate $G(t)$ by closing the contour with an appropriately chosen semicircle with radius $R \to \infty$ (again distinguishing between the different cases!). [Check your results for $G(t)$: (i) for $\Omega = 1$ and $\gamma = 0$, $G(\pi/2) = 1$; (ii) for $\Omega = \gamma = 1$, $G(1) = \mathrm{e}^{-1}$; (iii) for $\Omega = 4$ and $\gamma = 5$, $G(1/3) = \frac{1}{3}\mathrm{e}^{-5/3}\sinh(1)$.]

P.C9.5 Essential Singularities

P.C9.6 Riemann surfaces

V

Vector calculus

The third part of this book, labeled V for 'vector calculus', introduces the mathematics of smooth structures in higher-dimensional spaces. Methodologically, this requires a synthesis of concepts of linear algebra and calculus introduced in the previous two chapters, respectively. We discuss the mathematical description of curves, surfaces and more general geometric objects in higher-dimensional spaces. We will learn how to characterize these structures both from a global and a local perspective. So-called vector fields will emerge as an important tool in the description of geometric structures of any kind. We will learn how to differentiate and integrate vector fields to probe their local and global contents, respectively. In the final chapters of part V we introduce differential forms as a powerful concept generalizing the notion of vector fields and allowing for an intuitive description of geometric structures relevant to both mathematics and physics.

V1 Curves

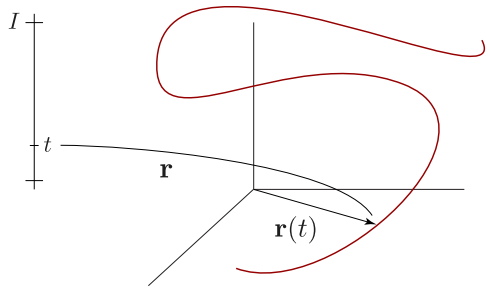
Curves in d-dimensional space play an important role in many areas of physics. This is true in particular in mechanics were they describe the motion of bodies through space. In this chapter we will discuss the mathematical definition of curves and introduce quantities describing them. We will learn how to differentiate and integrate with reference to curves.

V1.1 Definition

A curve can be imagined as a smooth line in d-dimensional space. To define this in mathematical terms we need the concept of a **vector-valued function**. This is a function

$$\mathbf{r} : I \ \to \mathbb{R}^d, \qquad t \mapsto \mathbf{r}(t), \tag{V1}$$

which smoothly assigns a vector $\mathbf{r}(t)$ to the parameter variable t. Here, $I \subset \mathbb{R}$ is some interval, which is taken to be $I = (0, 1)$, unless otherwise stated. It is often useful to interpret t as a time-like variable, in which case $\mathbf{r}(t)$ is a time-dependent position vector describing the motion of a point through $\mathbb{R}^d$. One may introduce an orthonormal basis $\{\mathbf{e}_i\}$ to parameterize $\mathbb{R}^d$ in Cartesian coordinates and represent $\mathbf{r}(t)$ in terms of a coordinate vector $\mathbf{x}(t) = (x^1(t), \ldots, x^d(t))$. This representation is described by d real functions $x^i(t)$ of the parameter t, which means that the mathematical description of vector-valued functions is not more difficult than that of scalar functions.



The **curve**, γ, corresponding to the function $\mathbf{r}$ is defined to be the image of $\mathbf{r}$, i.e.

$$\gamma \equiv \{\mathbf{r}(t) | t \in I\}, \tag{V2}$$

where the term 'image' is defined as in section L1.1. A *visual* image of γ in $\mathbb{R}^d$ is obtained by drawing a line passing through the points $\mathbf{r}(t) \in \mathbb{R}^d$ for all values of t (see figure).

The function $\mathbf{r}(t)$ defines a **parameterization of the curve** γ. A parameterization contains more 'information' than the curve itself, since it describes not only the shape of the curve, but also *how* the point $\mathbf{r}(t)$ moves (quickly/slowly?) along the curve as function of t. For example, a curve might be realized as a penciled route connecting two locations on a

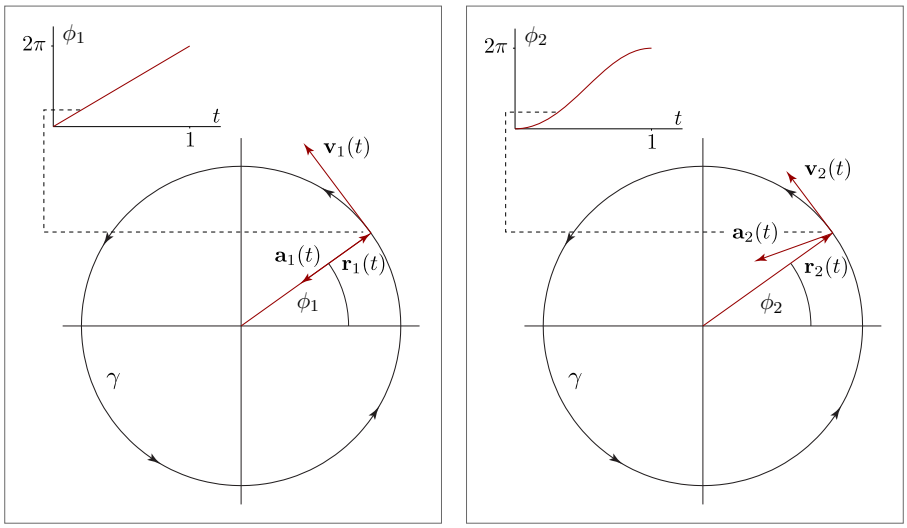


Figure V1: Schematic depiction of the two parameterizations (V3) of the unit circle. Left: the angle $\phi_1(t)$ increases uniformly with time. Right: the angle $\phi_2(t)$ increases non-uniformly with time. The difference shows in different velocity and acceleration vectors, as discussed in the text.

road map. Then a cyclist's schedule for reaching certain points $\mathbf{r}(t)$ at various specified times t would be a possible parameterization of the route.

Any curve has infinitely many distinct parameterizations. For example, the two functions $\mathbf{r}_1(t)$ and $\mathbf{r}_2(t)$ defined by

$$\mathbf{r}_i(t) = \begin{pmatrix} \cos(\phi_i(t)) \\ \sin(\phi_i(t)) \end{pmatrix}, \qquad \phi_1(t) = 2\pi t, \qquad \phi_2(t) = \pi[1 - \cos(\pi t)]\,, \tag{V3}$$

are different parameterizations of the same curve, namely a unit-circle in $\mathbb{R}^2$. To verify this, first note that $(r_i^1)^2 + (r_i^2)^2 = 1$ lies on the unit circle. In either parameterization $\phi_i(t)$ increases monotonically from 0 to 2π (cf. Fig. V1). This means that a circular curve is fully covered as previously stated.

INFO The function $\mathbf{r}(t)$ is often referred to as a curve without discriminating between the **curve and its parameterization**. This should not cause confusion as long as the relation between curves and parameterizations is kept in mind: A curve is an invariant geometric object in space and its various possible parameterizations are different languages for describing it.

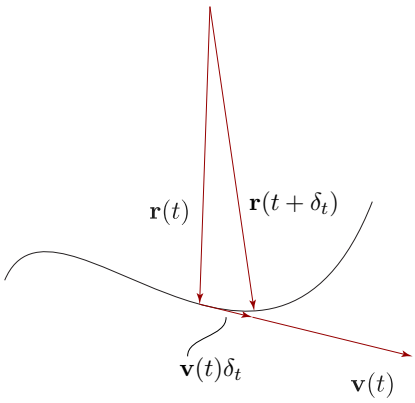
V1.2 Curve velocity

The point $\mathbf{r}(t)$ moves through space at a certain *velocity* (Geschwindigkeit). Velocity is a vectorial quantity, $\mathbf{v}$, whose direction is tangent to the curve and whose magnitude measures

the speed of the motion (see Fig. V1 where the different lengths of the velocity vector indicate that the two parameterizations traverse the curve at different speed).

Mathematically, the velocity, $\mathbf{v}(t)$, of the curve at time $t \in I$ is defined as

$$\mathbf{v}(t) = \lim_{\delta_t \to 0} \frac{\mathbf{r}(t+\delta_t) - \mathbf{r}(t)}{\delta_t} \equiv \frac{\mathrm{d}\mathbf{r}(t)}{\mathrm{d}t} \equiv \dot{\mathbf{r}}(t). \qquad \text{(V4)}$$



The differential quotient expresses the intuitive notion that the velocity describes the distance between two nearby points, $\mathbf{r}(t+\delta_t) - \mathbf{r}(t)$, in relation to the time, δ_t, that it took to traverse them (see figure).[1] Inserting the component representations $\mathbf{r}(t) = \mathbf{e}_i r^i(t)$ into Eq. (V4) we obtain $\mathbf{v} = \dot{\mathbf{r}} = \mathbf{e}_i \dot{r}^i \equiv \mathbf{e}_i v^i$, i.e. the derivative acting on the vector $\mathbf{r}$ is computed component-wise:

$$v^i(t) = \frac{\mathrm{d}r^i(t)}{\mathrm{d}t} \equiv \dot{r}^i(t).$$

To see that $\mathbf{v}$ lies tangent to the curve, rewrite (V4) as

$$\mathbf{r}(t+\delta_t) \simeq \mathbf{r}(t) + \delta_t \mathbf{v}(t).$$

Varying δ_t at fixed t we obtain a tangent, i.e. a straight line $\mathbf{r}(t) + \delta_t \mathbf{v}(t)$ which for small δ_t is a good local approximation to the curve near $\mathbf{r}(t)$.

INFO In the following we will often need to differentiate vector-valued functions. All these derivatives can be reduced to ordinary derivatives acting on the components of vectors. However, one should aim to keep the notation compact and avoid component representations where possible. Useful **vector differentiation rules** include:

$$\begin{aligned}
&\mathrm{d}_t(\mathbf{r}+\mathbf{s}) = \mathrm{d}_t\mathbf{r} + \mathrm{d}_t\mathbf{s},\\
&\mathrm{d}_t(a\mathbf{r}) = (\mathrm{d}_t a)\,\mathbf{r} + a(\mathrm{d}_t\mathbf{r}),\\
&\mathrm{d}_t(\mathbf{r}\cdot\mathbf{s}) = (\mathrm{d}_t\mathbf{r})\cdot\mathbf{s} + \mathbf{r}\cdot(\mathrm{d}_t\mathbf{s}),\\
&\mathrm{d}_t(\mathbf{r}\times\mathbf{s}) = (\mathrm{d}_t\mathbf{r})\times\mathbf{s} + \mathbf{r}\times(\mathrm{d}_t\mathbf{s}) \qquad (\text{for } d=3).
\end{aligned} \qquad \text{(V5)}$$

For the sake of transparency, we have omitted the time argument here, e.g. $\mathrm{d}_t a = \mathrm{d}_t a(t)$, etc. All these relations can be verified by expressing the vectors in terms of their components, $\mathbf{r}(t) = \mathbf{e}_i r^i(t)$, etc., applying standard rules of differentiation, and remembering that the Cartesian basis vectors are time-independent, $\dot{\mathbf{e}}_i = \mathbf{0}$.

[1] The dot notation is customary for derivatives with respect to a time-like parameter. For example, one does not write $\dot{f}(x) = \frac{\mathrm{d}f}{\mathrm{d}x}$ if x parameterizes length.

As an example, consider a time-dependent vector, $\mathbf{r}(t)$, of fixed norm $\mathbf{r}\cdot\mathbf{r} = l^2 = \text{const}$. Differentiation w.r.t. time yields:

$$0 = \mathrm{d}_t l^2 = \mathrm{d}_t(\mathbf{r}\cdot\mathbf{r}) = (\mathrm{d}_t\mathbf{r})\cdot\mathbf{r} + \mathbf{r}\cdot(\mathrm{d}_t\mathbf{r}) = 2\mathbf{r}\cdot(\mathrm{d}_t\mathbf{r}) = 2\mathbf{r}\cdot\mathbf{v}, \tag{V6}$$

where $\mathbf{v} = \mathrm{d}_t\mathbf{r}$ is the curve velocity. This shows that for a circular curve traced out by a position vector of fixed norm, the velocity vector is always perpendicular to the position vector.

If the the velocity along the curve changes in time, the motion is subject to **acceleration** (Beschleunigung). Acceleration is a vectorial quantity defined as the rate of change of velocity,

$$\mathbf{a}(t) \equiv \lim_{\delta_t\to 0}\frac{\mathbf{v}(t+\delta_t)-\mathbf{v}(t)}{\delta_t} = \dot{\mathbf{v}}(t) \equiv \ddot{\mathbf{r}}(t), \tag{V7}$$

or $a^i(t) = \dot{v}^i(t) = \ddot{r}^i(t)$ in components.

EXAMPLE Consider the two curves $\mathbf{r}_1(t)$ and $\mathbf{r}_2(t)$ defined in Eq. (V3). Their velocity and acceleration vectors read

$$\mathbf{v}_i(t) = \begin{pmatrix}-\sin(\phi_i(t))\\ \cos(\phi_i(t))\end{pmatrix}\dot{\phi}_i(t), \qquad \dot{\phi}_1(t) = 2\pi, \qquad \dot{\phi}_2(t) = \pi^2\sin(\pi t)\,,$$

$$\mathbf{a}_i(t) = -\begin{pmatrix}\cos(\phi_i(t))\\ \sin(\phi_i(t))\end{pmatrix}(\dot{\phi}_i(t))^2 + \begin{pmatrix}-\sin(\phi_i(t))\\ \cos(\phi_i(t))\end{pmatrix}\ddot{\phi}_i(t)\,, \qquad \ddot{\phi}_1(t) = 0, \qquad \ddot{\phi}_2(t) = \pi^3\cos(\pi t)\,.$$

A series of 'snapshots' of these vectors at different times is shown in Fig. V2. Notice that $\mathbf{v}_i\cdot\mathbf{r}_i = 0$, which was proved generally in Eq. (V6). Also notice that the speed is constant along the first curve, $\|\mathbf{v}_1(t)\| = 2\pi$, but changes along the second, $\|\mathbf{v}_2(t)\| = \pi^2|\sin(\pi t)|$. Correspondingly the acceleration vector for the first curve is directed towards the center ($\ddot{\phi}_1 = 0$ implies $\mathbf{a}_1 \parallel -\mathbf{r}_1$), whereas the acceleration vector for the second curve has a tangential component ($\ddot{\phi}_2 \neq 0$ implies $\mathbf{a}_2\cdot\mathbf{v}_2 \neq 0$, see red arrows), which acts to increase or decrease the speed along the curve.

INFO We conclude this section on curve velocity with a mathematical subtlety: in this text, we will always parameterize curves by *open*[2] parameter intervals, such as $(0,1)$. This is done to guarantee the global differentiability of the function $\mathbf{r}(t)$. For a closed interval, $[0,1]$, the parameterization would not be differentiable [3] at $t=0$ or $t=1$, and this would lead to unwanted side effects, both mathematical and physical. (For example, the velocity of a curve would not be defined at its end points.) For a curve defined on an open interval, $(0,1)$, the end points $\mathbf{r}(0)$ and $\mathbf{r}(1)$ are formally excluded from the curve. In practice, however, this omission is generally not of relevance, because for any continuous curve the endpoints can always be *defined* as limits, e.g. $\mathbf{r}(1) = \lim_{t\to 1}\mathbf{r}(t)$.

[2] The concept of an 'open interval' is explained in section L1.3, p. 16.

[3] The definition of differentiability requires the existence of the differential quotient (C1), $[f(t+\delta_t) - f(t)]/\delta_t$, irrespective of the sign of the incremental parameter, δ_t. This condition is violated at the boundary of a closed interval. For example, if $f(t)$ is defined on $[0,1]$, then $f(1+\delta_t)$ is not defined for positive δ_t.

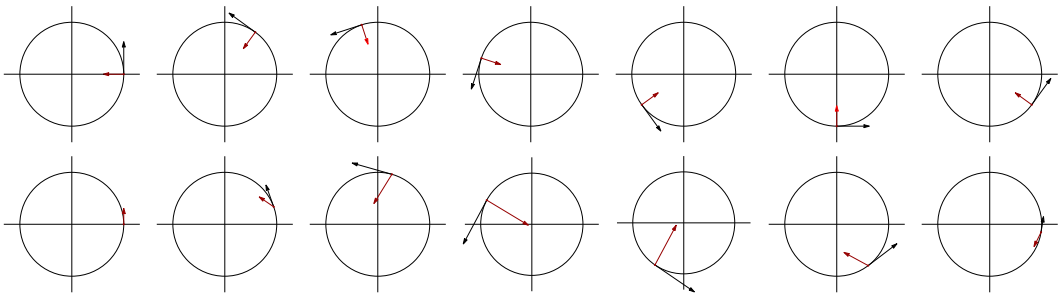
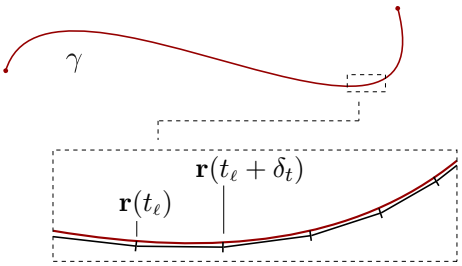


Figure V2: The velocity vectors (black arrows) and acceleration vectors (red arrows) for the two parameterizations $\mathbf{r}_1(t)$ (upper row) and $\mathbf{r}_2(t)$ (lower row) of a circle defined in Eq. (V3), shown at different times.

V1.3 Curve length

An important characteristic of a curve, γ, is its length. An estimate for the curve length may be obtained by approximating the curve as a concatenation of many short, straight line segments (see figure). The geometric length of each segment can be computed using the Euclidean scalar product on $\mathbb{R}^d$ and in the limit of an infinitely fine discretization, their sum converges to the length of the curve.



To make this strategy quantitative, we need a parameterization of the curve, say $\mathbf{r} : (0,1) \to \mathbb{R}^d$, $t \mapsto \mathbf{r}(t)$. We divide the parameter interval $(0,1)$ into $N \gg 1$ subintervals of width $\delta_t = 1/N$, bounded by the discrete parameter values $t_\ell = \ell\,\delta_t$, with $\ell = 0, \dots N$. Each difference vector $\mathbf{r}(t_\ell + \delta_t) - \mathbf{r}(t_\ell)$ then defines a line segment approximately tangent to the curve, and by adding the lengths of these segments,

$$L_{\delta_t} \equiv \sum_{\ell=0}^{N-1} \|\mathbf{r}(t_\ell + \delta_t) - \mathbf{r}(t_\ell)\|,$$

we obtain an estimate of the the length of the curve. For small δ_t, one may approximate $\|\mathbf{r}(t_\ell + \delta_t) - \mathbf{r}(t_\ell)\| \simeq \|\delta_t\,\dot{\mathbf{r}}(t_\ell)\| = \delta_t \|\dot{\mathbf{r}}(t_\ell)\|$ and this yields

$$L \equiv \lim_{\delta_t \to 0} L_{\delta_t} = \lim_{\delta_t \to 0} \delta_t \sum_{\ell=0}^{N-1} \|\dot{\mathbf{r}}((t_\ell)\| = \int_0^1 \mathrm{d}t\, \|\dot{\mathbf{r}}(t)\|,$$

where in the last step we recognized the appearance of a Riemann sum [cf. Eq. (C18)]. Denoting the **length of a curve** γ by $L[\gamma]$, we have thus have

$$\boxed{L[\gamma] = \int_0^1 \mathrm{d}t\, \|\dot{\mathbf{r}}(t)\|.} \tag{V8}$$

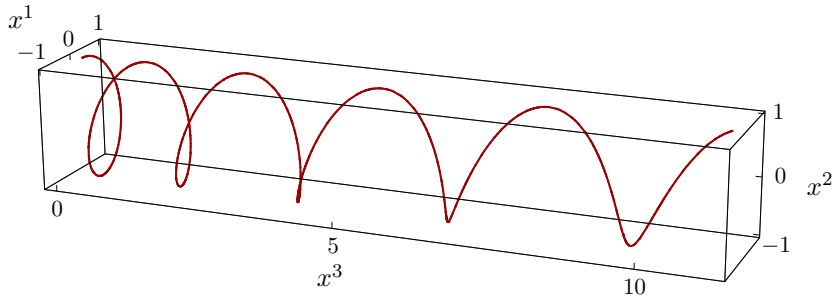


Figure V3: The curve parameterized by Eq. (V9).

This definition has been obtained by constructive geometric reasoning and therefore should not depend on the choice of parameterization. To verify its parameterization invariance, consider an arbitrary smooth and monotonically increasing function $t : (a, b) \to (0, 1), s \mapsto t(s)$ such that the function $\mathbf{r}' : (a, b) \to \mathbb{R}^d$, $s \mapsto \mathbf{r}'(s) \equiv \mathbf{r}(t(s))$ defines a different parameterization of the same curve. Applying the length formula in the new parameterization yields

$$\begin{aligned} L[\gamma] &= \int_a^b \mathrm{d}s \, \|\mathrm{d}_s \mathbf{r}'(s)\| = \int_a^b \mathrm{d}s \, \|\mathrm{d}_s \mathbf{r}(t(s))\| \overset{(C7)}{=} \int_a^b \mathrm{d}s \, \|\mathrm{d}_t \mathbf{r}(t)\big|_{t=t(s)} \mathrm{d}_s t(s)\| \\ &= \int_a^b \mathrm{d}s \, \frac{\mathrm{d}t(s)}{\mathrm{d}s} \, \|\mathrm{d}_t \mathbf{r}(t)\big|_{t=t(s)}\| \overset{(C26)}{=} \int_0^1 \mathrm{d}t \, \|\mathrm{d}_t \mathbf{r}(t)\|, \end{aligned}$$

where the chain rule was used at the end of the first line, and a variable substitution at the end of the second. Thus definition (V8) for the curve length is indeed parametrization invariant.

EXERCISE Compute the length of the curve Eq. (V3) in the two parameterizations given there, and show that the circumference of the unit circle is obtained in either case.

EXAMPLE Consider the curve γ shown in the figure above with parameterization

$$\mathbf{r} : (0, 5) \to \mathbb{R}^3, \qquad t \mapsto \mathbf{r}(t) \equiv \left(\sin(2\pi t), \cos(2\pi t), \tfrac{2}{3} t^{3/2}\right)^T. \tag{V9}$$

The norm of the velocity vector,

$$\frac{\mathrm{d}\mathbf{r}(t)}{\mathrm{d}t} = \left(2\pi \cos(2\pi t), -2\pi \sin(2\pi t), t^{1/2}\right)^T,$$

is given by $\|\mathrm{d}_t \mathbf{r}(t)\| = \sqrt{4\pi^2 + t}$ and this integrates to

$$L[\gamma] = \int_0^5 \mathrm{d}t \, (4\pi^2 + t)^{1/2} = \tfrac{2}{3}(4\pi^2 + t)^{3/2}\Big|_0^5 = \tfrac{2}{3}\left[(4\pi^2 + 5)^{3/2} - (2\pi)^3\right].$$

INFO For a curve with parameterization $\mathbf{r} : (0,1) \to \mathbb{R}$, $t \mapsto \mathbf{r}(t)$, consider the length, $s(t)$, of the curve segment corresponding to the partial interval $(0,t)$, $t \leq 1$,

$$s(t) \equiv \int_0^t \mathrm{d}u \, \|\mathrm{d}_u \mathbf{r}(u)\|. \tag{V10}$$

The function $s(t)$ grows monotonically with t from 0 at $t = 0$ to $L[\gamma]$ as $t \to 1$. It defines a bijection $s : (0,1) \to (0, L[\gamma])$ and may therefore be inverted to yield a function, $t(s)$, that assigns to each length $s \in (0, L[\gamma])$ the parameter $t(s)$ at which s is reached. This observation suggests parameterizing the curve by its own length function. The resulting parameterization,

$$\mathbf{r}_L : (0, L[\gamma]) \to \mathbb{R}^3, \qquad s \mapsto \mathbf{r}_L(s) \equiv \mathbf{r}(t(s)) \,,$$

is called the **natural parameterization** of the curve. The subscript 'L' is usually omitted and one writes $\mathbf{r}(s) \equiv \mathbf{r}(t(s))$ once it has been made clear that s refers to the length.

The distinguishing feature of the natural parameterization is that the resulting curve velocity, $\mathbf{v}(s) = \mathrm{d}_s \mathbf{r}(s)$, has unit magnitude:

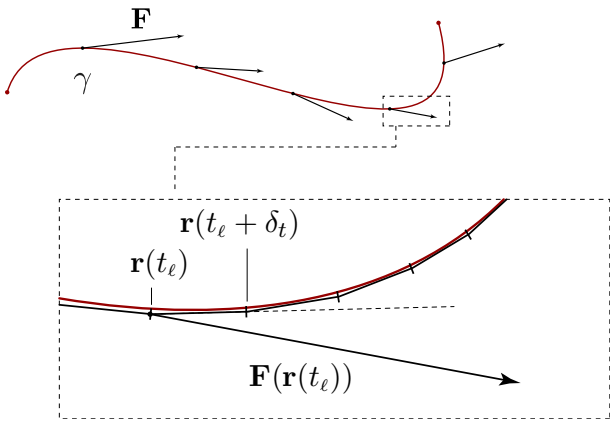
$$\begin{aligned} \|\mathrm{d}_s \mathbf{r}(s)\| = \|\mathrm{d}_s \mathbf{r}(t(s))\| &= \|\mathrm{d}_t \mathbf{r}(t)\big|_{t(s)}\| \, \frac{\mathrm{d}t(s)}{\mathrm{d}s} \\ &\overset{(C8)}{=} \|\mathrm{d}_t \mathbf{r}(t)\big|_{t(s)}\| \frac{1}{\left.\frac{\mathrm{d}s(t)}{\mathrm{d}t}\right|_{t=s(t)}} \overset{(V10)}{=} \frac{\|\mathrm{d}_t \mathbf{r}(t)|_{t(s)}\|}{\|\mathrm{d}_t \mathbf{r}(t)\big|_{t(s)}\|} = 1. \end{aligned} \tag{V11}$$

This fact implies the orthogonality, $\mathbf{a}(s) \perp \mathbf{v}(s)$, between the curve velocity and the acceleration vector $\mathbf{a}(s) = \mathrm{d}_s \mathbf{v}(s)$, cf. Eq. (V6).

Try to develop some intuition for why in the natural parameterization, $\mathbf{r}(s)$, the curve is traversed at a uniform velocity. If in some other parametrization, $\mathbf{r}(t)$, a curve segment is traversed very quickly (or slowly), what does this mean for the rate of change of the length function $s(t)$, and what is the consequence for $\mathbf{v}(s)$? Compute the natural parameterization of the curve (V9).

V1.4 Line integral

In physics, curves often appear as integration domains for a class of integrals known as *line integrals*. The idea of the line integral is best motivated via an application. In section **??** we defined the work done when a body subject to a constant force, $\mathbf{F}$, is moved along a straight path, $\mathbf{s}$, as $W = \mathbf{F} \cdot \mathbf{s}$. More generally, however, the force may *vary* along the path, and the path itself need not be straight (see the figure, where the path follows the curve γ).



The work done under these generalized conditions is computed by straightforward adaption of the previous construction for the curve length: let $\mathbf{r}(t)$, $t \in (0,1)$, be a parameterization of the path, γ, and $\mathbf{F}(\mathbf{r}(t))$ be the force acting at the point $\mathbf{r}(t)$. To determine the work done, we divide the curve into $N = \delta_t^{-1} \gg 1$ segments $\mathbf{s}_\ell = \mathbf{r}(t_\ell + \delta_t) - \mathbf{r}(t_\ell)$, where the discretization is defined as in section V1.3. The work along each of these (straight) segments is given by $W_\ell = \mathbf{s}_\ell \cdot \mathbf{F}_\ell$ with $\mathbf{F}_\ell = \mathbf{F}(\mathbf{r}(t_\ell))$,[4] i.e.

$$W_\ell = [\mathbf{r}(t_\ell + \delta_t) - \mathbf{r}(t_\ell)] \cdot \mathbf{F}(\mathbf{r}(t_\ell)) \simeq \delta_t \, \dot{\mathbf{r}}(t_\ell) \cdot \mathbf{F}(\mathbf{r}(t_\ell)).$$

The total work along the path is obtained by summation over all segments and in the limit $\delta_t \to 0$ of an infinitely fine segmentation one obtains

$$W \equiv \lim_{\delta_t \to 0} \sum_{\ell=0}^{N-1} W_\ell = \lim_{\delta_t \to 0} \delta_t \sum_{\ell=0}^{N-1} \dot{\mathbf{r}}(t_\ell) \cdot \mathbf{F}(\mathbf{r}(t_\ell)) = \int_0^1 \mathrm{d}t \, \dot{\mathbf{r}}(t) \cdot \mathbf{F}(\mathbf{r}(t)) \equiv \int_\gamma \mathrm{d}\mathbf{r} \cdot \mathbf{F}.$$

The last expression is symbolic notation for the line integral of the force along the curve; it is *defined* in terms of the integral over time given in the second-last expression.

The construction above is an example of the **line integral** of a general vector-valued function, $\mathbf{f} : \gamma \to \mathbb{R}^d, \mathbf{r} \mapsto \mathbf{f}(\mathbf{r})$, defined on a curve γ in $\mathbb{R}^d$. The line integral is built according to the following procedure:

1. Parameterize the curve by a vector-valued function $\mathbf{r} : (0,1) \to \mathbb{R}^d, t \mapsto \mathbf{r}(t)$.
2. Construct the real-valued function $\dot{\mathbf{r}}(t) \cdot \mathbf{f}(\mathbf{r}(t))$.
3. Integrate that function over the domain of the curve parameter,

$$\boxed{\int_\gamma \mathrm{d}\mathbf{r} \cdot \mathbf{f} \equiv \int_0^1 \mathrm{d}t \, \dot{\mathbf{r}}(t) \cdot \mathbf{f}(\mathbf{r}(t)).} \tag{V12}$$

Although the construction makes reference to a particular parametrization, the result is **independent of the choice of parameterization**. (Proceed as in section V1.3 to convince yourself that this is so.) This implies, for example, that the work invested to pull a body along a curve does not depend on the speed at which the curve is traversed.

EXAMPLE

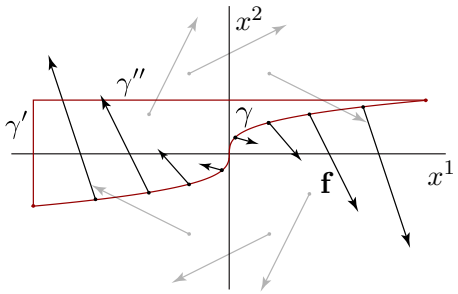
[4] For sufficiently small δ_t and a smooth force function, $\mathbf{F}(\mathbf{r}(t)) \simeq \mathbf{F}(\mathbf{r}(t + \delta_t))$, the specific choice of the 'readout point' at which the force is evaluated is not of importance.

Consider a vector-valued function

$$\mathbf{f}:\ \mathbb{R}^2 \to \mathbb{R}^2, \qquad \mathbf{r} = \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} \mapsto \mathbf{f}(\mathbf{r}) = \begin{pmatrix} x^2 \\ -x^1 \end{pmatrix},$$

and a two-dimensional curve, γ, parametrized as

$$\mathbf{r}:\ (-1,1) \to \mathbb{R}^2, \qquad t \mapsto \mathbf{r}(t) = \begin{pmatrix} x^1(t) \\ x^2(t) \end{pmatrix} = \begin{pmatrix} t^3 \\ 2t \end{pmatrix}.$$



To compute the line integral, $\int_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{f}$, we determine the curve velocity, $\dot{\mathbf{r}}(t)$, and evaluate the vector function along the curve, $\mathbf{f}(\mathbf{r}(t))$, obtaining, respectively,

$$\dot{\mathbf{r}}(t) = \begin{pmatrix} 3t^2 \\ 2 \end{pmatrix}, \qquad \mathbf{f}(\mathbf{r}(t)) = \begin{pmatrix} x^2(t) \\ -x^1(t) \end{pmatrix} = \begin{pmatrix} 2t \\ -t^3 \end{pmatrix}.$$

Their scalar product, $\dot{\mathbf{r}}(t)\cdot\mathbf{f}(\mathbf{r}(t)) = 6t^3 - 2t^3 = 4t^3$, integrated over the curve parameter, t, yields

$$\int_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{f} = \int_{-1}^{1} \mathrm{d}t\, \dot{\mathbf{r}}(t)\cdot\mathbf{f}(\mathbf{r}(t)) = \int_{-1}^{1} \mathrm{d}t\, 4t^3 = 0.$$

For the present choice of $\mathbf{f}$ and γ the integrand is an antisymmetric function of t, hence the integral vanishes.[5] This antisymmetry reflects the 'vortex-like' winding of the vectors $\mathbf{f}$ around the origin, as indicated in the figure. If $\mathbf{f}$ is interpreted as a force and the line integral as the work performed by it, then this work is zero, because the contributions where $\mathbf{f}$ acts 'along' the integration path cancel with those where it acts 'opposite' to it (for every point on the path for which the projection of $\mathbf{f}$ onto $\dot{\mathbf{r}}$ is positive, there is another point where it is negative, but with the same magnitude).

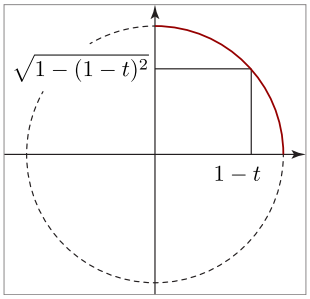
Now consider another path connecting the initial and final points of γ, say $\gamma' \cup \gamma''$, as shown in the figure. Compute the line integral over this path as the sum of the line integrals over γ' and γ'', respectively. Show that the integral does not vanish. This result demonstrates that the work done against a force along a path between two points can, in general, depend on the shape of that path.

INFO Some physics texts discuss line integrals using the notation $\mathrm{d}\mathbf{r} = \sum_{i=1}^{3} \mathbf{e}_i\, \mathrm{d}x^i$ for the 'line element' and $\int \mathrm{d}\mathbf{r}\cdot\mathbf{f} = \sum_{i=1}^{3} \int \mathrm{d}x_i\, f^i$ for line integrals. Such notation is OK if one is familiar with differential forms and really understands what one is doing, but otherwise is prone to errors. For a fault-proof interpretation of the 'line element' we refer to chapter V5 on differential forms.

[5] The integral $\int_{-a}^{a} \mathrm{d}t\, g(t)$ vanishes if $g(t) = -g(-t)$ (why?).

V2 Curvilinear Coordinates

In chapter L we argued that the Euclidean space $\mathbb{R}^d$ is best spanned by a fixed orthonormal basis. However, there are circumstances where it is preferable to abandon this principle and represent the vicinity of each point $\mathbf{r} \in \mathbb{R}^d$ by an individual basis that depends on that point. To understand why this may be a better choice, consider the curve



$$\mathbf{r}(t) = \left(1-t, \sqrt{1-(1-t)^2}\right)^T, \qquad t \in (0,1) \qquad \text{(V13)}$$

At first sight, it may not be obvious that $\mathbf{r}(t)$ describes a quadrant of the unit circle, $S^1 = \{\mathbf{r} \in \mathbb{R}^2 | \|\mathbf{r}\| = 1\}$, i.e. a set of points with unit distance to the origin. The problem is that due to the square root in the second component, this representation 'breaks the symmetry' between the 1- and 2-coordinates. However, the circle itself is symmetric under an exchange of these two coordinates. The representation (V13) thus has less symmetry than the object it describes, and consequently is generally inconvenient to work with.

As a rule, it is always more convenient to describe physical systems in a language reflecting the full symmetry of the problem. In the example above, the use of a fixed orthonormal basis does not appropriately describe the rotational symmetry and we should seek alternative descriptions.

V2.1 An example: polar coordinates

Let us begin our discussion with a simple yet important case study. Consider a problem defined in two-dimensional space. The coordinates, $\mathbf{x} \equiv (x,y)^T$, describing a point $\mathbf{r} = \mathbf{e}_x x + \mathbf{e}_y y$ with reference to a fixed orthonormal basis, $\{\mathbf{e}_x, \mathbf{e}_y\}$, are called **Cartesian coordinates**. Our discussion above indicated that Cartesian coordinates are not ideally suited to the description of problems possessing rotational symmetry. In such cases a more natural choice would be to characterize the same point, $\mathbf{r}$, by a pair of **polar coordinates**, $\mathbf{y} \equiv (\rho,\phi)^T$, describing its distance from the origin ρ, and the angle, ϕ, between $\mathbf{r}$ and a fixed reference direction, say $\mathbf{e}_x$ (cf. Fig. V4). The point $\mathbf{r}$ can then be represented using two different sets of coordinates,

$$\mathbf{r} = \mathbf{e}_x\, x + \mathbf{e}_y\, y = \mathbf{e}_x\, \rho\cos\phi + \mathbf{e}_y\, \rho\sin\phi\,, \qquad \text{(V14)}$$

where the second representation follows from the geometric definition of the polar coordinates. The correspondence between the two 'languages', Cartesian and polar, is established by the **coordinate transformation**

$$\begin{aligned} &\mathbf{x} : \mathbb{R}^+ \times (0, 2\pi) \longrightarrow \mathbb{R}^2 \backslash \mathbb{R}^+, \\ &\qquad \mathbf{y} = \begin{pmatrix} \rho \\ \phi \end{pmatrix} \longmapsto \mathbf{x}(\mathbf{y}) = \begin{pmatrix} x(\rho,\phi) \\ y(\rho,\phi) \end{pmatrix} = \begin{pmatrix} \rho\cos\phi \\ \rho\sin\phi \end{pmatrix}, \end{aligned} \tag{V15a}$$

and its inverse

$$\begin{aligned} &\mathbf{y} : \mathbb{R}^2 \backslash \mathbb{R}^+ \longrightarrow \mathbb{R}^+ \times (0, 2\pi), \\ &\qquad \mathbf{x} = \begin{pmatrix} x \\ y \end{pmatrix} \longmapsto \mathbf{y}(\mathbf{x}) = \begin{pmatrix} \rho(x,y) \\ \phi(x,y) \end{pmatrix} = \begin{pmatrix} \sqrt{x^2+y^2} \\ \arctan(y/x) \end{pmatrix}. \end{aligned} \tag{V15b}$$

A good way to visualize the polar coordinates is to plot the Cartesian coordinate representation $\mathbf{x}(\rho, \phi)$ as a function of ρ at fixed values of ϕ, and of ϕ at fixed values of ρ, respectively (see Fig. V4). This generates a system of **coordinate lines** in the form of a spider web. The main **advantage of polar coordinates** is that they afford an optimal representation of systems with rotational symmetry. In polar coordinates, points sitting at a fixed distance, R, from the origin have a simple representation, $(\rho, \phi)^T = (R, \phi)^T$, while in Cartesian coordinates we need to parameterize them as pairs, $(x, y)^T$ subject to the constraint $\sqrt{(x)^2 + (y)^2} = R$. Calculations in the latter language involve inconvenient square roots and are generally more complicated and less intuitive.

INFO Notice that in Eq. (V15) the variable ϕ is defined on the *open* interval, $(0, 2\pi)$. Openness is required to ensure differentiability of the coordinate map, including at the boundaries of the underlying intervals.[3] For example, global differentiability is needed to define basis vectors tailored to the coordinate system, as discussed in section V2.3. The price to be paid is that the map defined in this way does not cover the entire plane $\mathbb{R}^2$: its image excludes points of the form $(\mathbf{e}_x \rho\cos(\phi) + \mathbf{e}_y \rho\sin(\phi))_{\phi=0,2\pi} = \mathbf{e}_x\rho + \mathbf{e}_y 0$, i.e. the positive real axis, here denoted as $\mathbb{R}^+ \equiv \{\mathbf{e}_x\rho \,|\, 0 < \rho \in \mathbb{R}\}$ (see the wriggly line in Fig. V4). However, this deficiency does not really limit the practical utility of the map. The reason is that we will mostly work with continuous functions, $f(\rho, \phi)$, whose values at the excluded points can be understood as limits, $f(\rho, 0) \equiv \lim_{\phi\to 0} f(\rho, \phi)$. Although in this text we will follow the mathematics convention to exclusively work with open coordinate intervals, the physics literature frequently extends the ϕ-coordinate domain to the semi-open interval $[0, 2\pi)$. The positive real axis is now included,[1] but the map is no longer differentiable there. We finally refer to the info section on p. **??** where coordinate representations providing full coverage are discussed.

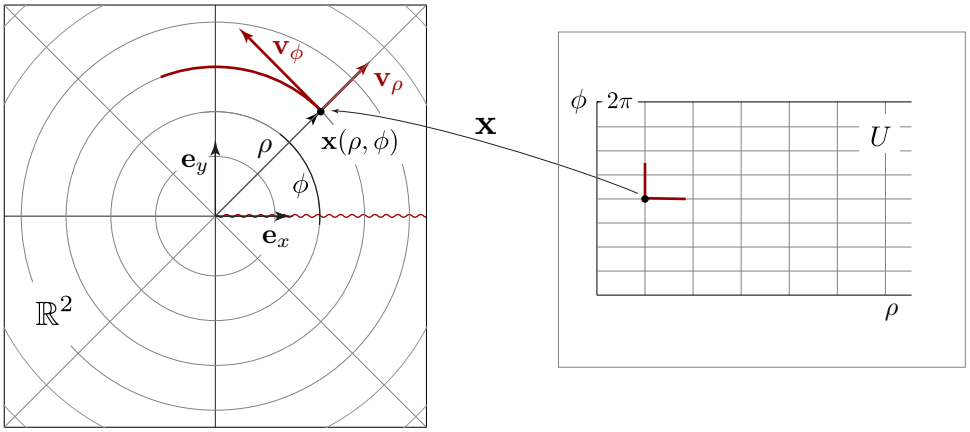


Figure V4: The construction of polar coordinates. Each coordinate pair, $(\rho,\phi)^T \in U$, describes a point, $\mathbf{x}(\rho,\phi) \in \mathbb{R}^2$, in the Cartesian coordinate plane. The concentric and radial lines are lines of constant radius ρ or angle ϕ, respectively. Tangent to these lines are the vectors of the coordinate basis discussed in section V2.3 (see Eq. (V23)). The wriggly line denotes the positive real axis, $\mathbb{R}^+$, which is not covered by the coordinate map.

V2.2 Coordinate transformations

The construction above motivates the following general definition of **curvilinear coordinates**: a system of coordinates is an invertible map,

$$\mathbf{r} : U \to M, \qquad \mathbf{y} \mapsto \mathbf{r}(\mathbf{y}) = \mathbf{r}(y^1, \ldots, y^d)\,, \tag{V16a}$$

between a coordinate domain $U \subset \mathbb{R}^d$, open in $\mathbb{R}^d$, and its image $M \subset \mathbb{R}^n$. [2] The inverse map assigns to each point $\mathbf{r} \in M$ its coordinates $\mathbf{y}(\mathbf{r}) \in U$ (see Fig. V5):

$$\mathbf{y} : M \to U, \qquad \mathbf{r} \mapsto \mathbf{y}(\mathbf{r}) = (y^1(\mathbf{r}), \ldots, y^d(\mathbf{r}))^T\,. \tag{V16b}$$

For example, for the case of polar coordinates discussed above, $M = \mathbb{R}^2 \backslash \mathbb{R}^+$ is the 'slit' two dimensional plane and $U = \mathbb{R}^+ \times (0, 2\pi)$ is its polar coordinate domain.

Note that in Eq. (V16a) the symbol $\mathbf{r}$ is used to denote both the transformation map $\mathbf{r} : U \to M$ and image points $\mathbf{r}(\mathbf{y}) \in M$. A similar statement holds for the symbol $\mathbf{y}$ in Eq. (V16b). Although such double assignments may appear a little confusing at first, they are perfectly consistent and generally used to keep the notation slim.

Now consider a second coordinate system for M, described by a different invertible map, [3]

$$\mathbf{r} : U' \to M, \qquad \mathbf{y}' \mapsto \mathbf{r}(\mathbf{y}') = \mathbf{r}(y'^1, \ldots, y^d)\,, \tag{V17a}$$

[1] However, the origin $(x,y)^T = (0,0)^T$ remains excluded because there the function ϕ is not defined.

[2] The image, M, of the coordinate domain U may be embedded in a space whose dimension is larger than that of the coordinate domain. For example, the description of a sphere (the surface of a three-dimensional ball) requires $d = 2$ coordinates, although the sphere is embedded in $(n = 3)$-dimensional space.

[3] To keep the notation slim, we use the *same* symbol, $\mathbf{r}$, for both the maps $\mathbf{r} : U \to M$ and $\mathbf{r} : U' \to M$, noting that they can be distinguished via the specified domains of definition, U vs. U', or arguments, y vs. y'.

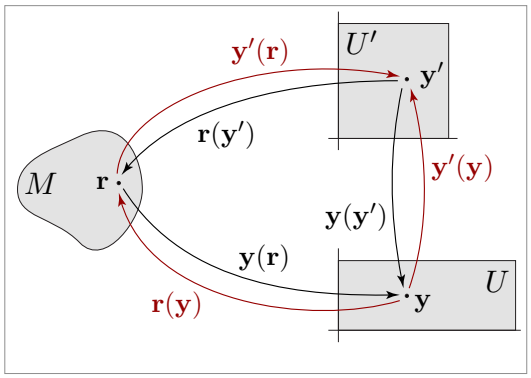


Figure V5: Schematic depiction of two coordinate representations of a subset $M \subset \mathbb{R}^n$ in terms of two coordinate systems, $\mathbf{y}$ and $\mathbf{y}'$, and the transformations between them.

with a different coordinate domain, $U' \subset \mathbb{R}^d$, open in $\mathbb{R}^d$, but the same image $M \subset \mathbb{R}^n$. Its inverse assigns to each point $\mathbf{r} \in M$ its coordinates $\mathbf{y}'(\mathbf{r}) \in U'$ in the second system:

$$\mathbf{y}' : M \to U', \qquad \mathbf{r} \mapsto \mathbf{y}'(\mathbf{r}) = (y'^1(\mathbf{r}), \ldots, y'^d(\mathbf{r}))^T . \tag{V17b}$$

For example, if we choose the second system to be **Cartesian coordinates** in the space $\mathbb{R}^d$, then $\mathbf{y}'$ would stand for the Cartesian coordinate vector $\mathbf{x} \equiv (x^1, \ldots, x^d)^T$, representing $\mathbf{r}$ in an orthonormal basis of $\mathbb{R}^d$.[4] (Unless otherwise specified, we will use the notation $\mathbf{x}$ exclusively for *Cartesian* coordinates.)

Given two such coordinate systems, each point in M can be described in two different ways, $\mathbf{r}(y) = \mathbf{r}(y')$. We may thus construct **coordinate transformations** between them,[5]

$$\mathbf{y}' = \mathbf{y}' \circ \mathbf{r} : U \to U', \qquad \mathbf{y} \mapsto \mathbf{y}'(\mathbf{y}), \tag{V18a}$$
$$\mathbf{y} = \mathbf{y} \circ \mathbf{r} : U' \to U, \qquad \mathbf{y}' \mapsto \mathbf{y}(\mathbf{y}'), \tag{V18b}$$

which express each coordinate point $\mathbf{y}'$ in U' in terms of a coordinate $\mathbf{y}$ in U, or vice versa. Eqs. (V15a) and (V15b) implement these coordinate transformations for the example of polar and Cartesian coordinates of the 2-plane, with $\mathbf{y} = (\rho, \phi)^T$ and $\mathbf{y}' = \mathbf{x} = (x, y)^T$. By construction, the maps $\mathbf{y}'(\mathbf{y})$ and $\mathbf{y}(\mathbf{y}')$ are invertible and smooth; these are the defining features of **diffeomorphic maps**.

Coordinates may be visualized in terms of **coordinate lines**. A coordinate line representing the jth coordinate is generated by varying y^j while keeping all remaining coordinates fixed.

[4] If M is embedded in a space $\mathbb{R}^n$ of dimension $n > d$, and one wants to describe it using Cartesian coordinates, $\mathbf{x} = (x^1, \ldots, x^n) \in \mathbb{R}^n$, then only d of these n components serve as independent coordinates for M, while the remaining $n - d$ ones are functions of the former. For example, a sphere with unit radius in $\mathbb{R}^3$ can be described by the Cartesian coordinates $(x^1, x^2, \sqrt{1 - (x^1)^2 + (x^2)^2})^T$.

[5] Following our predilection for slim notation, we again use the same symbols for maps defined on different domains, since the specified domains and arguments suffice to uniquely identify them. For example, when writing $\mathbf{y}' = \mathbf{y}' \circ \mathbf{r} : U \to U'$, it is understood that the first map in the composition refers to $\mathbf{r} : U \to M$, $\mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$, the second to $\mathbf{y}' : M \to U'$, $\mathbf{r} \mapsto \mathbf{y}'(\mathbf{r})$, and the net result to $\mathbf{y}' : U \to U'$, $\mathbf{y} \mapsto \mathbf{y}'(\mathbf{r}(\mathbf{y})) \equiv \mathbf{y}'(\mathbf{y})$.

This defines a *curve* in M,

$$\mathbf{r}_j : I \to M, \qquad y \mapsto \mathbf{r}_j(y) \equiv \mathbf{r}(y^1, \ldots, y, \ldots, y^d), \tag{V19}$$

where the argument y takes the place of y^j and I is an interval of y-values such that $(y^1, \ldots, y, \ldots, y^d)^T$ lies in U. In this way, each fixed choice for the remaining coordinates, $y^{i\neq j}$, generates its own j-coordinate line in M. If two different sets of coordinates, $\mathbf{y}'$ and $\mathbf{y}$ are defined, one may define the $\mathbf{y}'$-representation of the coordinate line associated with y^j,

$$\mathbf{y}'_j : I \to U', \qquad y \mapsto \mathbf{y}'_j(y) \equiv \mathbf{y}'(y^1, \ldots, y, \ldots, y^d), \tag{V20}$$

i.e. the curve in U' that traces out the $\mathbf{y}'$-coordinates traversed when varying y^j. For example, Fig. V4 shows lines $\mathbf{x}_\rho$ and $\mathbf{x}_\phi$ in the Cartesian coordinate plane traced out by varying the polar coordinates ρ and ϕ, respectively. (How would the coordinate lines $\mathbf{y}_j$ generated in the polar coordinate domain under variation of the Cartesian coordinates look like?)

INFO In many applications M is a subset of an affine space. Once a point of origin, O, has been chosen, the latter becomes identical to a vector space, V, and $M \subset V$. The specification of a fixed orthonormal basis of V then assigns to each $\mathbf{r} \in M$ a Cartesian coordinate vector, $\mathbf{x} \in U_\mathrm{C}$, via the map $\mathbf{x} : M \to U_\mathrm{C}$, $\mathbf{r} \mapsto \mathbf{x}(\mathbf{r})$. This identification is so natural that the **distinction between M and its Cartesian representation domain, U_C**, is easily forgotten. However, within the framework of the present discussion one should draw a clear conceptual distinction between points $\mathbf{r}$ in M (which have invariant meanings such as center points of planets in the solar system), and *any* of their coordinate representations (which are 'languages' in which to describe these points).

V2.3 Coordinate basis and local basis

General definitions

Every point $\mathbf{r}(\mathbf{y}) \in M$ lies at the intersection of d coordinate lines, $\mathbf{r}_j(y)$, as defined in Eq. (V19). We can obtain a tangent vector for the coordinate line $\mathbf{r}_j(y)$ at point $\mathbf{r}(\mathbf{y})$ by computing the corresponding curve velocity, defined as

$$(\mathbf{v}_j)_\mathbf{r} \equiv \mathbf{v}_{j,\mathbf{r}} = \frac{\mathrm{d}}{\mathrm{d}y}\mathbf{r}_i(y) = \frac{\partial}{\partial y^j}\mathbf{r}(\mathbf{y}). \tag{V21}$$

Since the directions of the coordinate lines generally vary with $\mathbf{r}$, the vectors $\mathbf{v}_{j,\mathbf{r}}$, too, depend on the base point $\mathbf{r}$ and a subscript will occasionally be used to emphasize this dependence. However, both in the physics and mathematics literature this subscript is not indicated unless necessary and we will follow this convention.

Since the map $\mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$ is defined to be invertible, the d vectors $\mathbf{v}_{j,\mathbf{r}}$ are all linearly independent.[6] They define a basis of $\mathbb{R}^d$, the **coordinate basis** corresponding to the $\mathbf{y}$-coordinates at $\mathbf{r}$. To obtain an explicit representation of the coordinate basis vectors, we may

[6] If the tangent vectors were linearly dependent, a non-trivial linear combination of these vectors would

expand $\mathbf{r}(\mathbf{y}) = \mathbf{e}_a x^a(\mathbf{y})$ in a *Cartesian* basis; we will temporarily label its basis vectors $\mathbf{e}_a$ by the symbol $a = 1, 2, \ldots, d$, for better discrimination from the index $j = 1, 2, \ldots, d$ labeling the coordinate basis vectors. The Cartesian components $x^a(\mathbf{y})$ of $\mathbf{r}(\mathbf{y})$ are functions of the curvilinear coordinates, but the Cartesian basis vectors $\mathbf{e}_a$ are not. Therefore Eq. (V21) yields

$$\mathbf{v}_j(\mathbf{y}) = \mathbf{e}_a \frac{\partial x^a(\mathbf{y})}{\partial y^j}. \tag{V22}$$

For example, in **polar coordinates**, the differentiation of $\mathbf{r}(\theta, \phi)$ in Eq. (V14) w.r.t. coordinates yields

$$\begin{aligned} \mathbf{v}_\rho &= \mathbf{e}_x \cos\phi + \mathbf{e}_y \sin\phi, \\ \mathbf{v}_\phi &= \rho(-\mathbf{e}_x \sin\phi + \mathbf{e}_y \cos\phi) \end{aligned} \tag{V23}$$

for the polar coordinate basis vectors (illustrated in Fig. V4). Note how these vectors emerge naturally as functions of the coordinates $\mathbf{y} = (\rho, \phi)^T$.

(Local) metric tensor

In general, the vectors $\{\mathbf{v}_{j,\mathbf{r}}\}$ of a coordinate basis are neither normalized, nor mutually orthogonal. However, many coordinate systems of practical relevance (polar, spherical, and cylindrical, to mention the most important ones) do have an orthogonal (although not normalized) coordinate basis. Systems possessing this feature are called **orthogonal coordinate system**.

In either case the local geometric structure (i.e norm and relative orientation) of the coordinate basis at a point $\mathbf{r}$ is described by the **metric tensor** Eq. (L47),

$$g_{ij,\mathbf{r}} \equiv \langle \mathbf{v}_{i,\mathbf{r}}, \mathbf{v}_{j,\mathbf{r}} \rangle \,, \tag{V24}$$

where $\langle\ ,\ \rangle$ is the standard scalar product in $\mathbb{R}^d$. For example, the **metric in polar coordinates** is given by

$$g_{\rho\rho} = 1, \qquad g_{\phi\phi} = \rho^2, \qquad g_{\rho\phi} = g_{\phi\rho} = 0, \tag{V25}$$

which shows how the norm of $\mathbf{v}_\phi$ grows with increasing distance from the origin while that of $\mathbf{v}_\rho$ remains constant. For later reference, we also state the components of the inverse metric, defined via Eq. (L53):

$$g^{\rho\rho} = 1, \qquad g^{\phi\phi} = \rho^{-2}, \qquad g^{\rho\phi} = g^{\phi\rho} = 0. \tag{V26}$$

---

exist that yields zero, $\mathbf{v}_j a^j = \partial_j \mathbf{r}\, a^j = \mathbf{0}$. Consequently the variation of $\mathbf{r}(\mathbf{y})$ upon a shift of its argument to $\mathbf{y} + \delta\,\mathbf{a}$ would vanish: $\mathbf{r}(\mathbf{y} + \delta\,\mathbf{a}) - \mathbf{r}(\mathbf{y}) \simeq \delta\, \partial_j \mathbf{r}\, a^j = \mathbf{0}$, where Eq. (C34) was used for each of the components r^j. Thus two different coordinates would be mapped onto the same image point, $\mathbf{r}(\mathbf{y} + \delta\,\mathbf{a}) = \mathbf{r}(\mathbf{y})$, in contradiction to the assumed invertibility of the map $\mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$.

Local basis

By construction, the coordinate basis vectors point in the direction of the coordinate lines and are computed via the straightforward derivative (V21). This makes them optimally suited to describe problems in the representation defined by the $\mathbf{y}$-coordinates. One may even argue that the lack of normalization that is characteristic for this basis is an intuitive feature. For example, the vector $\mathbf{v}_\phi$ defined in Eq. (V23) has norm $\|\mathbf{v}_\phi\| = \rho$. This expresses the fact that $\mathbf{v}_\phi = \partial_\phi \mathbf{r}$ describes the change in $\mathbf{r}$ induced by a change in the angular coordinate, which is the larger, the larger the norm $|\mathbf{r}| = \rho$ is (think about this point). However, in the physics community it is customary to *normalize* the vectors of the coordinate basis and in this way pass to what is called the **local basis**. The vectors of the local basis are defined as

$$\mathbf{e}_{j,\mathbf{r}} = \frac{\mathbf{v}_{j,\mathbf{r}}}{\sqrt{g_{jj}}} = \frac{\mathbf{v}_{j,\mathbf{r}}}{\|\mathbf{v}_{j,\mathbf{r}}\|}, \tag{V27}$$

and frequently denoted by the letter $\mathbf{e}$. In this case, they are distinguished from the vectors of the Cartesian basis by their subscript. For example the **local basis in polar coordinates** is given by

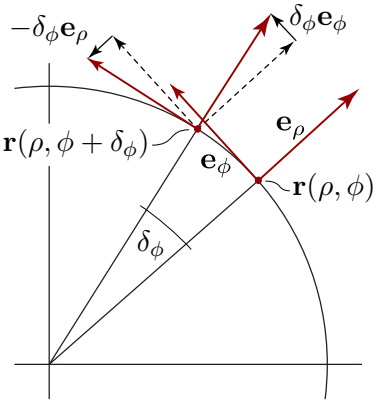
$$\begin{aligned} \mathbf{e}_\rho &= \mathbf{v}_\rho = \mathbf{e}_x \cos\phi + \mathbf{e}_y \sin\phi\,, \\ \mathbf{e}_\phi &= \frac{1}{\rho}\mathbf{v}_\phi = -\mathbf{e}_x \sin\phi + \mathbf{e}_y \cos\phi\,. \end{aligned} \tag{V28}$$

Although the normalization feature is convenient for some purposes, it comes with a price tag: the normalization factor, $(g_{jj}(\mathbf{y}))^{-1/2}$, is a function of $\mathbf{y}$. In mathematical (and physical) practice, the coordinate or local basis vectors usually appear as building blocks in operations involving several derivatives w.r.t. coordinates $\mathbf{y}$. These operations become more complicated in the presence of a $\mathbf{y}$-dependent normalization function. Therefore, one may reason that this is one of the cases where it would actually be advantageous to use *un*normalized basis vectors.

As an example of a relatively easy local basis vector derivative operation, consider the partial derivatives

$$\begin{aligned} \partial_\rho \mathbf{e}_\rho &= 0, \qquad & \partial_\phi \mathbf{e}_\rho &= \mathbf{e}_\phi, \\ \partial_\rho \mathbf{e}_\phi &= 0, \qquad & \partial_\phi \mathbf{e}_\phi &= -\mathbf{e}_\rho, \end{aligned} \tag{V29}$$

which follow directly from the definition Eq. (V28). These derivatives describe how the vectors vary under variations of coordinates (cf. the figure). Evidently a variation in ρ leaves both basis vectors unchanged, but a variation in ϕ changes $\mathbf{e}_\rho$ in a direction parallel to $\mathbf{e}_\phi$, and $\mathbf{e}_\phi$ in a direction anti-parallel to $\mathbf{e}_\rho$.



In applications such derivatives appear, e.g., when the local basis is employed to describe **physical motion along curves**. As an example, consider a two-dimensional curve with parameterization $\mathbf{r}(t)$. Expressed in Cartesian and local polar basis vectors, this vector assumes the form

$$\mathbf{r}(t) = \mathbf{e}_x x(t) + \mathbf{e}_y y(t) = \mathbf{e}_\rho(t)\, \rho(t) = \mathbf{e}_{\rho,\mathbf{r}(t)}\, \rho(t),$$

where the subscript $\mathbf{r}(t)$ in $\mathbf{e}_{\rho,\mathbf{r}(t)}$ emphasizes that the basis vector may change with time as the base point $\mathbf{r}(t)$ varies. The curve velocity thus takes the form

$$\dot{\mathbf{r}} = \mathbf{e}_\rho \, \dot{\rho} + \dot{\mathbf{e}}_\rho \, \rho, \tag{V30}$$

where the time arguments have been suppressed for notational compactness. It remains to compute the time derivative $\dot{\mathbf{e}}_\rho$ explicitly. Since the time dependence of a local basis vector $\mathbf{e}_i(t)$ comes from the time dependence of the coordinates at which it is evaluated, as $\mathbf{e}_i(t) = \mathbf{e}_{i,\mathbf{r}(t)} = \mathbf{e}_{i,\mathbf{r}(\rho(t),\phi(t))}$, the chain rule of calculus Eq. (C38) (with the identifications $\mathbf{f} \to \mathbf{e}$, $\mathbf{g} \to \mathbf{y} = (\rho, \phi)^T$, $x \to t$) yields

$$\dot{\mathbf{e}}_\rho = (\partial_\rho \mathbf{e}_\rho) \, \dot{\rho} + (\partial_\phi \mathbf{e}_\rho) \, \dot{\phi} \overset{(V29)}{=} \mathbf{e}_\phi \, \dot{\phi} \,, \qquad \dot{\mathbf{e}}_\phi = (\partial_\rho \mathbf{e}_\phi) \, \dot{\rho} + (\partial_\phi \mathbf{e}_\phi) \, \dot{\phi} \overset{(V29)}{=} -\mathbf{e}_\rho \, \dot{\phi} \,. \tag{V31}$$

The curve velocity (V30) can thus be written as

$$\dot{\mathbf{r}} = \mathbf{e}_\rho \, \dot{\rho} + \mathbf{e}_\phi \, \rho \, \dot{\phi} \,. \tag{V32}$$

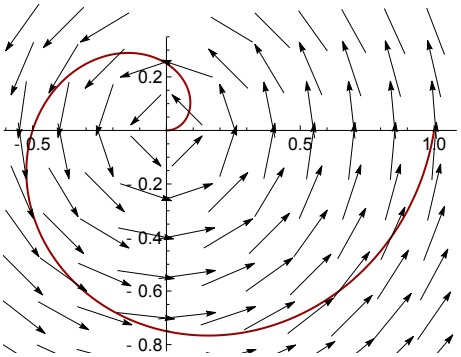
This equation states that $\dot{\rho}$ and $\dot{\phi}$, the rates of change of the radial or polar coordinates during the motion, define the corresponding components of the velocity vector. The proportionality of the polar component to the radial coordinate ρ accounts for the fact that changing ϕ shifts the point $\mathbf{r}(t)$ by an amount that increases with its distance from the origin.

INFO Occasionally, it becomes necessary to compute higher-order derivatives of curve parameterizations in curvilinear coordinates. As an example, consider the **curve acceleration for a curve in polar coordinates**. Differentiating $\dot{\mathbf{r}}$ w.r.t. time and using Eq. (V31) once more, we obtain

$$\begin{aligned} \mathbf{a} = \mathrm{d}_t(\dot{\mathbf{r}}) &\overset{(V32)}{=} \mathrm{d}_t(\mathbf{e}_\rho \, \dot{\rho} + \mathbf{e}_\phi \, \rho \, \dot{\phi}) = \dot{\mathbf{e}}_\rho \, \dot{\rho} + \mathbf{e}_\rho \, \ddot{\rho} + \dot{\mathbf{e}}_\phi \, \rho \, \dot{\phi} + \mathbf{e}_\phi \, \dot{\rho} \, \dot{\phi} + \mathbf{e}_\phi \, \rho \, \ddot{\phi} \\ &\overset{(V31)}{=} (\mathbf{e}_\phi \dot{\phi}) \, \dot{\rho} + \mathbf{e}_\rho \, \ddot{\rho} + (-\mathbf{e}_\rho \dot{\phi}) \, \rho \, \dot{\phi} + \mathbf{e}_\phi \, \dot{\rho} \, \dot{\phi} + \mathbf{e}_\phi \, \rho \, \ddot{\phi} = \mathbf{e}_\rho \, (\ddot{\rho} - \rho \, \dot{\phi}^2) + \mathbf{e}_\phi \, (2\dot{\rho} \, \dot{\phi} + \rho \, \ddot{\phi}). \end{aligned} \tag{V33}$$

To qualitatively interpret the different contributions to the velocity vector, consider different types of motion, e.g. purely radial motion with $\dot{\phi} = 0$, or purely angular motion with $\dot{\rho} = 0$, or motion at constant angular velocity with $\dot{\phi} = \mathrm{const}$.

The derivation of equation (V33) shows that computations with curvilinear coordinates require care. A useful safety check is to monitor the **physical dimensions** of terms at all stages of the computation. For example, the vector $\mathbf{r}$ has physical dimension 'length'. To express this compactly one writes $[\mathbf{r}] = \text{length}$, using square brackets as shorthand for 'dimension of'. Each time derivative divides this dimension by one dimension of time, i.e. $[\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}] = \text{length/time}$ and $[\mathbf{a}] = [\frac{\mathrm{d}^2\mathbf{r}}{\mathrm{d}t^2}] = \text{length/time}^2$. The different terms contributing to Eq. (V33) all have this dimension. Regardless of the context, the dimensional analysis of results is a potent aid in avoiding computational errors.



EXAMPLE As an example illustrating the usefulness of curvilinear coordinates, consider the **work done by a rotationally symmetric force field**, $\mathbf{F}(\mathbf{r}) = f\mathbf{e}_\phi$, $\mathbf{r} \neq \mathbf{0}$, along a spiral path, γ, in the plane. Except for the origin where the angular direction is not defined, the force is colinear to $\mathbf{e}_\phi$, and has constant strength, $f = \text{const.}$[7] Consider a path parameterized as $\mathbf{y}(t) = (\rho(t), \phi(t))^T = (\frac{tR}{t_0}, 2\pi\frac{t}{t_0})^T$, describing a spiral winding once around the origin between times $t = 0$ and t_0 and reaching a radial distance R at the final time (see the figure, where distance is plotted in units of R, such that the final separation corresponds to a unit distance). Substituting this parameterization into Eq. (V32) we obtain $\dot{\mathbf{r}} = \frac{R}{t_0}(\mathbf{e}_\rho + 2\pi\frac{t}{t_0}\mathbf{e}_\phi)$, and $\dot{\mathbf{r}} \cdot \mathbf{F} = \frac{2\pi Rft}{t_0^2}$. This yields the work integral

$$W = \int_\gamma \mathrm{d}r \cdot \mathbf{F} = \int_0^{t_0} \mathrm{d}t\, \dot{\mathbf{r}} \cdot \mathbf{F} = \int_0^{t_0} \mathrm{d}t\, \frac{2\pi Rft}{t_0^2} = \pi Rf.$$

The positive sign indicates that work is done *by* the force along a path approximately aligned with it. Also note that excluding the positive real axis from the definition of the variable ϕ implies excluding the points $\mathbf{r}(0)$ and $\mathbf{r}(t_0)$ from the curve, where $\phi = 0$ and 2π, respectively, i.e. restricting the curve parameter t to the *open* interval $(0, t_0)$ instead of using the closed interval $t \in [0, t_0]$. This, however, does not change the value of the integral.

Try doing the same calculation in Cartesian coordinates; you will find that it becomes technically more complicated and less intuitive.

V2.4 Cylindrical and spherical coordinates

In low dimensions, $d = 2, 3$, the continuous symmetry most frequently encountered is rotational symmetry, namely rotational symmetry about a point in $\mathbb{R}^2$, a fixed rotation axis in $\mathbb{R}^3$ or a point in $\mathbb{R}^3$. To describe these cases, tailor-made curvilinear coordinate systems have been devised. These are the polar coordinates discussed above, and the three-dimensional cylindrical and spherical coordinate systems, to be introduced next.

Cylindrical coordinates

Cylindrical coordinates are designed to describe problems which are rotationally symmetric around a fixed *axis*. For example, the axially symmetric magnetic field generated by a straight, current-carrying wire is conveniently described in cylindrical coordinates. The construction of

[7] In fact, since we excluded the entire positive real axis when defining polar coordinates [Eq. (V15)], we implicity do the same when expressing $\mathbf{F}$ in terms of $\mathbf{e}_\phi$. However, the computation of the work below shows that this omission is irrelevant, both from a mathematical and physical perspective.

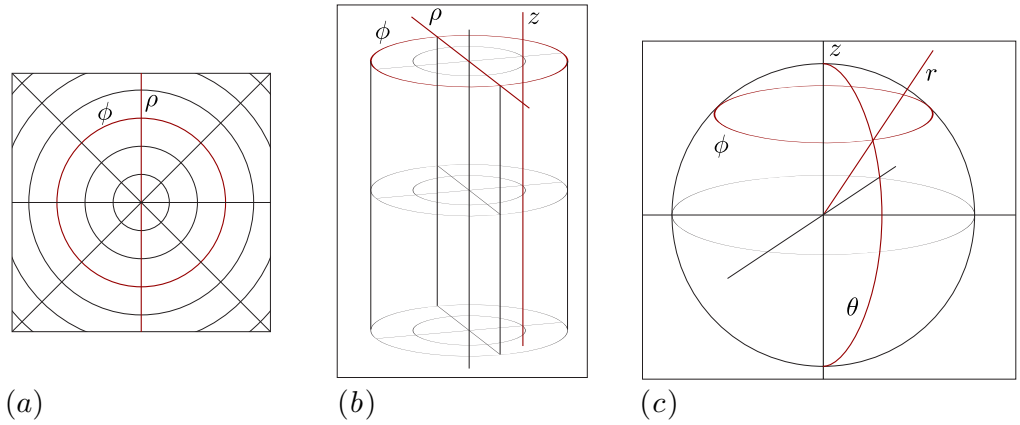


Figure V6: Coordinate lines of the three most frequently used curvilinear coordinate systems. (a) Two-dimensional polar coordinates, (b) cylindrical coordinates, and (c) spherical coordinates (sometimes called three-dimensional polar coordinates).

cylindrical coordinates is shown in figure V6: following standard conventions we define the x^3-axis of a Cartesian coordinate system as the symmetry axis of the problem. We next pick two directions orthogonal to it to define a three dimensional Cartesian system of coordinates (x, y, z). A vector $\mathbf{r}$ may then be decomposed as $\mathbf{r} = \mathbf{e}_z z + \mathbf{r}_\perp$, where $\mathbf{r}_\perp \perp \mathbf{e}_z$ lies in the xy-plane. Choosing polar coordinates, (ρ, ϕ), to parameterize this plane, we obtain a representation $\mathbf{r}_\perp = \mathbf{e}_x \rho\cos\phi + \mathbf{e}_y \rho\sin\phi$ for the transverse component, and the representation

$$\boxed{\mathbf{r}(\rho, \phi, z) = \mathbf{e}_x \rho\cos\phi + \mathbf{e}_y \rho\sin\phi + \mathbf{e}_z z,} \tag{V34}$$

for the three-dimensional vector. The corresponding transformation map between its **cylindrical coordinates** $\mathbf{y} = (\rho, \phi, z)^T$ and its Cartesian coordinates $\mathbf{x} = (x, y, z)^T$ is given by

$$\begin{aligned} \mathbf{x} : \mathbb{R}^+ \times (0, 2\pi) \times \mathbb{R} &\longrightarrow \mathbb{R}^3 \backslash (\mathbb{R}^+ \times \{0\} \times \mathbb{R}), \\ \mathbf{y} = \begin{pmatrix} \rho \\ \phi \\ z \end{pmatrix} &\longmapsto \mathbf{x}(\mathbf{y}) = \begin{pmatrix} x(\rho, \phi, z) \\ y(\rho, \phi, z) \\ z(\rho, \phi, z) \end{pmatrix} = \begin{pmatrix} \rho\cos\phi \\ \rho\sin\phi \\ z \end{pmatrix}, \end{aligned} \tag{V35a}$$

and the inverse map is

$$\begin{aligned} \mathbf{y} : \mathbb{R}^3 \backslash (\mathbb{R}^+ \times \{0\} \times \mathbb{R}) &\longrightarrow \mathbb{R}^+ \times (0, 2\pi) \times \mathbb{R}, \\ \mathbf{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} &\longmapsto \mathbf{y}(\mathbf{x}) = \begin{pmatrix} \rho(x, y, z) \\ \phi(x, y, z) \\ z(x, y, z) \end{pmatrix} = \begin{pmatrix} \sqrt{x^2 + y^2} \\ \arctan(\frac{y}{x}) \\ z \end{pmatrix}. \end{aligned} \tag{V35b}$$

As for polar coordinates, we ensure global differentiability by defining ϕ on an *open* interval, $\phi = (0, 2\pi)$. The image of the map $\mathbf{y} \to \mathbf{x}$ therefore excludes all image points of the form $(x, y, z)^T = (\rho, 0, z)^T$, which together define the half-plane of positive x-values at $y = 0$, $\mathbb{R}^+ \times \{0\} \times \mathbb{R} \equiv \{(x, y, z)^T | x \in \mathbb{R}^+, y = 0, z \in \mathbb{R}\}$ (see the shaded plane in figure V7).

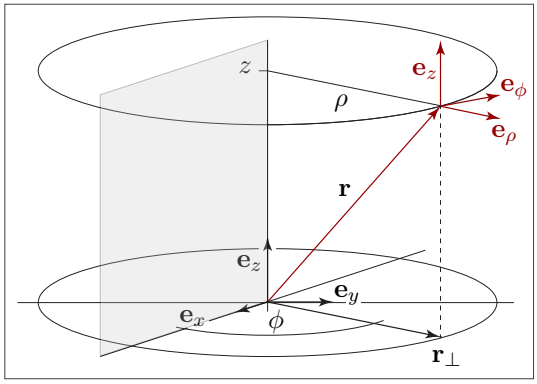


Figure V7: The definition of cylindrical coordinates [Eq. (V35)].

Eqs. (V22), (V24), and (V27) can be used to compute the **coordinate basis vectors for cylindrical coordinates**, $\{\mathbf{v}_\rho, \mathbf{v}_\phi, \mathbf{v}_z\}$, the metric tensor, and the **local basis vectors**, $\{\mathbf{e}_\rho, \mathbf{e}_\phi, \mathbf{e}_z\}$. One finds

$$\begin{aligned} \mathbf{v}_\rho &= \mathbf{e}_x \cos\phi + \mathbf{e}_y \sin\phi, & g_{\rho\rho} &= 1, & \mathbf{e}_\rho &= \mathbf{v}_\rho, \\ \mathbf{v}_\phi &= \rho(-\mathbf{e}_x \sin\phi + \mathbf{e}_y \cos\phi), & g_{\phi\phi} &= \rho^2, & \mathbf{e}_\phi &= \frac{1}{\rho}\mathbf{v}_\phi, \\ \mathbf{v}_z &= \mathbf{e}_z, & g_{zz} &= 1, & \mathbf{e}_z &= \mathbf{e}_z. \end{aligned} \tag{V36}$$

EXERCISE Verify the **orthogonality of the cylindrical coordinate basis**, $g_{ij} = 0, i \neq j$. Also verify that the local basis defines a right-handed system, $\mathbf{e}_\rho \times \mathbf{e}_\phi = \mathbf{e}_z$. The basis comprises a fixed vector in z-direction, $\mathbf{e}_z$, and the local basis, $\{\mathbf{e}_\rho, \mathbf{e}_\phi\}$, of a polar system spanning the plane perpendicular to z. Notice that the point $\mathbf{r}$ now affords the simple representation

$$\mathbf{r} = \mathbf{e}_\rho\, \rho + \mathbf{e}_z z. \tag{V37}$$

From here, the velocity of a time-dependent vector $\mathbf{r}(t)$ is obtained as

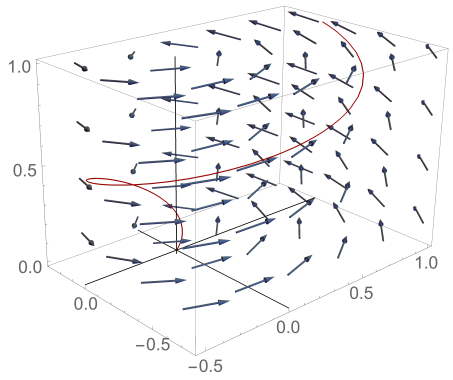
$$\dot{\mathbf{r}} = \mathbf{e}_\rho\, \dot\rho + \mathbf{e}_\phi\, \rho\, \dot\phi + \mathbf{e}_z \dot z. \tag{V38}$$

EXAMPLE Let us take another look at the spiral curve defined in (V9). In cylindrical coordinates, it is represented as $(\rho(t), \phi(t), z(t))^T = (1, 2\pi t, (2/3)t^{3/2})^T$. We may now use the representation (V37) to represent its velocity as

$$\dot{\mathbf{r}}(t) = \dot{\mathbf{e}}_\rho\, \rho + \mathbf{e}_\rho\, \dot\rho + \dot{\mathbf{e}}_z z + \mathbf{e}_z \dot z \overset{(V31)}{=} (\mathbf{e}_\phi\, \dot\phi)\rho + 0 + 0 + \mathbf{e}_z \dot z = \mathbf{e}_\phi\, 2\pi + \mathbf{e}_z\, t^{1/2}. \tag{V39}$$

This equation describes how the velocity vector winds around the z-axis while building up a growing z-component. In agreement with our previous analysis, the norm of this vector is obtained as $\|\dot{\mathbf{r}}\| = \sqrt{(2\pi)^2 + t}$. Although the expressions in cylindrical coordinates are not necessarily 'simpler' than their Cartesian counterparts, they are better suited to expose the geometry of the curve.

EXAMPLE As another example, consider a force $\mathbf{F} = f\mathbf{e}_\phi + c\,\mathbf{e}_z$ similar to that discussed on p. 404, but now with a constant component, c, in the z-direction. We aim to compute the work done along a three-dimensional spiral, which in a time t_0 winds once around the origin up to a maximal separation R from the central axis, while also climbing up to a height Z (see the figure, where ρ and z are indicated in units of R and Z, respectively). In cylindrical coordinates, this curve can be parameterized as $\mathbf{y}(t) = (\rho(t), \phi(t), z(t))^T = (R\frac{t}{t_0}, 2\pi\frac{t}{t_0}, Z\frac{t}{t_0})^T$. Eq. (V38) yields $\dot{\mathbf{r}} = \frac{R}{t_0}(\mathbf{e}_\rho + 2\pi\frac{t}{t_0}\mathbf{e}_\phi) + \frac{Z}{t_0}\mathbf{e}_z$, hence $\dot{\mathbf{r}}\cdot\mathbf{F} = \frac{2\pi Rft}{t_0^2} + \frac{Zc}{t_0}$, thus the work integral gives



$$W = \int_\gamma \mathrm{d}r\cdot\mathbf{F} = \int_0^{t_0} \mathrm{d}t\,\dot{\mathbf{r}}\cdot\mathbf{F} = \int_0^{t_0} \mathrm{d}t\,\left(\tfrac{2\pi Rft}{t_0^2} + \tfrac{Zc}{t_0}\right) = \pi Rf + Zc\,.$$

Spherical coordinates

Spherical coordinates are used to describe problems possessing rotational symmetry around a fixed point in Euclidean space. We choose this point as the origin of a Cartesian coordinate system. In cases where the problem possesses a particular axis of interest,[8] this axis is commonly chosen as the z-axis. The x- and y-axes then span the 'equatorial plane', as indicated in figure V8. A point $\mathbf{r}$ is now described in terms of the following three numbers: its distance, r, from the origin; the angle, θ, between the vector $\mathbf{r}$ and the z-axis; and the angle, ϕ, enclosed by the x-axis and the projection of $\mathbf{r}$ onto the equatorial plane.

Elementary geometry shows that the z-component of a vector can now be represented as $r\cos\theta$, where $\theta \in (0,\pi)$. Its perpendicular distance from the central axis is given by $r\sin\theta$, which means that the x- and y-components are given by, respectively, $(r\sin\theta)\cos\phi$ and $(r\sin\theta)\sin\phi$. This is summarized by the representation

$$\boxed{\mathbf{r}(r,\theta,\phi) = \mathbf{e}_x\, r\sin\theta\cos\phi + \mathbf{e}_y r\sin\theta\sin\phi + \mathbf{e}_z r\cos\theta.} \qquad \text{(V40)}$$

The map describing the change from **spherical coordinates** $\mathbf{y} = (r,\theta,\phi)^T$ to Cartesian coordinates $\mathbf{x} = (x,y,z)^T$ is thus given by

$$\mathbf{x} : \mathbb{R}^+ \times (0,\pi) \times (0,2\pi) \longrightarrow \mathbb{R}^3\backslash(\mathbb{R}^+ \times \{0\} \times \mathbb{R})\,, \qquad \text{(V41a)}$$

$$\mathbf{y} = \begin{pmatrix} r \\ \theta \\ \phi \end{pmatrix} \longmapsto \mathbf{x}(\mathbf{y}) = \begin{pmatrix} x(r,\theta,\phi) \\ y(r,\theta,\phi) \\ z(r,\theta,\phi) \end{pmatrix} = \begin{pmatrix} r\sin\theta\cos\phi \\ r\sin\theta\sin\phi \\ r\cos\theta \end{pmatrix},$$

[8] For the description of a planet, this might be the axis connecting its magnetic north and south poles, for example.

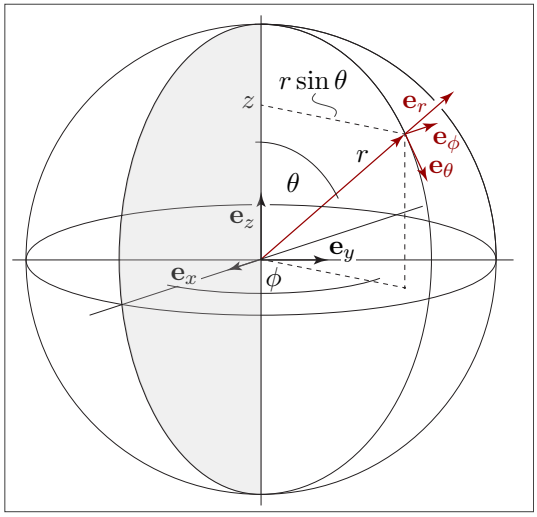


Figure V8: The definition of spherical coordinates [Eq. (**??**)].

and its inverse

$$\mathbf{y} : \mathbb{R}^3 \backslash \mathbb{R}^+ \times \{0\} \times \mathbb{R} \longrightarrow \mathbb{R}^+ \times (0,\pi) \times (0,2\pi), \tag{V41b}$$

$$\mathbf{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} \longmapsto \mathbf{y}(\mathbf{x}) = \begin{pmatrix} r(x,y,z) \\ \theta(x,y,z) \\ \phi(x,y,z) \end{pmatrix} = \begin{pmatrix} \sqrt{x^2+y^2+z^2} \\ \arccos\left(\frac{z}{\sqrt{x^2+y^2+z^2}}\right) \\ \arctan(y/x) \end{pmatrix}.$$

Since we take the intervals for ϕ and θ to be open, the image of the map $\mathbf{x}(\mathbf{y})$ excludes the half-plane $\mathbb{R}^+ \times \{0\} \times \mathbb{R}$, as for cylindrical coordinates.

EXERCISE Verify that the **coordinate basis vectors for spherical coordinates**, $\{\mathbf{v}_r, \mathbf{v}_\theta, \mathbf{v}_\phi\}$, the metric tensor, and the **local basis vectors**, $\{\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\phi\}$, are given by, respectively,

$$\begin{aligned}
&\mathbf{v}_r = \mathbf{e}_x \sin\theta\cos\phi + \mathbf{e}_y \sin\theta\sin\phi + \mathbf{e}_z\cos\theta, && g_{rr} = 1, && \mathbf{e}_r = \mathbf{e}_r, \\
&\mathbf{v}_\theta = r(\mathbf{e}_x\cos\theta\cos\phi + \mathbf{e}_y\cos\theta\sin\phi - \mathbf{e}_z\sin\theta), && g_{\theta\theta} = r^2, && \mathbf{e}_\theta = \frac{1}{r}\mathbf{v}_\theta, \\
&\mathbf{v}_\phi = r\sin\theta\,(-\mathbf{e}_x\sin\phi + \mathbf{e}_y\cos\phi), && g_{\phi\phi} = r^2\sin^2\theta, && \mathbf{e}_\phi = \frac{1}{r\sin\theta}\mathbf{v}_\phi,
\end{aligned} \tag{V42}$$

with $g_{i\neq j} = 0$. Again the off-diagonal elements of the metric tensor vanish, implying that the local basis vectors are mutually orthogonal. Verify that they form a right-handed system, $\mathbf{e}_r \times \mathbf{e}_\theta = \mathbf{e}_\phi$. In the local basis the point $\mathbf{r}$ has the simple representation

$$\mathbf{r} = \mathbf{e}_r\, r. \tag{V43}$$

Verify that the velocity of a time-dependent vector $\mathbf{r}(t)$, obtained by computing the time derivative of this expression, is given by

$$\dot{\mathbf{r}} = \mathbf{e}_r\,\dot{r} + \mathbf{e}_\theta\, r\dot{\theta} + \mathbf{e}_\phi\, r\dot{\phi}\sin\theta\,. \tag{V44}$$

INFO Curvilinear coordinates are tailored to describe structures of lower dimension, $n < d$, embedded in d-dimensional space. For example, the **surface of a sphere** of unit radius, S^2, is an $(n = 2)$-dimensional object embedded in $(d = 3)$-dimensional space. It can be parameterized by keeping the radius of the sphere, $r = 1$ fixed and letting the two angular coordinates θ and ϕ run through their domain of definition. In this way, we obtain a representation

$$(0, \pi) \times (0, 2\pi) \to S^2 \subset \mathbb{R}^3, \qquad (\theta, \phi) \mapsto \mathbf{r}(1, \theta, \phi),$$

playing a role analogous to the one-dimensional parameterization $t \mapsto \mathbf{r}(t)$ of a curve (which can be seen as a $(n = 1)$-dimensional object in d-dimensional space). In mathematical terminology, such generalizations of smooth n-dimensional 'surfaces' are called **differentiable manifolds** and their description in terms of generalized coordinates is a concept of great importance in physics and mathematics. We will return to this point in chapter V5 where advanced methods for the description of manifolds are introduced.

V2.5 Local coordinate bases and linear algebra

REMARK This section re-interprets the concepts introduced above from a linear algebraic perspective. It introduces methodology for working with curvilinear coordinates that will facilitate our later discussion of various geometric structures. The section requires familiarity with matrices, in particular the transformation matrices between different base (section L5.6). It is included for reference purposes and may be skipped at first reading.

Jacobi matrix

From the perspective of linear algebra, Eq. (V22) defines a linear transformation between the two bases $\{\mathbf{e}_a\}$ and $\{\mathbf{v}_j\}$, of the form $\mathbf{v}_j = \mathbf{e}_a J^a{}_j$. The matrix mediating this transformation,

$$J^a{}_j \equiv \left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right)^a{}_j \equiv \frac{\partial x^a(\mathbf{y})}{\partial y^j}, \tag{V45}$$

is called the **Jacobi matrix** of the map $\mathbf{y} \mapsto \mathbf{x}(\mathbf{y})$ that expresses Cartesian in terms of curvilinear coordinates. Its matrix elements are generally nonlinear functions of the coordinates y^j. However when considered at a fixed point $\mathbf{r}$, i.e. a fixed set of coordinates $\mathbf{y}$, the numbers $J^a{}_j$ define a fixed $d \times d$ matrix, and all the concepts of linear algebra can be applied to it.

The **inverse of the Jacobi matrix** is given by

$$(J^{-1})^j{}_a = \left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)^j{}_a \equiv \frac{\partial y^j(\mathbf{x})}{\partial x^a}, \tag{V46}$$

where the curvilinear coordinates $\mathbf{y} = \mathbf{y}(\mathbf{x})$ are now interpreted as functions of the Cartesian coordinates. That these matrices are inverse to each other can be checked as

$$J^a{}_j (J^{-1})^j{}_b = \frac{\partial x^a(\mathbf{y})}{\partial y^j}\frac{\partial y^j(\mathbf{x})}{\partial x^b} = \frac{\partial x^a}{\partial x^b} = \delta^a{}_b,$$

where the chain rule Eq. (C36) was used. The inverse matrix can then be used to switch from the coordinate basis back to the Cartesian basis using $\mathbf{e}_a = \mathbf{v}_j (J^{-1})^j{}_a$, i.e.

$$\mathbf{e}_a = \mathbf{v}_j(\mathbf{y}(\mathbf{x}))\frac{\partial y^j(\mathbf{x})}{\partial x^a}. \tag{V47}$$

Here, both factors on the right vary as functions of $\mathbf{x}$. However, they do so in such a way that their product yields the constant Cartesian basis vectors $\mathbf{e}_a$.

Now let $\mathbf{u}(\mathbf{r})$ be a generic vector at the point $\mathbf{r} = \mathbf{r}(\mathbf{x}) = \mathbf{r}(\mathbf{y})$. Depending on which basis is used, it affords the two representations, $\mathbf{u} = \mathbf{e}_a u^a(\mathbf{x}) = \mathbf{v}_j(\mathbf{y}) u^j(\mathbf{y})$, where the choice of subscript, a vs. j, indicates which basis is referred to. (In practice, the slightly ambiguous notation, using the same symbol u for the coefficients, $u^j(\mathbf{x})$ or $u^a(\mathbf{y})$, of a vector in different bases does not create problems, see the examples below.) From linear algebra we know that the corresponding **change between vector components** is given by the transformation matrix as $u^a = J^a{}_j u^j$, and $u^j = (J^{-1})^j{}_a u^a$, or

$$u^a(\mathbf{x}) = \frac{\partial x^a(\mathbf{y})}{\partial y^j} u^j(\mathbf{y})\bigg|_{\mathbf{y}=\mathbf{y}(\mathbf{x})}, \qquad u^j(\mathbf{y}) = \frac{\partial y^j(\mathbf{x})}{\partial x^a} u^a(\mathbf{x})\bigg|_{\mathbf{x}=\mathbf{x}(\mathbf{y})}. \tag{V48}$$

Here, the subscript $\mathbf{y} = \mathbf{y}(\mathbf{x})$ emphasizes that the expression on the r.h.s. of the first equality emerges as a function of the generalized coordinates, $\mathbf{y}$. However, when featuring in a coordinate change to Cartesian coordinates, $\mathbf{x}$, all $\mathbf{y}$-dependences should be expressed through $\mathbf{x}$ via the unique correspondence $\mathbf{y} = \mathbf{y}(\mathbf{x})$.

Example: Jacobi Matrix of polar coordinates

From Eq. (V15a) the **Jacobi matrix** of the polar coordinate system is readily obtained as[9]

$$J = \frac{\partial(x,y)}{\partial(\rho,\phi)} = \begin{pmatrix} \frac{\partial x}{\partial \rho} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial \rho} & \frac{\partial y}{\partial \phi} \end{pmatrix} = \begin{pmatrix} \cos\phi & -\rho\sin\phi \\ \sin\phi & \rho\cos\phi \end{pmatrix}, \tag{V49}$$

where $J = J^a{}_j$ now carries the indices $a = x, y$ and $j = \rho, \phi$. Inserting the elements of J into Eq. (V22), one indeed obtains Eq. (V23) for the transformation between the basis vectors $\{\mathbf{v}_\rho, \mathbf{v}_\phi\}$ and $\{\mathbf{e}_x, \mathbf{e}_y\}$.

The passage in opposite direction is mediated by the inverse Jacobi matrix, which from Eq. (V15b) is obtained as

$$J^{-1} = \frac{\partial(\rho,\phi)}{\partial(x,y)} = \begin{pmatrix} \frac{\partial \rho}{\partial x} & \frac{\partial \rho}{\partial y} \\ \frac{\partial \phi}{\partial x} & \frac{\partial \phi}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{x}{(x^2+y^2)^{1/2}} & \frac{y}{(x^2+y^2)^{1/2}} \\ -\frac{y}{x^2+y^2} & \frac{x}{x^2+y^2} \end{pmatrix}, \tag{V50}$$

[9] The notation $\frac{\partial(x^1,x^2,\dots)}{\partial(y^1,y^2,\dots)}$ is equivalent to $\frac{\partial \mathbf{x}}{\partial \mathbf{y}}$.

and Eq. (V47) yields

$$\mathbf{e}_x = \mathbf{v}_\rho \frac{x}{(x^2+y^2)^{1/2}} - \mathbf{v}_\phi \frac{y}{x^2+y^2},$$
$$\mathbf{e}_y = \mathbf{v}_\rho \frac{y}{(x^2+y^2)^{1/2}} + \mathbf{v}_\phi \frac{x}{x^2+y^2},$$

where this time everything is expressed in the $\mathbf{x} = (x, y)$ language. As an exercise, compute the coordinate basis vectors directly from Eqs. (V15a) and (V21) as $\mathbf{v}_j = \partial_j \mathbf{r}, j = \rho, \phi$. Which route do you find more intuitive, the direct one, or the one engaging the Jacobi matrix? Although the merits of the Jacobi matrix may not be immediately obvious from the present context, we will see how it becomes an important tool as we move along.

For a vector with Cartesian representation $\mathbf{u}(\mathbf{r}) = \mathbf{e}_a u^a(\mathbf{x})$, the polar coordinate representation $\mathbf{u}(\mathbf{r}) = \mathbf{v}_j(\mathbf{y}) u^j(\mathbf{y})$, with $\mathbf{y} = (\rho, \phi)^T$, is given by

$$\begin{pmatrix} u^\rho \\ u^\phi \end{pmatrix}(\mathbf{y}) = J^{-1}(\mathbf{x}) \begin{pmatrix} u^x \\ u^y \end{pmatrix}(\mathbf{x})\Big|_{\mathbf{x}=\mathbf{x}(\mathbf{y})},$$

where the argument $\mathbf{y}(\mathbf{x})$ on the left emphasizes that $(u^\rho, u^\phi)^T(\mathbf{y})$ is delivered as a function of Cartesian coordinates. In a second step, one will then typically express $\mathbf{x}$ in terms of the polar coordinates $\mathbf{y}$ via Eq. (V15a). As an example, consider the vector with Cartesian representation $\mathbf{u} = (-y\mathbf{e}_x + x\mathbf{e}_y)(x^2+y^2)^{-1/2}$ or, in components, $(x^2+y^2)^{-1/2} \left(\begin{smallmatrix} -y \\ x \end{smallmatrix}\right)$. We want to compute its representation in the polar basis at the point with Cartesian coordinates $\mathbf{x} = (x, y)^T$. (Do not forget that all formulas are specific to a fixed point $\mathbf{r} = \mathbf{r}(\mathbf{x}) = \mathbf{r}(\mathbf{y})$!) A quick calculation shows that $\left(\begin{smallmatrix} u^\rho \\ u^\phi \end{smallmatrix}\right) = J^{-1} \left(\begin{smallmatrix} u^x \\ u^y \end{smallmatrix}\right) = (x^2+y^2)^{-1/2} \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$. We can express this in terms of polar coordinates using $(x^2+y^2)^{1/2} = \rho$, which leads to $\left(\begin{smallmatrix} u^\rho \\ u^\phi \end{smallmatrix}\right) = \left(\begin{smallmatrix} 0 \\ \rho^{-1} \end{smallmatrix}\right)$, or $\mathbf{u} = \rho^{-1}\mathbf{v}_\phi = \mathbf{e}_\phi$.

Jacobi matrix and metric

It is sometimes useful to express the metric g_{ij} defined by the coordinate basis vectors in terms of the Jacobi matrix. To this end, we note that $g_{ij} = (v_i)^a \delta_{ab} (v_j)^b$. The expansion $\mathbf{v}_j = \mathbf{e}_a J^a{}_j$ implies $(v_j)^a = J^a{}_j$, so that we obtain $g_{ij} = J^a{}_i \delta_{ab} J^b{}_j = (J^T)_i{}^a J^a{}_j = (J^T J)_{ij}$, where the definition of the transpose of a matrix Eq. (L107) was used. This leads to the desired relation **connecting the metric with the Jacobi matrix**:

$$\boxed{g_{ij} = (J^T J)_{ij}.} \tag{V51}$$

Although it may sometimes be more economical (and intuitive) to calculate the metric directly by analyzing the scalar products (V24), this relation plays an important role in different contexts, notably in integration theory (cf. the discussion following Eq. (C58) in chapter C4 on multi-dimensional integration). Apply relation (V51) to the polar Jacobi matrix to verify that the metric (V24) is obtained.

EXERCISE

Apply Eq. (V35) to verify that the **Jacobi matrix in cylindrical coordinates** is given by

$$J = \frac{\partial(x,y,z)}{\partial(\rho,\phi,z)} = \begin{pmatrix} \cos\phi & -\rho\sin\phi & 0 \\ \sin\phi & \rho\cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad J^{-1} = \frac{\partial(\rho,\phi,z)}{\partial(x,y,z)} = \begin{pmatrix} \frac{x}{(x^2+y^2)^{1/2}} & \frac{y}{(x^2+y^2)^{1/2}} & 0 \\ -\frac{y}{x^2+y^2} & \frac{x}{x^2+y^2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{V52}$$

If further computing practice is needed, you may check the **Jacobi matrix in spherical coordinates** follows from Eq. (V41) as

$$J = \frac{\partial(x,y,z)}{\partial(r,\theta,\phi)} = \begin{pmatrix} \sin\theta\cos\phi & r\cos\theta\cos\phi & -r\sin\theta\sin\phi \\ \sin\theta\sin\phi & r\cos\theta\sin\phi & r\sin\theta\cos\phi \\ \cos\theta & -r\sin\theta & 0 \end{pmatrix},$$

$$J^{-1} = \frac{\partial(r,\theta,\phi)}{\partial(x,y,z)} = \begin{pmatrix} \frac{x}{(x^2+y^2+z^2)^{1/2}} & \frac{y}{(x^2+y^2+z^2)^{1/2}} & \frac{z}{(x^2+y^2+z^2)^{1/2}} \\ \frac{xz}{(x^2+y^2)^{1/2}(x^2+y^2+z^2)} & \frac{yz}{(x^2+y^2)^{1/2}(x^2+y^2+z^2)} & -\frac{(x^2+y^2)^{1/2}}{x^2+y^2+z^2} \\ -\frac{y}{x^2+y^2} & \frac{x}{x^2+y^2} & 0 \end{pmatrix}. \tag{V53}$$

Also verify explicitly that the expressions given in Eqs. (V52) and (V53) satisfy $J^{-1}J = 1$.

V3 Fields

Physical information is often encoded in functions mapping d-dimensional space into image domains such as the real or complex numbers, the vector spaces $\mathbb{R}^n$ or $\mathbb{C}^n$, groups, or other mathematical structures. When they appear in physical contexts, such functions are called **fields**.[1] Before defining fields in formal terms, let us give some examples of their use in physics.

- ▷ Local variations in the temperature in a volume $U \subset \mathbb{R}^3$ can be described by a **scalar field in three-dimensional space**, $T : U \to \mathbb{R}, \mathbf{r} \mapsto T(\mathbf{r})$, i.e. a map assigning to each point $\mathbf{r} \in U$ the local temperature, $T(\mathbf{r})$. Fields taking values in $\mathbb{R}$ or $\mathbb{C}$ are generally called real or complex **scalar fields**, respectively.
- ▷ If the temperature profile depends on time, a **time-dependent scalar field**, $T : U \times I \to \mathbb{R}, (\mathbf{r}, t)^T \mapsto T(\mathbf{r}, t)$, is required to describe the temperature variations over an interval of time $I \subset \mathbb{R}$. This field is defined on a subset of four-dimensional space-time, $U \times I \in \mathbb{R}^3 \times \mathbb{R}$.
- ▷ The flow of a fluid of homogeneous density is described by a field, $(\mathbf{r}, t)^T \mapsto \mathbf{v}(\mathbf{r}, t) \in \mathbb{R}^3$, where $\mathbf{v}$ describes speed and direction of the flow at a point in space, $\mathbf{r}$, and time, t. This is an example of a three-dimensional **vector field** defined on four-dimensional space-time.
- ▷ The state of a **ferromagnet** is described by a field that assigns to each space-time point $(\mathbf{r}, t)^T$ a unit-normalized vector $\hat{\mathbf{n}}(\mathbf{r}, t) \in \mathbb{R}^3$ describing the local magnetization of the material. For example, a ferromagnetic phase is distinguished by an approximately homogeneous magnetization, $\hat{\mathbf{n}}(\mathbf{r}, t) \simeq \text{const.}$, which generates the macroscopic magnetic field characteristic for magnetic substances. A unit-normalized vector, $\|\hat{\mathbf{n}}\| = 1$, may be identified with a point on the sphere of unit radius, S^2, so the field $\hat{\mathbf{n}} : \mathbb{R}^3 \times R \to S^2$ maps space-time onto the unit sphere.

Mathematically, a **field** is a smooth map

$$\mathbf{F} : M \to L, \qquad \mathbf{r} \mapsto \mathbf{F}(\mathbf{r}), \tag{V54}$$

assigning to points $\mathbf{r}$ of the **base manifold** (Basismannigfaltigkeit), M, values $\mathbf{F}(\mathbf{r})$ in the **target manifold** (Zielmannigfaltigkeit), L. We assume that $M \subset \mathbb{R}^d$ and $L \subset \mathbb{R}^n$ are open subset of d and n dimensional vector spaces, respectively.[2] If M is parameterized by a system

[1] These fields are unrelated to the (number-)fields of mathematics defined in section L1.3.

[2] Situations where this setting is too narrow will be discussed in section V4.1 below.

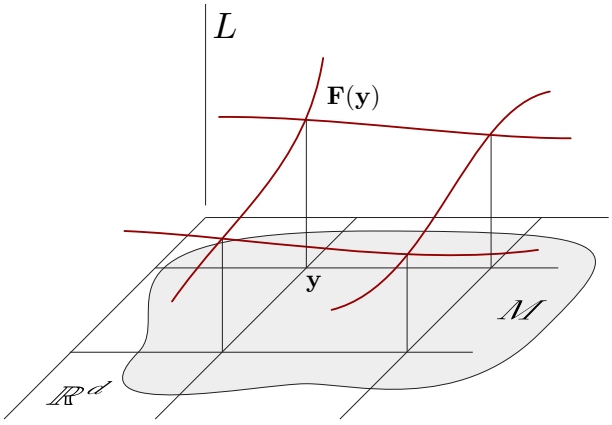


Figure V9: Schematic illustration of the concept of a field as a map, $\mathbf{F}$, from a base manifold M to a target manifold L.

of generalized coordinates the arguments $\mathbf{r} = \mathbf{r}(\mathbf{y})$ may then be parameterized by coordinate vectors $\mathbf{y} = (y^1, \ldots, y^d)^T$. Likewise, a system of coordinates on L implies a coordinate representation for $\mathbf{F}$. Throughout this introductory section we will not rigorously discriminate between points $\mathbf{r}$ and their coordinate vectors $\mathbf{y}$. Likewise, we will identify $\mathbf{F} = (F^1, \ldots, F^n)^T$ with its coordinate representation. This leads to descriptions of the field as

$$\mathbf{F} : M \to L, \qquad \mathbf{y} = (y^1, \ldots, y^d)^T \mapsto \mathbf{F}(\mathbf{y}) = (F^1, \ldots, F^n)(\mathbf{y}), \tag{V55}$$

which must be taken with a grain of salt but should not lead to confusion. We finally note that, as in previous chapters, we tend to reserve the symbol $\mathbf{x}$ for **Cartesian coordinates**. For example, a point in $(3+1)$-dimensional space-time has Cartesian representations as $\mathbf{x} = (x^0, x^1, x^2, x^3)^T$, where $x^0 = t$ parameterizes time, and $x^{1,2,3}$ are the b coordinates of a spatial vector.

If $n = 1$, then $\mathbf{F} = F$ is a real-valued function, and fields of this type are called **real scalar fields**. For $M = \mathbb{C} \cong \mathbb{R}^2$ we have a **complex scalar field**. If $M = \mathbb{R}^{n>1}$ we speak of a **vector field**.[3] Finally, $M \not\subset \mathbb{R}^n$ may be a genuine subset of $\mathbb{R}^n$, such as the sphere $S^2 \subset \mathbb{R}^2$ mentioned above. The general concept of all these maps is illustrated in Fig. V9 where the shaded gray area represents the base manifold U and thick lines symbolize the image values $\mathbf{F}(\mathbf{x})$.

Fields can be visualized in a variety of ways, as illustrated in Fig. V10 with three different examples. A scalar field in two-dimensional space can be imagined as a 'surface' floating over a plane (left panel) whose height relative to the plane is the field value. A vector field, $\mathbf{F}(\mathbf{r})$, mapping two-dimensional space points to two-dimensional vectors (center panel) can be visualized in terms of a 'swarm of arrows', where $\mathbf{F}(\mathbf{r})$ is indicated by an arrow representing $\mathbf{F}$ with base point at $\mathbf{r}$. Such representations are often used to describe, e.g., distributions

[3] Formally, a complex *scalar* field, $M \cong \mathbb{R}^2$ may be identified with a two dimensional real *vector* field. However, in the complex case, additional conditions discussed in chapter C9 are generally imposed. This means that a complex scalar field has more structure than a generic two-dimensional real vector field, and that the two classes should be distinguished.

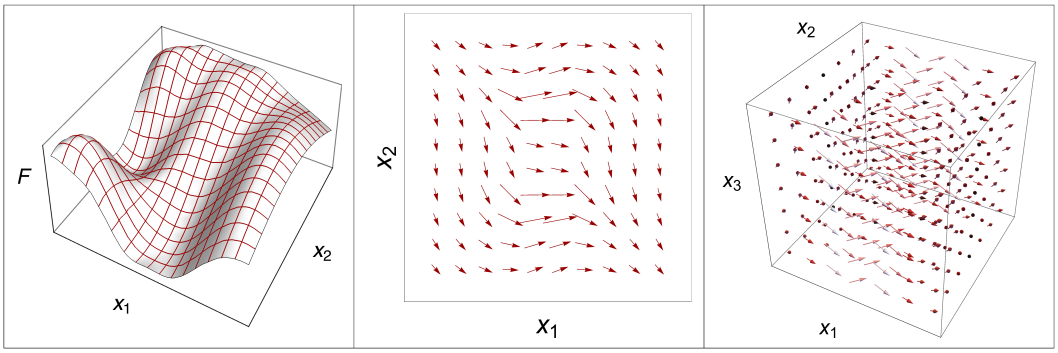


Figure V10: Visualization of a scalar field in two dimensions, $n = 1, d = 2$ (left), a two-dimensional vector field in two dimensions, $n = 2, d = 2$ (center), and a three-dimensional vector field in three dimensions, $n = 3, d = 3$ (right).

of current flow in the oceans. Likewise, three-dimensional vectors in three-dimensional space may be represented in terms of three-dimensional visualizations (right panel), depicting, e.g., the flow of a fluid in a vessel. However, the figure also illustrates how visual representations of three-dimensional vector fields tend to lack clarity.

In the rest of this chapter, we will learn how to describe fields in quantitative terms.

V3.1 Scalar fields

Scalar fields are real-valued functions depending on more than one argument, $f = f(\mathbf{y}) = f(y^1, \ldots, y^d)$. (Although an ordinary function $f(y)$ of one variable $(d = 1)$ may also be considered as a field, the term is usually restricted to functions with base manifolds of dimension $d \geq 2$.) As an example, consider the two-dimensional scalar field,

$$h : \mathbb{R}^2 \to \mathbb{R}, \qquad \mathbf{x} = (x, y)^T \mapsto h(\mathbf{x}) = \frac{1}{(x^2 + y)^2 + c}, \tag{V56}$$

where c is a positive constant. As mentioned in the previous section, such fields may be visualized as surfaces of local height, $h(\mathbf{x})$, floating over the two-dimensional plane (cf. Fig. V11). The surface analogy suggests an alternative, truly two-dimensional graphic representation the field. For a number of constant values, $h_n \equiv c \times n$, $n \in \mathbb{Z}, c = \text{const.}$, **contour lines** are drawn in the (x, y)-plane along which the function remains at a constant value, $h(\mathbf{x}) = h_n$. This yields the contour plot shown in the bottom of the figure. The contour plot indicates changes in the function in terms of the density of contour lines, where widely-spaced (or densely-spaced) lines are indicative of shallow (or steep) function changes. Contour representations are used frequently used, e.g., in geographic maps to indicate the altitude levels of the charted territory.

Total differential

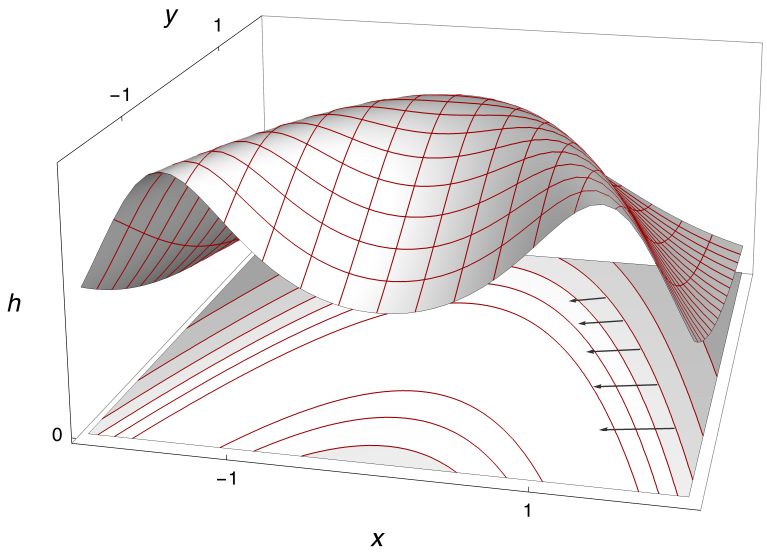
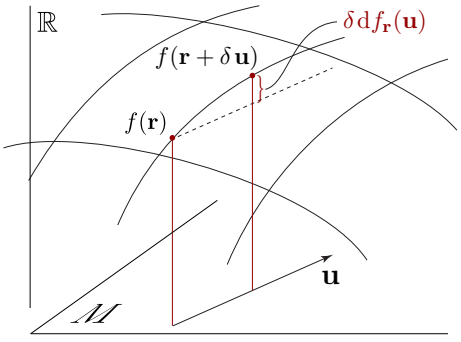


Figure V11: Representation of the field $h(\mathbf{x})$ of (V56) as a surface floating over the xy-plane. The bottom of the graph shows a contour plot of the function, in which the lines denote constant values of the function. Regions in which the contour lines are dense indicate that the slope of the function is steep there (why?). The arrows indicate the direction in which the function increases most steeply, and their length indicates the magnitude of the increase. Note that the length of the arrows is largest in regions where the contour lines are dense, and the function varies most strongly.



One frequently needs to describe how field values, $f(\mathbf{r})$, change under small variations of the argument, $\mathbf{r} \to \mathbf{r} + \delta\,\mathbf{u}$, where $\mathbf{u}$ is a vector describing the direction in which the change is observed and δ is an (infinitesimally) small variation parameter. The answer to such questions is provided by a quantity known as the **total differential** of the field. For a given point $\mathbf{r} \in M \subset \mathbb{R}^d$, the total differential, $\mathrm{d}f_{\mathbf{r}}$, is a linear map acting on vectors $\mathbf{u} \in \mathbb{R}^d$ to produce a number that describes the rate of change of f in the direction of $\mathbf{u}$.[4] It is defined as

$$\mathrm{d}f_{\mathbf{r}} : \mathbb{R}^d \to \mathbb{R}, \qquad \mathbf{u} \mapsto \mathrm{d}f_{\mathbf{r}}(\mathbf{u}) \equiv \lim_{\delta\to 0} \frac{1}{\delta}\big(f(\mathbf{r}+\delta\,\mathbf{u}) - f(\mathbf{r})\big)\,. \tag{V57}$$

An argument similar to that used to prove Eq. (C34) shows that the differential $\mathrm{d}f_{\mathbf{r}}$ at fixed $\mathbf{r}$ is *linear* in its vectorial argument,[5] i.e. $(a, b \in \mathbb{R},\ \mathbf{u}, \mathbf{w} \in \mathbb{R}^d)$

$$\mathrm{d}f_{\mathbf{r}}(a\mathbf{u} + b\mathbf{w}) = a\,\mathrm{d}f_{\mathbf{r}}(\mathbf{u}) + b\,\mathrm{d}f_{\mathbf{r}}(\mathbf{w}). \tag{V58}$$

[4] Notice that $\mathbf{u}$ need not necessarily lie in M. For example, if the field is defined on the disk of unit radius, $M = D \subset \mathbb{R}^2$, we may consider $\mathbf{u} = (100, 100)^T$ and $\mathbf{r} = (0, 0)^T$. For infinitesimal δ, $\mathbf{r} + \delta\,\mathbf{u}$ then lies in D although $\mathbf{u}$ does not.

[5] To see this explicitly, evaluate the differential on a sum of two vectors as
$\mathrm{d}f(\mathbf{u}+\mathbf{w}) \equiv \lim_{\delta\to 0} \delta^{-1}\big(f(\mathbf{r}+\delta\,\mathbf{u}+\delta\,\mathbf{w}) - f(\mathbf{r}+\delta\,\mathbf{w}) + f(\mathbf{r}+\delta\,\mathbf{w}) - f(\mathbf{r})\big)$

The definition of the total differential does not make reference to a coordinate system and therefore remains somewhat abstract. A more tangible representation is obtained by evaluating $\mathrm{d}f$ on the jth vector of a coordinate basis, $\mathbf{v}_j = \partial_{y^j}\mathbf{r}(\mathbf{y})$, at $\mathbf{r} = \mathbf{r}(\mathbf{y})$. According to definition (V57) this is $\mathrm{d}f_{\mathbf{r}}(\mathbf{v}_j) = \lim_{\delta\to 0}\delta^{-1}\big(f(\mathbf{r}+\delta\,\mathbf{v}_j) - f(\mathbf{r})\big) = \lim_{\delta\to 0}\delta^{-1}\big(f(\mathbf{r}(\mathbf{y}) + \delta\partial_j\mathbf{r}(\mathbf{y})) - f(\mathbf{r}(\mathbf{y}))\big)$. Compare this expression to the jth partial derivative of the coordinate representation, given by Eq. (C31): $\partial_{y^j} f(\mathbf{y}) = \partial_{y^j} f(\mathbf{r}(\mathbf{y})) = \lim_{\delta\to 0}\delta^{-1}\big(f(\mathbf{r}(\mathbf{y}+\delta\,\mathbf{e}_j)) - f(\mathbf{r}(\mathbf{y}))\big) = \lim_{\delta\to 0}\delta^{-1}\big(f(\mathbf{r}(\mathbf{y}) + \delta\partial_j\mathbf{r}(\mathbf{y})) - f(\mathbf{r}(\mathbf{y}))\big)$. The two expressions are equal and so we have the identification

$$\boxed{\mathrm{d}f_{\mathbf{r}(\mathbf{y})}(\mathbf{v}_j) = \partial_{y^j} f(\mathbf{y}).} \tag{V59}$$

This intuitive formula states that the change of a function along the jth coordinate vector equals the partial derivative of the function's coordinate representation. In the following, the differential will appear frequently, and we often use shorthand notations such as $\mathrm{d}f_{\mathbf{r}(\mathbf{y})} \equiv \mathrm{d}f_{\mathbf{r}} \equiv \mathrm{d}f_{\mathbf{y}} \equiv \mathrm{d}f$, where the last representation leaves the dependence of the differential on the coordinates implicit. For a general vector $\mathbf{u} = \mathbf{v}_j u^j$ expanded in the coordinate basis, the linearity of the differential, $\mathrm{d}f(\mathbf{u}) = \mathrm{d}f(\mathbf{v}_j u^j) = \mathrm{d}f(\mathbf{v}_j)u^j$, then implies the representation

$$\boxed{\mathrm{d}f_{\mathbf{y}}(\mathbf{u}) = \frac{\partial f(\mathbf{y})}{\partial y^j} u^j\,.} \tag{V60}$$

Comparison of Eq. (V57) with the definition of the one-dimensional derivative, Eq. (C1), shows that the differential $\mathrm{d}f_{\mathbf{r}}$ generalizes the concept of an ordinary derivative to higher dimensions. It describes the change of the function f by a linear approximation, as can be seen by evaluating the r.h.s. of the definition for small but finite δ. This leads to a formula analogous to the one-dimensional Eq. (C2),

$$f(\mathbf{r}+\delta\,\mathbf{u}) \simeq f(\mathbf{r}) + \mathrm{d}f_{\mathbf{r}}(\delta\,\mathbf{u}), \tag{V61}$$

showing how for small variations, $\delta\mathbf{u}$, the change in the function is described by a linear map, i.e. a map satisfying the condition (V58).

INFO The total differential plays an important role both in mathematics and physics, where it is applied to describe the changes of functions in convenient and versatile ways. Many of these applications rely on a representation of the total differential of a general function, f, in terms of the differentials of the coordinate functions: the ith coordinate, y^i, can be considered as a function, $y^i : U \to \mathbb{R}$, $\mathbf{y} \mapsto y^i(\mathbf{y}) = y^i$, assigning to the coordinate vector $\mathbf{y} \in U$ its ith component, y^i. Since $\frac{\partial y^i}{\partial y^j} = \delta^i{}_j$, we see from Eq. (V60) that this function has the total differential $\mathrm{d}y^i_{\mathbf{y}}(\mathbf{u}) = u^i$, so that Eq. (V60) can be written as

$$\mathrm{d}f_{\mathbf{y}}(\mathbf{u}) = \frac{\partial f(\mathbf{y})}{\partial y^j}\mathrm{d}y^j_{\mathbf{y}}(\mathbf{u})\,.$$

$= \lim_{\delta\to 0}\delta^{-1}\big(f(\mathbf{r}+\delta\,\mathbf{u}+\delta\,\mathbf{w}) - f(\mathbf{r}+\delta\,\mathbf{w})\big) + \lim_{\delta\to 0}\delta^{-1}\big(f(\mathbf{r}+\delta\,\mathbf{w}) - f(\mathbf{r})\big) = \mathrm{d}f(\mathbf{u}) + \mathrm{d}f(\mathbf{w})$.

In the first equality we inserted $0 = -f(\mathbf{r}+\delta\,\mathbf{w}) + f(\mathbf{r}+\delta\,\mathbf{w})$, and in the second we noted that the infinitesimal offset $\delta\,\mathbf{w}$ in the arguments of the first difference vanishes in the limit $\delta \to 0$.

This should be considered as a relation between the linear maps $\mathrm{d}f_{\mathbf{y}}$ and $\mathrm{d}y^j_{\mathbf{y}}$. Since it holds for arbitrary vectors $\mathbf{v}$, the maps themselves are equal in the sense that

$$\boxed{\mathrm{d}f = \frac{\partial f(\mathbf{y})}{\partial y^j}\mathrm{d}y^j\,,} \tag{V62}$$

where we followed the convention to omit the coordinate subscript, writing $\mathrm{d}f_{\mathbf{y}} = \mathrm{d}f$. For example, the function h defined in Eq. (V56) has the total differential

$$\mathrm{d}h = -\frac{2(x^2+y)}{((x^2+y)^2+c)^2}(2x\mathrm{d}x + \mathrm{d}y).$$

In principle, $\mathrm{d}f$ is a linear map that may be applied to a general vector $\mathbf{v}$ to produce the number $\mathrm{d}f(\mathbf{v})$. However, the above construction shows that one should rather think of the total differential as a map acting on a 'small' vector, $\delta\mathbf{v}$ to describe the change of a function under a small change of its argument, $\mathbf{y} \to \mathbf{y} + \delta\mathbf{v}$. To illustrate this point with a physically motivated example from **thermodynamics** (where the use of total differentials is pervasive), let $p(V,T)$ be the pressure of a gas in a container of volume V at temperature T. We now ask for the change in pressure under small variations, δV and δT, of volume and temperature, respectively. To answer this question, we set up the total differential

$$\mathrm{d}p = \frac{\partial p(V,T)}{\partial V}\mathrm{d}V + \frac{\partial p(V,T)}{\partial T}\mathrm{d}T. \tag{V63}$$

The corresponding change in pressure, $\delta p_{(V,T)} \equiv p(V+\delta V, T+\delta T) - P(V,T) \overset{\text{(V61)}}{\simeq} \mathrm{d}p_{V,T}(\delta V, \delta T)$ can now conveniently be represented as[6]

$$\delta p_{(V,T)} = \mathrm{d}p_{(V,T)}(\delta V, \delta T) = \frac{\partial p(V,T)}{\partial V}\delta V + \frac{\partial p(V,T)}{\partial T}\delta T.$$

For example, for an **ideal gas** Clapeyron's formula states that $pV = nRT$, where n is the amount of substance (in units of moles) and R the Avogadro constant. This may be represented as $p(V,T) = nRT/V$, with $\partial_V p = -nR\frac{T}{V^2}$ and $\partial_T p = nR\frac{1}{V}$, so that

$$\delta p_{(V,T)} = \mathrm{d}p_{(V,T)}(\delta V, \delta T) = nR\left(-\frac{T\delta V}{V^2} + \frac{\delta T}{V}\right). \tag{V64}$$

Unfortunately, physics parlance tends to describe the differential itself (and not the arguments on which it acts) as a 'small quantity'. For example, one frequently finds formulations such as 'let $\mathrm{d}p = \partial_V p\,\mathrm{d}V + \partial_T p\,\mathrm{d}T$ be the variation of pressure, $\mathrm{d}p$, under small variations of volume and temperature, $\mathrm{d}V$ and $\mathrm{d}T$, respectively'. Factually, this is nonsense — $\mathrm{d}p, \mathrm{d}V, \mathrm{d}T$ are linear maps which cannot be 'small' — but this misconception is quite pervasive in physics. However, if one keeps in mind that the formulation actually refers to the action of the differential on a small argument, $(\delta V, \delta T)^T$, i.e. $\delta p = \partial_V p\,\delta V + \partial_T p\,\delta T$, confusion can be kept to a minimum.

We finally note that in the terminology of mathematics, the differentials $\mathrm{d}f$ and $\mathrm{d}y^i$ are called **differential forms**. Differential forms play an increasingly important role in physics and they are discussed in more depth in chapter V5.

[6] In the last step, the total differentials $\mathrm{d}V$ and $\mathrm{d}T$ occurring in Eq. (V63) are applied to the vector $(\delta V, \delta T)^T$, yielding δV and δT, respectively.

Gradient

In physics, the local change of a scalar field, f, is often described in terms of a quantity which is derived from the differential, $\mathrm{d}f$, but is of a more 'geometric nature', the so called **gradient field**, $\boldsymbol{\nabla} f$,

$$\boldsymbol{\nabla} f : M \subset \mathbb{R}^d \to \mathbb{R}^d, \qquad \mathbf{r} \mapsto \boldsymbol{\nabla} f_{\mathbf{r}} \,. \tag{V65}$$

The gradient field assigns to each point $\mathbf{r} \in M \subset \mathbb{R}^d$, a vector, $\boldsymbol{\nabla} f_{\mathbf{r}} \in \mathbb{R}^d$, that has the same number of components as $\mathbf{r}$. As with the differential, the $\mathbf{r}$-dependence of the gradient vector is frequently left implicit and one uses the shorthand notation $\boldsymbol{\nabla} f$. The defining feature of the gradient vector is that it points in the direction of the steepest increase of the function f, and that its norm is set by the growth rate of the function in that direction. For an illustration, see Fig. V11, where the black arrows represent the two-dimensional gradient field of the function h at a few selected points.

The quantitative definition of the gradient field is formulated in terms of the function's differential: for each vector $\mathbf{u} \in \mathbb{R}^d$ one requires that

$$\mathrm{d}f_{\mathbf{r}}(\mathbf{u}) = \langle \boldsymbol{\nabla} f_{\mathbf{r}}, \mathbf{u} \rangle \,, \tag{V66}$$

where $\langle \ , \ \rangle$ is the standard scalar product in $M \subset \mathbb{R}^d$. This equation defines the gradient through the implicit condition that the scalar product of the gradient with any vector $\mathbf{u}$ must be equal to the function's differential evaluated on that vector. Eq. (V66) implies that the variation $\mathrm{d}f(\mathbf{u})$ (the left-hand side) is strongest along the direction of $\mathbf{u}$ for which the alignment of $\mathbf{u}$ with the gradient vector, $\boldsymbol{\nabla} f$, expressed through the scalar product $\langle \boldsymbol{\nabla} f, \mathbf{u} \rangle$ (the right-hand side), becomes maximal. In other words, the vector $\boldsymbol{\nabla} f$ points in the direction of strongest increase of the function f. Denoting this direction by the unit vector $\mathbf{e}$, we may thus write $\boldsymbol{\nabla} f = \mathbf{e} \|\boldsymbol{\nabla} f\|$. To obtain an interpretation of the *norm* $\|\boldsymbol{\nabla} f\|$, we substitute $\mathbf{u} = \boldsymbol{\nabla} f$ into the defining equation (V66), obtaining $\|\boldsymbol{\nabla} f\| \, \mathrm{d}f(\mathbf{e}) \overset{(V58)}{=} \mathrm{d}f(\boldsymbol{\nabla} f) \overset{(V66)}{=} \langle \boldsymbol{\nabla} f, \boldsymbol{\nabla} f \rangle = \|\boldsymbol{\nabla} f\|^2$, where in the first equality the linearity of the differential was used. Division by $\|\boldsymbol{\nabla} f\|$ leads to $\|\boldsymbol{\nabla} f\| = \mathrm{d}f(\mathbf{e})$, i.e. the norm of the gradient equals the value $\mathrm{d}f(\mathbf{e})$ of the differential in the direction of maximal increase, which gives the slope of f in that direction. To summarize,

> The gradient vector $\boldsymbol{\nabla} f_{\mathbf{r}}$ points in the direction along which the slope of the function f at $\mathbf{r}$ is maximal, and $\|\boldsymbol{\nabla} f_{\mathbf{r}}\|$ gives the magnitude of the maximal slope.

(V67)

To obtain explicit representations for the gradient vector, we expand it in the $\mathbf{y}$-coordinate basis $\{\mathbf{v}_i\}$, denoting the components by $\boldsymbol{\nabla} f^i$. If we insert $\boldsymbol{\nabla} f = \mathbf{v}_i \boldsymbol{\nabla} f^i$ and $\mathbf{u} = \mathbf{v}_j$ into Eq. (V66), the l.h.s. yields $\mathrm{d}f(\mathbf{v}_j) \overset{(V59)}{=} \partial_{y^j} f$, the r.h.s. $\langle \boldsymbol{\nabla} f, \mathbf{v}_i \rangle = \langle \mathbf{v}_i \boldsymbol{\nabla} f^i, \mathbf{v}_j \rangle \overset{(V24)}{=} \boldsymbol{\nabla} f^i g_{ij}$. Equating these expressions and using the index-lowering convention $\boldsymbol{\nabla} f_j \equiv \boldsymbol{\nabla} f^i g_{ij}$ of Eq. (L51), we obtain

$$\boxed{(\boldsymbol{\nabla} f_{\mathbf{r}(\mathbf{y})})_j = \partial_{y^j} f(\mathbf{y}).} \tag{V68}$$

Hence in the coordinate basis the gradient's **covariant components**, $\boldsymbol{\nabla} f_j$, are simply given by the partial derivatives of f w.r.t. to y^j. (If a different basis is used, e.g. the local basis, $\{\mathbf{e}_j\}$, then different, and generally more complicated expressions are obtained.)

The **contravariant components** of the gradient vector are obtained by raising the index using Eq. (L55) and Eq. (L53) for the inverse metric tensor,

$$\boldsymbol{\nabla} f^j = g^{ji} \boldsymbol{\nabla} f_i = g^{ji} \partial_{y^i} f \,. \tag{V69}$$

For a Cartesian basis, where $g_{ij} = \delta_{ij}$, these are inessential operations, since $\boldsymbol{\nabla} f^i = \boldsymbol{\nabla} f_i$. For a general coordinate basis, co- and contravariant components are different. Notice though, that when the gradient appears in a scalar product with another vector, say $\mathbf{u} = \mathbf{v}_i u^i$, with

$$\langle \boldsymbol{\nabla} f, \mathbf{u} \rangle = \boldsymbol{\nabla} f_i u^i = (\partial_{y^i} f) u^i, \tag{V70}$$

only the covariant components, given by the simple Eq. (V68), are needed.

INFO The gradient vector is often used to describe the **rate of change of a function along a curve**, $t \mapsto \mathbf{r}(t) = \mathbf{r}(\mathbf{y}(t))$, where in the second equality a parameterization in coordinates $\mathbf{y}$ is assumed. Application of the chain rule (C36) then yields

$$\frac{\mathrm{d} f(\mathbf{y}(t))}{\mathrm{d}t} = \partial_{y^j} f(\mathbf{y}(t)) \frac{\mathrm{d} y^j(t)}{\mathrm{d}t} \overset{\text{(V68)}}{=} \boldsymbol{\nabla} f_j \, \dot{y}^j = \boldsymbol{\nabla} f_{\mathbf{r}(\mathbf{y}(t))} \cdot \dot{\mathbf{r}}(\mathbf{y}(t)) \,. \tag{V71}$$

This formula states that the rate at which f changes along the curve is determined by its slope in the direction of the curve velocity.

In a Cartesian basis, where $\partial^j = \partial_j = \partial_{x^j}$, the gradient vector can be represented in the following form, which is often found in the physics literature:

$$\boldsymbol{\nabla} f = \mathbf{e}_j \boldsymbol{\nabla} f^j = \begin{pmatrix} \partial^1 f \\ \vdots \\ \partial^d f \end{pmatrix} . \tag{V72}$$

In this representation, $\boldsymbol{\nabla} f$ can be interpreted as the action of a **gradient operator** (also called '**nabla operator**'), $\boldsymbol{\nabla}$, on the function f. The nabla operator is a formal vector defined as

$$\boldsymbol{\nabla} \equiv \mathbf{e}_j \partial^j = \begin{pmatrix} \partial^1 \\ \vdots \\ \partial^d \end{pmatrix} . \tag{V73}$$

It is a 'differential operator' in the sense that it acts on the function to its right (it never occurs alone) as $f \mapsto \boldsymbol{\nabla} f$, where the r.h.s. is defined through (V72). The denotations 'nabla f' and 'gradient f' are synonyms.

EXAMPLE As an example, consider the field $h(\mathbf{x})$ of Eq. (V56) shown in Fig. V11. Evaluating its partial derivatives, we find

$$\boldsymbol{\nabla} h_{(x,y)} = \begin{pmatrix} \partial_x h(x,y) \\ \partial_y h(x,y) \end{pmatrix} = -\frac{2(x^2+y)}{\left[(x^2+y)^2 + c\right]^2} \begin{pmatrix} 2x \\ 1 \end{pmatrix} . \tag{V74}$$

In the contour plot at the bottom of the figure, a few arrows representing this gradient field indicate how it stands orthogonal to the contour lines of the function (and thus points in a direction of maximal variation). For example, for any point on the line $x = 0$, the vector $(2x, 1)^T$ points in the y-direction. At $(x, y)^T = (0, 0)^T$ the gradient vanishes, reflecting the absence of a direction of increase, i.e. this point is a local maximum.

The **gradient in the local basis of a curvilinear system** is computed by inserting the elements g^{ij} of the inverse metric tensor, Eq. (L53), into Eq. (V69). In the standard coordinate systems, polar, cylindrical, spherical, these representations assume a relatively simple form, thanks to the diagonal form of the metric tensor, $g_{ij} = 0$, $i \neq j$. As a consequence, the inverse elements required to formulate the contravariant components of the metric tensor are trivially obtained as $g^{jj} = g_{jj}^{-1}$. For example, in polar coordinates we have the expansions

$$\begin{aligned}\boldsymbol{\nabla} f = \mathbf{v}_\rho \, \boldsymbol{\nabla} f^\rho + \mathbf{v}_\phi \, \boldsymbol{\nabla} f^\phi &\overset{(V69)}{=} \mathbf{v}_\rho \, g^{\rho\rho} \partial_\rho f + \mathbf{v}_\phi \, g^{\phi\phi} \partial_\phi f \overset{(V26)}{=} \mathbf{v}_\rho \, \partial_\rho f + \mathbf{v}_\phi \frac{1}{\rho^2} \partial_\phi f \\ &\overset{(V27)}{=} \mathbf{e}_\rho \, \partial_\rho f + \mathbf{e}_\phi \frac{1}{\rho} \partial_\phi f . \end{aligned} \tag{V75}$$

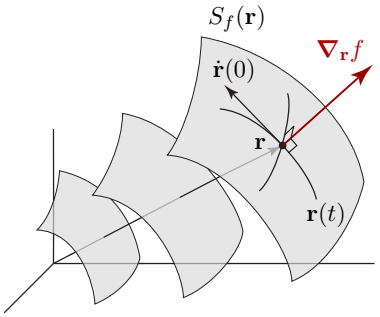
EXERCISE Compute the **gradient in spherical coordinates**, i.e. a system of coordinates (r, θ, ϕ) with diagonal metric $g_{rr} = 1$, $g_{\theta\theta} = r^2$, $g_{\phi\phi} = r^2 \sin^2 \theta$. Show that the result is given by

$$\nabla f^r = \partial_r f , \qquad \nabla f^\theta = \frac{1}{r^2} \partial_\theta f , \qquad \nabla f^\phi = \frac{1}{r^2 \sin^2 \theta} \partial_\phi f . \tag{V76}$$

The general representation of the gradient in an orthogonal (diagonal metric tensor) system reads as

$$\boldsymbol{\nabla} f = \mathbf{v}_j \, g^{jj} \partial_{y^j} f = \mathbf{e}_j \frac{1}{\sqrt{g_{jj}}} \partial_{y^j} f . \tag{V77}$$

Although the right-most version of this formula is the one most frequently encountered in the physics literature, the presence of square-root normalization factors looks awkward. From a geometric perspective, it is more natural to work in the un-normalized coordinate basis (center representation), or to avoid the usage of contravariant gradient indices altogether, in which case the simple covariant formula Eq. (V68) suffices to describe the gradient.



INFO It is sometimes useful to characterize the geometry of the gradient vector in terms of so called **contour surfaces**. Contour surfaces generalize the contour lines describing functions $f : \mathbb{R}^2 \to \mathbb{R}$ to functions in arbitrary dimensions, $f : \mathbb{R}^d \to \mathbb{R}$. A contour surface, $S_c \equiv \{\mathbf{r}' \in \mathbb{R}^d | f(\mathbf{r}') = c\}$, $c \in \mathbb{R}$ is defined as the set of all points $\mathbf{r}'$ for which f assumes the fixed value, c. Every point $\mathbf{r}$ lies on such a contour surface, namely the surface $S_{f(\mathbf{r})}$ defined by all points on which f assumes the value $f(\mathbf{r})$.

For $d = 2$, these 'surfaces' reduce to the contour lines illustrated in Fig. V11. In higher dimensions, the equation $f(\mathbf{r}') = f(\mathbf{r})$ is one real equation that constrains a set of d variables, say the coordinates $\mathbf{y} = (y^1, \ldots, y^d)^T$ of $\mathbf{r}'$. This constraint allows one to express one of them, say $y^d = y^d(y^1, \ldots, y^{d-1})$, in terms of the other $d-1$ free variables, $y^1, \ldots, y^{d-1}$, which may then be interpreted as coordinates parameterizing the surface. This shows that the contour surfaces are $(d-1)$-dimensional objects in d-dimensional space. (Exceptions to this rule occur at extremal points of the function f. For example, the contour surface corresponding to a global maximum $f(\mathbf{r}_{\max}) = f_{\max}$ is just a single point, $S_{f_{\max}} = \{\mathbf{r}_{\max}\}$.)

The geometry of these surfaces is equivalently described by the statement that

> the gradient vector $\boldsymbol{\nabla}_{\mathbf{r}} f$ stands perpendicular to the contour surface $S_{f(\mathbf{r})}$ through $\mathbf{r}$.

To see this, let $\mathbf{r}(t)$ be a curve lying within the contour surface $S_{f(\mathbf{r})}$, running through the point $\mathbf{r}$ at $\mathbf{r}(0) = \mathbf{r}$. The function f then remains stationary along the curve, i.e. $\frac{\mathrm{d}}{\mathrm{d}t} f(\mathbf{r}(t)) = 0$. Application of Eq. (V71) at $t = 0$ thus yields $0 = \boldsymbol{\nabla} f_{\mathbf{r}(t)} \cdot \dot{\mathbf{r}}(t)\big|_{t=0} = \boldsymbol{\nabla} f_{\mathbf{r}} \cdot \dot{\mathbf{r}}(0)$. From this we conclude that the gradient vector is perpendicular to the tangent vector at $\mathbf{r}$ of an arbitrary curve running within the surface and passing through $\mathbf{r}$, and therefore is perpendicular to the surface as such.

V3.2 Gradient fields

REMARK Throughout this section, Cartesian coordinates, $\mathbf{x}$, are used.

As mentioned above, vector fields can be imagined as 'swarms' of vectors in space. They often contain universal (i.e. independent of details) features which determine the structure of the swarm at large scales. For example, the field describing the steady flow of a fluid in a cylinder resembles a regular 'stream' of vectors, cf. Fig. V11(a). The (electric) field created by charged particles contains regions from which vectors emanate, Fig. V11(b). The vector field describing a fluid with vortices contains centers around which the vectors rotate, Fig. V11(c). Other fields may show all these features simultaneously..

In the following three sections, we will introduce concepts to describe the universal features of vector fields. We begin with a discussion of the simplest type of vector fields, those describing regular flow. In the subsequent two sections, we will learn how to identify whether a vector field contains sources or centers of rotation, respectively.

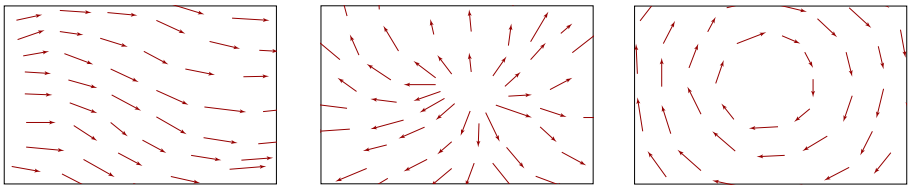


Figure V12: (a) Source-free and rotation-free vector field. (b) Vector field containing a source. (c) Vector field with vorticity.

Definition of gradient fields

Gradient fields are the simplest type of vector fields. Their defining feature is that they can be represented as the gradient of a function. Given a smooth vector field, $\mathbf{v} : U \subset \mathbb{R}^d \to \mathbb{R}^d, \mathbf{x} \mapsto \mathbf{v}(\mathbf{x})$, a natural first question to ask is whether $\mathbf{v}$ is a **gradient field**, i.e. whether there exists a smooth scalar field, $\varphi(\mathbf{x})$, such that $\mathbf{v}(\mathbf{x}) = \boldsymbol{\nabla}\varphi_{\mathbf{x}}$. If so, the function φ is called the **potential** of the field.[7] Notice that for a gradient field, the target space $\mathbb{R}^d$ and the base manifold U must have the same dimension, e.g. a field of planar vectors, $\mathbf{v}(\mathbf{x}) \in \mathbb{R}^2$, defined in three-dimensional space, $\mathbf{x} \in \mathbb{R}^3$, cannot be a gradient field.

If $\mathbf{v}$ is a gradient field, its Cartesian components can be written as $v^i = \partial^i\varphi = \partial_i\varphi$, where we noted that in an orthonormal basis the positioning of indices is immaterial, and $\partial_i = \partial^i$. Now compute the difference of 'mixed' derivatives,

$$\partial_i v^j - \partial_j v^i = \partial_i\partial_j\varphi - \partial_j\partial_i\varphi = 0, \tag{V78}$$

where the last equality follows from the commutativity of partial derivatives acting on a smooth function [Eq. (C32)]. Eq. (V78) represents a *necessary* condition for $\mathbf{v}$ to be a gradient field, meaning that if a field fails the condition, it cannot be a gradient field. However, the condition is not *sufficient*, i.e. there exist fields for which Eq. (V78) holds although they are not gradient fields. This point, and the extension of (V78) to a full criterion for ensuring that a vector field is a gradient field, will be discussed later in this section.

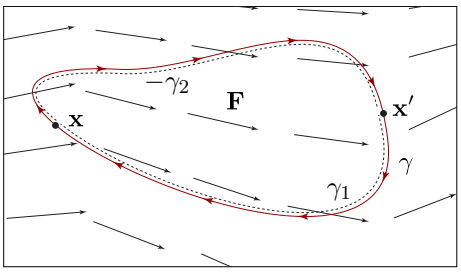
Gradient fields play an important role in **physics**. For example, physical forces are described by vector fields, $\mathbf{F}$, where the vector $\mathbf{F}(\mathbf{x})$ represents the force acting at point $\mathbf{x}$. As discussed in section V1.4, the work done by such a force along a path γ is described by the line integral

$$W[\gamma] = \int_\gamma \mathrm{d}\mathbf{r} \cdot \mathbf{F} \ .$$

Many forces occurring in physics have the property that no work is done if a body is moved along a *closed* path (cf. figure), $\oint_\gamma \mathrm{d}\mathbf{r} \cdot \mathbf{F} = 0$, where we used the standard symbol, $\oint$, to denote the **line integral along a closed path**. This happens if the work done against the force along some portions of the path balances against the work done by the force along

[7] In physics, it is customary to include a minus sign in the definition of the potential, writing $\mathbf{v} = -\boldsymbol{\nabla}\varphi$.

others. A vector field $\mathbf{F}$ whose line integral along an arbitrary closed path vanishes is called a **conservative vector field**. Gravitational forces, electrostatic forces, and several others are examples of conservative force fields.



Another way of expressing the fact that a force field $\mathbf{F}$ is conservative is to say that its line integral along *any* path connecting two points, say $\mathbf{x}'$ and $\mathbf{x}$, is independent of the choice of path. To see this, consider two different curves, say γ_1 and γ_2, that both run from $\mathbf{x}'$ to $\mathbf{x}$ (cf. the dashed lines in the figure). Let $-\gamma_2$ denote the curve γ_2 traversed in reverse order, from $\mathbf{x}$ to $\mathbf{x}'$. The line integral along γ_2 is the negative[8] of that along $-\gamma_2$, $W[-\gamma_2] = -W[\gamma_2]$. The curves γ_1 and $-\gamma_2$ may now be combined to a single *closed* curve, γ. The integral along γ is the sum of the integrals along the two segments, $W[\gamma] = W[\gamma_1] + W[-\gamma_2] = W[\gamma_1] - W[\gamma_2]$. Now, if the field is conservative, then $W[\gamma] = 0$, implying that $W[\gamma_1] = W[\gamma_2]$, thus the value of the line integral is indeed independent of the choice of path.

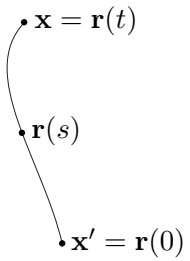
The above construction shows that if the line integral of a vector field around any closed path vanishes, then its line integral along any path connecting two arbitrary points is independent of the choice of the connecting path. It is easy to show (try it!) that the converse is also true, so that we have the equivalence:

$$\forall\, \mathbf{x}', \mathbf{x} \in U: \quad \int_{\gamma_{\mathbf{x}'\to\mathbf{x}}} \mathrm{d}\mathbf{r}\cdot\mathbf{v} \quad \text{is independent of } \gamma \quad \Longleftrightarrow \quad \oint_{\gamma} \mathrm{d}\mathbf{r}\cdot\mathbf{v} = 0\,. \tag{V79}$$

It turns out that there is another equivalence which connects these criteria to the gradientness of a field:

$$\forall\, \mathbf{x}', \mathbf{x} \in U: \quad \int_{\gamma_{\mathbf{x}'\to\mathbf{x}}} \mathrm{d}\mathbf{r}\cdot\mathbf{v} \quad \text{is independent of } \gamma \quad \Longleftrightarrow \quad \mathbf{v} \text{ is a gradient field.} \tag{V80}$$

This is a non-trivial statement whose two different directions, $\Rightarrow$ and $\Leftarrow$, need to be proven separately. We first assume that $\mathbf{v}(\mathbf{x}) = \boldsymbol{\nabla}\varphi_{\mathbf{x}}$ is a gradient field. Let $\gamma_{\mathbf{x}'\to\mathbf{x}}$ be a curve parametrized by $\mathbf{r}: [0,t] \to \mathbb{R}^d$, $s \mapsto \mathbf{r}(s)$, with $\mathbf{r}(0) = \mathbf{x}'$, $\mathbf{r}(t) = \mathbf{x}$. The line integral of the gradient field is then computed as



$$\begin{aligned}\int_{\gamma_{\mathbf{x}'\to\mathbf{x}}} \mathrm{d}\mathbf{r}\cdot\mathbf{v} &= \int_0^t \mathrm{d}s\, \frac{\mathrm{d}\mathbf{r}(s)}{\mathrm{d}s}\cdot\boldsymbol{\nabla}\varphi_{\mathbf{r}(s)} \overset{(V71)}{=} \int_0^t \mathrm{d}s\, \frac{\mathrm{d}\varphi(\mathbf{r}(s))}{\mathrm{d}s} \\ &= \varphi(\mathbf{r}(t)) - \varphi(\mathbf{r}(0)) = \varphi(\mathbf{x}) - \varphi(\mathbf{x}').\end{aligned}$$

This expression depends on $\mathbf{x}'$ and $\mathbf{x}$, but not on the choice of the connecting path $\gamma_{\mathbf{x}'\to\mathbf{x}}$.

[8] Verify this statement from the definition of the line integral, using the fact that if $\mathbf{r}(t)$, $t \in (0,1)$ is a parametrization of γ_2, then the reverse path $-\gamma_2$ can be parametrized by $\mathbf{r}(1-t)$, $t \in (0,1)$.

Conversely, let us assume that the line integral between any two points $\mathbf{x}', \mathbf{x} \in U$ is independent of the connecting path $\gamma_{\mathbf{x}'\to\mathbf{x}}$. Pick a fixed point $\mathbf{x}'$ and define the function

$$\varphi(\mathbf{x}) = \int_{\gamma_{\mathbf{x}'\to\mathbf{x}}} \mathrm{d}\mathbf{r}\cdot\mathbf{v}\,. \tag{V81}$$

This is a valid definition of a function of $\mathbf{x}$ because φ does not depend on the choice of $\gamma_{\mathbf{x}'\to\mathbf{x}}$. Using the same path parametrization as above, $\varphi(\mathbf{r}(t))$ may be represented as

$$\varphi(\mathbf{r}(t)) = \int_{\gamma_{\mathbf{x}'\to\mathbf{r}(t)}} \mathrm{d}\mathbf{r}\cdot\mathbf{v} = \int_0^t \mathrm{d}s\,\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}s}\cdot\mathbf{v}(\mathbf{r}(s))\,.$$

Differentiating this expression w.r.t. t and processing its left and right sides by the chain rule (V71) and the fundamental theorem of calculus Eq. (C19), respectively, we obtain

$$\dot\varphi(\mathbf{r}(t)) = \dot{\mathbf{r}}(t)\cdot\boldsymbol{\nabla}\varphi_{\mathbf{r}(t)} = \dot{\mathbf{r}}(t)\cdot\mathbf{v}(\mathbf{r}(t)). \tag{V82}$$

This relation must hold for any value of $\dot{\mathbf{r}}(t)$ and any $\mathbf{r}(t)\equiv\mathbf{x}$, which requires $\mathbf{v}(\mathbf{x}) = \boldsymbol{\nabla}\varphi_{\mathbf{x}}$, showing that $\mathbf{v}$ is a gradient field. This construction also provides a constructive method for computing the potential, through (V81). Notice that the potential of a vector field is defined only up to a constant, i.e. $\varphi(\mathbf{x})+c$, with $c\in\mathbb{R}$, is a potential too. The freedom to add a constant reflects the arbitrariness of the starting point $\mathbf{x}'$ in the definition, i.e. a different starting point would lead to a potential differing from φ only by a constant (why?).

A topological criterion for gradient fields

Above, we have argued that Eq. (V78) must necessarily hold if $\mathbf{v}$ is a gradient field. Whether or not this condition is *sufficient* depends on the 'topology' (see info section below) of the domain, U, of definition of $\mathbf{v}$:

> A vector field, $\mathbf{v}: U\to\mathbb{R}^d$ is a gradient field if its components obey the condition
>
> $$\partial_i v^j - \partial_j v^i = 0, \qquad i=1,\ldots,d \tag{V83}$$
>
> *and* its domain of definition, U, is *simply connected*.

The meaning of the attribute 'simply connected' is defined as follows: a subset $U\subset\mathbb{R}^d$ is called **connected** if any two of its elements can be connected by a continuous path in U. For example, the set shown in the left panel of Fig. V13 is not connected because it contains pairs of points which cannot be connected by a path inside the set. The set shown in the center panel is connected but not **simply connected**: Although all points are connectible, there exist closed paths which cannot be contracted to a point-like trivial path inside the set. The set shown in the right panel is connected and simply connected: All points are connectible and every closed path in the set is contractible to a trivial one.

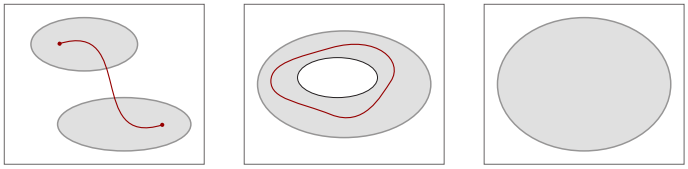


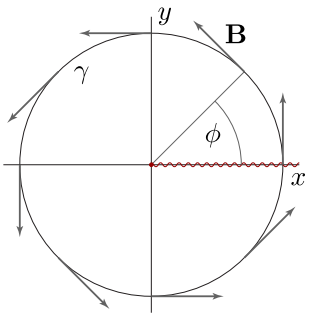
Figure V13: Left panel: a disconnected subset of $\mathbb{R}^2$. Points in separate subsets cannot be connected by a path that lies fully in the set. Center panel: a connected but not simply connected set. Closed paths exist which cannot be contracted to a point-like path inside the set. Right panel: a simply connected set. All points are connectible inside the set, and all paths are contractible.

INFO The connectedness of a subset is an example of a *topological criterion*. **Topology** is the discipline of mathematics addressing structures which do not change under continuous deformation. Topological features of a set remain invariant unless it is subjected to discontinuous operations such as tearing or gluing. (Of course, the terms 'continuous', 'tearing', and 'gluing' all require a precise mathematical definition. However, these are closely related to the meanings that these words have in daily life.) For example, a simply connected set remains simply connected unless a hole is drilled into it, which would be an example of a discontinuous change. In particular, topological features do not depend on notions related to geometric distance, angles, etc. Topology often describes mathematical structures in terms of integer-valued topological 'indices'. For example, the number of holes contained in a surface defines a topological invariant. Topological structures are of interest to physics because they are the most 'universal' (independent of details) features a system can have, and explaining universality is a prime objective of physics. For example, the vortex shown in Fig. V12(c) is an example of a topological structure in a two-dimensional vector field — it cannot be removed by any continuous operation and the number of times the field rotates around the center (once in the figure) is an example of a topological invariant. For their explanation of the important role played by such vortices in real two-dimensional materials, J.M. Kosterlitz and D.J. Thouless were awarded the 2016 Nobel prize in physics (shared with D. Haldane).

The proof showing that simple connectedness and Eq. (V83) define a criterion for gradient fields is beyond the scope of this text. However, the following counter-example demonstrates that the vanishing of the mixed derivative Eq. (V83) is not sufficient to establish that a vector field is a gradient field.

EXAMPLE Consider the vector field,

$$\mathbf{B} : U = \mathbb{R}^2 \backslash \{(0,0)\} \mapsto \mathbb{R}^2, \qquad \begin{pmatrix} x \\ y \end{pmatrix} \mapsto \frac{1}{x^2+y^2} \begin{pmatrix} -y \\ x \end{pmatrix}, \tag{V84}$$



defined in the 'punctured plane', $\mathbb{R}^2\backslash\{(0,0)\}$. The origin $\{(0,0)\}$ needs to be excluded from the domain of definition, U, because denominator in Eq. (V84) diverges at this point. Due to the exclusion of the origin, U is a non-simply connected set: paths winding around the origin cannot be contracted to a trivial point-like path.

The vector field $\mathbf{B}$ rotates around origin, as indicated in the figure. In physics, fields of this type are realized as **magnetic fields** generated by currents. For example, an infinitely long, straight wire carrying a uniform current will generate a magnetic field whose profile in the plane perpendicular to the wire equals our $\mathbf{B}$. We now ask whether $\mathbf{B}$ is a gradient field.

It is straightforward to verify that $\partial_x B_y - \partial_y B_x = 0$ everywhere in U, so Eq. (V83) holds. However, the domain of definition, U, is not simply connected, and so $\mathbf{B}$ may still turn out not to be a gradient field. To see that this is indeed the case, we compute the line integral along a circular closed path in the xy-plane, of radius R and centered on the origin. Parameterizing this path as $\mathbf{r}(t) = R(\cos(2\pi t), \sin(2\pi t))^T$, we have $\dot{\mathbf{r}}(t) = 2\pi R(-\sin(2\pi t), \cos(2\pi t))^T$ and $\mathbf{B}(\mathbf{r}(t)) = (1/R)(-\sin(2\pi t), \cos(2\pi t))^T$, and hence

$$\int_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{B} = \int_0^1 \mathrm{d}t\,\dot{\mathbf{r}}(t)\cdot\mathbf{B}(\mathbf{r}(t)) = \int_0^1 \mathrm{d}t\,(2\pi R)\frac{1}{R}\big[\sin^2(2\pi t)+\cos^2(2\pi t)\big] = 2\pi.$$

We have thus identified a closed path along which $\mathbf{B}$ integrates to give a non-vanishing result; according to Eqs. (V79) and (V80), this means that $\mathbf{B}$ cannot be a gradient field.

It is instructive to modify the above setup slightly so as to convert $\mathbf{B}$ into a proper gradient field. To this end, we choose a more restricted domain of definition $\tilde{U} = \mathbb{R}^2\backslash\mathbb{R}^+$, i.e. we remove the positive real axis (indicated by a wavy line in the figure). This manipulation has two notable consequences: first, the domain of definition now *is* simply connected, since any path in $\tilde{U}$ (i.e. any path not intersecting the now forbidden wavy line) can be contracted to a point. Second, $\tilde{U}$ represents the domain of definition of a polar coordinate system, $\mathbf{y} = (\rho,\phi)^T$, which allows us to formulate calculations in more intuitive ways. It is straightforward to verify (try it!) that in the coordinate basis for polar coordinates, $\mathbf{B}$ can be expressed as $\mathbf{B}(\mathbf{y}) = \mathbf{v}_\phi \frac{1}{\rho^2}$. This equals the gradient, $\boldsymbol{\nabla}\varphi_{\mathbf{y}}$, of the function $\varphi(\mathbf{y}) = \varphi(\rho,\phi) \equiv \phi$, as can be checked using Eq. (V75): $\boldsymbol{\nabla}\phi = (\mathbf{v}_\rho\partial_\rho + \mathbf{v}_\phi\frac{1}{\rho^2}\partial_\phi)\phi = \mathbf{v}_\phi\frac{1}{\rho^2}$.

We conclude that $\boldsymbol{\nabla}\phi = \mathbf{B}$, i.e. $\mathbf{B}$ is indeed a gradient field on the domain $\tilde{U}$. Notice that the non-vanishing of its line integral along γ does not contradict the conditions Eqs. (V79) and (V80) requiring the vanishing of the integral of a gradient field along closed curves. The reason is that the restriction of the path γ to the domain $\tilde{U}$ yields a path that is *not* closed. This restriction implies the removal of the boundary points of the un-restricted path and a parametrization $\mathbf{r} : (0,1) \to \tilde{U}$, $t \mapsto \mathbf{r}(t)$. The removal of the boundary points, $t = 0$ and 1, ensures that the curve does not touch the positive real axis and hence stays inside the domain of definition. In effect this means that the previously closed curve is now cut open, so that the gradient condition does not apply to it.

The cutting of a curve at a single point should not affect the value for the line integral over the continuous field $\mathbf{B}$. To verify this statement, we note that in polar coordinates, $\mathbf{r}(t) = R(\mathbf{v}_\rho)_{(R,\phi(t))}$. This implies $\dot{\mathbf{r}} = R(\partial_\phi\mathbf{v}_\rho)\dot{\phi} = \mathbf{v}_\phi(2\pi)$. On the integration contour we have $\mathbf{B} = R^{-2}\mathbf{v}_\rho$ and hence $\mathbf{B}\cdot\dot{\mathbf{r}} = 2\pi R^{-2}g_{\phi\phi} = 2\pi$, where Eq. (V28)] was used. From these relations we readily recover the

result obtained above:

$$\int_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{B} = \int_0^1 \mathrm{d}t\,\dot{\mathbf{r}}(t)\cdot\mathbf{B}(\mathbf{r}(t)) = \int_0^1 \mathrm{d}t\,2\pi = 2\pi.$$

To conclude this section, let us summarize the **criteria for a vector field being a gradient field**. A vector field $\mathbf{v}$ is a gradient field

- ▷ if there exists a potential, φ, such that $\mathbf{v} = \boldsymbol{\nabla}\varphi$; or
- ▷ if its line integral around any closed loop, γ, in its domain of definition vanishes, $\oint_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{v} = 0$; or
- ▷ if the line integral between any two points in its domain of definition does not depend on the choice of the path connecting these two points; or
- ▷ if the criterion (V83) holds.

V3.3 Sources of vector fields

REMARK Requires chapter C4. Readers who have not read that chapter in full may consult the first subsection of section C4.4 for a definition of the integral of functions over two-dimensional surfaces embedded in three-dimensional space.

In the beginning of section V3.2, we introduced a number of qualitative characteristics describing a vector field. We pointed out that a vector field may contain 'sources' from which vectors appear to emanate, or 'vortices', i.e. centers of circulation (cf. Fig. V12). In the following we introduce tools to detect such structures. In fact, we already know one test criterion — a gradient field cannot contain vortices: if a vortex were present, as in Fig. V12(c), the field vectors' approximate alignment with a closed curve encircling the vortex center would imply a non-vanishing line integral along that curve. This would be in violation of the criterion that gradient fields have vanishing line integrals along closed curves. The argument also conveys another lesson: there appears to be a connection between 'local structures' of vector fields (such as point-like vortex centers), and 'global structures' (such as the integrals around curves surrounding the center).

In this section and the next, we discuss these connections and learn how to apply them to characterize the sources and the vorticity of vector fields, respectively.

Divergence in Cartesian coordinates

Let $\mathbf{u} : \mathbb{R}^d \supset M \to \mathbb{R}^d$, $\mathbf{x} \mapsto \mathbf{u}(\mathbf{x})$ be a smooth d-component vector field in d-dimensional space where a Cartesian parameterization of the argument domain $\mathbf{u}(\mathbf{r}) = \mathbf{u}(\mathbf{r}(\mathbf{x})) \equiv \mathbf{u}(\mathbf{x})$ is

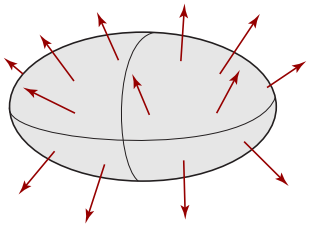
assumed. Its **divergence** is a scalar field defined as

$$\operatorname{div}\mathbf{u} \equiv \boldsymbol{\nabla}\cdot\mathbf{u} : M \to \mathbb{R}, \qquad \mathbf{x} \mapsto (\operatorname{div}\mathbf{u})(\mathbf{x}) = (\boldsymbol{\nabla}\cdot\mathbf{u})(\mathbf{x}) \equiv \sum_{i=1}^{d} \partial_i u^i(\mathbf{x}), \tag{V85}$$

where u^i are the Cartesian components of $\mathbf{u} = \mathbf{e}_i u^i$. The generalization of the divergence to curvilinear coordinate systems is discussed in the info section on p. 433.

The divergence of a vector field is a scalar function that measures its source content, i.e. to what extent it can be associated with the presence of sources. To understand this statement, imagine a vector field containing a point source, as in Fig. V12(b). The figure shows how the x-component u^x grows in the x-direction ($\partial_x u^x > 0$) and the y-component grows in the y-direction ($\partial_y u^y > 0$). According to Eq. (V85), the divergence $\operatorname{div}\mathbf{u}$ will thus be positive at the source. This observation indicates that the divergence is a *local* probe for the presence of sources. It is local in the sense that it describes $\mathbf{u}(\mathbf{x})$ in terms of derivatives taken at $\mathbf{x}$. In the following, we will discuss sources from the complementary *global* perspective, and then connect the global and local views to obtain a powerful unified description.

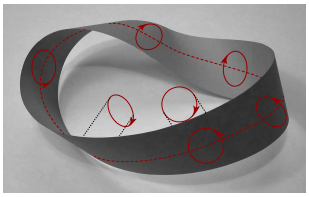
Surface integrals of vector fields



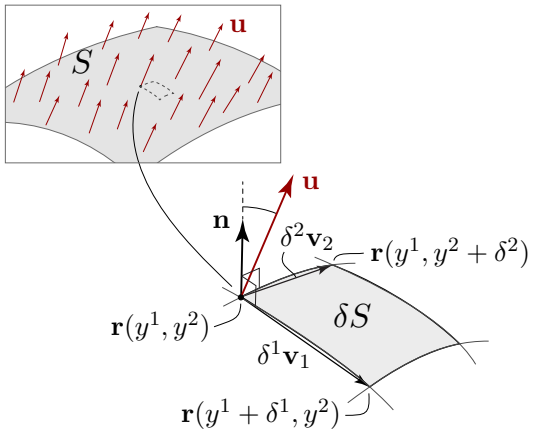
Consider a two-dimensional surface, $S \subset M$, embedded in a three-dimensional domain M, and a vector field $\mathbf{u}$ defined on M. For a given $\mathbf{r} \in S$ one may picture $\mathbf{u}(\mathbf{r})$ as a vector specifying the direction and velocity of a 'liquid' streaming through the surface (as if the latter were a sieve). If S is a *closed* surface and the net amount of outward flow is positive/negative then the vector field must contain sources/sinks inside S. The non-vanishing of the flux through closed surfaces therefore is a measure for the presence of sources, where a sink is interpreted as a 'negative source'.

To make this statement quantitative, we need to determine the flux of vector fields through surfaces (open or closed) via a suitably-defined surface integral. We start by giving a surface an *orientation*. By definition, the **orientation of a surface** is a convention identifying one of its faces as the 'outside' and the opposite face as the 'inside'. Not all surfaces admit such an assignment (see info section below), however most of practical relevance do. For example, the closed surface of a sphere has a natural out- and inside, and for a planar sheet one may assign one side to be the outside.

INFO A surface is called **orientable** if it permits the global assignment of an 'inside' and an 'outside' face. Planes, spheres, cylinders, and 'most' other surfaces are orientable in this sense. By contrast, the Möbius strip (see figure) is an example of a non-orientable surface. Inspection of the figure shows that it has just one face, not two. However it it not entirely obvious how to cast this pictorial observation into sound mathematical language. One of several equivalent ideas is



as follows: a surface is non-orientable if it is possible to continuously deform a closed curve which is traversed anticlockwise, into one which is traversed clockwise. The figure illustrates how this is achieved for the Möbious strip. By contrast, the direction of traversal of a closed curve on a sphere cannot be altered. For further discussion of orientability, see p 476.



Quantitatively, the flux of $\mathbf{u}$ through a surface element δS at $\mathbf{r}$ is defined as $\delta\Phi \equiv |\delta S|\,(\mathbf{n}\cdot\mathbf{u})$, where $\mathbf{n}(\mathbf{r})$ is the outward-pointing unit vector orthogonal to δS (see figure). The scalar product $\mathbf{n}\cdot\mathbf{u}$ is the component of $\mathbf{u}$ perpendicular to δS, and multiplication of this component with the geometric area, $|\delta S|$, of the surface element *defines* the flux through this element. Concrete expressions for these quantities may be obtained by parameterizing the surface as $\mathbf{r} : U \subset \mathbb{R}^2 \to S$, $\mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$, in terms of a two-component coordinate vector, $\mathbf{y} \equiv (y^1, y^2)^T$ (cf. section C4.4). For a coordinate domain discretized via a rectangular grid with spacings δ^1 and δ^2, the induced surface element δS at $\mathbf{r}(\mathbf{y})$ is then spanned by the two vectors $\delta^i\partial_{y^i}\mathbf{r}(\mathbf{y}) \equiv \delta^i\mathbf{v}_i$ ($i = 1, 2$, no summation). It has geometric area $|\delta S| = \delta^1\delta^2\|\mathbf{v}_1\times\mathbf{v}_2\|$, and $\mathbf{n} \equiv \frac{\mathbf{v}_1\times\mathbf{v}_2}{\|\mathbf{v}_1\times\mathbf{v}_2\|}$ is its normal unit vector. We thus obtain the **flux through the surface element** as[9]

$$\delta\Phi = |\delta S|\,(\mathbf{n}\cdot\mathbf{u}) = \delta^1\delta^2(\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{u}. \tag{V86}$$

Note that $\delta\Phi = \delta\Phi(\mathbf{r})$ depends on the point $\mathbf{r}$ through the choice of the corner point used in its construction. There is arbitrariness in this choice, we might have picked a different corner, or taken any other point in δS as a reference point. However, all these different choices, $\mathbf{r}'$, are close to each other in the sense that $\|\mathbf{r}-\mathbf{r}'\| = \mathcal{O}(\delta)$. Since all $\mathbf{r}$-dependent functions entering the construction of $\delta\Phi$ are smooth, the differences $\delta\Phi(\mathbf{r}) - \delta\Phi(\mathbf{r}') = \mathcal{O}(\delta^3)$ ($\delta\Phi$ is $\mathcal{O}(\delta^2)$ and a third power in δ comes from the Taylor expansion of the smooth function $\Phi(\mathbf{r}')$ around $\mathbf{r}$) are negligibly small in the limit $\delta^1, \delta^2 \to 0$. **Local approximations** during which smooth functions will be read out at arbitrary points of convenience within infinitesimally small geometric structures will be used frequently throughout.

The total **flux of $\mathbf{u}$ through the surface**, Φ_S, is obtained as the (Riemann) sum over all such elements, leading to a **vector field surface integral**, or **flux integral**, of the following form:

$$\boxed{\Phi_S \equiv \int_S \mathrm{d}\mathbf{S}\cdot\mathbf{u} \equiv \int_U \mathrm{d}y^1\mathrm{d}y^2\,(\partial_{y^1}\mathbf{r}\times\partial_{y^2}\mathbf{r})\big|_{\mathbf{r}=\mathbf{r}(\mathbf{y})}\cdot\mathbf{u}(\mathbf{r}(\mathbf{y}))}. \tag{V87}$$

[9] In the physics literature $\delta\mathbf{S} \equiv |\delta S|\,\mathbf{n} = \delta^1\delta^2(\mathbf{v}_1\times\mathbf{v}_2)$ is often called an **oriented surface element**. This denotation emphasizes that $\delta\mathbf{S}$ contains information on both, the geometric area and the orientation of the surface element.

Here, $\int_S \mathrm{d}\mathbf{S}\cdot\mathbf{u}$ is a formal symbol for the flux, whose concrete meaning is given by the coordinate integral on the right.

Gauss' theorem

Our discussion above identified two different criteria for the presence of sources in a vector field: a non-vanishing flux through a closed surface, and a non-vanishing divergence at the sources of a vector field, respectively. There must be a connection between the two.

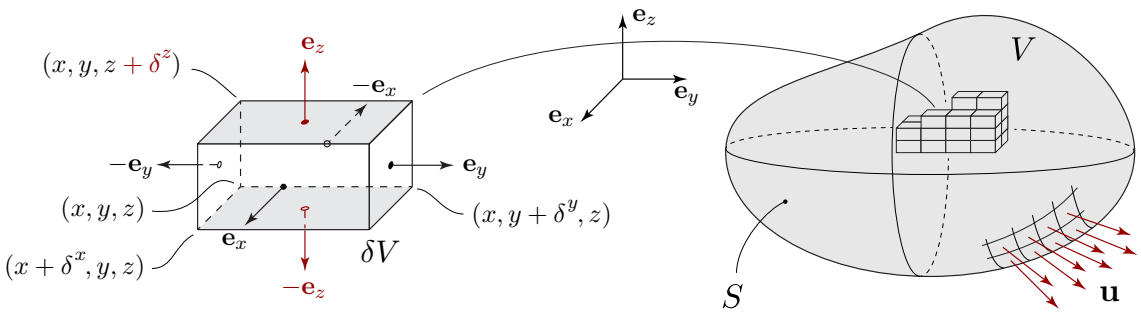


Figure V14: On the derivation of Gauss' theorem.

To establish a relation between vector field divergence and surface integrals, we consider an infinitesimal volume element, δV, shaped as the box shown in Fig. V14. Imagine the box sits inside the domain of definition of a smooth vector field $\mathbf{u}$. Let us calculate the outward flux of $\mathbf{u}$ over the surface, δS, of the box. Choosing coordinates as indicated in the figure, $\mathbf{e}_z$ is a unit vector normal to the top surface of the box and its opposite, $-\mathbf{e}_z$, is normal to the bottom surface. Since the vector field is smooth, we can choose the box so small that the variation of $\mathbf{u}$ across the extension of the box is very weak. Therefore the surface integral over each of the faces of the box can be accurately described by the local approximation, Eq. (V86).For example, the sum of the integrals over the top and bottom faces is given by

$$\delta\Phi_{\mathrm{top}}+\delta\Phi_{\mathrm{bot}} \simeq \delta^x\delta^y\Big[\mathbf{e}_z\cdot\mathbf{u}(x,y,z+\delta^z)-\mathbf{e}_z\cdot\mathbf{u}(x,y,z)\Big] \simeq \delta^x\delta^y\delta^z\partial_z u^z(x,y,z). \quad \text{(V88)}$$

Here, the differences in the values of the z-coordinate, although of $\mathcal{O}(\delta)$ are of importance because a function difference $\mathbf{u}(\ldots,z+\delta)-\mathbf{u}(\ldots,z)$ is at hand. However, once this difference has been evaluated to obtain a result of $\mathcal{O}(\delta^3)$ the precise choice of the coordinates x,y within the box faces become irrelevant, due to the local approximability principle discussed above.

Adding analogous contributions from the remaining surfaces one arrives at the result

$$\int_{\delta S}\mathrm{d}\mathbf{S}\cdot\mathbf{u} \simeq \delta^x\delta^y\delta^z(\partial_x u^x+\partial_y u^y+\partial_z u^z)=\delta^x\delta^y\delta^z(\boldsymbol{\nabla}\cdot\mathbf{u})\simeq\int_{\delta V}\mathrm{d}V\,\boldsymbol{\nabla}\cdot\mathbf{u}. \quad \text{(V89)}$$

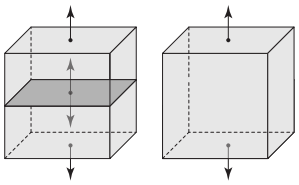
Johann Carl Friedrich Gauss (1777-1855)

German astronomer, physicist and mathematician. Gauss made breakthrough contributions to a wide spectrum of mathematical disciplines. He worked on non-Euclidean geometry, algebra, the theory of special functions, and may be regarded the founding father of modern statistics. Gauss was one of the last 'universal scholars'. His interests extended beyond the boundaries of physics and mathematics into the realm of geography, literature, cartography, and other fields of science.

In the first step we observed that the contributions of the three surfaces combine to give the divergence of $\mathbf{u}$. For the final equality we once more used the assumed near-constancy of the vector field over the extension of the box to identify the term $\delta^x\delta^y\delta^z(\boldsymbol{\nabla}\cdot\mathbf{u})$ with a volume integral. The result (V89) confirms the expectation that a non-vanishing flux of a vector field through a closed surface implies a non-vanishing divergence inside the surface, and vice versa.

Although this correspondence has been established only for the case of an infinitesimally small box, a simple argument shows that the result carries over to more general volumes, such as the extended structure shown in Fig. V14. Imagine a volume V, with boundary surface (outer hull) S, filled up with a large number of infinitesimal boxes, δV_ℓ, bounded by surfaces δS_ℓ. By a standard Riemann sum type argument, the volume integral of $\boldsymbol{\nabla}\cdot\mathbf{u}$ over the full volume V can be expressed as

$$\int_V \mathrm{d}V\,\boldsymbol{\nabla}\cdot\mathbf{u} \simeq \sum_\ell \int_{\delta V_\ell} \mathrm{d}V\,(\boldsymbol{\nabla}\cdot\mathbf{u}) = \sum_\ell \int_{\delta S_\ell} \mathrm{d}\mathbf{S}\cdot\mathbf{u} \simeq \int_S \mathrm{d}\mathbf{S}\cdot\mathbf{u}\,. \tag{V90}$$



In the crucial last step we observed that the sum of the surface integrals over all boxes approximately equals the surface integral over the outer hull, S. To understand this, consider the sum of the surface integrals over just two adjacent boxes. The contributions to the integral from their touching faces cancel.[10] The sum of the two surface integrals thus equals the integral over the outer surface of the two merged boxes. By the same argument, the integral over a stacked array of boxes equals the integral over its outer hull, and this fact was exploited for the last step in Eq. (V90). In the limit of an infinitely fine box decomposition, the approximate equalities in Eq. (V90) become exact.

Summarizing, we have found that the volume integral of a divergence equals the flux integral over the volume's outer hull,

$$\boxed{\int_V \mathrm{d}V\,\boldsymbol{\nabla}\cdot\mathbf{u} = \int_S \mathrm{d}\mathbf{S}\cdot\mathbf{u}\,,} \tag{V91}$$

a result known as **Gauss' theorem**. The theorem states that non-vanishing flux integrals over closed surfaces – obtained for surfaces surrounding sources of outward/or inward directed flow – reflect a non-vanishing vector field divergence. We reiterate that the choice of the

[10] The reason is that the two touching faces have equal area, but normal vectors pointing in opposite directions. The surface integrals over these two faces thus have equal magnitude but opposite sign.

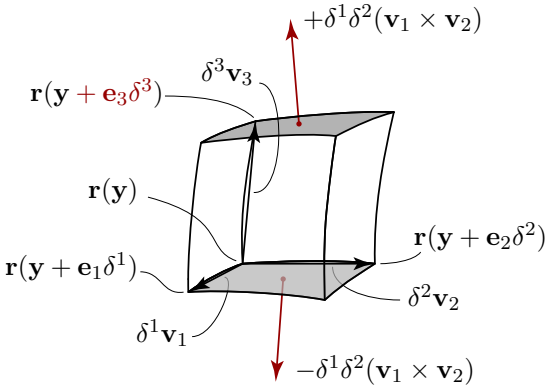
volume bounded by S is arbitrary, as long as it remains within the domain of definition of the vector field. This result may actually be used to *define* the divergence as the outward flux of the underlying vector field per unit volume. To this end, let δV be an infinitesimal test volume of unspecified shape, with outer surface δS and geometric volume $|\delta V|$. Then, $\int_{\delta V} \mathrm{d}V\, \mathrm{div}(\mathbf{u}) \simeq |\delta V|\, \mathrm{div}(\mathbf{u})$, so that we may define

$$\boxed{\mathrm{div}(\mathbf{u}) \equiv \lim_{|\delta V|\to 0} \frac{1}{|\delta V|} \int_{\delta S} \mathrm{d}\mathbf{S}\cdot\mathbf{u}\,.} \tag{V92}$$

This definition has the advantage of not being tied to a specific system of coordinates. It may thus be used to express the divergence in arbitrary coordinates, see the info section below.

Divergence in general coordinates

Eq. (V85) describes the divergence of a vector field in Cartesian coordinates. However, the presence or absence of sources in a vector field is an 'invriant' feature not depending on coordinates. Indeed, the derivation of Gauss' theorem can be straightforwardly adapted to arbitrary coordinates, and as a result yields a generalized representation of the divergence. Such representations are useful if the symmetry of a problem disfavors Cartesian coordinates.



Equation (V92) may be applied to derive a formula for the **divergence in generalized coordinates**. Assume V to be described by a three-dimensional coordinate map $\mathbf{r}: U \to V$, $\mathbf{y} \mapsto \mathbf{r}(\mathbf{y})$. An infinitesimal cuboid in U, with corner points $\mathbf{y}$ and $\mathbf{y}+\mathbf{e}_i\delta^i$ (with $i=1,2,3$, no summation), then maps onto a distorted cuboid, δV, as shown in the figure. The edges of δV are approximately defined by the vectors $\delta^i\partial_{y^i}\mathbf{r}(\mathbf{y}) = \delta^i\mathbf{v}_i(\mathbf{y})$, evaluated at the appropriate corners. We aim to compute $\int_{\delta S}\mathrm{d}\mathbf{S}\cdot\mathbf{u}$, the outward flux of $\mathbf{u}$ through the surface, δS, of δV. In analogy to Eq. (V88), the top and bottom faces yield a contribution $\delta\Phi_{\mathrm{top}} + \delta\Phi_{\mathrm{bot}} = \big(|\delta S|\,\mathbf{n}\cdot\mathbf{u}\big)_{\mathrm{top}} + \big(|\delta S|\,\mathbf{n}\cdot\mathbf{u}\big)_{\mathrm{bottom}}$ where, however, the Cartesian surface elements $\delta^x\delta^y u^z$ of (V88) need to be replaced by the more general triple products, $\delta^1\delta^2(\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{u}$, of Eq. (V86). This leads to the expression

$$\delta^1\delta^2\Big[((\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{u})(\mathbf{y}+\mathbf{e}_3\delta^3) - ((\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{u})(\mathbf{y})\Big] \simeq \delta^1\delta^2\delta^3\partial_{y^3}\Big[((\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{u})(\mathbf{y})\Big].$$

To simplify the right-hand side, we expand $\mathbf{u} = \sum_i \mathbf{v}_i u^i$ in the coordinate basis. Only the 3-component survives in the triple product, yielding[11] $(\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{u} = (\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{v}_3\, u^3 = \sqrt{g}\,u^3$. Here we recalled the connection (C58) to the metric tensor and used the shorthand notation $\sqrt{g} \equiv \sqrt{|\det g|}$. Thus, the net contributions from the top and bottom faces is

[11] We assume a right-handed coordinate system, so that the triple product $(\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{v}_3$ is positive.

$\delta^1\delta^2\delta^3\partial_{y^3}\big(\sqrt{g}u^3\big)$. Adding the contributions from the remaining surface pairs we obtain the total outward flux as $\int_{\delta S}\mathrm{d}\mathbf{S}\cdot\mathbf{u} = \delta^1\delta^2\delta^3\sum_i\partial_{y^i}(\sqrt{g}\,u^i)$. Since the volume of the distorted cuboid is given by $|\delta V| \simeq \delta^1\delta^2\delta^3|(\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{v}_3| = \delta^1\delta^2\delta^3\sqrt{g}$ (see Eq. (L89)), we can express the flux as $|\delta V|\frac{1}{\sqrt{g}}\sum_i\partial_{y^i}(\sqrt{g}\,u^i)$. Division by $|\delta V|$ and comparison with Eq. (V92) leads to

$$\boxed{\mathrm{div}(\mathbf{u}) = \frac{1}{\sqrt{g}}\sum_i\partial_{y^i}(\sqrt{g}\,u^i)} \tag{V93}$$

for the **divergence** of a vector field, expanded in the **coordinate basis** of a generic coordinate system. For example, in spherical coordinates, where Eq. (V36) yields $\sqrt{g} = r^2\sin\theta$, one obtains

$$\mathrm{div}(\mathbf{u}) = \frac{1}{r^2}\partial_r(r^2\,u^r) + \frac{1}{\sin\theta}\partial_\theta(\sin\theta u^\theta) + \partial_\phi u^\phi. \tag{V94}$$

INFO The sources of vector fields describing physical quantities generally have a clearly-defined physical meaning. For example, **Gauss'** (!) **law** of electromagnetism states that

$$\boldsymbol{\nabla}\cdot\mathbf{E} = 4\pi\rho, \tag{V95}$$

where $\mathbf{E}$ is the electric field, ρ the charge density, i.e. the amount of charge per unit volume, and so-called CGS units are used. Integrating Eq. (V95) over a volume V bounded by a surface S and using Gauss' theorem (V91), one obtains an equivalent statement of Gauss' law,

$$\int_S\mathrm{d}\mathbf{S}\cdot\mathbf{E} = 4\pi Q, \tag{V96}$$

where $Q = \int_V\mathrm{d}V\rho$ is the charge contained in the volume V. Eqs. (V95) and (V96) are called the differential and the integral formulations of Gauss' law, respectively. Both state that electic fields are created by electric charge. While Eq. (V96) may be easier to understand intuitively, the differential representation Eq. (V95) does not make reference to a specific volume and hence is better suited to the mathematical description of electrodynamics.

Another (independent) statement of electrostatics is that a static charge distribution, ρ, generates an electric field which is a gradient field, $\mathbf{E} = -\boldsymbol{\nabla}\varphi$, where φ is the so-called electrostatic potential. (For time-varying charge distributions, $\rho(\mathbf{x},t)$, the electric field need no longer be a gradient field.) Gauss' law then assumes the form $\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\varphi = -4\pi\rho$, known as the **Poisson equation**.

Laplace operator

The second-order differential operator

$$\Delta = \boldsymbol{\nabla}\cdot\boldsymbol{\nabla} \tag{V97}$$

is known as the **Laplace operator** or **Laplacian**. In Cartesian coordinates it assumes the form $\Delta\phi = \sum_i\partial_i(\partial_i\phi)$, or just $\Delta = \sum_i\partial_i^2$. The Laplacian governs many important equations in physics, including (f, q are functions depending on space and/or time)

Pierre Simon Laplace (1749-1827)

French mathematician, physicist and astronomer. Important contributions include a five volume work on celestial mechanics, the development of Bayesian statistics (which is of paramount importance to current date statistical analysis in all sciences), the formulation of the Laplace equation and the Laplace transform, and many others. Laplace is remembered as one of the greatest scientists of all times, and sometimes referred to as the 'French Newton'.

$$\Delta f = 0 \qquad \textbf{Laplace equation},$$
$$\Delta f = q \qquad \textbf{Poisson equation},$$
$$\Delta f - \partial_t^2 f = q \qquad \textbf{wave equation}.$$

It is also a central building block of the Schrödinger equation of quantum mechanics. An expression for the **Laplace operator in general coordinates** is obtained by applying the covariant divergence operation Eq. (V93) to the covariant gradient,

$$\Delta f = \operatorname{div}(\boldsymbol{\nabla} f) = \frac{1}{\sqrt{g}} \sum_i \partial_{y^i} (\sqrt{g}\, (\boldsymbol{\nabla} f)^i),$$

If we then apply Eq. (V77) to represent the latter in coordinates, we arrive at the generalized representation of the Laplace operator:

$$\boxed{\Delta f = \frac{1}{\sqrt{g}} \sum_{ij} \partial_{y^i} (\sqrt{g}\, g^{ij} \partial_{y^j} f)\,.} \tag{V98}$$

For example, the **Laplace operator in spherical coordinates** is given by

$$\Delta f = \frac{1}{r^2} \partial_r \big(r^2 \partial_r f\big) + \frac{1}{r^2 \sin^2\theta} \partial_\theta \big(\sin\theta \partial_\theta f\big) + \frac{1}{r^2 \sin^2\theta} \partial_\phi^2 f, \tag{V99}$$

and this formula is heavily used in electrodynamics and quantum mechanics.

EXERCISE Consider a radially symmetric charge distribution characterized by a density $\rho(r)$. The electric field generated by this distribution will have the radial form $\mathbf{E} = \mathbf{v}_r E^r(r)$ in the coordinate basis, where the absence of components in θ and ϕ directions reflects the rotational symmetry of the distribution. For the same reason, the strength of the field, $E^r(r)$, depends only on the radial coordinate. A formula for the field strength is obtained by applying the integral version of Gauss' law, Eq. (V96), to a ball, B, of radius r centered around the charge. The charge contained in the ball is then obtained as

$$Q(r) = \int_B dV\, \rho = 4\pi \int_0^r \mathrm{d}s\, s^2 \rho(s).$$

The l.h.s. of Gauss' law (V96) contains an integral over the surface, ∂B, of the ball, i.e. a sphere of radius r. Computing this integral using Eq. (V87), with $\partial_\theta \mathbf{r} = \mathbf{v}_\theta$ and $\partial_\phi \mathbf{r} = \mathbf{v}_\phi$, we obtain

$$\int_{\partial B} \mathrm{d}\mathbf{S} \cdot \mathbf{E} = \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, (\mathbf{v}_\theta \times \mathbf{v}_\phi) \cdot \mathbf{v}_r E^r(r) = \int_0^\pi \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, r^2 \sin\theta\, E^r(r) = 4\pi r^2 E^r(r),$$

where we used $(\mathbf{v}_\theta \times \mathbf{v}_\phi) \cdot \mathbf{v}_r \overset{(C64)}{=} \sqrt{g} \overset{(C65)}{=} r^2 \sin\theta$. Equating the two sides of Eq. (V96) we obtain

$$E^r(r) = \frac{Q(r)}{r^2} = \frac{4\pi}{r^2} \int_0^r \mathrm{d}s\, s^2 \rho(s). \tag{V100}$$

Finally, one may apply Eq. (V94) to compute $\mathrm{div}(\mathbf{E})$ and verify that this solution satisfies the differential form of Gauss' law, Eq. (V95). Notice that if r lies outside the support of the charge distribution (i.e. if $\rho(s) = 0$ for $s \geq r$), the charge $Q(r)$ within the ball equals the total charge of the distribution, say Q, so that $E^r(r) = Q/r^2$. This is the **electric Coulomb field** generated by a charge Q.

V3.4 Circulation of vector fields

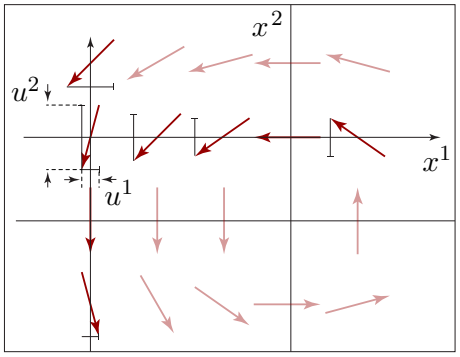
The presence of circulation (see Fig. V12(c)) can be addressed by methods similar to those introduced in the previous section. The defining characteristic of a vector field $\mathbf{u}$ winding around a region in space is that there exist closed curves, γ, (encircling the region in question) such that the line integrals $\oint_\gamma \mathrm{d}\mathbf{s} \cdot \mathbf{u}$, assume non-vanishing values. These line integrals now assume a role similar that of the surface integrals in the previous section. As with the divergence, the non-vanishing of these 'test integrals' is equivalent to the non-vanishing of a differential quantity, the 'curl' of a vector field:

Curl

Let $\mathbf{u} : \mathbb{R}^3 \supset M \to \mathbb{R}^3$, $\mathbf{x} \mapsto \mathbf{u}(\mathbf{x})$ be a three-dimensional vector field defined in three dimensional space where a Cartesian parameterization of the argument domain is assumed, $\mathbf{u}(\mathbf{r}) \equiv \mathbf{u}(\mathbf{r}(\mathbf{x})) \equiv \mathbf{u}(\mathbf{x})$. Its **curl** is a vector field, defined as

$$\mathrm{curl}\,\mathbf{u} \equiv \boldsymbol{\nabla} \times \mathbf{u} : M \to \mathbb{R}^3, \qquad \mathbf{x} \mapsto (\mathrm{curl}\,\mathbf{u})(\mathbf{x}) = (\boldsymbol{\nabla} \times \mathbf{u})(\mathbf{x}) = \mathbf{e}_i \epsilon^{ijk}\, \partial_j u^k\big|_{\mathbf{x}}. \tag{V101}$$

Notice the erratic appearance of co– and contravariant indices on the right hand side. As in previous cases (e.g. the definition of the cross product) this is a sure sign that elements of a metric tensor are missing and that we are working with a formula that makes sense only in Cartesian coordinates (where $g_{ij} = \delta_{ij}$). We will return to this point below, when we discuss the curl in generalized coordinates.



A few comments: the symbol $\boldsymbol{\nabla} \times \mathbf{u}$ serves as a mnemonic indicating that the curl looks like the cross product of the 'vector' $\boldsymbol{\nabla} = (\partial_1, \partial_2, \partial_3)^T$ and $\mathbf{u}$. However, one shouldn't read too much into this interpretation. To get the gist of the definition, consider the 3-component, $(\boldsymbol{\nabla} \times \mathbf{u})^3 = \partial_1 u^2 - \partial_2 u^1$. A positive curl means that u^2 has a tendency to grow in the 1-direction, while u^1 tends to diminish in 2-direction. Now, this is what we would expect from a vector field showing finite circulation in the 12-plane (see the figure, where vertical and horizontal bars indicate how u^1 and u^2 change with position). As in the previous section, we now have two tentative criteria for the presence of circulation, a global one (the non-vanishing of closed loop line integrals) and a local one (the non-vanishing of the curl). It remains to establish a connection between these two.

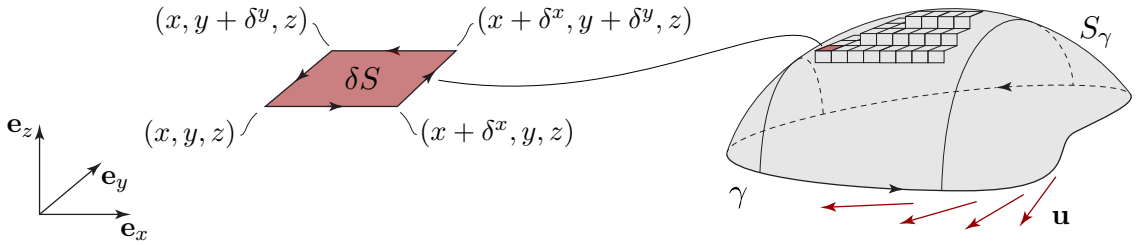


Figure V15: On the derivation of Stokes theorem. For a discussion, see the text.

Stokes theorem

Consider an infinitesimally small rectangle, δS, in the xy-plane of a three-dimensional coordinates system as indicated in Fig. V15. We aim to compute the line integral $\oint_{\gamma_{\delta S}} \mathrm{d}\mathbf{s}\cdot\mathbf{u}$ of a smooth vector field $\mathbf{u}$ around the closed rectangular boundary, $\gamma_{\delta S}$, of δS. The integral is done in mathematically positive orientation, i.e. the integration path winds in counterclockwise direction around the z-axis. As is obvious from the figure, the integration path γ consists of two pairs of parallel edges. Since these edges are traversed in opposite direction, we expect the respective integrals to nearly cancel against each other. For example, the integral along the pair of edges parallel to the x-axis yields

Sir George Gabriel Stokes (1819-1903)

Irish physicist and mathematician. Stokes worked on the theory of hydrodynamics, wave propagation, and the theory of sound. He was the first to understand the principles of fluorescence.

$$\int_{\text{front}} \mathrm{d}\mathbf{r}\cdot\mathbf{u} + \int_{\text{back}} \mathrm{d}\mathbf{r}\cdot\mathbf{u} \simeq \delta^x \underbrace{\mathbf{e}_x\cdot\mathbf{u}}_{u^x}(x,y,z) - \delta^x \mathbf{e}_x\cdot\mathbf{u}(x, y+\delta^y, z) \simeq -\delta^x\delta^y\partial_y u^x(x,y,z).$$

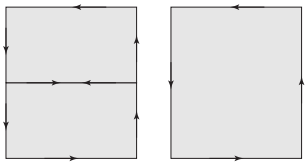
Once more, the local approximation principle discussed on p. 430 implies near constancy of $\mathbf{u}$ along the edges, and this justifies the first approximation. In the second step, we perform a first order Taylor expansion in the small difference of the vector field component u^x on the opposing edges with their slightly different y-coordinate. In doing so, the precise value of the readout coordinate x is of no significance, once more due to the locality principle. Adding to this expression the sum of integrals, $\int_{\text{left}} + \int_{\text{right}}$ of the other edge pair, we obtain

$$\oint_{\gamma_{\delta S}} \mathrm{d}\mathbf{r}\cdot\mathbf{u} \simeq \delta^x\delta^y(-\partial_y u^x + \partial_x u^y)(x,y,z) = \delta^x\delta^y(\boldsymbol{\nabla}\times\mathbf{u})\cdot\mathbf{e}_z \simeq \int_{\delta S}\mathrm{d}\mathbf{S}\cdot(\boldsymbol{\nabla}\times\mathbf{u}), \tag{V102}$$

where in the final step we noted that the third expression is approximately equal to the area integral of $\boldsymbol{\nabla}\times\mathbf{u}$ over the surface element. Here, the orientation is such that the positively oriented traversal of the line integral corresponds to a surface normal vector pointing in the *positive* z-direction (give this point some consideration).

As in the discussion of Gauss' law the construction above is straightforwardly generalized from infinitesimal rectangular to arbitrarily shaped extended integration domains: consider the curve γ shown in Fig. V15. Let $S_\gamma \subset M$ be an arbitrary surface bounded by γ. Imagine an approximate 'tiling' of S_γ by infinitesimal, rectangular surface elements, δS_ℓ, as indicated in the figure. We then obtain (cf. the analogous Eq. (V90))

$$\int_{S_\gamma}\mathrm{d}\mathbf{S}\cdot(\boldsymbol{\nabla}\times\mathbf{u}) \simeq \sum_\ell \int_{\delta S_\ell}\mathrm{d}\mathbf{S}\cdot(\boldsymbol{\nabla}\times\mathbf{u}) = \sum_\ell \oint_{\gamma_{\delta S_\ell}}\mathrm{d}\mathbf{r}\cdot\mathbf{u} \simeq \oint_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{u}. \tag{V103}$$



In the crucial last step we observed that the sum of the line integrals round all rectangles approximately equals the line integral over the boundary, γ, of the surface S_γ. To understand this, consider the sum of the line integrals over just two adjacent rectangles. The contributions to the integral from their touching edges cancel, because they are traversed in opposite directions. The sum of the two line integrals thus equals the line integral around the outer boundary of the two merged rectangles. By the same argument, the sum of line integrals around a set of rectangles tiling a more complex surface equals the line integral along the outer perimeter of the surface. In Eq. (V103) that perimeter approximately equals γ, so we obtain the last equality of the equation. In the limit that the tile size goes to zero, the approximate equalities Eq. (V103) become exact.

Summarizing, we have found that the surface integral of a curl equals the line integral around the boundary of the surface,

$$\boxed{\int_{S_\gamma}\mathrm{d}\mathbf{S}\cdot(\boldsymbol{\nabla}\times\mathbf{u}) = \oint_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{u},} \tag{V104}$$

a result known as **Stokes' theorem**. It states that non-vanishing line integrals around closed curves – obtained for curves surrounding regions of circulating flow – reflect a non-vanishing

vector field curl. We reiterate that the choice of the surface bounded by γ is arbitrary, as long as it remains within the domain of definition of the vector field. This result may actually be used to *define* the curl of a vector field in a manner that does not make reference to a particular system of coordinates (cf. the analogous Eq. (V92)): for an infinitesimal surface element δS, bounded by the curve $\gamma_{\delta S}$ and with normal unit vector $\mathbf{n}$, we define

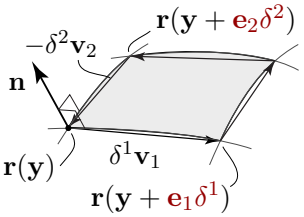
$$\boxed{\mathbf{n}\cdot(\boldsymbol{\nabla}\times\mathbf{u}) \equiv \lim_{|\delta S|\to 0} \frac{1}{|\delta S|} \oint_{\gamma_{\delta S}} \mathrm{d}\mathbf{r}\cdot\mathbf{u}.} \tag{V105}$$

Curl in generalized Coordinates

As with the divergence before, the infinitesimal-area Eq. (V105) can be applied to derive a formula for the **curl in general coordinates**. We assume a three-dimensional coordinate system, $\mathbf{r} : U \subset \mathbb{R}^3 \to \mathbb{R}^3$, $\mathbf{y} = (y^1, y^2, y^3)^T \mapsto \mathbf{r}(\mathbf{y})$. An infinitesimal rectangle in U with corner points $\mathbf{y}$ and $\mathbf{y} + \mathbf{e}_i\delta^i$ (with $i = 1, 2$, no summation) then maps onto a distorted rectangle, δS, as shown in the figure. The edges of δS are approximately defined by the vectors $\delta^i\partial_{y^i}\mathbf{r}(\mathbf{y}) = \delta^i\mathbf{v}_i(\mathbf{y})$, evaluated at the appropriate corners. Its geometric area is $|\delta S| = \delta^1\delta^2\|\mathbf{v}_1\times\mathbf{v}_2\|$, and $\mathbf{n} \equiv \frac{\mathbf{v}_1\times\mathbf{v}_2}{\|\mathbf{v}_1\times\mathbf{v}_2\|}$ is its normal unit vector. Rearranging Eq. (V105), we thus obtain the following relation:

$$\oint_{\gamma_{\delta S}} \mathrm{d}\mathbf{r}\cdot\mathbf{u} \simeq |\delta S|\,\mathbf{n}\cdot(\boldsymbol{\nabla}\times\mathbf{u}) \simeq \delta^1\delta^2(\mathbf{v}_1\times\mathbf{v}_2)\cdot(\boldsymbol{\nabla}\times\mathbf{u})\,. \tag{V106}$$

We now expand the curl in the coordinate basis, $\boldsymbol{\nabla}\times\mathbf{u} = \mathbf{v}_i(\boldsymbol{\nabla}\times\mathbf{u})^i$. Using $(\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{v}_{1,2} = 0$ and recalling the relation $(\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{v}_3 = \sqrt{|\det g|} \equiv \sqrt{g}$, Eq. (C58), we can represent the r.h.s. as



$$\delta^1\delta^2(\mathbf{v}_1\times\mathbf{v}_2)\cdot\mathbf{v}_3(\boldsymbol{\nabla}\times\mathbf{u})^3 = \delta^1\delta^2\sqrt{g}\,(\boldsymbol{\nabla}\times\mathbf{u})^3.$$

Next we consider the l.h.s. of Eq. (V106), involving the line integral round the perimeter, $\gamma_{\delta S}$. The contribution of the 'front' and 'back' edges can be obtained using the local approximation in a manner analogous to Eq. (**??**), yielding $\delta^1(\mathbf{v}_1\cdot\mathbf{u})(\mathbf{y}) - \delta^1(\mathbf{v}_1\cdot\mathbf{u})(\mathbf{y}+\delta^2\mathbf{e}_2) \simeq -\delta^1\delta^2\partial_{y^2}(\mathbf{v}_1\cdot\mathbf{u})(\mathbf{y})$. Adding a similar contribution from the right and left edges, we find that $\oint_{\gamma_{\delta S}}\mathrm{d}\mathbf{r}\cdot\mathbf{u}$ is given by

$$\delta^1\delta^2\Big[\partial_{y^1}(\mathbf{v}_2\cdot\mathbf{u}) - \partial_{y^2}(\mathbf{v}_1\cdot\mathbf{u})\Big] = \delta^1\delta^2\epsilon^{3jk}\partial_{y^j}(\mathbf{v}_k\cdot\mathbf{u}) = \delta^1\delta^2\epsilon^{3jk}\partial_{y^j}(\mathbf{v}_k\cdot\mathbf{v}_l u^l) = \delta^1\delta^2\epsilon^{3jk}\partial_{y^j}(g_{kl}u^l).$$

For the first equality we used the antisymmetric tensor, $\epsilon^{3jk}a_jb_k = a_1b_2 - a_2b_1$, to simplify the alternating sum, for the second expanded $\mathbf{u}$ in the coordinate basis, and for the last inserted $\mathbf{v}_k\cdot\mathbf{v}_l = g_{kl}$. Equating the left- and right-hand sides of Eq. (V106) we obtain $\sqrt{g}\,(\boldsymbol{\nabla}\times\mathbf{u})^3 = \epsilon^{3jk}\partial_{y^j}(g_{kl}u^l)$. Analogous relations hold for the 1- and 2-components, so that

we have the representation

$$\boxed{(\boldsymbol{\nabla}\times\mathbf{u})^i = \frac{1}{\sqrt{g}}\epsilon^{ijk}\partial_{y^j}(g_{kl}u^l),} \tag{V107}$$

for the **components of the curl in arbitrary coordinates**. For Cartesian coordinates, with $g_{kl} = \delta_{kl}$ and $g = 1$, the formula reduces to Eq. (V101). Explicit representations in other coordinate systems are somewhat more complicated. For example, a short calculation (try it!) shows that **the curl in spherical coordinates** is given by,

$$\begin{aligned}
(\boldsymbol{\nabla}\times\mathbf{u})^r &= \frac{1}{\sin\theta}\partial_\theta\big(\sin^2\theta u^\phi\big) - \partial_\phi u^\theta,\\
(\boldsymbol{\nabla}\times\mathbf{u})^\theta &= \frac{1}{r^2\sin\theta}\partial_\phi u^r - \frac{\sin\theta}{r^2}\partial^r\big(r^2u^\phi\big),\\
(\boldsymbol{\nabla}\times\mathbf{u})^\phi &= \frac{1}{r^2\sin\theta}\partial^r r^2u^\theta - \frac{1}{r^2\sin\theta}\partial^\theta\big(u^r\big).
\end{aligned} \tag{V108}$$

	Gauss' theorem	**Stokes' theorem**
addresses	sources of vector fields	circulation of vector fields
local description	$\boldsymbol{\nabla}\cdot\mathbf{u}$	$\boldsymbol{\nabla}\times\mathbf{u}$
global description	$\int_S \mathrm{d}\mathbf{S}\cdot\mathbf{u}$	$\oint_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{u}$
correspondence	Eq. (V91)	Eq. (V104)

Table V3.1: Parallels between Stokes' and Gauss' theorem

	addresses	local	global	correspondence
Gauss' theorem	$\boldsymbol{\nabla}\cdot\mathbf{u}$	$\int_S \mathrm{d}\mathbf{S}\cdot\mathbf{u}$		
Stokes	circulation	$\boldsymbol{\nabla}\times\mathbf{u}$	$\oint_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{u}$	$\int_{S_\gamma}\mathrm{d}\mathbf{S}\cdot(\boldsymbol{\nabla}\times\mathbf{u}) \overset{(V104)}{=} \oint_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{u}$

Table V3.2: Parallels between Stokes' and Gauss' theorem

Finally notice the striking parallels between Stokes' theorem and Gauss' theorem, summarized in Tab. V3.2. In fact, the two theorems are special cases of a more general mathematical law, known as the **generalized Stokes' theorem**. (The basic identity $\int_a^b \frac{\mathrm{d}f}{\mathrm{d}x} = f(b) - f(a)$ is another variant of that theorem. Like the higher dimensional variants of Stokes' theorem, it establishes a connection between the behavior of a function on the 'boundary' $\{a, b\}$, to the integral of the derivative of that function over the interior $[a, b]$.) The general version of Stoke's theorem is discussed in section **??** (see Eq. (V184) there) after the required mathematical terminology has been introduced.

INFO The curl of physically relevant vector fields generally carries **physical significance** itself. Let us illustrate this point on the example of magnetism: **Ampère's law** states that the line integral of the magnetic field, $\mathbf{B}$, along a closed loop, γ, equals the electric current I_{S_γ} (i.e. the charge per unit time) flowing through *any* area, S_γ, bounded by that loop.[12] This equality is expressed by the formula

$$\oint_\gamma \mathrm{d}\mathbf{r} \cdot \mathbf{B} = \frac{4\pi}{c} I_{S_\gamma}, \tag{V109}$$

where c is the speed of light and so-called CGS units are used. The current may be expressed as a surface integral,

$$I_{S_\gamma} = \int_{S_\gamma} \mathrm{d}\mathbf{S} \cdot \mathbf{j}, \tag{V110}$$

over the **current density**, $\mathbf{j}$. (In fact, the current density is *defined* through the condition that its integral over any surface equal the physical current flowing through that surface.) Stokes' law states that

$$\oint_\gamma \mathrm{d}\mathbf{r} \cdot \mathbf{B} = \int_{S_\gamma} \mathrm{d}\mathbf{S} \cdot (\boldsymbol{\nabla} \times \mathbf{B}). \tag{V111}$$

Comparing Eqs. (V109), (V110), and (V111), we arrive at

$$\boldsymbol{\nabla} \times \mathbf{B} = \frac{4\pi}{c} \mathbf{j}. \tag{V112}$$

This equation, known as the **differential form of Ampère's law**, states that the circulation of the magnetic field is caused by a flow of current.

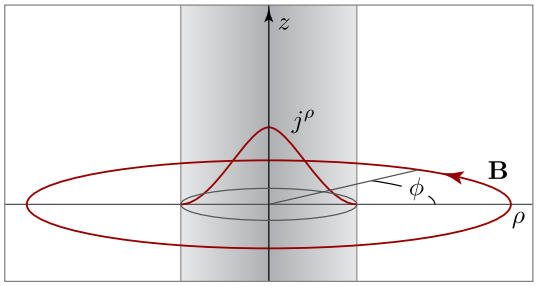


Figure V16: Current distribution and magnetic field of an infinite cylindrical wire (shaded).

EXERCISE Apply Eq. (V107) to verify that the **curl in cylindrical coordinates**, Eq. (V35), is given by

$$(\boldsymbol{\nabla} \times \mathbf{u})^\rho = \frac{1}{\rho} \partial_\phi u^z - \rho \partial_z u^\phi,$$

[12] We here assume time-independent current flow. If it is time-dependent, the situation becomes more complicated, cf. discussion in chapter V7.

$$(\boldsymbol{\nabla}\times\mathbf{u})^{\phi}=\frac{1}{\rho}\partial_z u^{\rho}-\frac{1}{\rho}\partial_\rho u^{z},$$
$$(\boldsymbol{\nabla}\times\mathbf{u})^{z}=\frac{1}{\rho}\partial_\rho\rho^2 u^{\phi}-\frac{1}{\rho}\partial_\phi u^{\rho}. \tag{V113}$$

Consider an infinite cylindrical wire as in Fig. V16, carrying a radially dependent current profile, $\mathbf{j}=\mathbf{v}_z f(\rho)$. (For example, $f(\rho)=c\Theta(R-\rho)$ would describe a wire of radius R and constant current density, $|\mathbf{j}|=c$.) Let D be a disk of radius ρ in the xy-plane centered on the axis of the wire. Confirm that the current flowing through D, $I=\int_D \mathrm{d}\mathbf{S}\cdot\mathbf{j}$, is given by $I=2\pi\int_0^\rho \mathrm{d}\rho'\,\rho' f(\rho')$.

The magnetic field generated by this current distribution winds circularly around the axis of the wire, $\mathbf{B}=\mathbf{v}_\phi B^\phi(\rho)$, where the translational symmetry of the problem in z-direction (the current does not depend on the z-coordinate) and the rotational symmetry in ϕ-direction (the current profile does not depend on ϕ) implies that the coefficient $B^\phi(\rho)$ can only depend on the radial coordinate ρ. Compute the line integral along the boundary ∂D (i.e. a circle of radius ρ) and confirm that $\int_{\partial D}\mathrm{d}\mathbf{r}\cdot\mathbf{B}=2\pi\rho^2 B^\phi(\rho)$. According to Eq. (V109) this must be proportional to the current, i.e. we have the identification

$$B^\phi(\rho)=\frac{4\pi}{c\rho^2}\int_0^\rho \mathrm{d}\rho'\,\rho' f(\rho').$$

Compute the curl of this magnetic field to confirm that the current density is given by Eq. (V112).

INFO In the previous two sections we discussed the sources and the circulation of vector fields. When employing general coordinates to describe these, the basis of coordinate vectors, $\mathbf{v}_i=\partial_i\mathbf{r}$, is most convenient, both from a conceptual and methodological point of view. However, in the physics community, the **local basis**, $\mathbf{e}_i=\mathbf{v}_i/\|\mathbf{v}_i\|$, is more widely used, since its vectors have unit length. For reference purposes, we here summarize the form of the essential vector analysis operations, gradient, divergence, curl, and the Laplace operator in their local basis representation. The spherical and cylindrical systems in which these formulas are generally applied are special in that their metric is *diagonal*, $g_{ij}=g_{ii}\delta_{ij}=\|\mathbf{v}_i\|^2\delta_{ij}$, so that $\mathbf{v}_i=\sqrt{g_{ii}}\,\mathbf{e}_i$. We assume this property throughout in what follows. We will distinguish between local and coordinate basis representations by temporarily denoting vector components of the latter by $\tilde{v}^i$. The expansions $\mathbf{u}=\sum_i \mathbf{e}_i u^i=\sum_i \mathbf{v}_i\tilde{u}^i$ then imply $u^i=\sqrt{g_{ii}}\,\tilde{u}^i$ (no summation). From this formula we can anticipate that the covariant structure of pairwise index contractions will be lost in the local basis representation.

The components of the **gradient** in the local basis are obtained from those in the coordinate basis as $\boldsymbol{\nabla}f^i=\sqrt{g_{ii}}\,\widetilde{\boldsymbol{\nabla}f}^i$. Using that $\widetilde{\boldsymbol{\nabla}f}^i \overset{(V69)}{=} g^{ij}\partial_{y^j}f$, and $g^{ij}=\delta^{ij}/g_{ii}$ we obtain leading to

$$\boldsymbol{\nabla}f^i=\frac{1}{\sqrt{g_{ii}}}\partial_{y^i}f.$$

The **divergence** is obtained from Eq. (V93) a replacement $u^i\equiv\tilde{u}^i\to u^i/\sqrt{g_{ii}}$:

$$\boldsymbol{\nabla}\cdot\mathbf{u}=\frac{1}{\sqrt{g}}\sum_i\partial_{y^i}\left(\sqrt{\frac{g}{g_{ii}}}\,u^i\right).$$

In an analogous manner the components of the **curl**, Eq. (V107), are transcribed to the local basis as

$$(\boldsymbol{\nabla}\times\mathbf{u})^i = \sqrt{\frac{g_{ii}}{g}}\sum_{jk}\epsilon_{ijk}\partial_{y^j}\left(\sqrt{g_{kk}}\,u^k\right).$$

Finally, the Laplace operator, $\Delta = \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}$, makes no reference to vector components and hence retains the form given by Eq. (V98):

$$\Delta f = \frac{1}{\sqrt{g}}\sum_i \partial_i\left(\frac{\sqrt{g}}{g_{ii}}\,\partial_i\phi\right).$$

The representations of these formulas in cylindrical and spherical coordinates are frequently needed in courses of theoretical physics and we summarize them for reference purposes:[13]

Cylindrical coordinates (local basis): $(\sqrt{g_{\rho\rho}}=1,\ \sqrt{g_{\phi\phi}}=\rho,\ \sqrt{g_{zz}}=1,\ \sqrt{g}=\rho)$

$$\begin{aligned}
\text{gradient:}\quad & \boldsymbol{\nabla}f = \mathbf{e}_\rho\,\partial_\rho f + \mathbf{e}_\phi\,\frac{1}{\rho}\partial_\phi f + \mathbf{e}_z\,\partial_z f,\\
\text{divergence:}\quad & \boldsymbol{\nabla}\cdot\mathbf{u} = \frac{1}{\rho}\partial_\rho\big(\rho u^\rho\big) + \frac{1}{r}\partial_\phi u^\phi + \partial_z u^z,\\
\text{curl:}\quad & \boldsymbol{\nabla}\times\mathbf{u} = \mathbf{e}_\rho\left[\frac{1}{\rho}\partial_\phi u^z - \partial_z u^\phi\right] + \mathbf{e}_\phi\left[\partial_z u^\rho - \partial_\rho u^z\right] + \mathbf{e}_z\frac{1}{\rho}\left[\partial_\rho\big(\rho u^\phi\big) - \partial_\phi u^\rho\right],\\
\text{Laplacian:}\quad & \Delta f = \frac{1}{\rho}\partial_\rho\big(\rho\,\partial_\rho f\big) + \frac{1}{\rho^2}\partial_\phi^2 f + \partial_z^2 f.
\end{aligned}\tag{V114}$$

Spherical coordinates (local basis): $(\sqrt{g_{rr}}=1,\ \sqrt{g_{\theta\theta}}=r,\ \sqrt{g_{\phi\phi}}=r\sin\theta,\ \sqrt{g}=r^2\sin\theta)$

$$\begin{aligned}
\text{gradient:}\quad & \boldsymbol{\nabla}f = \mathbf{e}_r\partial_r f + \mathbf{e}_\theta\,\frac{1}{r}\partial_\theta f + \mathbf{e}_\phi\,\frac{1}{r\sin\theta}\partial_\phi f,\\
\text{divergence:}\quad & \boldsymbol{\nabla}\cdot\mathbf{u} = \frac{1}{r^2}\partial_r\big(r^2u^r\big) + \frac{1}{r\sin\theta}\partial_\theta\big(\sin\theta u^\theta\big) + \frac{1}{r\sin\theta}\partial_\phi u^\phi,\\
\text{curl:}\quad & \boldsymbol{\nabla}\times\mathbf{u} = \mathbf{e}_r\,\frac{1}{r\sin\theta}\left[\partial_\theta(\sin\theta u^\phi) - \partial_\phi u^\theta\right] + \mathbf{e}_\theta\,\frac{1}{r}\left[\frac{1}{\sin\theta}\partial_\phi u^r - \partial_r\big(ru^\phi\big)\right] +\\
& \qquad + \mathbf{e}_\phi\,\frac{1}{r}\left[\partial_r\big(ru^\theta\big) - \partial_\theta u^r\right],\\
\text{Laplacian:}\quad & \Delta f = \frac{1}{r^2}\partial_r\big(r^2\,\partial_r f\big) + \frac{1}{r^2\sin\theta}\partial_\theta\big(\sin\theta\,\partial_\theta f\big) + \frac{1}{r^2\sin^2\theta}\partial_\phi^2 f.
\end{aligned}\tag{V115}$$

[13] When deriving these formulas, notice that when ∂_{y^i} acts on $\sqrt{g}$ or $\sqrt{g_{ii}}$, those factors independent of the variable y^i can be pulled upfront; e.g. for spherical coordinates, $\partial_r\sqrt{g} = \sin\theta\,\partial_r r^2$, $\partial_\phi\sqrt{g} = r^2\sin\theta\,\partial_\phi$, etc.

V4 Basic concepts of differential geometry

REMARK This chapter requires familiarity with chapter L11. As in that chapter, we abandon the boldface notation for vectors, e.g. we write r instead of $\mathbf{r}$. As in previous chapters, the components of coordinate vectors will mostly be denoted by $y \in \mathbb{R}^d$ and their components by y^j. If no confusion is possible, a fixed coordinate system y has been chosen, and different points r, p, q on a manifold are under consideration, we will label their coordinates as $r^j \equiv y^j(r), p^j, q^j$, etc. In this way, the introduction of ever new symbols for coordinate vectors is avoided. However, this notation must be used with due care. Throughout the chapter we will frequently need to differentiate curves $y(t)$ at $t = 0$. To keep the notation slim, we will often abbreviate $\mathrm{d}_t y(0) \equiv \mathrm{d}_t\big|_{t=0} y(t)$.

Smooth geometric structures define the 'arena' for the formulation of various fields of physics and mathematics. Many of these structures are easy to understand on an intuitive level, consider empty space, a two-dimensional sphere, or a circle as examples. Others can be more challenging to visualize — a sphere in five dimensional space — or may have no obvious visualization at all. For example, we have seen that the set of all rotations of three dimensional space defines a group. There is a sense of 'smoothness' in this set, because any rotation can be generated by a continuous deformation of any other rotation, and clearly the set of rotations is 'geometrical' in some sense. Yet it may not be evident how to conceptualize its geometry in any obvious way.

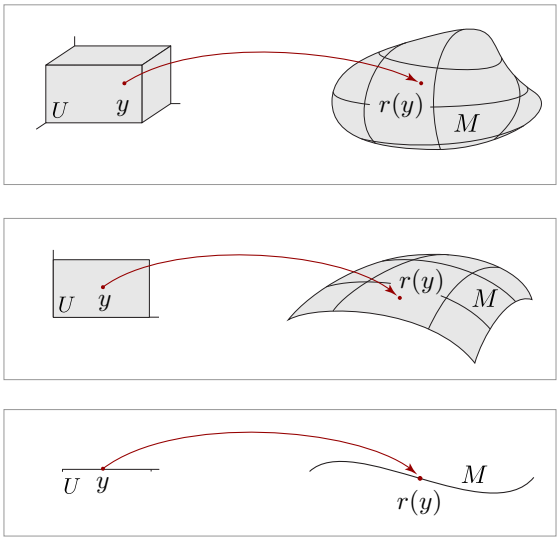
In this chapter, we will introduce the foundations of **differential geometry**, a comprehensive framework to understand smooth geometric objects in a unified fashion. The gateway into differential geometry is the realization that all the structures alluded to above have in common that they look *locally* (but in general not globally) like some $\mathbb{R}^d$. A circle looks locally like a segment of a line, i.e. a subset of $\mathbb{R}^1$. *Globally*, however, the circle is different from a segment of a line, and this difference between the global and the local level is of defining importance to its geometric description. Likewise, the set of rotations of three-dimensional space may be parameterized by three rotation angles, and this set of angles defines a three-dimensional cuboid, a subset of $\mathbb{R}^3$. Globally, however, there is a difference between the set of rotations and a cuboid, etc.

Building on our earlier discussion of curvilinear coordinates, we here introduce the framework for to describe smooth geometric structures both locally and globally. In the next chapter we will then introduce *differential forms* as a key tool to actively work with these objects in mathematical and physical contexts.

V4.1 Differentiable manifolds

The overarching mathematical terminology for 'smooth geometric structures' is **differentiable manifolds** (differenzierbare Mannigfaltigkeit), or just manifolds for short. Prominent examples of manifolds are spheres, tori, balls, smooth curves, various group structures, and many others more. In this section we elaborate on the local and the global description of such objects and show how to advance from one to the other.

The local and the global perspective of manifolds



A reasonable first attempt to define what a manifold, M, is might be to consider it as the image of a **diffeomorphic** (infinitely often differentiable, and bijective) map $r : U \to M, y \mapsto r(y)$, where $U \subset \mathbb{R}^d$ is an *open* coordinate domain in $\mathbb{R}^d$. This approach introduces what we will later understand as the 'local view'; it provides a 1-to-1 identification between M and an open subset of $\mathbb{R}^d$. A few examples of manifolds for which this local perspective is sufficient are shown in the figure.

For others, however, it falls short of providing the full picture. As a simple example, consider the $(d = 1)$-dimensional circle S^1 of unit radius. If the sole intention is to perform integral operations, then S^1 may be described as a circular curve parametrized on an open interval in such a way that its end points (almost) touch (see Fig. V17 below). In other cases, however, we need to describe a circle as what it is, a *closed curve*. For example, this distinction played a key role in our discussion of gradient fields on non-simply connected domains on p. 426. The closed circle cannot be represented as the diffeomorphic image of an open, i.e. end-point-excluding, parameter interval (think about this point). In the next subsection we explain how extended coordinate descriptions can be designed to obtain a 'global' definition, including objects that cannot be represented as images of single coordinate maps.

However, before turning to this generalization let us mention a second aspect key to the general understanding of manifolds: without even noticing, many people conceptualize the unit circle as a circle embedded in $\mathbb{R}^2$, such as a circle drawn on a piece of paper. However, circles may be realized in different ways. Think of a circle in $\mathbb{R}^3$, or in a space of even higher dimensionality; the set of rotations around a fixed axis can be understood as a circle where the rotation angle is a one-dimensional coordinate and a full rotation gets one back to the origin; we saw that the set of unit-modular complex numbers $\exp(i\phi), \phi \in \mathbb{R}$ is a circle in the

complex plane, etc. These are examples of circles 'embedded' in different sets. Now suppose we defined the circle as the *diffeomorphic* image of a map $U \to S^1 \subset X$, where X is one of these embedding sets. This approach would make reference to differentiability in the 'host medium' X. In this way, X would become an essential part of the definition, and different realizations of X would lead to different definitions. Clearly, we should aim to avoid this excess baggage. Rather we should aim for a 'universal' definition not referring to any specific embedding and describing the circle as a 'stand-alone object'.

In the next subsection we introduce a powerful definition of manifolds which includes objects that cannot be described in terms of a single coordinate map, and avoids the problems mentioned above by not making reference to host media. This definition will provide us with a solid foundation on which all further discussion will be based.

Definition of manifolds

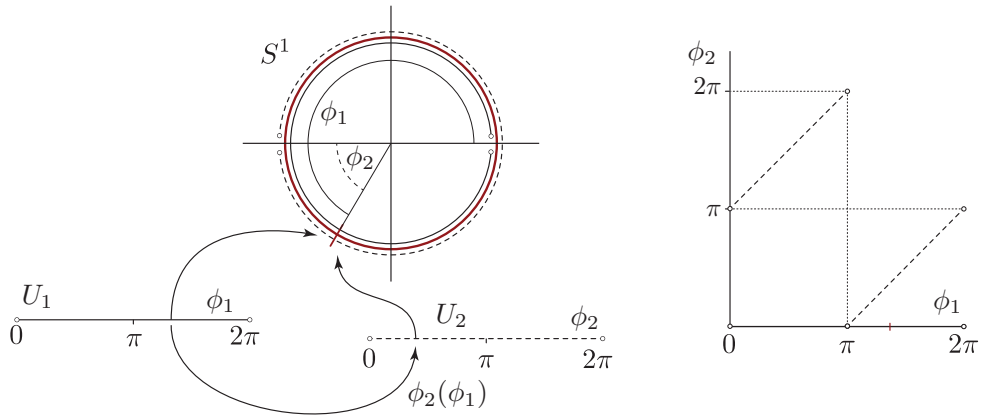


Figure V17: Coordinate representation of a circle employing two coordinate maps. Discussion, see text.

The key to a comprehensive description of manifolds lies in the realization that more than one coordinate map may be needed to parameterize M. The situation is illustrated in Fig. V17 on the example of the unit circle, $M = S^1$, embedded in $\mathbb{R}^2$ for graphical representability. One coordinate, $\phi_1 \in U_1 \equiv (0, 2\pi)$, is chosen to parameterize the circle as $r_1(\phi_1) \equiv (\cos\phi_1, \sin\phi_1)^T$. This map does not reach the point $(1,0)^T \in S^1$, because U_1 is an open interval and the end-points 0 and 2π are excluded. However, a second coordinate, $\phi_2 \in U_2 \equiv (0, 2\pi)$,[1] may now be engaged to parameterize a different portion of S^1 as $r_2(\phi_2) \equiv (\cos(\phi_2 - \pi), \sin(\phi_2 - \pi))^T$. This map *does* reach the previously excluded point, since $(1,0)^T = r(\phi_2 = \pi)$; however, it excludes the point $(-1,0)^T$. We conclude that each point on the circle is included in at least one of the images $r_1(U_1)$ and $r_2(U_2)$ of the coordinate maps, and the majority, i.e., all except $(\pm 1, 0)^T$, lie in both images.

[1] Although the two coordinate intervals $U_1 = U_2 = (0, 2\pi)$ are identical, it is expedient to think of them as separate domains and label them differently.

Let $M_{12} \equiv r_1(U_1) \cap r_2(U_2) = S^1 \setminus \{(1,0)^T, (-1,0)^T\}$ be the intersection of the two coordinate images, i.e. the set of points reached by both maps. For each $r \in M_{12}$, we have two coordinate representations, $r = r_1(\phi_1) = r_2(\phi_2)$. This defines a map $r_1^{-1}(M_{12}) \to r_2^{-1}(M_{12})$, $\phi_1 \mapsto \phi_2(\phi_1) = r_2^{-1}\big(r_1(\phi_1)\big)$, assigning to each coordinate ϕ_1 the corresponding coordinate ϕ_2. By construction, the transition map $r_2^{-1} \circ r_1$ is a diffeomorphic map from $r_1^{-1}(M_{12})$ to $r_2^{-1}(M_{12})$. It defines the change from the r_1 to the r_2 language in the description of S^1.

EXERCISE Verify that $r_1^{-1}(M_{12}) = (0, 2\pi) \setminus \{\pi\} = (0, \pi) \cup (\pi, 2\pi)$. Show that on this union of (open) intervals, $\phi_2(\phi_1) = \phi_1 + \pi$ for $\phi_1 < \pi$ and $\phi_2 = \phi - \pi$ for $\phi_1 > \pi$. The switch between the two branches occurs at the limiting point between two almost touching open intervals. However this point is excluded from the definition of the transition map. Within their respective open domains of definition the maps $\phi_2 = \phi_1 \pm \pi$ are trivially invertible and infinitely often differentiable, i.e. they represent diffeomorphisms. Notice that nowhere in the construction did we require differentiability in the space $\mathbb{R}^2$ within which the manifold S^1 is embedded.

The circle as discussed above serves as a role model for the general definition of differentiable manifolds. Referring for a rigorous discussion to the literature, a **differentiable d-dimensional manifold**, M, is a set covered by the combined image, $M = \bigcup_{a=1}^{k} r_a(U_a)$, of k coordinate maps, $r_a : U_a \to M, y \mapsto r_a(y)$, where U_a are open coordinate domains in $\mathbb{R}^d$.[2] Each individual coordinate map, r_a, is called a **chart** of the manifold and a collection of charts, $\{r_1, r_2, \ldots, r_k\}$ that fully covers the manifold is called an **atlas**. In the above example, we parameterized $M = S^1$ through an atlas involving two charts, r_1 and r_2.

The maps $r_a : U_a \to M_a \subset M$ between the coordinate domains and their images in $r_a(U_a) \equiv M_a \subset M$ are required to be invertible and continuous.[3] We introduce their inverses, $y_a \equiv r_a^{-1}$, as $y_a : M_a \to U_a, r \mapsto y_a(r) = r_a^{-1}(r)$. The images M_a of different charts in M generally overlap. Where this happens the intersections $M_{ab} \equiv M_a \cap M_b$ define regions with more than one coordinate representation, $r = r_a(y_a) = r_b(y_b)$ (see Fig. V18 for an illustration with two charts). The crucial condition of smoothness now is that the **transition functions**

$$y_b \circ r_a : y_a(M_{ab}) \to y_b(M_{ab}), \qquad y_a \mapsto y_b(y_a) \equiv y_b(r_a(y_a)), \tag{V116}$$

must be diffeomorphic maps between their domains of definition $y_a(M_{ab})$ and $y_b(M_{ab})$. In the above example of the unit circle S^1 we had just one such function, $\phi_2(\phi_1)$, one overlap region, $M_{12} \subset S^1$, and the intersection domain of coordinates was $(0, \pi) \cup (\pi, 2\pi)$. If the above condition is met, M is a differentiable manifold. Notice that the differentiability criterion applies to maps $y_b(y_a)$ *between* different coordinates, but not to the maps $r(y_a)$ from

[2] To avoid confusion between the vector-valued maps, r_a, and covariant components, r_i, we index the former with early Latin letters, $a, b, \ldots$.

[3] A technical remark: if M is embedded in a vector space such as $\mathbb{R}^c$, the continuity of the maps r_a may be defined using the mathematical structure of that embedding space. However, even if this is not the case it is still possible to define continuity, provided M does possess the mathematical structure of a so-called **topological space**. Although a comprehensive discussion of topological spaces at this point would lead too far, and the manifolds relevant to our discussion *are* embedded in vector space structures, it may be worth keeping in mind that the definition of manifolds has a more general scope. For further discussion we refer to textbooks on differential geometry.

coordinate domains into M. This is an important feature, which makes it possible to define manifolds which need not be embedded in $\mathbb{R}^c$.

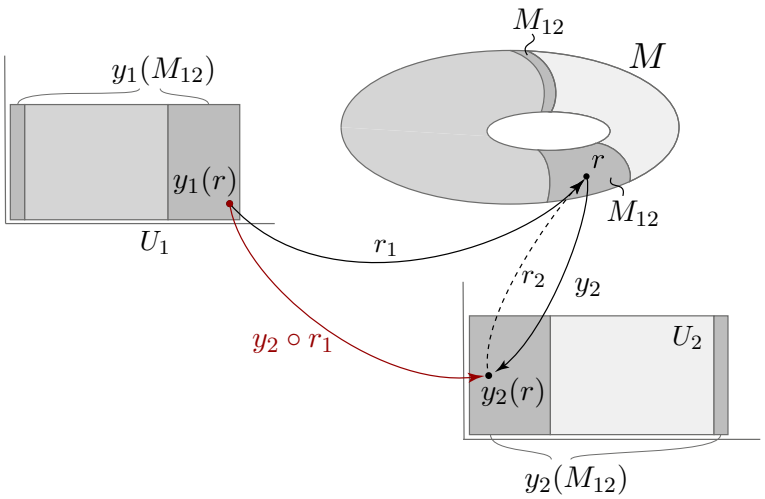


Figure V18: On the coverage of manifolds by multiple charts. Discussion, see text.

How important are multi-chart representations of manifolds in practice? The answer depends on the context. As discussed previously, single-chart coverages are often sufficient to 'approximately' cover manifolds, i.e. to cover them up to subsets of lower dimensionality. For example, the description of a circle by polar coordinats misses an isolated point, and the description of the two-sphere by spherical coordinates misses a line connecting the north and south poles along a great half-circle, cf. section (V2.1). Incomplete or 'local'[4] coverages of this type are often sufficient to compute integrals over manifolds (cf. discussion on p. 229 in section C4.2), or to describe their local geometric structure. In such cases, no extension to a complete coordinate description is required.

By contrast, full coverages provided by multi-chart atlases and their transition functions become important when 'global' or topological aspects play a role. (For example, a Möbius strip is 'locally' diffeomorphic to a rectangular strip, but is 'globally' different. This difference shows in the transition functions mediating between a minimal atlas of two charts parameterizing the Möbius strip, think about this point.)

In either context, **differential forms** will emerge as powerful tools to describe the geometry of manifolds, and that of physically relevant structures defined on them. In the following the focus will be put more on the local perspective, and we will mostly work with the local descriptions provided by single charts. The extension to a global framework is left for lecture courses in topology, differential geometry, or advanced courses in theoretical physics.

[4] A remark on a possibly disconcerting wording convention: single charts of manifolds are often said to provide a 'local' description, even if 'local' means everything-except-one-point. Confusion can be avoided if one accepts that mathematicians define the attribute 'local' as 'non-global'.

V4.2 Tangent space

Much like a smooth function looks locally linear, a smooth manifold looks locally flat. For example, the surface of earth is globally a sphere, but looks locally planar. The planes locally approximating a general d-dimensional manifold are d-dimensional vector spaces called tangent spaces. In the example of earth, this is all easy to imagine: the neighborhood of each location on earth is locally approximated by a two-dimensional plane in the embedding three-dimensional space. These planes differ from point to point, and it may also be intuitively evident that the infinite collection of all of them, a set called the 'tangent bundle' and to be defined in the next subsection, contains exhaustive information on the geometric structure of earth's surface.

Tangent spaces and the tangent bundle play a very important role in the geometric description of manifolds. In the following, we will learn how to describe them, both intuitively and in more formal mathematical terms. Our approach will be flexible enough to encompass manifolds not embedded in a host vector space, and for which the visual picture of tangent spaces may be not quite as obvious as in the example above.

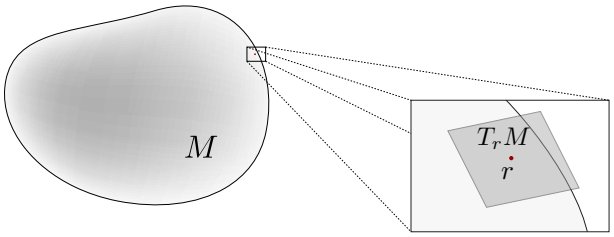


Figure V19: The setup considered in this section. A manifold is a 'smooth' object, which means that locally it looks flat (much like the surface of earth looks locally flat). The asymptotic vicinity of any point r in a d-dimensional manifold M can be approximated by a d-dimensional vector space, called the tangent vector space to r at M and denoted by T_rM. Differential forms will emerge as objects describing the geometry of tangent spaces and, upon extrapolation, the geometry of M at large.

Smooth functions on manifolds

The principal tool required for the description of tangent space (and, in fact, that of *any* other geometric structure on manifolds, too) are **smooth functions** $f : M \to \mathbb{R}$. Although the concept of a smooth real valued function seems innocent enough, it may not be entirely evident how the attribute 'smooth' is actually defined in the present context. We agreed to refrain from differentiating (the principal operation required to detect smoothness) in M, and so we define the smoothness of a function with reference to a coordinate system, see Fig. V20: a function $f : M \to \mathbb{R}$, $r \mapsto f(r)$, is smooth if its coordinate representation, $f(r(y))$ is a smooth function of the coordinates y. More precisely, the composition of f with a coordinate map $y : U \to M \ni r$ enclosing the point r, namely $f : U \to \mathbb{R}$, $y \mapsto f(r(y)) \equiv f(y)$, must

be a smooth function from $U \subset \mathbb{R}^d$ into the real numbers. Following common conventions we denote $f : M \to \mathbb{R}$ and its coordinate representation, $f : U \to \mathbb{R}$, by the same symbol.[5]

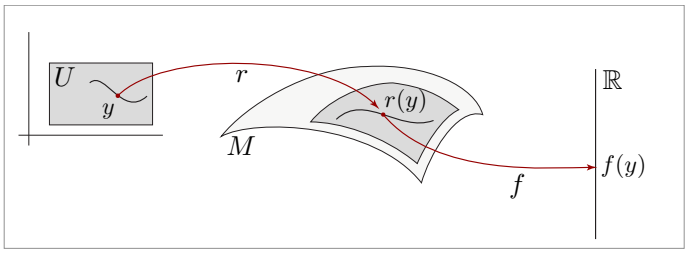


Figure V20: A function on a manifold $f : M \to \mathbb{R}$, $r \mapsto f(r)$ is smooth if its coordinate representations $f : U \to \mathbb{R}$, $y \mapsto f(y) \equiv f(r(y))$ are smooth functions from $U \subset \mathbb{R}$ into the real numbers. Likewise, a curve in a manifold is smooth if its coordinate representation is a smooth curve.

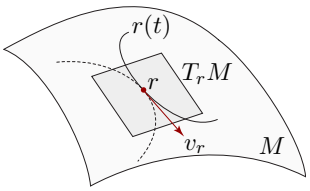
Likewise, a curve $r : \mathbb{I} \to M$, $t \mapsto r(t)$ is smooth if its coordinate representation $r : \mathbb{I} \to U$, $t \mapsto y(t) \equiv y(r(t))$ is smooth. The smoothness of other objects defined on M is defined in similar ways. Perhaps a good way to think about the situation is to consider functions, curves, etc. as absolute objects, and their coordinate representations as descriptions of these objects in a given language (different coordiantes means different languages). Mathematical calculations require a language description and are therefore performed in coordinates. The functions $f(y) = f(r(y))$ and $f(y') = f(r(y'))$ are descriptions of the same $f(r)$ in different languages, and $f(y') = f(y(y'))$ is the translation from one to the other.

INFO The seemingly indirect definition of smoothness via coordinate representations is motivated by quite practical considerations. To understand why, consider $M = S^2 \subset \mathbb{R}^3$, i.e. the two-sphere embedded in $\mathbb{R}^3$. Let $f : S^2 \to \mathbb{R}$ be a function defined on the sphere, and *only* on the sphere, such that f does not have any meaningful extension into the embedding space. For concreteness, consider a sphere coated by a material of varying mass distributions, and let f describe the corresponding surface mass density. Assume $\mathbb{R}^3$ to be parameterized by Cartesian coordinates, (x^1, x^2, x^3). The function f is then defined on the subset of coordinates obeying the condition $\sum_j (x^j)^2 = 1$. This implies that its partial derivatives Eq. (C30) cannot be defined in $\mathbb{R}^3$. (If x is on the sphere, then $x+\delta x^j$ is not, no matter how small δ, i.e. the difference quotient $\delta^{-1}(f(x+\delta x^j)-f(x))$ is not defined. (Why does this problem not arise with partial derivatives $\partial_{y^j} f(x(y))$ in coordinate representations?)

Tangent vectors as equivalence classes of curves

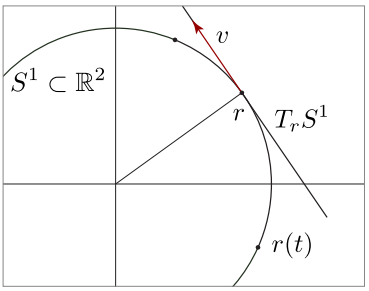
[5] Note that if f passes the smoothness criterion in one coordinate representation, then it will be smooth in all other representations, too. This is because the transition maps mediating between different coordinates are smooth functions, so $f(y') \equiv f(y(y'))$ will be a smooth function of the coordinates y' if $f(y)$ is a smooth function of y.

Let $r(t)$ be a smooth curve in M passing through the point r at $t = 0$, i.e. $r(0) = r$ (see figure). The velocity vector at $t = 0$,



$$v_r \equiv \mathrm{d}_t r(0) \equiv \mathrm{d}_t\big|_{t=0} r(t), \tag{V117}$$

is tangent to the curve at r and therefore tangent to M. Intuitively, it is tempting to define the tangent space at r as the set of all tangent velocity vectors that can be built in this way.



This is indeed almost, but not quite, what we are going to do. A drawback of Eq. (V117) is that it is breaking the promise to not differentiate in M: the derivative $\mathrm{d}_t r(t) = \lim_{\delta\to 0}(r(t+\epsilon) - r(t))$ can only be built if the manifold is embedded in a vector space, $M \subset \mathbb{R}^n$, and differences of vectors $r(t)$ are taken within that space. As a consequence, the tangent space to a circle, for example, would depend on whether the circle is embedded in $\mathbb{R}^2$ (see the figure for a realization of one of its tangent spaces as a one-dimensional subspace of $\mathbb{R}^2$) or in $\mathbb{R}^3$, and this is a complication we would prefer to avoid.

As a first step towards a better definition we note that different curves passing through r can have the same tangent vector. For example, the dashed curve indicated in the figure above will have the same tangent vector at r as the solid curve $r(t)$ if it is traversed at the same speed. This observation motivates the following construction: let $f : M \to \mathbb{R}$ be a smooth function on M (or at least in a neighborhood containing r). We may then build the **directional derivative** of f along $r(t)$ as $\mathrm{d}_t f(r(0))$, i.e. the ordinary derivative of the real function $t \mapsto f(r(t))$, evaluated at $t = 0$. Two curves $r(t)$ and $r'(t)$ are called 'equivalent', $r(t) \sim r'(t)$, at $r = r(0) = r'(0)$ if they lead to the same directional derivative, $\mathrm{d}_t f(r(0)) = \mathrm{d}_t f(r'(0))$, for any smooth function f. The set of all curves which are equivalent in this sense define an **equivalence class of curves**, $[r(t)]$, and this equivalence class in turn defines a tangent vector, which we denote as $\hat{v}_r$.

Although this definition may seem abstract, it is in fact very 'geometric'. It associates tangent vectors with 'bushels' of curves in M touching at a point r where they are all traversed in the same direction and at the same speed. Intuitively, the vector $\hat{v}_r$ is the common tangent vector of these curves at this point. To make the description quantitative and give the vector $\hat{v}_r$ a **coordinate representation** in terms of d components, we need to employ a system of coordinates $y = (y^1, \ldots, y^d)^T$ of the manifold. The components, v_r^j, are then defined as

$$v_r^j = \mathrm{d}_t y^j(r(0)). \tag{V118}$$

i.e. each component is the directional derivative of a coordinate function y^j along any of $\hat{v}_r$'s representing curves. The resulting set of d components defines the coordinate representation $v_r \equiv (v_r^1, \ldots, v_r^d)^T$ of $\hat{v}_r$, which, of course, is specific to the coordinate system used.

We emphasize that the values obtained for the components do not depend on the choice of the representing curve. The coordinate functions $y^j(r)$ are smooth in a neighborhood of r and by virtue of the equivalence relation any other curve $r'(t) \in [r(t)]$ will give the same

value, $\mathrm{d}_t y^j(r(0)) = \mathrm{d}_t y^j(r'(0))$. Notice also that definition (V118) is equivalent to, and in fact generalizes the 'naive' definition (V117). This formula is recovered if the d-dimensional M is embedded in a vector space $\mathbb{R}^d$ of equal dimension, and Cartesian coordinates are used parameterize the latter. In this case, $r = \{r^j\}$ may be identified with its Cartesian coordinate representation. For these coordinates, $y^j = r^j$, and $v_r^j = \mathrm{d}_t r^j(t)$ is the coordinate representation of the tangent vector according to both Eqs. (V117) and (V118).

EXERCISE Consider $M = \mathbb{R}^2$ and the point $r = (R, 0)^T$ in a Cartesian coordinate system. Show that the curves $r_1(t) = R(\cos(t), \sin(t))^T$, $r_2(t) = R(2 - \cos(t), \sin(t))^T$, and $r_3(t) = R(1, t)^T$ satisfy the conditions $r_a(0) = r$ and $\mathrm{d}_t f(r_a(0))$ for any smooth function, i.e. that they all lie in the same equivalence class at r. (Hint: check that in the chosen coordinates, $\mathrm{d}_t f(r_a(0))$ for all curves.) Verify that the components of the tangent vector in Cartesian coordinates are given by $(v^1, v^2) = (0, R)$, and in polar coordinates by $(v^r, v^\phi) = (0, 1)$. Why is the curve $r_4(t) = (\cos(2t), \sin(2t))^T$ *not* equivalent to the curve $r_1(t)$, although it looks identical when sketched on paper?

Tangent vectors as directional derivative operators

The constructions above illustrate how tangent vectors and the curves representing them always (!) appear in the context of directional derivatives of functions $f : M \to \mathbb{R}$; indeed, the sole purpose of working with 'equivalence classes of curves' is to have a means of taking directional derivatives of functions along these curves. This suggests another way of thinking of a tangent vector $\hat{v}_r$: it may be identified with a **differential operator**, $\partial_{v,r}$. By definition, this operator acts on functions as $f \mapsto \partial_{v,r} f$, where $\partial_{v,r}$ is the directional derivative of f at r along any of the curves in the class $[r(t)]$ of $\hat{v}_r$:

$$\partial_{v,r} : f \mapsto \partial_{v,r} f = \mathrm{d}_t f(r(0)). \tag{V119}$$

The two definitions of tangent vectors, as equivalence classes of curves or as directional derivative operators, are equivalent to each other and will be used interchangeably throughout this text. Both require a bit of getting used to but in fact are quite intuitive. In fact, we will mostly work with the directional derivative notation and identify $\hat{v}_r = \partial_{v,r}$, where the subscript v is a reference to the vector $\hat{v}_r$ defined through a class of representing curves.

Two more **remarks on notation**: first, the definition of a tangent vector is specific to its base point, r, as emphasized by the notation $\partial_{v,r}$. However, the identity of this base point is usually evident from the context, and in such cases the subscript r is omitted to arrive at the slimmer notation $\partial_{v,r} \to \partial_v$ (much like coordinate basis vectors in section V2.3 where usually denoted in the abbreviated notation $\mathbf{v}_j$, rather than $\mathbf{v}_{j,r}$). Second, the object ∂_v must not be confused with a partial derivative. As emphasized above, the definition of partial derivatives requires coordinates, whereas ∂_v is a geometric object. However, we will observe below that formulas in which ∂_v features have undeniable similarity to those involving partial derivatives, and this is the likely origin of the denotation ∂_v for tangent vectors.

Irrespective of which representation for $\hat{v}_r$ is used, $\partial_{v,r} \leftrightarrow [r(t)]$, the components v_r^j representing the vector in a coordinate system $\{y^j\}$ are obtained by (applying the differential

operator to) $\leftrightarrow$ (taking the directional derivative of) the functions y^j

$$\boxed{v^j_r = \partial_{v,r} y^j(r) = \mathrm{d}_t y^j(r(0)).} \tag{V120}$$

In the next section we will describe how the present definition of tangent vectors can be applied to obtain an efficient description of the geometry of tangent space.

Tangent space bases

The set of all tangent vectors, $\partial_{v,r}$, defined as above defines a vector space, the **tangent space** to M at r,

$$T_r M \equiv \{\partial_{v,r} | \partial_{v,r} \text{ tangent to } M \text{ at } r\}. \tag{V121}$$

Above we introduced a geometric picture of individual tangent vectors, ∂_v, and gave a prescription for computing their components (relative to a coordinate system). Building on this discussion we now show how to understand $T_r M$ as a d-dimensional vector space, and how to construct suitable bases for this space. All this is best done by shifting as much of the discussion as possible to the representing coordinate domain. Indeed our construction above was based on curves $r(t)$ in M, and each such curve has a coordinate representation, $y(t) = y(r(t))$, in U. Now consider the special curves $y_j(t) = y + e_j t$, where y is the coordinate representation of the base point $r(y) = r$ and e_j is the jth standard unit vector in U. These curves in U have images $r(y_j(t))$ which define 'coordinate lines' in M (cf. Fig. V21). In section V2.2 we had introduced the concept of coordinate lines for the special case of manifolds embedded in $\mathbb{R}^2$ or $\mathbb{R}^3$, cf. Eq.(V19), or Fig. V4, which shows polar coordinate lines for $M = \mathbb{R}^2 \backslash \{0\}$.

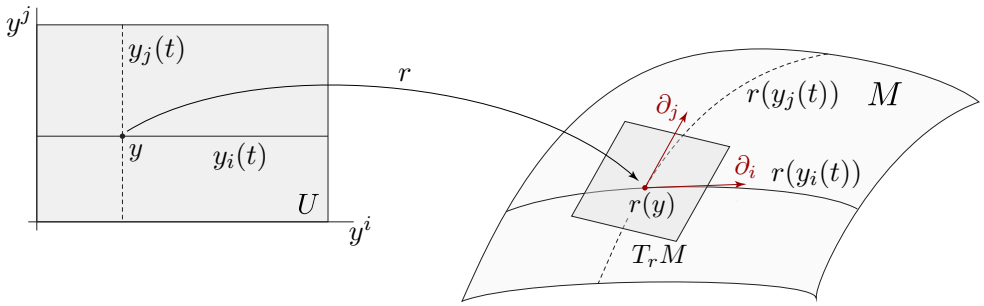


Figure V21: Curves $y_j(t)$ in U along which all but the jth coordinate are kept constant define 'coordinate lines' $r(y_j(t))$ in M. The tangent vectors, ∂_j, defined by these curves define the holonomic basis for the tangent space $T_r M$. If M is embedded in $\mathbb{R}^c$, the c-dimensional representatives of the vectors ∂_j correspond to the coordinate basis vectors $\mathbf{v}_j$ discussed in section V2.2.

The tangent vector defined by the coordinate curve $y_j(t)$ running in the e_j direction is denoted by the symbol ∂_j:

$$\partial_j : f \mapsto \partial_j f \equiv \mathrm{d}_t f(r(y_j)) \equiv \mathrm{d}_t f(y_j(0)), \tag{V122}$$

where we continue to use the shorthand notation $f(y) \equiv f(r(y))$ for the coordinate dependence of smooth functions. Observe that ∂_j acts on functions as a partial derivative in y^j-direction: $\partial_j f = \mathrm{d}_t f(y_j(0)) = \mathrm{d}_t\big|_{t=0} f(y+e_j t) = \partial_j f(y)$, where on the left side ∂_j denotes the vector (represented as differential operator), and on the right side the standard definition of the partial derivative. In view of this equality it makes perfect sense to denote the tangent vector associated with the jth coordinate line by the symbol ∂_j.

The coordinate representation of the tangent vector ∂_j is given by the jth standard vector, $e_j = (0,\dots,1,\dots,0)^T$. This is seen by computing its ith component $(\partial_j)^i$ via Eq. (V120): we apply ∂_j to the ith coordinate function $y^i = y^i(r)$,

$$(\partial_j)^i = \partial_j(y^i(r)) = \mathrm{d}_t\big|_{t=0} y^i(y + e_j t) = \delta^i{}_j, \tag{V123}$$

which may be identified as either the jth partial derivative of y^i, or equivalently as the derivative of y^i along the jth coordinate curve. Either way we identify $(\partial_j)^i = (e_j)^i = \delta^i{}_j$ as the i-component of the standard vector e_j.

The collection of the d vectors $\{\partial_j\}$ defines a **basis of tangent space**. To understand why, let us try a tentative expansion $\partial_v = v^j\partial_j$ of a generic tangent vector in terms of the vectors ∂_j. The expansion coefficients may be identified by applying both sides to a coordinate function, y^j. On the l.h.s. this yields $\partial_v y^j$, and on the r.h.s., $(v^i\partial_i)(y^j) = v^i(\partial_i y^j) \overset{(V123)}{=} v^j$, implying $v^j = \partial_v y^j$. We conclude that a generic tangent vector can be expanded as

$$\boxed{\partial_v = v^j\partial_j, \qquad v^j = (\partial_v y^j),} \tag{V124}$$

where the components v^j are obtained by taking directional derivatives of the coordinate functions y^j. Notice that this definition of vector components v^j coincides with the earlier prescription (V118), so that $\partial_v = v^j\partial_j \in T_rM$ and $v = v^j e_j \in \mathbb{R}^d$ are equivalent representations of the same geometric object. Also notice that the notation ∂_v is nicely compatible with the understanding of ∂_j as a partial derivative in the j-direction: the relation

$$\partial_v f(y) = v^j\partial_j f(y) = \frac{\partial f(y)}{\partial y^j}(\partial_v y^j) \tag{V125}$$

can either be understood as the expansion of ∂_v in the basis ∂_j, or, equivalently, as the chain rule applied to the directional derivative of the function $f(y)$.

Bases $\{\partial_j\}$ defined with reference to a local coordinate system are called **holonomic bases** of tangent spaces. In most cases the holonomic basis associated to a conveniently chosen coordinate system will be the preferred basis in the geometric description of a manifold.

INFO While our general discussion does not require any embedding, let us now discuss the important case of a **manifold embedded in a vector space**, $\mathbb{R}^n$. Notice that the embedding dimension, n, need not be equal to the manifold dimension, d (think of a $(d=2)$-dimensional surface embedded in $\mathbb{R}^{(n=3)}$, etc.). As discussed earlier, the tangent space T_rM to a point $r \in M$ now is a d-dimensional subspace of $\mathbb{R}^n$. In a Cartesian basis of $\mathbb{R}^n$, each point $r \equiv (r^1,\dots,r^n) \in M$ is described by an n-component coordinate representation, where $r^i(y)$ are smooth functions of M's local coordinates.

This setup leads to another representation of tangent vectors: to a vector $\partial_v \in T_r M$ we assign the coordinate vector $v = (v^1, \ldots, v^n)^T$, with components $v^j \equiv \partial_v r^j = \mathrm{d}_t r^j(y(0)) \equiv \mathrm{d}_t r^j(0)$, where $r^j(y(t)) = r^j(t)$ is the Cartesian representation of a curve $r(t)$ representing ∂_v. Each tangent vector is thus represented by an n-component vector, $v \equiv e_j v^j$, in the embedding space $\mathbb{R}^n$. This is nothing but a somewhat more elaborate formulation of the picture behind the intuitive formula (V117) discussed in the beginning of the section. Specifically, the vectors of the holonomic basis ∂_j now have the coordinate representation

$$v_j = \mathrm{d}_t r(y_j(0)) = \frac{\partial r(y)}{\partial y^j}. \tag{V126}$$

In these vectors we recognize the elements of the **coordinate basis** of M at r introduced in section V2.3 (there denoted in boldface fonts as $\mathbf{v}_j$). Fig. V22 offers a visual recapitulation of this connection on the example of cylindrical coordinates.

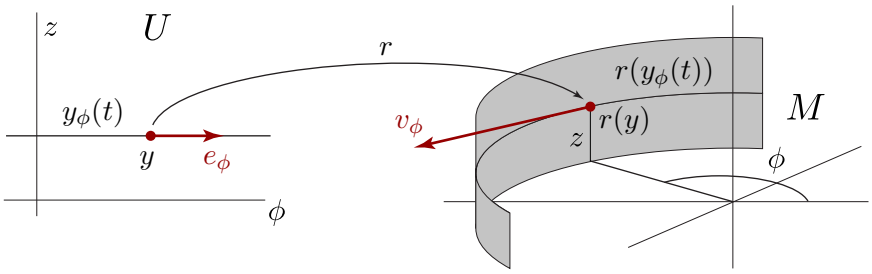


Figure V22: A two-dimensional cylinder $M \subset \mathbb{R}^3$ of unit radius can be locally described by cylindrical coordinates, $r(y)$, with two-dimensional coordinate vectors $y = (\phi, z)^T \equiv \phi e_\phi + z e_z$ where $e_\phi = (1, 0)^T$, $e_z \equiv (0, 1)^T$. (Do not confuse e_ϕ, a vector in the coordinate domain, with the local basis vectors $\mathbf{e}_\phi$ of section V2.3.) The tangent vector ∂_ϕ at $r(y)$ is generated by the curve $y_\phi(t) = (\phi + t, z)^T = y + t e_\phi$, (cf. Eq. (V123)). In the embedding space $\mathbb{R}^3$, ∂_ϕ is represented by a three-component vector, v_ϕ. If $r = (r^1, r^2, r^3)^T$ is represented in Cartesian coordinates, the components of v_ϕ are obtained by differentiating the coordinate functions $r^j(\phi, z)$ along $y_\phi(t)$, i.e. $(v_\phi)^j = \mathrm{d}_t r^j(y_\phi(0)) = \partial_\phi r^j(\phi, z)$. In this way one obtains $v_\phi = (-\sin\phi, \cos\phi, 0)^T$ for the Cartesian representation of ∂_ϕ in $\mathbb{R}^3$. This equals the vector $\mathbf{v}_\phi$ introduced in section V2.3 as one of the elements of the cylindrical coordinate basis, cf. Eq. (V36).

Now consider the trivial yet important case that the manifold and its embedding space have equal dimensionality, $d = n$, but that the former is an open *subset* of the latter, $M \subset \mathbb{R}^d$ (think of a two-dimensional disk in $\mathbb{R}^2$, etc.). Although such a manifold is smaller than the embedding space, the tangent space at any point is actually *equal* to the embedding space, $T_r M = \mathbb{R}^d$. The intuitive reason for this is that although the points of a disk are confined to it, the vectors tangent to curves in the disk may assume arbitrarily large values if only the curves are traversed sufficiently fast (think about this!). If a Cartesian basis, $\{e_j\}$, is used to span $\mathbb{R}^d$, both points $r \in M$ in the manifold and vectors $\partial_v \in T_r M$ in the tangent space are represented by d-component coordinate vectors, $r = e_j r^j$ and $v = e_j v^j$, respectively. One might then be tempted to not distinguish conceptually between points $r \in M$ and tangent vectors $\partial_v \in T_r M$. However, such conceptual sloppiness can be counterproductive and lead to confusion. In the present context it is best to avoid it.

Finally, let us explore how vector components $v^i(y)$ change under a **change of coordinates** $y \mapsto y'(y)$ where y and y' are two systems with finite overlap on M. The components of a vector,[6] $\partial_v = v^j(y)\partial_{y^j} = v^i(y')\partial_{y'^i}$, in these two systems are obtained by application of the vector to the respective coordinate functions, $v^j(y) = \partial_v y^j$ and $v^i(y') = \partial_v y'^i$. Given the components $v^j(y)$ the components $vi(y')$ are obtained by application of the chain rule: $v^i(y') = \partial_v y'^i = \partial_v y'^i(y) = \frac{\partial y'^i(y)}{\partial y^j}\partial_v y^j = \frac{\partial y'^i(y)}{\partial y^j}v^j(y)$. The right hand side of this expression yields the components $v^i(y')$ expressed as functions of y. However, one may express all coordinates $y = y(y')$ in terms of y' to obtain the representation

$$v^i(y') = \left.\frac{\partial y'^i(y)}{\partial y^j}v^j(y)\right|_{y=y(y')} . \tag{V127}$$

Note how Eq. (V127) generalizes the earlier result Eq. (V48). That relation described how the components of vectors defined on a subset $M \subset \mathbb{R}^d$ change if one switches from a Cartesian basis to a general coordinate basis. Equation (V127) describes the change of components for more general transformations between arbitrary holonomic bases of (not necessarily embedded) manifolds. It is also used to transcribe vector components from one coordinate language to another in cases where a manifold cannot be covered by a single chart, cf. Fig. V18. In either case, the **Jacobi matrix**, $J^i{}_j = \frac{\partial y'^i}{\partial y^j}$, and its inverse, $(J^{-1})^j{}_i = \frac{\partial y^j}{\partial y'^i}$, are the central ingredients of the transformation formulas associated with the map $y \mapsto y'(y)$.

To summarize, under coordinate transformations vector field expansions behave as

$$\boxed{\partial_v = v^j(y)\partial_{y^j} = v^i(y')\partial_{y'^i} = \left[v^j(y)\,\frac{\partial y'^i}{\partial y^j}\right]_{y=y(y')}\partial_{y'^i}.} \tag{V128}$$

Notice the structural similarity of the transformation formula (V128) to a 'chain rule formula' where ∂_{y^j} is understood as a partial derivative, and $\partial_{y^j} = \frac{\partial y'^i}{\partial y^j}\,\partial_{y'^i}$ is the chain rule for partial derivatives, in the form needed to compute the action of ∂_{y^j} on a function $f(y'(y))$.

EXERCISE Consider the set $M = \{(x,y)|\, y > 0, |x| < y\}$ (the shaded region in the figure). Parameterize M by the **hyperbolas**,

$$x = \rho\sinh(\alpha), \qquad y = \rho\cosh(\alpha), \tag{V129}$$

where the set $U = \{(\rho,\alpha)|\rho,\alpha \in \mathbb{R}^+\}$ defines the coordinate domain. Construct the vector fields ∂_ρ and ∂_α, i.e. the fields defining the holonomic frame of the hyperbolic coordinate system, and find their components in Cartesian coordinates, $((\partial_\rho)^x, (\partial_\rho)^y)^T$ and $((\partial_\alpha)^x, (\partial_\alpha)^y)^T$.

[6] A word on **notational conventions**: vector fields can be expanded in different coordinate bases as $v = v^j(x)\partial_{x^j} = v^j(y)\partial_{y^j} = v^j(z)\partial_{z^j}, \ldots$. In this text, we will use a convention where the *argument* of the coefficient functions in $v^j(y)\partial_{y^j}$ indicates which coordinate system they refer to. It is important to keep this point in mind when coordinate changes are discussed. For example, in the relation $v^i(y'(y)) = \frac{\partial y'^i}{\partial y^j}v^j(y)$, the y-coefficient functions $v^j(y)$ should be carefully distinguished from the functions $v^i(y'(y))$, which are the y'-coefficient functions expressed in terms of the y-coordinates. Although expressions such as $v^i(y'(y))$ may be unwieldy, the systematic use of this notation avoids errors which often occur in more implicit formulations of coordinate changes.

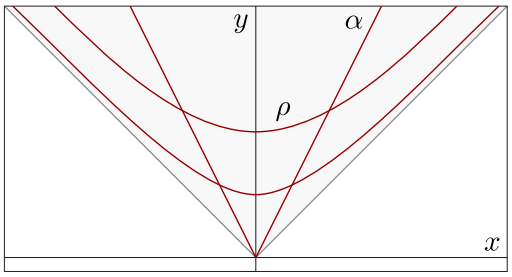


Figure V23: Hyperbolic coordinates parameterizing a 'cone' (shaded region) in the two-dimensional plane.

To **summarize** our so far discussion, we have seen how to construct tangent vector spaces T_rM describing the asymptotic neighborhoods of individual points r on a manifold. The vectors of these spaces are in one-to-one relation to equivalence classes of curves, $[r(t)]$, traversing r 'in the same direction and at the same speed'. Tangent vectors can be thought of as pointers along these curves. However, in most applications it is more expedient to understand them as directional derivatives, ∂_v, monitoring how smooth functions $f(r)$ change along these curves. All three pictures are equivalent, and the connection is made quantitative by representing tangent vectors through their components in a system of coordinates, y, as discussed above. We learned how a system of coordinates, y^i, defines basis vectors, ∂_j, for these tangent spaces, and how generic tangent vectors ∂_v can be expanded in terms of these. Although it is tempting to visualize tangent vectors within the framework of an embedding of M in a 'larger' space, the tangent space construction as such does not require this additional structure.

Tangent bundle and vector fields

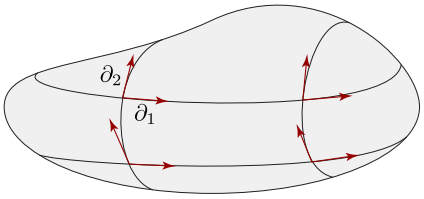
The discussion of the previous subsection was specific to individual points, r, on a manifold. Ultimately, however, we aim to employ tangent spaces as a means to describe the geometry of manifolds at large. Although tangent spaces at different points all have the same dimensionality, d, they differ from point to point (much like differently oriented planes in $\mathbb{R}^3$ are different two-dimensional vector spaces). This motivates the introduction of a 'container set', the **tangent bundle**

$$TM \equiv \bigcup_{r\in M} T_rM, \tag{V130}$$

as the formal union of all tangent spaces. The most important function of the tangent bundle is that it accommodates the vector *fields* of a manifold. A **vector field** ∂_v is a smooth map,

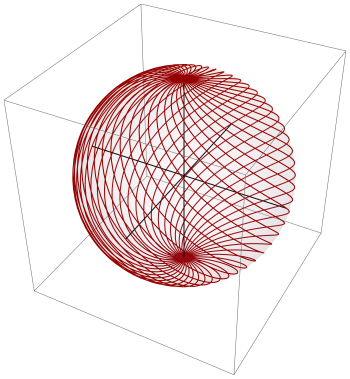
$$\partial_v : M \to TM, \qquad r \mapsto \partial_{v,r}, \tag{V131}$$

that assigns a vector $\partial_{v,r}$ to each point r. The set of all vector fields on M is often denoted $\mathrm{vect}(M)$. When M is embedded in a vector space $\mathbb{R}^n$, this definition coincides with our earlier understanding of vector fields (think about this point).



A set of vector fields, $\{\partial_{v_j}\}$, $j = 1, \ldots, d$, such that for all r, the vectors $\{\partial_{v_j,r}\}$ define a basis of T_rM, is called a **frame** of M. Our preferred frames will be **holonomic frames**, i.e. frames formed by the vectors $\{(\partial_j)_r\}$ for a chosen coordinate system (see figure). In a coordinate frame, any vector field ∂_v can be expanded as $\partial_v = v^j\partial_j$, where the d components v^j are now smooth *functions* on the manifold, $v^j : M \to \mathbb{R}$, $r \mapsto v^j_r$. The values of these functions at r are obtained by taking the directional derivatives, $v^j_r = \partial_{v,r}y^j$, of the coordinate functions according to the prescriptions discussed in the previous subsection (cf. Eq. (V124)).

INFO In practice, vector fields on manifolds are often defined through a **flow on the manifold**. A flow, $\Phi : I \times X \mapsto M$, $(t, r) \mapsto \Phi_t(r)$, $X \subset M$, $I \subset \mathbb{R}$ is a family of curves (locally) covering the manifold. These curves, called field lines, can be parameterized such that $\Phi_0(r) = r$, i.e. for fixed r, $\Phi_t(r)$ is a curve passing thorough r at time $t = 0$. The metaphorical analogy is that of a liquid streaming through the manifold, hence the name flow. For example, the coordinate lines of the jth coordinate of a local chart can be understood as a system of field lines with $\Phi_t(r) = r(y + e_jt)$, where $y = y(r)$ is the coordinate representation of r. Likewise, the flow of a system of n differential equations introduced in section C7.5 defines a system of field lines, where the domain of definition of the equations, $X \subset \mathbb{R}^n$, assumes the role of the manifold. A given flow $\Phi_t(r)$ defines a vector field, say ∂_v, via the following construction: For each $r \in X$ in the domain of definition of the flow, we view $\Phi_t(r)$ as a representative curve for a vector tangent to the corresponding field line at $t = 0$, and denote this vector by $\partial_{v,r} \in T_rM$. We then define ∂_v as the set, $\{\partial_{v,r}\}$, of all such vectors as r traverses X. For example, each of the fields ∂_i that define the coordinate frame itself is generated by such a 'coordinate flow', namely that along the coordinate lines of the corresponding ith coordinate.



As an example, let $M = S^2$ be the unit sphere, locally parametrized by spherical coordinates $y = (\theta, \phi)^T$ (we do not forget that the standard spherical coordinate chart does not reach all points in M). Consider the flow locally defined through $y(\Phi_t(r)) = (\theta + at, \phi+t)^T$, $a \in \mathbb{R}$. This is a system of spiraling curves on the sphere, as shown in the figure for $a = 0.2$. The corresponding vector field, say ∂_v, has the local coordinate representation $v^\theta_r = \partial_t\Phi^\theta_t\big|_{t=0}(r) = a$ and analogously $v^\phi_r = 1$. Its expansion in the holonomic basis thus reads $\partial_v = a\partial_\theta + \partial_\phi$.

V5 Alternating differential forms

REMARK What follows builds on chapter L11; recapitulate, if necessary.

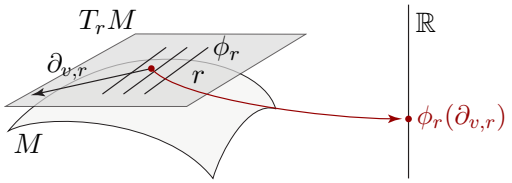
In this chapter, we introduce differential forms as a powerful tool to work with the geometry of manifolds, both from a mathematical and a physical perspective. Our discussion so far has shown how manifolds can be described by local linearizations – the system of tangent spaces. The focus was on the construction of the vectorial elements of these spaces, the tangent vectors, and on their description in terms of coordinates. We now take an essential next step and add to our previous description the elements of *multi*linear algebra. Adapting the concepts introduced in chapter L11 for general vector spaces to the bundle of tangent vector spaces, we will introduce dual vectors and tensors of higher degree on manifolds.

These constructions will lead to a synthesis of elements of multilinear algebra and of calculus. Much like tensors generalize the concept of vectors, smoothly varying (i.e. differentiable) tensor fields emerge as generalizations of vector fields. Differential forms are a subclass of tensor fields which play an important role in calculus and differential geometry, and are becoming increasingly important as a tool of modern physics. Indeed, many physical objects traditionally described as vector fields – force fields, vector potentials (sic), magnetic fluxes, etc. – are in fact differential forms. It is increasingly recognized that a language using differential forms provides cleaner and more natural descriptions of the physical phenomena related to these objects. Some of these applications will be touched upon in the final chapter of part V, chapter V7, where we outline how classical electrodynamics can be formulated in the language of differential forms.

V5.1 Cotangent space and differential one-forms

In section L11.2 we introduced the *dual space* of a vector space. Its elements, the dual vectors, are linear maps of vectors into the reals. In the following, we will explore a particular class of dual spaces, namely those dual to the tangent spaces of a manifold. We will see that these spaces play an important role both in the description of manifolds and in applications in physics.

Cotangent space



The dual space of the tangent space, T_rM, of a manifold is called the **cotangent space**, T_rM^*, to M at r. Its elements,

$$\phi_r : T_rM \to \mathbb{R}, \qquad \partial_{v,r} \mapsto \phi_r(\partial_{v,r}), \tag{V132}$$

are linear maps of tangent vectors into the real numbers and are called **one-forms**. In the figure, a form ϕ_r is represented by a pattern of parallel lines, as in Fig. L21(b) (such visualizations are useful for illustrative purposes but not widely used in concrete applications).

Since each tangent space, T_rM, of a manifold is defined with reference to a base point, r, the dual space, T_rM^*, too, is specific to this point. This dependence is emphasized by the definition, where both the argument vectors, $\partial_{v,r}$, and the one-forms, ϕ_r, carry a base point subscript. However, it is customary to suppress this subscript ($\partial_{v,r} \to \partial_v$ and $\phi_r \to \phi$) if the identity of the base point is clear from the context.

In analogy to the tangent bundle, we define the **cotangent bundle** of the manifold,

$$TM^* \equiv \bigcup_{r\in M} T_rM^*, \tag{V133}$$

as the union of its cotangent spaces. Much like a vector field, $\partial_v : M \to TM$, $r \mapsto \partial_{v,r}$ (cf. Eq. (V131)) is a smooth map which assigns a vector, $\partial_{v,r} \in T_rM$, to each point r in M, a **differential one-form**, or just one-form, is a smooth map,

$$\phi : M \to TM^*, \qquad r \mapsto \phi_r, \tag{V134}$$

which assigns a dual vector, $\phi_r \in T_rM^*$, to each r. The assignment is 'smooth' in the sense that if the form acts on a smooth vector field, ∂_v, then $\phi_r(\partial_{v,r})$ is a smooth function of r. We denote the set of all one-forms satisfying this condition by $\Lambda^1(M)$.

The definition above states that forms may be understood as maps

$$\phi : \mathrm{vect}(M) \to \Lambda^0(M), \qquad \partial_v \mapsto \phi(\partial_v), \tag{V135}$$

assigning to vector fields smooth functions $\phi(\partial_v) : M \to \mathbb{R}$, $r \mapsto \phi_r(\partial_{v,r})$. In the present context, it is customary to denote smooth functions as '**zero-forms**', and to denote the set of all these functions by the symbol $\Lambda^0(M)$. The rationale behind this notation will become evident a little further down.

Note that the two equations, Eqs. (V134) and (V135) emphasize different aspects of the differential form. The first defines the differential form as a smooth assignment of points, r, to one-forms, ϕ_r, while the second defines it via its action on vector fields. These are two faces of the same coin and it makes sense to use the same symbol ϕ in both equations although, strictly speaking, slightly different mappings are described.

Differential of functions

Consider a smooth function $f : \mathbb{R}^d \mapsto \mathbb{R}$ defined in $\mathbb{R}^d$. In section **??** we introduced the total differential $\mathrm{d}f_x$ as a map acting on vectors v as $\mathrm{d}f_x(v) = \partial_v f \equiv \mathrm{d}_t\big|_{t=0} f(x+tv)$. This

definition is readily generalized to that of the differential of functions on manifolds acting on vectors of their tangent spaces. We introduce the **differential of a function** $f : M \to \mathbb{R}$ as

$$\mathrm{d}f_r : T_rM \to \mathbb{R}, \qquad \partial_{v,r} \mapsto \mathrm{d}f_r(\partial_{v,r}) \equiv (\partial_v f)(r) = \mathrm{d}_t f(r(0)). \tag{V136}$$

This equation describes the local action of $\mathrm{d}f_r$ on vectors $\partial_{v,r} \in T_rM$, where the directional derivative appearing on the right is the same as that in Eq. (V119). The corresponding **differential one-form**, $\mathrm{d}f$, extends the definition to an action on vector fields as

$$\boxed{\mathrm{d}f : \mathrm{vect}(M) \to \Lambda^0(M), \qquad \partial_v \mapsto \mathrm{d}f(\partial_v) = \partial_v f,} \tag{V137}$$

where $(\mathrm{d}f(\partial_v))_r = \mathrm{d}f_r(\partial_{v,r}) = (\partial_v f)(r)$ is defined locally as usual. Note that the definition $\mathrm{d}f(\partial_v) = \partial_v f$ given in Eq. (V136) can be read in two ways. We may consider $\mathrm{d}f(\partial_v)$ as the action of a fixed *function* on different vectors via the differential. Previously, in Eq. (V119), the same expression was interpreted as $\partial_v f$, i.e. the action of a fixed *vector* on different functions. In either interpretation the directional derivative of the function along the vector is taken. The differential is linear in its arguments, $\mathrm{d}f_r(\partial_u + \partial_v) = \mathrm{d}f_r(\partial_u) + \mathrm{d}f_r(\partial_v)$, and it varies smoothly with r if $\partial_v \in \mathrm{vect}(M)$ is a smooth vector field. This identifies $\mathrm{d}f$ as a proper differential form.

Coordinate bases of cotangent space

Consider the differentials $\mathrm{d}y^i$ of the coordinate functions, $y^i : M \to \mathbb{R}$. These differentials define the *dual* basis corresponding to the holonomic basis ∂_j, i.e. they form a **basis of cotangent space**. To see why, consider the action of $\mathrm{d}y^i$ on ∂_j, i.e. the directional derivative of the ith coordinate in the direction of the jth coordinate basis vector,

$$\mathrm{d}y^i(\partial_j) = \partial_j y^i = \delta^i{}_j, \tag{V138}$$

which is the defining relation for a dual basis, cf. Eq. (L254). Arbitrary forms $\phi \in \Lambda^1(M)$ can be expanded in the dual basis as $\phi = \phi_i \mathrm{d}y^i$. As with general dual basis expansions (Eq. (L256)), the components of the form are found by evaluating the form on elements of the direct basis. This yields $\phi_i = \phi(\partial_i)$, i.e. we have the result

$$\boxed{\phi = \phi_i \mathrm{d}y^i, \qquad \phi_i = \phi(\partial_i),} \tag{V139}$$

where the components $\phi_i \in \Lambda^0(M)$ are smooth functions, $\phi_i(r)$, on M. Expansions of this type are called **coordinate representations of forms**.[1]

In the specific case where the form is the differential of a function, $\phi = \mathrm{d}f$, the components are obtained as $\mathrm{d}f(\partial_i) = \partial_i f = \partial_{y^i} f(y)$. The expansion then assumes the form

$$\boxed{\mathrm{d}f = \frac{\partial f(y)}{\partial y^i}\, \mathrm{d}y^i,} \tag{V140}$$

[1] A d-component representation of forms as 'dual vectors' can be obtained, if desired, by representing $\mathrm{d}y^i$ by the ith standard vector e^i, in which case ϕ is represented by $\phi_i e^i = (\phi_1, \ldots, \phi_d)$.

and generalizes Eq. (V62) from section V3.1 to the context of general differentiable manifolds.

As with coordinate representations of tangent vectors, one often needs to **change coordinates in the representations of forms**. Consider a coordinate change expressing y' through y-coordinates via the map $y \mapsto y'(y)$, and the expansions of a form, $\phi = \phi_i(y')\mathrm{d}y'^i = \phi_j(y)\mathrm{d}y^j$, in these two systems.[2] The component functions in the y-system, $\phi_j(y)$, are obtained from those of the y'-representation as $\phi_j(y) = \phi(\partial_{y^j}) = (\phi_i(y')\mathrm{d}y'^i)(\partial_{y^j}) \overset{(V137)}{=} \phi_i(y')\frac{\partial y'^i}{\partial y^j}$. Expressing the r.h.s. in terms of y-coordinates we are led to

$$\boxed{\phi = \phi_i(y')\,\mathrm{d}y'^i = \left[\phi_i(y')\,\frac{\partial y'^i}{\partial y^j}\right]_{y'=y'(y)} \mathrm{d}y^j.} \tag{V141}$$

This formula is the twin of Eq. (V128) for the change of representation of vector fields: whereas the components of a vector field transform *contra*variantly with the Jacobi matrix, $J^i{}_j = \frac{\partial y'^i}{\partial y^j}$, of the map $y \mapsto y'(y)$, i.e. $v^i(y') = [J^i{}_j v^j(y)]_{y=y(y')}$, the components of the form transform *co*variantly with the inverse Jacobi matrix, $\phi_i(y') = [\phi_j(y)(J^{-1})^j{}_i]_{y=y(y')}$. These transformation properties leave the action of a form on a vector invariant, $\phi(\partial_v) = \phi_i(y')v^i(y') = \phi_j(y(y'))v^j(y(y'))$, as they should.

EXAMPLE Let $U = \mathbb{R}^+ \times (0, 2\pi)$ be the polar coordinate domain of the slit plane, $M = \mathbb{R}^2\backslash\mathbb{R}^+$. Consider the differential form $\mathrm{d}\phi$ generated by the angular coordinate function ϕ. We now switch to a parameterization of M by Cartesian coordinates, $x = (x^1, x^2)^T$, with associated holonomic frame $\{\partial_1, \partial_2\}$. The coordinate representations of these vectors are identical to the standard Cartesian basis vectors, $v_i = e_i$, and the corresponding dual vectors are the differential forms $\mathrm{d}x^i$. They form a basis of TM^*, and hence there is an expansion $\mathrm{d}\phi = \phi_1\mathrm{d}x^1 + \phi_1\mathrm{d}x^2$, with coordinate-dependent coefficients $\phi_i(x)$. To identify the latter, we have to evaluate $\mathrm{d}\phi(\partial_i) = \partial_i\phi$ for $\phi(x) = \arctan(x^2/x^1)$. This gives $\phi_1 = -x^2/((x^1)^2 + (x^2)^2)$ and $\phi_2 = x^1/((x^1)^2 + (x^2)^2)$, or

$$\mathrm{d}\phi = \frac{-x^2\mathrm{d}x^1 + x^1\mathrm{d}x^2}{(x^1)^2 + (x^2)^2}. \tag{V142}$$

INFO Consider a point particle moving on a manifold M under the influence of a potential function, $\varphi : M \to \mathbb{R}$. This function describes how the energy of the particle varies with its position. We define the **force** acting on the particle as the differential one-form,

$$f = -\mathrm{d}\varphi = -\frac{\partial\varphi(y)}{\partial y^i}\mathrm{d}y^i, \tag{V143}$$

where y is a coordinate vector and $\varphi(y) = \varphi(r(y))$, as usual. To understand the meaning of this form, let $r_1 = r(y)$ and $r_2 = r(y + \Delta)$ be two points infinitesimally close to each other on the manifold, where the displacement $\Delta = \delta^j e_j$ denotes the difference in their coordinates. The infinitesimal

[2] As for vectors,[6] the argument of a coefficient function indicates which coordinate systems it refers to.

tangent vector $\partial_\Delta \equiv \delta^j \partial_j$ in the tangent space $T_{r_1}M$ to r_1 then is a vector, with infinitesimal components δ^j, 'pointing in the direction' of r_2.[3] Equivalently, we may view ∂_Δ as a tangent vector corresponding to a curve connecting the points r_1 and r_2 on the manifold. The energy difference $\delta\phi \equiv \varphi(r_2) - \varphi(r_1)$ can then be expressed as

$$\delta\phi = \varphi(y+\Delta) - \varphi(y) \simeq \frac{\partial\varphi(y)}{\partial y^j}\,\delta^j \overset{(V138)}{=} \left(\frac{\partial\varphi(y)}{\partial y^i}\mathrm{d}y^i\right)(\delta^j\partial_j) = -f(\partial_\Delta). \tag{V144}$$

This shows how the potential difference between nearby points equals the (negative of the) force form applied to the tangent vector, ∂_Δ, describing their separation. The definition (potential difference) = (force form acting on vector) differs from the traditional view where force is a vector. Representing this vector in a boldface notation $\mathbf{f}$, potential differences between points separated by a small vector $\boldsymbol{\Delta}$ are scalar products, $\delta\phi = -\langle \mathbf{f}, \boldsymbol{\Delta}\rangle$. We will return to the discussion of the differences between the two formulations in chapter V6 below.

Finally, a comment on **potentially confusing notation**: in the physics literature formulations like 'let $\mathrm{d}\varphi = \varphi(r_2) - \varphi(r_1)$ be the small potential difference between nearby points' are frequently used. Here, we express the same difference as $\mathrm{d}\varphi(\partial_\Delta)$. In the present approach, $\mathrm{d}\varphi$ is a differential form and not 'small' in any sense. The smallness is in the argument vector, ∂_Δ. What the more casual physics formulation actually refers to is the differential of the function, $\mathrm{d}\varphi$, applied to a small argument vector. If one is aware of this interpretation, confusion can be avoided.

V5.2 Pushforward and Pullback

At this stage, we have introduced the basic structures used to describe the geometry of manifolds, coordinates, tangent and co-tangent space, vector fields and forms. We now take the next step to consider *maps* on manifolds. This will include maps $F : M \to L$ establishing connections between different manifolds whose dimensions, $\dim(M) \equiv d$ and $\dim(L) \equiv c$, need not even be the same, or maps $F : M \to M$ describing structures on a single manifold. An example with $d = c$ is a coordinate map for the manifold L of the form $F \equiv r : U \to L$, $y \mapsto r(y)$, with $M \equiv U \subset \mathbb{R}^d$ being the coordinate domain. Further examples include the flow, Φ_t, on a manifold (cf. discussion on p. V4.2), described by a map of the form $F = \Phi_t : M \to M$, $r \mapsto \Phi_t(r)$; real-valued functions on a manifold, $F : M \to L \equiv \mathbb{R}$ $r \mapsto F(r)$; and many others.

Our goal in this section is to understand how the two fundamental geometric structures defined on manifolds, namely vectors fields and forms, behave under the action of a map. The general situation is illustrated in Fig. V24: given a map

$$F : M \to L, \qquad r \mapsto q(r), \tag{V145}$$

we can 'pushforward'[4] a vector field $\partial_v \in \mathrm{vect}(M)$ to a vector field $F_*\partial_v \in \mathrm{vect}(L)$ on the

[3] Quotes are used because the construction does *not* require M to be embedded in a vector space. All concrete vector operations are performed in the coordinate domain. Keep an eye on this point.

[4] The operation is commonly denoted as 'pushforward', although 'push-forward' or 'push forward' would seem to be more natural ways of writing.

image domain. Likewise, a differential form $\omega \in \Lambda^1(L)$ defined on the image of F can be 'pulled back' to a differential form $F^*\omega \in \Lambda^1(M)$ on M.

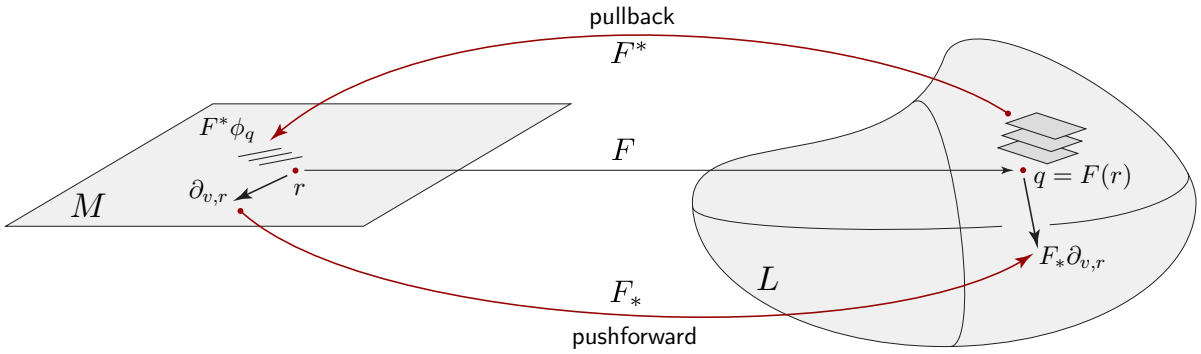
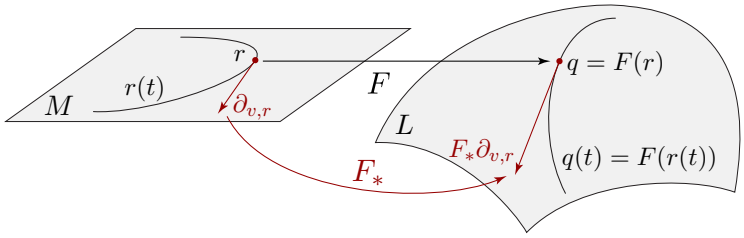


Figure V24: Pushforward of vectors and pullback of forms: under pushforward, vectors $\partial_{v,r}$ on M map to vectors $F_*\partial_{v,r}$ on L. Forms ω_q on L get pulled back to forms $F^*\omega_q$ on M. For illustrative purposes, we have visualized the 1-forms as lines in a two-dimensional manifold M, or as planes in a three-dimensional manifold L, cf. section L11.6.

Pushforward



The **idea of pushforward** is easily explained: assume that a vector $\partial_{v,r} \in T_rM$ describes the separation between two nearby points on the manifold M (such as the separation of two neighboring points on a curve). Under F these points get mapped to points which now are close in L. The image of $\partial_{v,r}$ under pushforward is the vector $F_*\partial_{v,r} \in T_qL$ describing the separation between these image points.

To make this definition quantitative, let $\partial_{v,r} \in T_rM$ be represented by a curve $r(t)$. The vector **pushforward**, $F_*\partial_{v,r} \in T_qL$, is then represented by the curve $q(t) \equiv F(r(t))$. Pushforward is linear in its arguments,[5] $F_*(\partial_u + \partial_v) = F_*(\partial_u) + F_*(\partial_v)$, and so we will usually write $F_*\partial_v$ (as with linear maps of vector spaces). For later reference we note that the pushforward of a vector under a **composite map**, $E \circ F : M \to K$, where $E : L \to K$ is a second map acts as

$$(E \circ F)_*\partial_v = E_*(F_*\partial_v), \tag{V146}$$

i.e. we push in two steps, first by F_* from M to the intermediate manifold, L, and from there by E_* on to the final destination, K. This composition feature is a direct consequence of the definition of pushforward.

[5] Intuitively, the linearity of this map should be evident. An economic way to verify it explicitly is by inspection of the coordinate representation to be discussed momentarily.

Component representations of the pushforward vector $F_*\partial_v$ are computed in the usual way: pick a coordinate system x on L and in this way define a holonomic basis ∂_{x^i}. The coefficients of the expansion $F_*\partial_v = (F_*\partial_v)^i\partial_{x^i}$ are then obtained by applying $F_*\partial_v$ to the coordinate functions, $(F_*\partial_v)^i = (F_*\partial_v)x^i = \mathrm{d}_t x^i(q(0)) = \mathrm{d}_t x^i(F(r(0))) \equiv \mathrm{d}_t F^i(r(0))$, where the shorthand $F^i = x^i(F)$ was used for the coordinate components of F. One often wants to express these components in terms of those of the vector $\partial_v = v^j\partial_{y^j}$, where a coordinate system y on M is assumed. This can be done by representing the map F itself in a coordinate language as $F(y) = F(r(y))$. Curves $r(t) = r(y(t))$ representing ∂_v then have coordinate representations $y(t)$, and $v^j = \partial_v y^j = \mathrm{d}_t y^j(0)$, as before. In this way, the components of the pushforward vector are obtained as $(F_*\partial_v)^i = \mathrm{d}_t F^i(y(0)) = \frac{\partial F^i(y(0))}{\partial y^j}\mathrm{d}_t y^j(0) = \frac{\partial F^i(y)}{\partial y^j}v^j$, and we have the expansion[6]

$$\boxed{F_*\partial_v = \partial_{x^i}\left[\frac{\partial F^i(y)}{\partial y^j}v^j\right]_{y=y(x)}}. \tag{V147}$$

The architecture of this formula underpins the qualitative definition of pushforward given above: under F, a vector ∂_v representing an 'infinitesimal' separation on M gets mapped to a vector $F_*\partial_v$ whose coordinate representation has components $\frac{\partial F^i}{\partial y^j}v^j$. Here, the **Jacobi matrix** $\frac{\partial F^i}{\partial y^j}$ is a generalization of those appearing in Eqs. (V45) and (V128). It describes how the coordinates $F^i(y)$ change under infinitesimal variations of their arguments y, and $\frac{\partial F^i}{\partial y^j}v^j$ is the change in F^i corresponding to the change in y described by the displacement vector ∂_v.

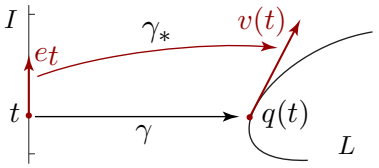
If $\partial_v : M \to TM$, $r \mapsto \partial_{v,r}$ is a **vector field**, the pushforward $F_* : TM \to TL$ may be applied to all vectors $\partial_{v,r}$. If, and only if, F is injective, this yields a vector field, $F_*\partial_v$, defined on the image $F(M) \subset L$. The injectivity condition is essential, for if F would map different points to the same image, $F(r_1) = F(r_2) = q$, a given vector field ∂_v could lead to two different image tangent vectors, $F_*\partial_{v,r_1}$ and $F_*\partial_{v,r_2}$, in the tangent space T_qL, i.e. the image vector field would be ill-defined at q. The **pushforward operation defined by injective maps** F,

$$F_* : \mathrm{vect}(M) \to \mathrm{vect}(F(M)), \qquad \partial_v \mapsto F_*\partial_v, \tag{V148}$$

can therefore be understood as a map from the space of vector fields on M to those on $F(M)$.

Various mathematical operations routinely applied in physics are pushforwards, although they are usually not understood in this way. Let us illustrate this point on two **examples.**

[6] Here, ∂_{x^i} is a vector, *not* a partial derivative. We write it to the left to emphasize the structure of the indices that are pairwise contracted.



▷ Consider a **curve**, $\gamma : I \to L \subset \mathbb{R}^c$, $t \mapsto q(t)$, where $I \subset \mathbb{R}$ is an open interval. We now have the identifications $M = I$, and $F = \gamma$. In the present context it does not make sense to distinguish between the one-dimensional 'manifold', I, and its coordinate representation, [7] and the curve parameter t may be considered as an element of I and as a coordinate at the same time.

The manifold I has a one-dimensional tangent space, T_tI, spanned by a vector ∂_t. We may represent this vector via the representing curve $t(s) = t+s$, such that the single component of ∂_t is obtained as $\mathrm{d}_s\big|_{s=0}(t+s) = 1$. The pushforward of ∂_t under γ, namely $\gamma_*\partial_t$, has the coordinate representation $\mathrm{d}_s\big|_{s=0} q(t+s) = \mathrm{d}_t\, q(t) = v(t)$, which is just the **curve velocity** in L. We conclude that the velocity vector tangent to a curve can be interpreted as the pushforward of the single 'unit vector' tangent to the parameter interval.

▷ Consider $M = L = \mathbb{R}^d$ and let $F = A$ be a **linear map**. As in the previous example, we do not distinguish between $M = \mathbb{R}^d$ and its (Cartesian) coordinate representation. The map then has the coordinate representation $y \mapsto y' = A(y) \equiv Ay$ with $y'^i = A^i{}_j y^j$. The Jacobi matrix of the transformation is given by $J^i{}_j = \frac{\partial y'^i}{\partial y^j} = A^i{}_j$, showing that the Jacobi matrix of a linear map equals that map. The pushforward of a tangent vector under a linear map, $A_*\partial_v \equiv \partial_{v'}$, has a coordinate transformation given by $v'^i = A^i{}_j v^j$, as follows from Eq. (V147). As one might have expected, tangent vectors transform contravariantly under the map.

As an example of physical importance, consider $M = L = \mathbb{R}^4$ and let $F = \Lambda$ be a **Lorentz transformation**, i.e. an element of the special orthogonal group, $\mathrm{O}(1,3)$, of linear maps $\Lambda^T\eta\Lambda = \eta$ leaving the Minkovski metric $\eta = \mathrm{diag}(1,-1,-1,-1)$ invariant (cf. p. 111). The Lorentz transformations $\Lambda : \mathbb{R}^4 \to \mathbb{R}^4$ are linear and the above discussion implies that $v'^\mu = \Lambda^\mu{}_\nu v^\nu$ under the pushforward by these maps. In physics parlance it is said that space-time vectors v^μ transform contravariantly under Lorentz transformations, and this is a well-known statement of special relativity.

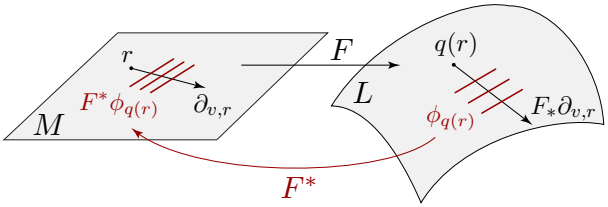
Pullback

The reciprocal operation, pullback F^*, acts on forms, and it works in the reverse direction: a form $\phi \in \Lambda^1(F(M))$ defined on the image of $F(M) \subset L$ is 'pulled back' to a form $F^*\phi \in \Lambda^1(M)$ on the pre-image M.

[7] Fomally, one may consider I parameterized by a 'coordinate domain' $U = I$, where $U \ni y(t) = t \in I$ is an identity coordinate assignment. Clearly, however, this type of overhead is excessive and does not make much sense, *unless* different parameterizations of the same 'manifold' I are considered, e.g. using a parameter $s(t)$. This illustrates how in some cases it can be expedient to identify a manifold with its coordinate representation. (Think how a different choice of parameterization, $t \mapsto s(t)$, may be considered as a change of coordinates of the manifold I. As an instructive exercise, discuss how the formulas below change if the different 'coordinate' s is used to parameterize I.)

The action of the pullback form is defined by the relation

$$(F^*\phi_{q(r)})_r(\partial_{v,r}) \equiv \phi_{q(r)}(F_*\partial_{v,r}), \quad \text{(V149)}$$



i.e. the action of the form $(F^*\phi_{q(r)})_r$ on a vector $\partial_{v,r} \in T_rM$ is found by reading out the action of the form $\phi_{q(r)}$ on the pushforward of $\partial_{v,r}$. This operation is linear, $F^*\phi(\partial_u + \partial_v) = F^*\phi(\partial_u) + F^*\phi(\partial_v)$, and hence defines a one-form. Since it is evident that pullback connects forms at $q(r)$ with forms at r, reference to the base points are usually omitted in the notation, i.e. we just write $F^*\phi$, etc. The extension of the pointwise pullback over the full image of F yields a map between differential forms,

$$F^* : \Lambda^1(F(M)) \to \Lambda^1(M), \qquad \phi \mapsto F^*\phi.$$

For later reference we note that the pullback of a form by a **composite map** $E \circ F : M \to K$, where $E : L \to K$ is a second map acts as

$$(E \circ F)^*\omega = F^*(E^*\omega), \quad \text{(V150)}$$

i.e. we first pull ω from the final target, K, to the intermediary manifold L, and from there in a second step back to M. This feature is a direct consequence of the definition.

Let us now find the **coordinate representation** of the pullback. Given coordinate representations $r(y)$ for M and $q(x)$ for L, a form ϕ and its pullback $F^*\phi$ can be expanded in their respective cotangent spaces as $\phi = \phi_i\,\mathrm{d}x^i$ and $F^*\phi = (F^*\phi)_j\,\mathrm{d}y^j$, respectively. We seek to establish a relation between the components $\phi_i(x)$ and $(F^*\phi)_j(y)$. To this end, we recall from Eq. (V139) that the components of ϕ are found by letting it act on L's tangent basis vectors, $\phi_i = \phi(\partial_{x^i})$. Likewise, the components of the pullback form, $F^*\phi$, are obtained by applying it to M's tangent basis vectors, $(F^*\phi)_j = (F^*\phi)(\partial_{y^j}) \overset{\text{(V149)}}{=} \phi(F_*\partial_{y^j})$. We expand the argument vector as $F_*\partial_{y^j} = (F_*\partial_{y^j})^i\partial_{x^i} \overset{\text{(V147)}}{=} \frac{\partial F^i}{\partial y^k}(\partial_{y^j})^k\partial_{x^i} \overset{\text{(V123)}}{=} \frac{\partial F^i}{\partial y^j}\partial_{x^i}$ to obtain $(F^*\phi)_j = \phi(\frac{\partial F^i}{\partial y^j}\partial_{x^i}) = \frac{\partial F^i}{\partial y^j}\phi_i$. This shows that the expansion of the pullback form is given by

$$\boxed{F^*\phi = \phi_i(x(y))\frac{\partial F^i}{\partial y^j}\,\mathrm{d}y^j.} \quad \text{(V151)}$$

Note the structural similarity of this formula to Eq. (V147) for the pushforward. Again the Jacobian matrix features as the central building block. The difference is that this time it is contracted with the covariant components, ϕ_i, of the argument form, whereas for the pushforward the contraction was with the contravariant components, v^j, of the argument vector.

Let us discuss a few **examples of pullback operations**:

- ▷ Consider the force one-form, $f = f_i\mathrm{d}q^i$, defined in the vicinity of a **curve** $\gamma : I \to \mathbb{R}^c$, $t \mapsto q(t)$. (Here, $F \equiv \gamma$ plays the role of the map, $M = I$ is its one-dimensional argument manifold, $L = \mathbb{R}^c$ the image manifold, and we do not discriminate between these sets and

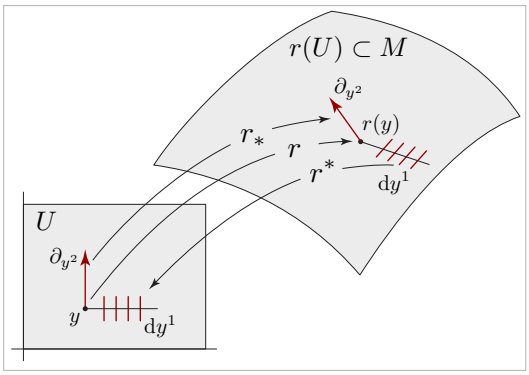
their coordinate representations.) The form f may be pulled back to a form $\gamma^* f$ defined on the parameter interval I. According to Eq. (V151), this form is given by

$$\gamma^* f = f_i \frac{\mathrm{d}q^i}{\mathrm{d}t}\,\mathrm{d}t. \tag{V152}$$

Notice how this expression is reminiscent of that appearing in Eq. (V12) in the computation of the line integral of a force. The difference is that in that context $\mathrm{d}t$ referred to an integration measure, whereas here it is a one-form. We will explain the correspondence between the two expressions in section V5.4 when we discuss the *integration* of forms.

▷ As in the analogous pushforward example, consider $M = L = \mathbb{R}^d$, let $F = A$ be a **linear map** with coordinate representation $y'^i = A^i{}_j y^j$ and ϕ' be a form. Then the pullback form, $\phi \equiv A^* \phi'$, has a coordinate representation whose components, found using Eq. (V151), are given by $\phi_j = \phi'_i A^i{}_j$, showing that the components of forms transform *co*variantly under linear maps.

EXERCISE Discuss in what sense the pullback of linear algebra (section L11.9) is a special case of the pullback defined here.



INFO Let us briefly address a subtlety concerning the **pushforward, pullback and the coordinate representations of forms and vectors**. Consider the differential of a coordinate function, $\mathrm{d}y^i$. We can think of this form in two different ways: the first is as the differential $\mathrm{d}y^i$ of a coordinate function $y^i : r(U) \mapsto \mathbb{R}$, where $r(U)$ is the image of a coordinate domain under the coordinate map, $r : U \to r(U) \subset M$, $y \mapsto r(y)$, of the manifold (see figure). In this way, $\mathrm{d}y^i$ becomes a differential form on the tangent bundle $Tr(U)^* \subset TM^*$, and this is the interpretation we have emphasized above. Alternatively, we may consider the differential $\mathrm{d}y^i$ of the function $y^i : U \mapsto \mathbb{R}$, $y \mapsto y^i$ defined on the coordinate domain itself. The function y^i is now trivial, it just projects a vector $y \in U$ to its ith coordinate. Nevertheless, it is a valid function and $\mathrm{d}y^i$ is a valid differential form, now defined on the cotangent bundle of the coordinate domain, TU^*. Of course the two definitions are closely related: $\mathrm{d}y^i$ defined on TU^* is the *pullback* of $\mathrm{d}y^i$ defined on $Tr(U)^*$ under the coordinate map, $r : U \to r(U)$. Conversely, $\mathrm{d}y^i$ defined on $Tr(U)^*$ is the pullback of that on TU^* under the inverse of the coordinate map, $y : r(U) \to U$, $r \mapsto y(r)$. To see this in explicit terms let us, for once, discriminate between objects defined on U and $r(U)$ by a subscript. For example, the two coordinate functions are denoted by y^i_U and $y^i_{r(U)}$ and their relation is given by $y^i_U(y) = y^i_{r(U)}(r(y))$. If ∂_{v_U} is a vector in U with generating curve $y(t)$, we then have $\mathrm{d}y^i_U(v) = \mathrm{d}_t y^i_U(y(0)) = \mathrm{d}_t y^i_{r(U)}(r(y(0))) = \mathrm{d}y^i_{r(U)}(r_* \partial_v)$, where in the last equality we used the fact that the pushforward vector of ∂_v is generated by the curve $r(y(t))$. According to the definition of pullback, their equality means that $\mathrm{d}y^i_U = r^* \mathrm{d}y^i_{r(U)}$, as stated above.

The two forms $\mathrm{d}y^i_U$ and $\mathrm{d}y^i_{r(U)}$ are so closely related that they are generally denoted by the same symbol, $\mathrm{d}y^i$, and this can sometimes be a source of confusion. (For example, the symbol $\mathrm{d}\theta$ may either refer to a differential form defined in the tangent bundle of a two-sphere, or a differential form in the domain of spherical coordinates, (θ, ϕ), of the sphere, two subtly different objects.) Mathematically, there is practically no difference between the two forms, and its is perhaps best to think of the two definitions above as different incarnations of the same object.

Before discussing why it can nevertheless be useful to discriminate between the two views, let us consider the analogous situation with the coordinate basis vectors. We have defined $\partial_{y^j} \equiv \partial_{y^j,r(U)}$ as basis vectors on the tangent bundle $Tr(U)$, generated by the curves $r(y + te_j)$. These curves are in correspondence to curves $y + te_j$ in the coordinate domain, U, where they generate vectors, $\partial_{y^j} \equiv \partial_{y^j,U}$, of TU commonly denoted by the same symbol. The notation really is to the point because the vector-differential operator in TU acts on functions as $\partial_{y_j} f(y) \equiv \mathrm{d}_t\big|_{t=0} f(y + te_j)$, i.e. as the ordinary partial derivative in the coordinate domain. The fact that $\partial_{y^j,r(U)}$ defined in $Tr(U)$ is obtained from the curve $r(y+te_j)$ means that it is the pushforward of $\partial_{y^j,U}$ defined in TU under the coordinate map. Combining the pushforward and pullback relation between the vectors and forms, we obtain identical actions in U and $r(U)$, $\delta^i{}_j = \mathrm{d}y^i_U(\partial_{y^j,U}) = r^*\mathrm{d}y^i_{r(U)}(\partial_{y^j,U}) = \mathrm{d}y^i_{r(U)}(r_*\partial_{y^j,U}) = \mathrm{d}y^i_{r(U)}(\partial_{y^j,r(U)})$, etc.

In the same way, we can think of a form expanded as in (V139) as a form in the cotangent bundle of the manifold, $Tr(U)^*$, or in the cotangent bundle TU^* of the coordinate domain. With vectors expanded as in Eq. (V124) the situation is analogous. This bivariate picture of forms and vectors suggests alternative interpretations of operations of differentiable geometry, notably those relating to coordinate changes. For example, when deriving Eq. (V141) above we interpreted it as a change of basis in the cotangent bundle TU^*. Alternatively, if we think of $\phi_U \equiv \phi_{i,U}(y)\mathrm{d}y^i_U$ as a form in the U-domain of y-coordinates, then $\phi_{U'} \equiv \phi_{i,U'}(y')\mathrm{d}y'^i_{U'}$ is the form represented in the U'-domain of y'-coordinates, and the discussion above implies that the two are related as $\phi_U = (y' \circ y^{-1})^*\phi_{U'}$, i.e. one is the pullback of the other under the map describing the coordinate change, $y' \circ y^{-1} : U \to U', y \mapsto y'(y)$. Of course, the two pictures are fully consistent with each other. For example, one may verify that the pullback formula (V151) applied to the case $F = (y' \circ y^{-1})$ is identical to the basis change formula Eq. (V141). As an exercise, discuss the analogous situation with vectors. Clarify how (V128) is obtained from (V147) if the change of vector expansions under a change of holonomic bases is interpreted as the pushforward of vector representations between coordinate domains.

Generally speaking, the form/vector–expanded–on–manifold view may be somewhat more geometrical, while the form/vector–expanded–in–coordinate domain is closer to the safe grounds of calculus as it is defined relative to open subsets of $\mathbb{R}^d$. It is often useful to switch between the two interpretations or to think about an operation in both ways at the same time.

Pushforward and pullback summary

To summarize, a map $F : M \to L, r \mapsto q(r)$ sends vectors $\partial_v \in TM$ to vectors $F_*\partial_v \in TL$ and forms $\phi \in TL^*$ to forms $F^*\phi \in TM^*$. If coordinates are used to represent elements of the manifolds as $r(y) \in M$ and $q(x) \in L$, respectively, and F defines a map of coordinates

as $F : y \mapsto x(y)$, the two basic formulas describing these operations read

$$\boxed{\begin{aligned} F_*(v^j \partial_{y^j}) &= \partial_{x^i} \frac{\partial x^i}{\partial y^j}\, v^j, \\ F^*(\phi_i \mathrm{d}x^i) &= \phi_i \frac{\partial x^i}{\partial y^j}\, \mathrm{d}y^j. \end{aligned}} \tag{V153}$$

The structure of these formulas is easy to remember: simply contract the matrix elements of the Jacobian $\frac{\partial x^i}{\partial y^j}$ with the components of either v^j or ϕ_i.

V5.3 Forms of higher degree

In section **??** we introduced alternating p-forms in vector spaces, i.e. anti-symmetric tensors acting on sets of p-argument vectors. (If you no longer remember this section well, now would be a good time to recapitulate.) *Differential* p-forms are forms of degree p on manifolds, much like differential one-forms were one-forms on manifolds.

In differential geometry, there is a matching between the degree of a differential form and the dimensionality of the geometric or physical objects it describes. Specifically, the one-forms discussed so far are tailored to the representation of one-dimensional objects. For example, the force form describes a directed quantity (the force), which is to be paired with another directed quantity (a displacement) to yield a scalar (work). Later on, we will see that one-forms can be integrated over one-dimensional manifolds (i.e. smooth curves), etc. In this section, we will first construct the extension to differential p-forms and then discuss how these objects are applied to the description of higher dimensional structures.

An alternating p-form, or just p-form, ω_r, defined with reference to a point r of a manifold is an antisymmetric map, $\omega_r : \otimes^p(T_rM) \to \mathbb{R}$, $((\partial_{v_1})_r, \ldots, (\partial_{v_p})_r) \mapsto \omega_r((\partial_{v_1})_r, \ldots, (\partial_{v_p})_r)$, assigning to p tangent vectors a number. The map is antisymmetric, i.e. the exchange of any two argument vectors yields a minus sign. We denote the set of all p-forms by $\Lambda^p(T_rM)$.

Differential p-forms are smooth extensions of pointwise-defined p-forms to forms defined on all of M,

$$\omega : \otimes^p \mathrm{vect}(M) \to \Lambda^0(M), \qquad (\partial_{v_1}, \ldots, \partial_{v_p}) \mapsto \omega(\partial_{v_1}, \ldots, \partial_{v_p}), \tag{V154}$$

where the function $\omega(\partial_{v_1}, \ldots, \partial_{v_p}) \in \Lambda^0(M)$ is defined through the pointwise construction, $\omega(\partial_{v_1}, \ldots, \partial_{v_p})(r) = \omega_r((\partial_{v_1})_r, \ldots, (\partial_{v_p})_r)$. The space spanned by all these forms is denoted by $\Lambda^p(M)$ (although $\Lambda^p(TM)$ would be a more accurate, if lengthier, notation).

For a tangent space of dimension $d = \dim(T_rM) = \dim(M)$, the space $\Lambda^p(T_rM)$ is a vector space of dimension $\binom{d}{p}$ (recall section **??**), hence $\binom{d}{p}$ 'coordinate functions' are required to specify a differential p-form. (We will see momentarily how these functions are obtained.) Since a d-dimensional vector space cannot support forms of degree higher than d, we have $\Lambda^{p>d}(M) = \{\,\}$.

Wedge product

All operations introduced in section **??** for p-forms of single vector spaces can be generalized to manifolds by smooth extension of pointwise definitions for the individual tangent spaces T_rM. Specifically, the wedge product, introduced in section **??**, is one such operation. Two forms $\phi_r \in \Lambda^p(T_rM)$ and $\psi_r \in \Lambda^q(T_rM)$ can be wedge-multiplied together to obtain $\phi_r \wedge \psi_r \in \Lambda^{p+q}(T_rM)$, where the action of the product form on $p+q$ vectors, $\partial_{v_1}, \ldots, \partial_{v_{p+q}}$, is defined by Eq. (L277). For example, for two one-forms $\phi_r, \psi_r \in \Lambda^1(T_rM)$, we have $(\phi_r \wedge \psi_r)(\partial_v, \partial_w) = \phi_r(\partial_v)\psi_r(\partial_w) - \phi_r(\partial_w)\psi_r(\partial_v)$, etc. Recall the most important properties of the wedge product, listed on p. 154.

The extension of this operation over the full manifold defines the **wedge product of differential forms**,

$$\wedge : \Lambda^p(M) \otimes \Lambda^q(M) \to \Lambda^{p+q}(M), \qquad (\phi, \psi) \mapsto \phi \wedge \psi, \tag{V155}$$

where $\phi \wedge \psi$ acts on pairs of vectors fields $(\phi \wedge \psi)(\partial_v, \partial_w)$ through the point-wise action $((\phi \wedge \psi)(\partial_v, \partial_w))_r = (\phi_r \wedge \psi_r)(\partial_{v,r}, (\partial_w)_r)$.

Coordinate representation

The wedge product is the key to the hierarchical construction of forms of higher degree from one-forms. In particular, it can be used to represent forms in a coordinate language (cf. Eq. (L280)).

Suppose we have a coordinate system y on a d-dimensional manifold M, with an associated set of coordinate forms $\{\mathrm{d}y^i\}$. A general form, $\omega \in \Lambda^p(M)$, can then be expanded as

$$\boxed{\omega = \frac{1}{p!}\omega_{i_1,\ldots,i_p}(y)\,\mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p},} \tag{V156}$$

where the components $\omega_{i_1,\ldots,i_p}(y)$, antisymmetric in their indices, are smooth functions of the coordinates. These functions are obtained by acting with the form on the basis vector fields,

$$\omega_{i_1,\ldots,i_p} = \omega(\partial_{i_1}, \ldots, \partial_{i_p}). \tag{V157}$$

Occasionally, it is expedient use the index permutation symmetry of the sum (both the coefficients and the wedge products are antisymmetric under exchange, so their product is symmetric) to convert it into one over ordered indices but without the prefactor $1/p!$, i.e. $\omega = \sum_{i_1<\cdots<i_p} \omega_{i_1,\ldots,i_p}(y)\,\mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p}$. (cf. Eq. (L281)).

As with one-forms, the change of representation under a **change of coordinates**, $y \mapsto y'(y)$, is obtained by letting the y'-representation of the form act on the basis vectors ∂_{y^j}. Using $\mathrm{d}y'^i(\partial_{y^j}) = \frac{\partial y'^i(y)}{\partial y^j}$, we obtain

$$\boxed{\omega = \frac{1}{p!}\omega_{i_1,\ldots,i_p}(y')\,\mathrm{d}y'^{i_1} \wedge \cdots \wedge \mathrm{d}y'^{i_p} = \frac{1}{p!}\left[\omega_{i_1,\ldots,i_p}(y')\frac{\partial y'^{i_1}}{\partial y^{j_1}} \cdots \frac{\partial y'^{i_p}}{\partial y^{j_p}}\right]_{y'=y'(y)} \mathrm{d}y^{j_1} \wedge \cdots \wedge \mathrm{d}y^{j_p},} \tag{V158}$$

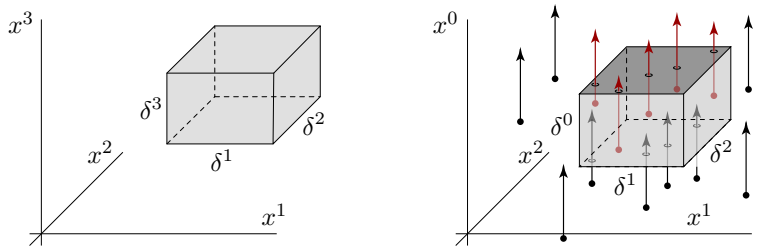


Figure V25: On the definition of density and current flow via differential forms. Discussion see text

which generalizes the one-form transformation rule (V141).

EXAMPLE In $M = \mathbb{R}^2$ consider the **Cartesian area two-form**, $\omega = \mathrm{d}x^1 \wedge \mathrm{d}x^2$. When this form acts on a pair of vectors, it yields $\omega(\partial_u, \partial_v) = \mathrm{d}x^1(\partial_u)\mathrm{d}x^2(\partial_v) - \mathrm{d}x^2(\partial_u)\mathrm{d}x^1(\partial_v) = u^1v^2 - u^2v^1$, the oriented area spanned by these vectors. The expansion of ω in a basis of polar coordinate vectors, $\{\partial_\rho, \partial_\phi\}$, has only a single component, $\omega_{\rho,\phi}$ (why?), which can be computed using Eq. (V157):

$$\omega_{\rho,\phi} = \omega(\partial_\rho, \partial_\phi) = \mathrm{d}x^1(\partial_\rho)\mathrm{d}x^2(\partial_\phi) - \mathrm{d}x^2(\partial_\rho)\mathrm{d}x^1(\partial_\phi) = (\partial_\rho x^1)(\partial_\phi x^2) - (\partial_\rho x^2)(\partial_\phi x^1) \overset{(V15a)}{=} \rho.$$

The polar representation of the area form is therefore given by

$$\omega = \rho\, \mathrm{d}\rho \wedge \mathrm{d}\phi. \tag{V159}$$

Similarly, in a basis $\{\partial_{y^1}, \partial_{y^2}\}$ corresponding to a general coordinate system y, the area form reads

$$\omega = \left(\frac{\partial x^1}{\partial y^1}\frac{\partial x^2}{\partial y^2} - \frac{\partial x^2}{\partial y^1}\frac{\partial x^1}{\partial y^2} \right) \mathrm{d}y^1 \wedge \mathrm{d}y^2. \tag{V160}$$

Here, the expression in parenthesis is the area of the parallelogram spanned by the two coordinate basis vectors $v_j = \partial_{y^j} x$ $(j = 1, 2)$ representing the tangent vectors ∂_{y^j} in Cartesian coordinates.

INFO The wedge product can be applied to construct differential forms of immediate physical significance. Let us illustrate this point on the example of the **current three-form**. Consider a situation where a large number of particles is confined to a region of space, V. Add a time axis to obtain a four-dimensional manifold, $M = \mathbb{R} \times V$, parameterized by Cartesian coordinates as $x = (x^0, x^1, x^2, x^3)$, where $x^{1,2,3}$ are Cartesian coordinate of V and $x^0 \equiv t$ is a time-like coordinate.[8]

The **density** of particles, $\rho(x)$, is a space-time dependent function defined such that the number of particles in an infinitesimal cubical box with geometric volume $\delta^1\delta^2\delta^3$, located at the space-time point t, x^1, x^2, x^3, is given by $\rho(x)\delta^1\delta^2\delta^3$. In form language this is described by a **density form**, whose application to the three vectors spanning the box yields the number of particles in it. This leads to the definition of a differential three-form with coordinate representation

$$\rho = j_{123}\, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3,$$

[8] In applications, time, t, is often multiplied with a characteristic velocity, c (such as the speed of light), to give all four coordinates, x^μ, with $\mu = 0, 1, 2, 3$, the same dimension of length. However, we will set $c = 1$ for simplicity throughout.

and $j_{123}(x) \equiv \rho(x)$. Applied to three infinitesimal tangent vectors $\partial_{\Delta_i} = \delta^i \partial_i$ (no summation), this form yields $j_{123}\,\mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3(\partial_{\Delta_1}, \partial_{\Delta_2}, \partial_{\Delta_3}) = j_{123}(x)\delta^1\delta^2\delta^3 = \rho(x)\delta^1\delta^2\delta^3$, as required. (Of course the construction is not specific to cubical boxes. Show that the application of the density form to three generic, positively oriented, infinitesimal vectors, $\partial_{\delta u}, \partial_{\delta v}, \partial_{\delta w}$, with Cartesian representations $\delta u, \delta v, \delta w$, yields j_{123} times the geometric volume of the parallelepiped spanned by these vectors. If necessary, recapitulate section L11.6 on the geometric meaning of volume forms.)

The construction above may be slightly modified to describe the flow of current. The **current density** in the 3-direction, $j_{012}(x)$, is a function defined such that the number of particles passing through an rectangular surface of area $\delta^1\delta^2$ in the 12-plane within time δ^0 at x equals $j_{012}(x)\delta^0\delta^1\delta^2$. This number equals the number of particles contained in a space-time box of volume $\delta^0\delta^1\delta^2$, i.e. a box of spatial area $\delta^1\delta^2$ and temporal extension δ^0, see figure V25. In analogy to the density form, we thus define a **current form**,

$$j = j_{012}\,\mathrm{d}x^0 \wedge \mathrm{d}x^1 \wedge \mathrm{d}x^2,$$

whose application to the tangent vectors, ∂_{Δ_0}, ∂_{Δ_1}, ∂_{Δ_2} yields the current density $j_{012}\,\delta^0\delta^1\delta^2$ at x.

In the same manner, current flow through area elements in the 23 and 31 plane is described by forms with weight functions j_{023} and j_{031}, respectively. Application of the form $\frac{1}{2}j_{0ij}\,\mathrm{d}x^0 \wedge \mathrm{d}x^i \wedge \mathrm{d}x^j$ to an argument $(\partial_{\Delta_0}, \partial_{\delta v}, \partial_{\delta w})$, where δv and δw now are Cartesian coordinate vectors pointing in spatial directions, with general components δv^i and δw^i, then yields $j_{0ij}\,\delta^0\delta v^i\delta w^j$. (Verify this result. In doing so, keep the the anti-symmetry of form-coefficients, $j_{0ij} = -j_{0ji}$ in mind and recall that summations over Latin indices $1 \leq i, j \leq 3$ are confined to the spatial sector of the space-time manifold.) This should be understood as the flow of particles in time δ^0 through the spatial area element spanned by the coordinate vectors δv and δw.

We finally note that the full information on particle densities and currents is contained in the **general current three-form**,

$$j = \frac{1}{3!}j_{\mu\nu\sigma}\,\mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \wedge \mathrm{d}x^\sigma, \tag{V161}$$

where $0 \leq \mu, \nu \leq 3$ now run over temporal and spatial indices. This form contains four independent coefficient functions, viz. j_{123} for the particle density, and j_{0ij} for the current. We finally note that while the current form has been defined with reference to a Cartesian system, one may subject Eq. (V161) to a coordinate change $x \mapsto y(x)$ to obtain representations of the current in other systems.

In an info section on p. 500 below we will discuss how the above form-characterization of current relates to the traditional physics description of the current in terms of vectors. We are not yet in a position to address this point because the translation between the two languages requires a *metric*.

EXERCISE The **stereographic coordinates** are a coordinate system $z = (z^1, z^2)^T$ alternative to the standard polar coordinates $y = (\theta, \phi)^T$ of the unit sphere S^2. As indicated in Fig. V26, they are defined by projecting points r on the sphere onto points q lying in a plane tangent to the southpole. (Sometimes, a plane through the equator is used as a projection plane instead.) In this way, the surface of the sphere gets mapped to a plane. Projections of this type find applications in diverse fields, including in cartography, geology, or differential geometry.

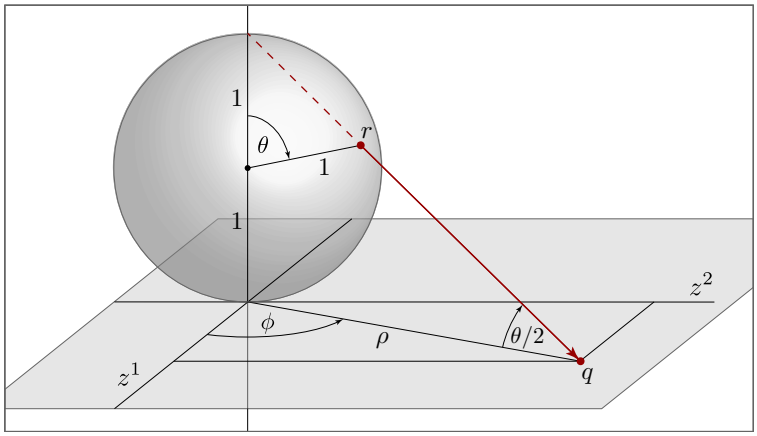


Figure V26: Stereographic projection of the sphere. To each point r on the sphere we assign a point q in a plane tangent to the southpole by shining a light from the northpole through r. The projection point q is defined as the intersection of the light ray with the plane. Further discussion, see text.

Verify by elementary geometric construction that the transition function between spherical and stereographic coordinates is given by[9]

$$
\begin{aligned}
&y : \mathbb{R}^2 \setminus (\mathbb{R}^+ \times \{0\}) \longrightarrow (0,\pi) \times (0,2\pi),\\
&\qquad z = \begin{pmatrix} z^1 \\ z^2 \end{pmatrix} \longmapsto \begin{pmatrix} \theta \\ \phi \end{pmatrix}(z) = \begin{pmatrix} 2\arctan\left(\frac{2}{\rho}\right) \\ \arctan\left(\frac{z^2}{z^1}\right) \end{pmatrix}, \qquad \rho \equiv \sqrt{(z^1)^2 + (z^2)^2},\\
&z : (0,\pi) \times (0,2\pi) \longrightarrow \mathbb{R}^2 \setminus (\mathbb{R}^+ \times \{0\}),\\
&\qquad y = \begin{pmatrix} \theta \\ \phi \end{pmatrix} \longmapsto \begin{pmatrix} z^1 \\ z^2 \end{pmatrix}(y) = \rho \begin{pmatrix} \cos\phi \\ \sin\phi \end{pmatrix}, \qquad \rho = \frac{2}{\tan\left(\frac{\theta}{2}\right)}\,.
\end{aligned}
\tag{V162}
$$

Also verify that $\sin(\theta) = \frac{4\rho}{4+\rho^2}$. On the sphere, we define the so-called **area two-form**

$$\omega \equiv \sin\theta \mathrm{d}\theta \wedge \mathrm{d}\phi. \tag{V163}$$

Notice the structural similarity between the area two-form and the 'area-element' $\sin\theta\,\mathrm{d}\theta\mathrm{d}\phi$ featuring in the integration over spheres (cf. example on p. 241). In chapter V6 (cf. discussion on p. 493) we will address the meaning of this connection and discuss how the form ω assigns to pairs of tangent vectors on the sphere the geometric area spanned by them, hence the name *area* form and the connection to the 'area-element' of spherical surface integration.

Apply Eq. (V158) to the case of stereographic coordinates, $y' = z$, and verify that the z-coordinate representation of the area form is given by

$$\omega = -\frac{1}{\left(1 + \left(\frac{z^1}{2}\right)^2 + \left(\frac{z^2}{2}\right)^2\right)^2}\,\mathrm{d}z^1 \wedge \mathrm{d}z^2. \tag{V164}$$

[9] Note that the projection excludes the positive z^1-axis, $\{z^1 > 0, z^2 = 0\}$, corresponding to the set $(\rho,\phi) \in \mathbb{R}^+ \times \{0\}$ which is excluded when using polar coordinates. Likewise, the points $z = (0,0)^T$ and '$z = \infty$' (i.e. the horizon of infinitely large z-values, $\rho = \infty$), corresponding to $\theta = \pi$ and $\theta = 0$, are also excluded.

Observe how stereographic projection maps 'small areas' around the north pole on the sphere, where θ is small, onto large regions in the outer plane, where ρ is large. This explains why the weight function of the form decreases for large values of the coordinates: large values of z represent only small geometric areas on the spere. For the same reason, the weight function enters with negative sign: positive increments in the θ-coordinate, corresponding to positive values of the area form, lead from north to south and are represented by negative increments in the stereographic coordinates. This relative sign change is compensated by the sign of the weight functions. If you find this wording too vague, it may be a good exercise to apply the area form to the pair of spherical basis vectors $(\partial_\theta, \partial_\phi)$, in both the polar coordinate representation (V163) and the spherical one, Eq. (V164). To compute the latter, first use Eq. (V162) to change basis vectors as $\partial_\theta = \frac{\partial \theta}{\partial z^i}\partial_{z^i}$, and then apply Eq. (V164). Monitor the appearance of signs in the course of the calculation.

Pullback

The pullback of forms $\omega \in \Lambda^p(L)$ under a map $F : M \to L$ is computed by an obvious generalization of the rule for one-forms:

$$\boxed{F^*\omega(\partial_{v_1}, \dots, \partial_{v_p}) \equiv \omega(F_*\partial_{v_1}, \dots, F_*\partial_{v_p}),} \tag{V165}$$

where the left hand side defines a form $F^*\omega \in \Lambda^p(M)$. Let

$$\omega = \frac{1}{p!} \sum_{i_1,\dots,i_p=1}^{c} \omega_{i_1,\dots,i_p}(x) \mathrm{d}x^{i_1} \wedge \cdots \wedge \mathrm{d}x^{i_p},$$

be a p-form on L expanded in local coordinates, $(x^1, \dots, x^c)$. The coordinate representation of its pullback, $F^*\omega$, to M, is found following the same logic as in the case of one-forms (cf. Eq.(V151)): application of the pullback form $F^*\omega$ to the basis vectors, $\partial_j \equiv \partial_{y^j}$ of a y-coordinate system on M yields the components as $(F^*\omega)_{j_1,\dots,j_d} = F^*\omega(\partial_{y_{j_1}}, \dots, \partial_{y_{j_d}}) = \omega(F_*\partial_{y_{j_1}}, \dots, F_*\partial_{y_{j_d}})$. Using $F_*\partial_{y_j} = \frac{\partial F^i}{\partial y^j}\partial_{x^i}$, a **formula for the pullback in coordinates**,

$$\boxed{F^*\omega = \frac{1}{p!} \sum_{j_1,\dots,j_p=1}^{d} \sum_{i_1,\dots,i_p=1}^{c} \omega_{i_1,\dots,i_p}(x(y)) \frac{\partial F^{i_1}}{\partial y^{j_1}} \cdots \frac{\partial F^{i_p}}{\partial y^{j_p}} \mathrm{d}y^{j_1} \wedge \cdots \wedge \mathrm{d}y^{j_p},} \tag{V166}$$

is obtained. This expression shows that the pullback of a p-form essentially follows from the pullback of its constituent one-forms, $F^*\mathrm{d}x^i = \frac{\delta F^i}{\partial y^j}\mathrm{d}y^j$.

EXERCISE Consider the **volume form**, $\omega = \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3$. of three-dimensional space $\mathbb{R}^3$. (The denotation 'volume form' will be justified in section V5.4.) We aim to find the representation of this form in spherical coordinates. To this end, apply the Cartesian coordinate forms to the spherical basis vectors as

$$\mathrm{d}x^1(\partial_\theta) = \partial_\theta(x^1) = \partial_\theta(r \sin\theta \cos\phi) = r \cos\theta \sin\phi,$$

etc. From these relations compute the change of representation of one-forms,

$$\mathrm{d}x^1 = \cdots + r\cos\theta\sin\phi\,\mathrm{d}\theta + \ldots,$$

etc. Substitute these relations into the definition of the Cartesian volume form to obtain the **volume form in spherical coordinates**,

$$\omega = r^2\mathrm{d}r \wedge \sin\theta\mathrm{d}\theta \wedge \mathrm{d}\phi. \tag{V167}$$

Top-dimensional forms and orientation

Much like one-forms, forms of highest degree, so-called **top-dimensional forms** are simple, in that they are characterized by a single coefficient function: for a form of degree d on an d-dimensional manifold, the coordinate representation (V156) reduces to[10]

$$\omega = \omega(y)\mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^d. \tag{V168}$$

Top-dimensional forms play an important role in the 'global' characterization of manifolds, notably in the theory of integration to be discussed in section V5.4. They also serve to describe the **orientation of a manifold**.

The heuristic meaning of orientation is that of a global sense of 'inside and outside', the best known example of a non-orientable manifold being the Möbius strip (cf. p 429). A manifold is orientable if, and only if, a globally non-vanishing top-dimensional form exists, i.e. a form whose weight function $\omega(y)$ is globally non-vanishing. The condition $\omega(y) \neq 0$ is actually independent of the chosen coordinate system: under a coordinate change $y \mapsto y'(y)$, the top-form (V168) changes according to (V158), which for $p = d$ simplifies to

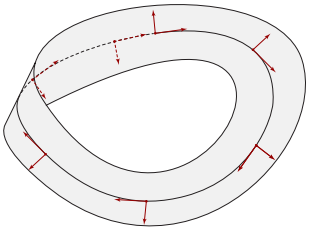
$$\begin{aligned}\omega &= \omega(y')\,\mathrm{d}y'^1 \wedge \cdots \wedge \mathrm{d}y'^d = \omega(y'(y))\frac{\partial y'^1}{\partial y_{i_1}} \ldots \frac{\partial y'^d}{\partial y_{i_d}}\mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_d} \\ &= \omega(y'(y))\frac{\partial y'^1}{\partial y_{i_1}} \ldots \frac{\partial y'^d}{\partial y_{i_d}}\epsilon^{i_1\ldots i_d}\mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^d \\ &= \det\left(\frac{\partial y'}{\partial y}\right)\omega(y'(y))\mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^d,\end{aligned} \tag{V169}$$

$\epsilon^{i_1\ldots i_n}$ is the antisymmetric tensor, in the second line we used the antisymmetry of the exterior product and, and in the last line $\frac{\partial y'}{\partial y}$ is the Jacobi matrix of the mapping $y \mapsto y'(y)$. The last line defines the coefficient $\omega(y)$ of the form in the y-representation, i.e. we have

$$\boxed{\omega(y) = \omega(y'(y))\det\left(\frac{\partial y'}{\partial y}\right).} \tag{V170}$$

The determinant of the Jacobi matrix describing a coordinate change never vanishes. If $\omega(y')$ is non-vanishing, $\omega(y)$ will therefore be non-vanishing, too, and vice versa.

[10] Top-forms on higher dimensional manifolds are often (but certainly not always) denoted by with the symbol ω. We will adopt this convention here.



An orientable manifold can be covered by coordinate charts $\{y^i\}$, $\{y'^i\}$, ... such that the weight functions $\omega(y)$, $\omega(y')\cdots > 0$ are all globally *positive*.[11] The result (V170) then shows that the Jacobi matrices $\left(\frac{\partial y'}{\partial y}\right)$ corresponding to the transformations all have positive determinant. At the same time, these matrices describe the change of tangent space bases, $\partial_{y^j} = \frac{\partial y'^i}{\partial y^j}\partial_{y'^i}$ (cf. Eq. (V128)), and the positivity of their determinants means that the bases are oriented in the same way. This shows how the existence of a globally non-vanishing d-form can be used to provide the entire manifold with a uniform orientation. The Möbius strip introduced on p. 429 is a basic example of a manifold lacking orientability. Any attempt to extend a basis to one covering its full tangent space leads to an orientation conflict, see the figure.

Exterior derivative

So far, we did little more than lifting operations of multi-linear algebra from single vector spaces to the bundles of tangent spaces of of manifolds. This was achieved by the straightforward smooth extension of definitions applicable to isolated tangent spaces, T_rM, to all of M. The operation to be introduced next is different in that it essentially relies on the *differentiability* of smooth structures on manifolds: we will introduce the *exterior derivative*, d, of forms, i.e. an operation describing how a differential form changes along specified directions on the manifold. Being a directional operation, this derivative will need a p-form, ω, and a directional tangent vector, ∂_v, as arguments. The exterior derivative, $\mathrm{d}\omega$, of a p-form ω then is an object acting on $(p+1)$ vectors, comprising the p-arguments of the p-form, and the directional specifier, ∂_v. More precisely, $\mathrm{d}\omega$ will be a $(p+1)$-form, i.e. the action on all of its arguments is linear and antisymmetric.

The exterior derivative plays a very important role in establishing relations between forms of different degree, p, and $p+1$. It is so important to the present formalism, that the theory of differential forms is sometimes called **exterior calculus**. In physics contexts d maps, e.g., one-forms probing changes of physical quantities under directional increments to two-forms whose arguments are area elements. In the sections below we will see how these connections play an important role both in the geometry of manifolds and in the formulation of physical theories.

In concrete terms, the **exterior derivative** is an operator

$$\mathrm{d} : \Lambda^p(M) \to \Lambda^{p+1}(M), \qquad \phi \mapsto \mathrm{d}\phi, \tag{V171}$$

subject to the following conditions:

▷ d is **linear**,

$$\mathrm{d}(a\phi + b\psi) = a\,\mathrm{d}\phi + b\,\mathrm{d}\psi, \tag{V172}$$

for $a, b \in \mathbb{R}$.

[11] If a coordinate system is such that $\omega(y) < 0$, just sign-invert one of the coordinates, e.g. $y^1 \to -y^1$, which will effect a sign change of $\omega(y)$.

▷ d obeys the **graded Leibniz rule**

$$\mathrm{d}(\phi \wedge \psi) = \mathrm{d}\phi \wedge \psi + (-)^{\mathrm{degree}(\phi)} \phi \wedge (\mathrm{d}\psi). \tag{V173}$$

▷ d is **nilpotent**,

$$\mathrm{d} \circ \mathrm{d} = 0. \tag{V174}$$

▷ When acting on a zero-form, $\phi \in \Lambda^0(M)$, i.e. a function, d reduces to the **differential** discussed in section V5.1 above.

The definitions above uniquely specify d. This is best seen by letting d act on the coordinate representation of a form, $\phi = \frac{1}{p!}\phi_{i_1,\ldots,i_p}\,\mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p}$. Application of the Leibniz rule yields $\mathrm{d}(\phi_{i_1,\ldots,i_p}\,\mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p}) = \mathrm{d}\phi_{i_1,\ldots,i_p} \wedge \mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p} + \phi_{i_1,\ldots,i_p}\,\mathrm{d}(\mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p}) = \mathrm{d}\phi_{i_1,\ldots,i_p} \wedge \mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p}$ where in the last step the nilpotency $\mathrm{d}^2 = 0$ was noted. The expansion $\mathrm{d}\phi_{i_1,\ldots,i_p} = \partial_j \phi_{i_1,\ldots,i_p} \mathrm{d}y^j$ then yields

$$\boxed{\mathrm{d}\left(\frac{1}{p!}\phi_{i_1,\ldots,i_p}\,\mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p}\right) = \frac{1}{p!}\partial_j \phi_{i_1,\ldots,i_p}\,\mathrm{d}y^j \wedge \mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p}.} \tag{V175}$$

Note that the exterior derivative form $\mathrm{d}\phi$ contains the derivatives of the coefficient functions $\partial_j \phi_{i_1,\ldots,i_p}$. This shows how d monitors the rate of change of the form ϕ along the manifold, different from the form–operations discussed so far which where defined locally with reference to individual points in M.

EXAMPLE

▷ In $M = \mathbb{R}^3$ consider the one-form $\phi = \phi_1 \mathrm{d}x^1 + \phi_2 \mathrm{d}x^2 + \phi_3 \mathrm{d}x^3$. Application of Eq. (V175) yields $\mathrm{d}\phi = (\partial_1\phi_2 - \partial_2\phi_1)\mathrm{d}x^1 \wedge \mathrm{d}x^2 + (\partial_2\phi_3 - \partial_3\phi_2)\mathrm{d}x^2 \wedge \mathrm{d}x^3 + (\partial_3\phi_1 - \partial_1\phi_3)\mathrm{d}x^3 \wedge \mathrm{d}x^1$. Does the structure of the coefficients remind you of a familiar operation of vector calculus?

▷ In $M = \mathbb{R}^3$ consider the two-form $j = j_1 \mathrm{d}x^2 \wedge \mathrm{d}x^3 + j_2 \mathrm{d}x^3 \wedge \mathrm{d}x^1 + j_3 \mathrm{d}x^1 \wedge \mathrm{d}x^2$. We observe that $\mathrm{d}j = (\partial_1 j_1 + \partial_2 j_2 + \partial_3 j_3)\mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3$.

It is a straightforward exercise (do it!) to apply the pullback formula (V166) to compute the pullback $F^*(\mathrm{d}\phi)$ of the exterior derivative of a form Eq. (V175). The same formulas may be applied to the computation of the exterior derivative $\mathrm{d}(F^*\phi)$ of the pullback of the form. The results agree, i.e. the computation proves that **pullback and exterior derivative commute**:

$$\boxed{\mathrm{d}F^*\phi = F^*\,\mathrm{d}\phi.} \tag{V176}$$

This identity can be applied to compute combinations of pullbacks and derivatives in arbitrary and most economic orders.

EXAMPLE The area two-form in polar coordinates, $\omega = \rho \mathrm{d}\rho \wedge \mathrm{d}\phi$ (cf. Eq. (V159)), can be written as the exterior derivative, $\omega = \mathrm{d}\kappa$, of the one-form $\kappa = \frac{1}{2}\rho^2 \mathrm{d}\phi$. Now consider the pullback y^* to Cartesian coordinates $x = (x^1, x^2)^T$ under the map $x \mapsto y(x) = (\theta, \phi)^T(x)$. Eq (V176) implies the relation $y^*\omega = \mathrm{d}y^*\kappa = y^*\mathrm{d}\kappa$, i.e. we may first pull back κ and then differentiate in Cartesian coordinate, $\mathrm{d}y^*\kappa$, or first differentiate and then pull back, $y^*\mathrm{d}\kappa$. Let us verify the equality of the operations by explicit computation: the pullback of κ is computed by application of Eq. (V151), $y^*\kappa = \frac{1}{2}\rho^2(x)\frac{\partial\phi(x)}{\partial x^j}\mathrm{d}x^j = \frac{1}{2}(x^1\mathrm{d}x^2 - x^2\mathrm{d}x^1)$, and the subsequent exterior derivative is $\mathrm{d}(y^*\kappa) = \mathrm{d}x^1 \wedge \mathrm{d}x^2$. Now check that $y^*\omega$, computed from ω using Eq. (V170), yields the same result. Which of the two routes do you find more economical?

EXERCISE Consider the area two-form on the sphere, $\omega = \sin\theta \mathrm{d}\theta \wedge \mathrm{d}\phi$ (cf. Eq. (V163)). It can be represented as (why?) the exterior derivative of a one-form, $\omega = \mathrm{d}\kappa$, where $\kappa = -\cos\theta \mathrm{d}\phi$. Apply Eq. (V162) to verify that its pullback, $z^*\kappa$, to the stereographic plane (cf. Exercise on p. 473) is

$$z^*\kappa = \frac{1 - \left(\frac{\rho}{2}\right)^2}{\left(1 + \left(\frac{\rho}{2}\right)^2\right)\rho^2}(z^2\mathrm{d}z^1 - z^1\mathrm{d}z^2), \qquad \rho^2 = (z^1)^2 + (z^2)^2.$$

Now compute $\mathrm{d}(z^*\kappa)$ to check that it coincides with $z^*\omega \overset{(V176)}{=} z^*(\mathrm{d}\kappa)$, as given by Eq. (V164).

V5.4 Integration of forms

In previous chapters, we have introduced different types of integrals, beginning with the elementary one-dimensional integral of functions, then moving on to higher-dimensional integrals of functions and integrals of vector fields. Some of these integrals required the construction of specific 'area and volume elements' (cf. chapter C4) or the presence of a metric.[12] Looking at the situation at large, one may get the impression that each particular environment requires its own custom-made integral.

In this section we will see that a much nicer, unified understanding of integration can be developed using differential forms: (i) with few exceptions, in mathematics integration is always understood as an integration of forms. Specifically, (ii) the objects to integrate over a d-dimensional manifold are d-dimensional forms, i.e. one-forms over curves, two-forms over surfaces, three-forms over volumes, etc. (iii) No metric is required to define these integrals, and (iv) and all variants introduced previously become special cases[13] of the unified concept.

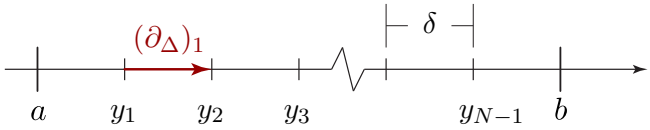


Figure V27: On the identification of the integral of one-forms with the Riemann integral.

Integration of one-dimensional forms in one-dimensional space

Fortunately, no added work is required to introduce the integration of forms. To start with, consider a one-dimensional form, $\phi = \phi(y)\mathrm{d}y$, defined on an interval $I = (a, b) \in \mathbb{R}$. We *define* the integral of this form over I as the ordinary Riemann integral of the function $\phi(y)$ over I:

$$\int_I \phi \equiv \int_I \phi(y)\mathrm{d}y = \int_a^b \phi(y)\mathrm{d}y. \tag{V177}$$

For example, if $\phi = y\,\mathrm{d}y$, and $I = (0, 1)$, then $\int_I \phi = \int_0^1 y\,\mathrm{d}y = \frac{1}{2}$. To understand the rationale behind this identification, we view the interval $I = (a, b)$ as a straight, one-dimensional 'curve', partitioned into N infinitesimal segments $(y_\ell, y_{\ell+1})$, with $y_\ell = \ell\,\delta$ and $\delta = (b - a)/N$. With each such segment we associate a vector, $\partial_{\Delta,\ell} = \delta\,\partial_y$, in the corresponding tangent space $T_{y_\ell}I$. This vector is defined so as to 'connect' the segment's endpoints, i.e. its single component in the y-coordinate system is given by δ, and $y_\ell + \delta = y_{\ell+1}$. In this way the curve can be identified with a 'concatenation' of infinitesimal tangent vectors, see Fig. V27. The application of the form ϕ to each such vector yields an infinitesimal number, $\phi(\partial_{\Delta,\ell}) = \phi(y_\ell)\mathrm{d}y(\partial_{\Delta,\ell}) = \phi(y_\ell)\delta$, and it is natural to *define* the integral of the form over I as the sum of these,

$$\int_I \phi \equiv \lim_{\delta\to 0} \sum_\ell \phi(\partial_{\Delta,\ell}) = \lim_{\delta\to 0} \delta \sum_\ell \phi(y_\ell).$$

This is a Riemann sum, which shows the identity of the form integral and the Riemann integral.

As a **physics example**, consider a force form $\phi = f$, and let $\partial_{\delta r,\ell}$ be the tangent vector associated with an infinitesimal displacement along a path. The associated work, i.e. the integral of the force along the path, is the sum of the works done along all displacements, $\sum_\ell f(\partial_{\delta r,\ell})$. Notice that the incremental 'smallness' in the construction is not associated with $f = f(y)\mathrm{d}y$ (there is no such thing as a 'small form'). Instead, it resides in the smallness of the infinitesimal tangent vectors. This job division may seem odd if one has been exposed to physics parlance such as, 'let $\mathrm{d}y$ be a small increment of length', etc. To avoid confusion, keep in mind that where differential forms are concerned, d does not mean smallness.

[12] The integral of a vector field over a surface in three-dimensional space involved a vector field normal to that surface, cf. Eq. (**??**). The definition of 'normal' requires a metric.

[13] In cases where the identification of a 'traditional integral' with its more natural form-definition seems awkward, the former is to blame; e.g. it may require the presence of a metric even when the latter does not.

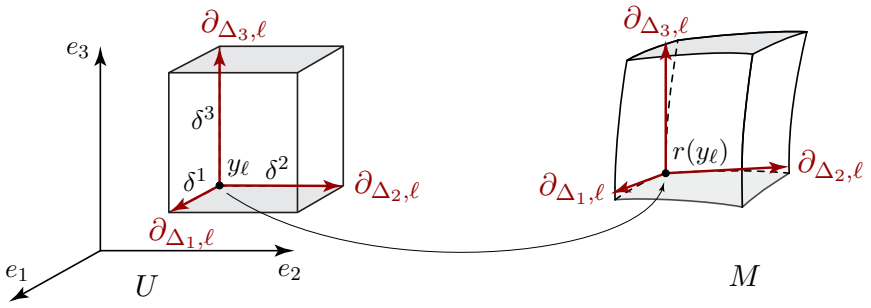


Figure V28: The identification of the integral of d-forms with d-dimensional Riemann integrals, illustrated for $d = 3$.

Integration of top-dimensional forms

Let ω be a **top-dimensional** d-form on a d-dimensional manifold M, e.g. a one-form on a line, a two-form on a surface, or a three-form in space, etc. Further, let $r : U \to M$, $y \mapsto r(y)$ be a system of coordinates providing an approximate[14] coverage of M. The form ω then affords the coordinate representation $\omega = \omega(y)\,\mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^d$.
Following the logic of the previous section, it is natural to define the integral of ω over M as

$$\int_M \omega = \int_M \omega(y)\,\mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^d \equiv \int_U \omega(y)\,\mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^d \equiv \int_U \omega(y)\,\mathrm{d}y^1 \ldots \mathrm{d}y^d, \tag{V178}$$

where the individual representations emphasize slightly different aspects of the integral: the first is the expression we aim to define, and in the second we use the expansion of the form in coordinates. In the third, we identify the integration of the form over M with the integral of the pullback of the form to the coordinate domain (see discussion in the info section on p. 468 for added motivation for this identification). In the crucial final definition, the integral of the form over the open subset $U \subset \mathbb{R}^d$ is identified with a multi-dimensional Riemann integral, where the role of the wedge product of coordinate forms is taken by the d-dimensional volume element, $\mathrm{d}y^1 \wedge \mathrm{d}y^2 \wedge \ldots \wedge \mathrm{d}y^d \to \mathrm{d}y^1 \mathrm{d}y^2 \ldots \mathrm{d}y^d$.

The latter interpretation of the **coordinate volume form as a Riemann volume element** replicates the logic of the previous discussion and extends it to higher dimensions. We consider the coordinate domain U partitioned into a large number of d-dimensional cuboids at coordinates y_ℓ, with infinitesimal side lengths δ^j ($j = 1, \ldots, d$) (cf. Fig. **??**, left, and section C4.3 on volume integrals). The edges of these cuboids are represented by tangent vectors, $\partial_{\Delta_j,\ell} = \delta^j \partial_{j,\ell}$ (no summation), in $T_{y_\ell}U$, and their volume is $(\mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^d)(\partial_{\Delta_1,\ell}, \ldots, \partial_{\Delta_d,\ell}) = \delta^1 \ldots \delta^d$. We define the integral over the form in the coordinate domain as the sum of these expressions multiplied by their respective weights, $\omega(y_\ell)$,

[14] Here, as always in integration theory, we tolerate situations where the coordinates exclude sets of lower dimension, isolated points on a circle, lines on a sphere, etc. As discussed in the info section on p. 229, such deficiencies do not affect integrals. In rare cases, where no single coordinate system suffices to represent M even under these relaxed conditions, the different coordinate domains of a covering atlas need to be treated separately.

i.e. as the sum $\sum_\ell \omega(y_\ell)\delta^1 \dots \delta^d$. In the limit $\delta^i \to 0$ this becomes the Riemann integral, $\int_U \omega(y)\,\mathrm{d}y^1 \dots \mathrm{d}y^d$.

As an aside, we note that the 'distorted volume elements' discussed extensively in chapter C4 (cf. Fig. C7, and several other related figures in that chapter) are spanned by the pushforwards of the tangent vectors $\partial_{\Delta_j} = \delta^j \partial_{y^j}$ from the coordinate domain TU to the tangent bundle TM (cf. Fig. V28, right). As discussed in the info section on p. 468 the tangent vectors in TU and TM are denoted by the same symbol, and so are the corresponding coordinate forms, $\mathrm{d}y^j$. The coordinate form $\mathrm{d}y^1 \wedge \dots \wedge \mathrm{d}y^d$ defined in TU^* or TM^* acts identically on the corresponding vectors and this identity is expressed by the second equality in Eq. (V178), which identifies the integral of ω over M with that of the integral of the pullback of ω to U.

EXAMPLE As a simple example, let $M = S^2$ be the surface of the unit sphere, parametrized by polar coordinates (θ, ϕ), and consider the integral of the area form, $\omega = \sin(\theta)\mathrm{d}\theta \wedge \mathrm{d}\phi$. The integral formula then gives

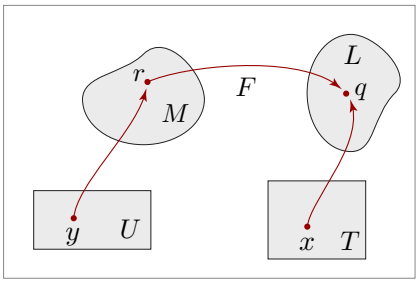
$$\int_{S^2} \sin(\theta)\mathrm{d}\theta \wedge \mathrm{d}\phi \equiv \int_{U=(0,\pi)\times(0,2\pi)} \sin(\theta)\mathrm{d}\theta \wedge \mathrm{d}\phi = \int_0^\pi \sin\theta\,\mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi = 4\pi. \qquad \text{(V179)}$$

Changes of coordinates and general integral transforms

Of course, the definition of the integral must be independent of the choice of coordinates. Under a **change of coordinates**, $y \mapsto y'(y)$, the representation of the form changes as specified by Eq. (V170). The integral formula then becomes

$$\begin{aligned}\int_{U'} \omega(y')\mathrm{d}y'^1 \dots \mathrm{d}y'^d &= \int_{U'} \omega(y')\mathrm{d}y'^1 \wedge \dots \wedge \mathrm{d}y'^d \\ = \int_U \omega(y'(y)) \det\left(\frac{\partial y'}{\partial y}\right) \mathrm{d}y^1 \wedge \dots \wedge \mathrm{d}y^d &= \int_U \omega(y'(y)) \det\left(\frac{\partial y'}{\partial y}\right) \mathrm{d}y^1 \dots \mathrm{d}y^d,\end{aligned}$$

and outermost equalities establish the compatibility with the general formulas for the change of variables in multi-dimensional Riemann integrals, cf. Eq. (C73). The inner equality connects the two integrals over coordinate form representations. It is instructive to read the integral $\int_U \omega(y)\mathrm{d}y^1 \wedge \dots \wedge \mathrm{d}y^d$ as the integral of the *pullback* of the form $\omega(y')\mathrm{d}y'^1 \wedge \dots \wedge \mathrm{d}y'^d$ from U' to the domain of U-coordinates.



The latter interpretation suggests a more general and extremely useful **connection between integrals of forms over different integration domains**: consider two orientable manifolds of equal dimension, M and L, represented by coordinate maps $r : U \to M$, $y \mapsto r(y)$ and $q : T \to L$, $x \mapsto q(x)$, respectively. Let $F : M \to L$ be an orientation-preserving *diffeomorphism* between the manifolds, i.e. a diffeomorphism such that its coordinate representations, $y \mapsto x(y) \equiv F(x)$, have positive Jacobi matrix, $\det\left(\frac{\partial F}{\partial y}\right) > 0$. For a top-form ω, defined on L, we then have the important formula

$$\boxed{\int_M F^*\omega = \int_L \omega.} \tag{V180}$$

This identity follows from the fact that the map $F \circ r : U \to L$, $y \mapsto F(r(y))$, can be seen as a coordinate representation of L, i.e. a system of coordinates alternative to x. The definition (V178) applied to this system then states that $\int_L \omega = \int_U (F \circ r)^*\omega = \int_U r^*(F^*\omega)$. For the second equality we used the composition property of pullback, Eq. (V150). $F^*\omega$ is a top-form on M, and the integral of its pullback $r^*(F^*\omega)$ to U, again according to Eq. (V178), equals the integral of this form over its ambient manifold M, $\int_U r^*(F^*\omega) = \int_M F^*\omega$. Combining these equalities, we obtain the statement (V180). As a side remark, notice how 'non-technical' this proof is: it is very general, and at the same time does not involve complicated-looking formulas. This combination of generality and structural elegance is a hallmark of differential form integration theory.

EXERCISE Consider the area form on the two-sphere, $\omega = \sin(\theta)\,\mathrm{d}\theta \wedge \mathrm{d}\phi$. Its pullback, $y^*\omega$, to the stereographic plane is given by Eq. (V164), where $y : \mathbb{R}^2 \to S^2$ is the coordinate transformation from the plane (modulo singular points) to the two-sphere, defined in Eq. (V162). Show that

$$\int_{S^2} \omega = \int_{\mathbb{R}^2} y^*\omega = 4\pi. \tag{V181}$$

Integration of lower rank forms

Finally, let us discuss how to integrate a form of degree d, defined on a manifold L of higher dimension, $n > d$, over a d-dimensional submanifold, $M \subset L$. Without much loss of generality, we may assume the embedding manifold to be given by an open subset $L \subset \mathbb{R}^n$, although this identification will not be used throughout. For example, we may consider a one-form in three-dimensional space ($d = 1$, $n = 3$) and integrate it over a curve; or a two-form in three-dimensional space ($d = 2$, $n = 3$) and integrate it over a surface.

The definition of such integrals readily follows from the previous constructions. Let M be parametrized by a coordinate mapping $F : U \to M$. A form, ϕ, defined on L is then

integrated over M by pulling it back to U and integrating there,

$$\boxed{\int_M \phi \equiv \int_U F^*\phi.} \tag{V182}$$

This makes sense, because in the d-dimensional domain U the d-form $F^*\phi$ is top-dimensional and therefore integrable via (V178).

For example, consider a one-form, $\phi = \phi_i(x)\mathrm{d}x^i$, defined in an n-dimensional manifold L with coordinates x. To compute its integral over a **curve**, $\gamma = M$, one parameterizes the latter by a coordinate, $r : I \to L$, $t \mapsto r(t)$. We then have $r^*\phi = \phi_i(r(t))\dot{r}^i(t)\mathrm{d}t$ and hence

$$\int_\gamma \phi = \int_I \phi_i(r(t))\dot{r}^i(t)\mathrm{d}t. \tag{V183}$$

In this formula we recognize the familiar structure of a line integral, cf. Eq. (V12). The difference between the two expressions is that Eq. (V183) contains a form acting on the velocity vector, $\phi(\partial_{\dot{r}}) = \phi_i\dot{r}^i$, whereas the traditional line integral contains the scalar product of a vector with the velocity vector, $\mathbf{f}\cdot\dot{\mathbf{r}} = f^j g_{ji}\dot{r}^i$. From a mathematical and – as will be argued below – also from a physical perspective, the form-variant formulation of the line integral is the more natural. At least, it does not require the excess baggage of a scalar product. For example, we have argued above that the force one-form, $\phi = f$, provides a definition of work along infinitesimal path segments that is very natural, since close to experimental protocols. Eq. (V183) shows how such a form may be integrated to compute the work done along curves of finite length. All this does not require the presence of a scalar product which one may argue is conceptual and methodological ballast in the present context.

EXAMPLE As an example, let us compute the work done against the force $f = x^2\mathrm{d}x^1 - x^1\mathrm{d}x^2$ (Cartesian coordinates in $\mathbb{R}^3$) along one revolution of a spiral curve, γ, with parameterization $r(t) = (\cos t, \sin t, ct)^T$. This force form has components $f_1 = x^2$, $f_2 = -x^1$ and $f_3 = 0$, hence Eq. (V183) yields

$$\int_\gamma f = \int_0^{2\pi} \left[x^2(t)\dot{x}^1(t) - x^1(t)\dot{x}^2(t)\right]\mathrm{d}t = \int_0^{2\pi} \left[(\sin t)(\sin t) - \cos t(-\cos t)\right]\mathrm{d}t = 2\pi.$$

EXERCISE A uniform current density in z-direction (in $\mathbb{R}^3$) is described by the differential 2-form $j = j_0\,\mathrm{d}x^1 \wedge \mathrm{d}x^2$. Find the current flowing through (a) the northern hemisphere of a sphere of radius R, (b) the full sphere. First try to find the answers using simple arguments, then check your results by explicitly integrating j over the (hemi)sphere.

Stokes' theorem

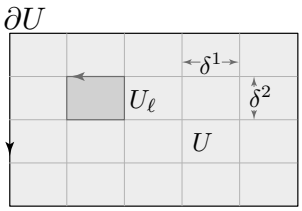
In the previous sections V3.2, **??** and **??** we discussed various integral identities which were all of the form (integral of X over the d-dimensional boundary of Y) = (integral of derivative

of X over the $(d+1)$-dimensional interior of Y). In all these cases, integrals over vector fields where involved. However, the fundamental law of calculus, $f(b) - f(a) = \int_a^b \mathrm{d}x\, f'(x)$, too, is of this form if we interpret $\{a, b\}$ as the boundary of the interval $[a, b]$. The common structure of these identities suggests that a general principle is behind the scenes.

Indeed, all the formulas alluded to above are special cases of one master-identity, the **general Stokes' theorem**. It states that for a $(d-1)$-form, ϕ, defined on a d-dimensional orientable manifold, M, with $(d-1)$ dimensional boundary, ∂M, the integral of ϕ over the boundary equals the integral of the exterior derivative of the form, $\mathrm{d}\phi$, over M itself:

$$\boxed{\int_{\partial M} \phi = \int_M \mathrm{d}\phi.} \tag{V184}$$

Notice the beauty of this formula: an expression containing just a few symbols subsumes all the different variants of boundary-bulk integral identities discussed previously.



INFO The **proof of Stokes' theorem** follows the same logic as those of its more specialized cousins. Thanks to the flexibility of the form-integration machinery, it can be formulated with minimal technical effort: let $r : U \to M$, $y \to r(y)$ be a coordinate representation of M. The domain boundary, ∂U, then parameterizes the boundary ∂M. The definition of form integrals means that Stokes' theorem assumes the form

$$\int_{\partial U} \omega = \int_U \mathrm{d}\omega, \tag{V185}$$

where $\omega = r^*\phi$ is the pullback of ϕ to U, and on the r.h.s. we used the commutativity of pullback and exterior derivative, $r^*\mathrm{d}\phi = \mathrm{d}r^*\phi = \mathrm{d}\omega$. Without loss of generality, we assume $U \subset \mathbb{R}^d$ to be a cuboid in $\mathbb{R}^d$ (see the figure for a two-dimensional representation). Following the general strategy of the more specialized proofs discussed earlier, we partition U into many infinitesimal cuboids, U_ℓ with boundary extensions δ^j, $j = 1, \ldots, d$. The boundary integral over ∂U can then be written as $\int_{\partial U} \omega = \sum_\ell \int_{\partial U_\ell} \omega$, where we used the fact that all contributions from integrals over 'internal' boundaries (the light gray lines in the figure) of the U_ℓ's cancel, because the touching boundaries of adjacent cuboids have opposite orientations. At the same time, we have $\int_U \mathrm{d}\omega = \sum_\ell \int_{U_\ell} \mathrm{d}\omega$, and so the proof of the theorem reduces to the the verification of $\int_{\partial U_\ell} \omega = \int_{U_\ell} \mathrm{d}\omega$ for infinitesimal domains. Let us expand the form ω with its $(d-1)$ independent coefficients as

$$\omega = \omega_{2,\ldots,d}\, \mathrm{d}y^2 \wedge \cdots \wedge \mathrm{d}y^d + \ldots + \omega_{1,\ldots,d-1}\, \mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^{d-1}.$$

The above discussion of form integrals implies that the integral of ω over the pair of faces of cuboid U_ℓ normal to the 1-direction is given by $\big[\omega_{2,\ldots,d}(y^1 + \delta^1, y^2, \ldots, y^d) - \omega_{2\ldots d}(y^1, y^2, \ldots, y^d)\big]\delta^2 \ldots \delta^d \simeq \partial_1 \omega_{2,\ldots,d}(y_\ell)\delta^1\delta^2 \ldots \delta^d$. Adding to this the contribution of the $(d-1)$ remaining pairs of faces we obtain $\int_{\partial U_\ell} \omega = \big[\partial_1 \omega_{2,\ldots,d} + \cdots + \partial_d \omega_{1,\ldots,d-1}\big]_\ell\, \delta^1 \ldots \delta^d$, which is equal to $\int_{U_\ell} \mathrm{d}\omega$, the integral of the exterior derivative, $\mathrm{d}\omega$, of the form over the interior of the cuboid U_ℓ. This proves Stokes' theorem for each infinitesimal cuboid and, upon extension, for the full integration domain.

As an example, consider the integral of a one-form $\phi = \phi_i \mathrm{d}y^i$ over a closed curve, γ, i.e. a curve which is the boundary, $\gamma = \partial S$, of some area S. Stokes's theorem applied to this situation, $\oint_\gamma \phi = \int_S \mathrm{d}\phi$, then implies the equality of the coordinate integrals

$$\oint_\gamma \phi_i \mathrm{d}y^i = \int_S \partial_j \phi_i \, \mathrm{d}y^j \wedge \mathrm{d}y^i. \tag{V186}$$

The l.h.s. is a line integral of the form Eq. (V183). On the r.h.s, the antisymmetric components $\partial_j \phi_i - \partial_i \phi_j$ of the two-form have a structure reminiscent of the curl of a vector field. Eq. (V186) thus is a formulation, in the language of differential forms, of Stokes' theorem from vector analysis, Eq. (V104). In chapter V6 we will discuss how a scalar product may be applied to relate differential forms to vectors. This tool can then be applied to establish the full connection between the general Stokes' theorem and those of vector analysis. For the moment, we just note that the general theorem works in all dimensions, and does not require a scalar product. The generality of the theorem reflects that forms, rather than vectors, are the more natural objects to integrate.

EXERCISE Write down a three-dimensional version of Stokes' theorem, i.e. one for a two-form with expansion $\phi = \frac{1}{2}\phi_{ij}\mathrm{d}y^i \wedge \mathrm{d}y^j$, defined on a 2-dimensional surface, $S = \partial V$, bounding a three-dimesional volume, V. Although there are no vector fields involved, try to identify structures reminiscent of **Gauss' theorem**. How many different components does the two-form have, and how many has its exterior derivative? Do you see index structures similar to those appearing in the vector field divergence? Can you suggest the construction of a vector field from the components of the form such that the three-dimensional Stokes' theorem assumes a form similar to the familiar Gauss theorem?

EXAMPLE Stokes' theorem can be applied to compute the volume of an object via a surface integral over its bounding surface. To illustrate this statement, consider a ball, B_R, of radius $r = R$. Its volume can be obtained by computing the integral of $\omega = r^2 \mathrm{d}r \wedge \sin(\theta)\mathrm{d}\theta \wedge \mathrm{d}\phi$, the volume form in spherical coordinates found in Eq. (V167), over the interior of the ball:

$$V_R = \int_{B_R} \omega \overset{(V178)}{=} \int_0^R r^2 \mathrm{d}r \int_0^\pi \sin\theta \, \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi = \frac{1}{3} 4\pi R^3 \,.$$

Alternatively, note that the volume form can be viewed as the exterior derivative, $\omega = \mathrm{d}\phi$, of the form $\phi = \frac{1}{3} r^3 \sin\theta \mathrm{d}\theta \wedge \mathrm{d}\phi$. We may thus evoke Stoke's theorem to compute the volume of B_R via an integral of ϕ over its surface, ∂B_R, i.e. a sphere of radius R:

$$V_R = \int_{B_R} \mathrm{d}\phi \overset{(V184)}{=} \int_{\partial B_r} \phi \overset{(V178)}{=} \frac{1}{3} R^3 \int_0^\pi \sin\theta \, \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi = \frac{1}{3} 4\pi R^3.$$

V6 Riemannian differential geometry

Beginning with section L3.3, metric structures have appeared several times in the text and were discussed from different perspectives. In this chapter, we introduce the metric into the framework of differential geometry, and this will reveal its full significance. Specifically, we will discuss

- ▷ how the metric describes geometric structures in terms of lengths, angles, and curvature;
- ▷ how it enables us to 'translate' between forms and vectors, and also between forms of different degrees;
- ▷ how it defines a unique top-dimensional form on a manifold and along with it ways to determine the 'volume' of the latter.

V6.1 Definition of the metric on a manifold

A **metric** on a d-dimensional manifold M is a covariant tensor field of second degree,

$$g : M \to TM^* \otimes TM^*, \qquad r \mapsto g_r, \tag{V187}$$

smoothly assigning to each point r in M a *bilinear form* g_r on the tangent space T_rM. Much like a differential two-form, a bilinear form g_r takes two tangent vectors $\partial_v, \partial_w \in T_rM$ as arguments to produce a number, $g_r(\partial_v, \partial_w)$. In this way, one may interpret a metric as a map

$$g : \mathrm{vect}(M) \times \mathrm{vect}(M) \to \mathbb{R}, \qquad (\partial_v, \partial_w) \mapsto g(\partial_v, \partial_w), \tag{V188}$$

assigning to two vector fields a function via the assignment $g(\partial_v, \partial_w)_r = g_r(\partial_{v,r}, \partial_{w,r})$. As with the two interpretations of forms (cf. Eqs. (V134) and (V135)), Eqs. (V187) and (V188) are equivalent but emphasize slightly different aspects of the metric.

The crucial difference distinguishing a metric from a 2-form is that it is *symmetric* in its arguments. More specifically, g is required to be

- ▷ **symmetric**, $\forall \partial_v, \partial_w \in T_rM$, $g_r(\partial_v, \partial_w) = g_r(\partial_w, \partial_v)$, and
- ▷ **non-degenerate**, $\forall \partial_w \in T_rM$, $g_r(\partial_v, \partial_w) = 0 \Rightarrow \partial_v = 0$.

If a metric is positive, i.e. $g(\partial_v, \partial_v) > 0$ if $\partial_v \neq 0$, it is called **positive definite**. More general situations are described via the **signature** of a metric, i.e. a variable specifying its number of negative eigenvalues. For a metric with q negative eigenvalues, the signature is sometimes written as (q, p) where $q + p = d$, or as $(+, +, \dots, -, -, \dots)$ with q pluses and p minuses. For example, the Lorentz metric of special relativity (see info section below) has signature $(+, -, -, -)$. As with metrics on single vector spaces, only the *sign* of the eigenvalues matters here. (One may change the norm of mutually orthogonal basis vectors to change the magnitude of the diagonal entries of a metric, but not their sign.) Manifolds equipped with a positive definite metric, i.e. a metric of signature $(+, \dots, +)$ are called **Riemannian manifolds**.

A convenient way of specifying a metric is in terms of the coordinate basis forms of cotangent space, i.e. the basis $\{\mathrm{d}y^i\}$. The expansion

$$\boxed{g = g_{ij}(y)\, \mathrm{d}y^i \otimes \mathrm{d}y^j \equiv g_{ij}(y)\, \mathrm{d}y^i\, \mathrm{d}y^j,} \tag{V189}$$

then defines the components of the **metric tensor** $g(y) = \{g_{ij}(y)\}$. The second representation, omitting the tensor product sign, is not particularly clean but prevalent in the physics literature. For example, in Cartesian coordinates the **standard metric of** $\mathbb{R}^d$ has the form $g_{ij} = \delta_{ij}$, i.e.

$$g = \mathrm{d}x^1 \otimes \mathrm{d}x^1 + \cdots + \mathrm{d}x^d \otimes \mathrm{d}x^d, \tag{V190}$$

and in this case, no reference to the metric tensor is made (resulting in an awkward two-index-upstairs summation).

In the coordinate representation the action of a general metric on two vector fields, with expansions $\partial_v = v^i \partial_i$ and $\partial_w = w^j \partial_j$, yields the function

$$g(\partial_v, \partial_w) = v^i g_{ij} w^j.$$

Under a **coordinate change** $y \mapsto y'(y)$, which expresses y' through y, with $\mathrm{d}y'^i = \frac{\partial y'^i}{\partial y^k} \mathrm{d}y^k$, the metric changes covariantly, i.e. as a covariant tensor of second degree, or a bilinear form:

$$g = g_{ij}(y')\, \mathrm{d}y'^i \otimes \mathrm{d}y'^j = g_{ij}(y'(y)) \frac{\partial y'^i}{\partial y^k} \frac{\partial y'^j}{\partial y^l}\, \mathrm{d}y^k \otimes \mathrm{d}y^l \equiv g_{kl}(y)\, \mathrm{d}y^k \otimes \mathrm{d}y^l. \tag{V191}$$

The representation on the r.h.s. side implies the **covariant change of metric coefficients**,

$$g_{kl}(y) \equiv g_{ij}(y') \frac{\partial y'^i}{\partial y^k} \frac{\partial y'^j}{\partial y^l} \bigg|_{y' = y'(y)}, \tag{V192}$$

Defining the Jacobi matrix matrix as $J^i{}_k = \frac{\partial y'^i}{\partial y^k}$, the covariant change of metric components assumes the form $g_{kl}(y) = g_{ij}(y'(y)) J^i{}_k J^j{}_l = (J^T)_k{}^i g_{ij}(y'(y)) J^j{}_l$, and this is sometimes abbreviated in a matrix notation as

$$g(y) = J^T g(y'(y)) J. \tag{V193}$$

For later reference, we note that this equation implies

$$\det g(y) = \left(\det J^T \det\left(g(y')\det J\right)\right)_{y'=y'(y)} = \left(\det\left(g(y')\det J^2\right)\right)_{y'=y'(y)}, \tag{V194}$$

where the notation emphasizes that all y'-dependences on the r.h.s. need to be expressed through y and $\det g$ denotes the **determinant of the metric tensor**, often abbreviated by g:[1]

$$g \equiv \det g = \epsilon^{i_1 i_2 \dots i_d} g_{i_1 1} g_{i_2 2} \dots g_{i_d d}. \tag{V195}$$

For an orientable manifold, $\det J$ can be chosen positive. Then Eq. (V194) implies the relation

$$\boxed{\sqrt{|g(y)|} = \sqrt{|g(y'(y))|}\det J,} \tag{V196}$$

which we will need below for the transformation properties of forms involving the metric tensor.

INFO Notation as in Eq. (V193) treats the metric as a matrix an should be used with care (or even avoided at all). The metric tensor is not a matrix, although it is often treated as one in the physics literature. Matrices are tensors of mixed co-contravariant degree $(1,1)$, cf. discussion in section **??**, while the metric is a bilinear form (degree $(0,2)$). This difference manifests itself in appearance of a *transposition* in the 'matrix' representation of the transformation Eq. (V193) whereas no transposition appears in the transformation law for matrices, Eq. (L271).

Within the context of differential geometry it is generally more efficient, and certainly less prone to errors, to work with the representation (V191), and to avoid the potentially confusing matrix notation.

EXAMPLE Consider the standard metric of two-dimensional space in Cartesian coordinates, $g = \mathrm{d}x^1 \otimes \mathrm{d}x^1 + \mathrm{d}x^2 \otimes \mathrm{d}x^2$. The polar representation $x^1 = \rho\cos\phi$ and $x^2 = \rho\sin\phi$, implies $\mathrm{d}x^1 = \mathrm{d}(\rho\cos\phi) = \cos\phi\,\mathrm{d}\rho - \rho\sin\phi\,\mathrm{d}\phi$, and similarly for $\mathrm{d}x^2$. Substituting these expressions into the metric, we obtain the **standard metric of $\mathbb{R}^2$ in polar coordinates**,

$$g = \mathrm{d}\rho \otimes \mathrm{d}\rho + \rho^2\,\mathrm{d}\phi \otimes \mathrm{d}\phi.$$

Notice that the coefficients $g_{\rho\rho} = 1$ and $g_{\phi\phi} = \rho^2$ appearing in this expression agree with those defined in Eq. (V25) of section V2.3. There we had defined the coefficients of the metric as $g_{ij} = g(\mathbf{v}_i, \mathbf{v}_j) = \langle \mathbf{v}_i, \mathbf{v}_j\rangle$, i.e. as the standard scalar products taken between elements of the coordinate basis. In the notation of the present formalism, this equals $g_{ij} = g(\partial_i, \partial_j)$. The latter formula isolates the coefficients g_{ij} in the expansion (V189), showing the equivalence of the formulations. Let us also verify Eq. (V196): For the map $y \mapsto x(y)$ expressing Cartesian in terms of polar coordinates, $\sqrt{|g(y)|} = \sqrt{g_{\rho\rho}g_{\phi\phi}} = \rho$ is indeed consistent with $\sqrt{|g(x(y))|}\det\left(\frac{x}{y}\right) \overset{(V49)}{=} 1\cdot\rho$.

[1] The overloading of the symbol 'g', which is simultaneously used for the abstract metric, its representation as a tensor, and the determinant of that tensor, should be no cause for concern. The notation is standard and which particular g is meant generally follows from the context.

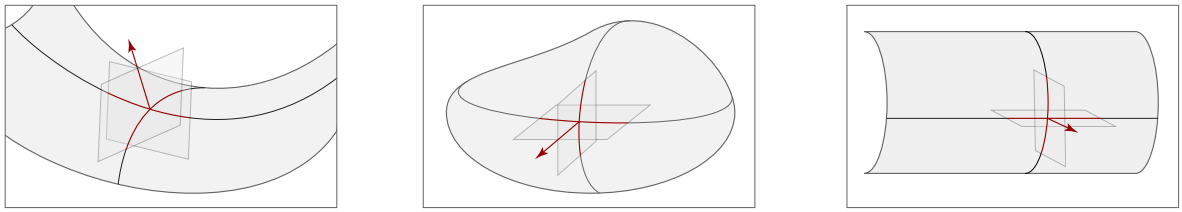


Figure V29: On the definition of the Gaussian curvature of surfaces S in $\mathbb{R}^3$. For a given point $r \in S$, one considers the set of curves defined by the intersection of all planes containing the normal to S at r. The Gaussian curvature, $\kappa = \kappa_{\min}\kappa_{\max}$, is defined as the product of the minimum and maximum curvatures, $\kappa_{\min}$ and $\kappa_{\max}$, of these curves. Left/center/right: surface of negative/positive/vanishing curvature.

EXERCISE Show that the **standard metric of $\mathbb{R}^3$ in spherical coordinates** (r, θ, ϕ) is given by

$$g = \mathrm{d}r \otimes \mathrm{d}r + r^2 \mathrm{d}\theta \otimes \mathrm{d}\theta + r^2 \sin^2\theta \, \mathrm{d}\phi \otimes \mathrm{d}\phi. \tag{V197}$$

Check that this result is consist with Eq. (V196) applied to the map $y \mapsto x(y)$ between Cartesian and spherical coordinates.

V6.2 Norm, angles, curvature

Given a metric, we can introduce concepts such as lengths and angles, etc. to the linear algebra of tangent spaces. For example, the **norm of tangent vectors**, $\|\partial_v\| = \sqrt{g(\partial_v, \partial_v)}$ may be determined to obtain normalized vectors, $\partial_n \equiv \frac{\partial_v}{\|\partial_v\|}$, and by extension normalized vector fields. A basis $\{\partial_{e_i}\}$ of normalized and mutually orthogonal vector fields, $g(\partial_{e_i}, \partial_{e_j}) = \eta_{ij}$, with $|\eta_{ij}| = \delta_{ij}$, is called an **orthonormal basis**. For a positive definite metric, orthonormal bases have $\eta_{ij} = \delta_{ij}$, while for a signature $(q, d-q)$ metric, they have $\eta_{ii} = -1$ for $i = 1, \ldots, q$ and $\eta_{ii} = 1$ for $i = q+1, \ldots, d$, with $\delta_{i\neq j} = 0$.

The curvilinear bases discussed in section V2.3 were orthonormal bases, obtained by normalization of a holonomic basis. For example, in spherical coordinates the holonomic basis vectors ∂_r, ∂_θ and ∂_ϕ have norm 1, r and $r\sin\theta$, respectively, and this yields $\partial_{e_r} = \partial_r$, $\partial_{e_\theta} = r^{-1}\partial_\theta$ and $\partial_{e_\phi} = (r\sin\theta)^{-1}\partial_\phi$. Likewise, we can define the local angle between vectors, $\cos(\theta) = g(\partial_v, \partial_w)/(\|\partial_v\| \, \|\partial_w\|)$ and hence introduce, for example, a vector normal to a 2-dimensional surface embedded in 3-dimensional space.

INFO The metric is instrumental to the description of the elementary geometry of manifolds. For example, it can be used to quantify the **curvature of surfaces** in three-dimensional space. To define the curvature at a surface point $r \in S$ one first constructs a normal vector to S at r (how can this be done?) and then considers the set of all planes containing that normal, see Fig. V29. The intersection of any such plane with the surface defines a curve in S, and each of these curves has a local curvature, κ, at r. As discussed in `problem xx` that curvature is a number, viz. the inverse of

the radius of a circle locally approximating the curve at r. Denote the maximum and the minimum of these curvatures over the set of all curves through r by $\kappa_{\min}$ and $\kappa_{\max}$, respectively. The product of these two numbers, $K \equiv \kappa_{\min}\kappa_{\max}$, defines the so-called **Gaussian curvature** of the surface at r. The Gaussian curvature is given a positive or negative sign depending on whether the two 'principal' curves with extremal curvature bend in the same direction or in opposite directions. Fig. V29 shows situations with negative, positive, and vanishing curvature. For example, a cylinder, although different from a plane, is a surface of globally vanishing curvature since $\kappa_{\min} = 0$ everywhere. Generic surfaces have regions of positive and negative curvature separated by lines of vanishing curvature.

A manifold with globally vanishing curvature is called a **flat manifold**. A manifold is flat if coordinate systems with constant metric tensor $g_{ij} = \eta_{ij}$ can be found. The coordinate lines of these coordinates are curves of vanishing curvature, and they define the vanishing Gaussian curvature of the manifold. For example, a cylinder of radius R centered along the z-axis may be parameterized by the coordinates coordinates $(\varphi = R\phi, z)$ ((ρ, ϕ, z) are standard cylindrical coordinates.) The coordinate vectors corresponding to these vectors read (cf. Eq. (V126)) $\partial_\varphi = -\sin(R^{-1}\varphi)\partial_1 + \cos(R^{-1}\varphi)\partial_2$, and $\partial_z = \partial_3$, where $\partial_{1,2,3}$ are cartesian coordinate vectors in $\mathbb{R}^3$. (We here assume the cylinder to be embedded in three dimensional space.) The 2×2 diagonal metric tensor defined by these vectors reads $g_{\varphi\varphi} = g_{zz} = 1$, i.e. $g_{ij} = \delta_{ij}$, and this demonstrates the flatness of the cylinder. The condition of the existence of a *global* representation of this type is of importance here. On a curved manifold, M, local transformations with representation $g_{r,ij} = \eta_{r,ij}$ at any point $r \in M$ can be found. However, it is not possible to extend them to a globally constant metric.

In an orthonormal frame, the metric assumes the form

$$g \equiv \eta = \sum_i \eta_{ii}\, \mathrm{d}x^i \otimes \mathrm{d}x^i, \tag{V198}$$

where $\eta_{ii} = \pm 1$ according to the signature, and η is standard notation for the metric in orthonormal representations. We here introduce the convention to label coordinates which are orthonormal in this sense by the symbol x. The notation generalizes the concept of Cartesian coordinates (orthonormal coordinates of a positive definite metric) to positive indefinite metrics.

Once a metric has been brought to a diagonal representation, η, it is often expedient to consider the restricted set of basis transformations which leave this form invariant. According to Eq. (V193), the corresponding Jacobi matrices satisfy the condition

$$J^T \eta J = \eta.$$

The set of these transformation matrices, 'stabilizing' the metric in this sense defines the **invariance group** of the metric. (Why do these matrices form a group?) For example, the invariance group of the standard metric $\eta_{ii} = 1$ in three-dimensional space is the group $\mathrm{O}(3)$ of three-dimensional matrices obeying the constraint $J^T J = \mathbb{1}$.

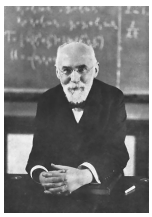
INFO The **Minkovski metric** of four-dimensional space time $\mathbb{R}^4 = \mathbb{R} \oplus \mathbb{R}^3$ is a metric of signature

$(-,+,+,+)$ and has the orthonormal representation[2]

$$g = \eta = \eta_{\mu\nu}\, \mathrm{d}x^\mu \otimes \mathrm{d}x^\nu = +\mathrm{d}x^0 \otimes \mathrm{d}x^0 - \sum_i \mathrm{d}x^i \otimes \mathrm{d}x^i. \tag{V199}$$

Here x^i are space-like coordinates and x^0 is understood as a time-like coordinate. It is customary to set $x^0 = ct$, where t is time and c a characteristic velocity, usually chosen to be the speed of light. We follow a widespread convention in which Greek indices $\mu, \nu = 0, 1, 2, 3$ run through all coordinates, while Latin indices $i, j = 1, 2, 3$ are space-like.

Hendrik Antoon Lorentz
1853–1928



Dutch physicist and recipient of the 1902 Nobel prize (with Peter Zeeman) for the explanation of the Zeeman effect. Lorentz identified the coordinate transformation equations stabilizing the Minkovski metric, and in this way laid the mathematical foundations of special relativity. The importance of his work reflects in Einstein's quotation (1953): "For me personally he meant more than all the others I have met on my life's journey."

The invariance group of the Minkovski metric is called the **Lorentz group** $\mathrm{O}(1,3)$. Its transformations, conventionally denoted by $\Lambda \in \mathrm{O}(1,3)$, obey

$$\Lambda^T \eta \Lambda = \eta, \tag{V200}$$

and are called **Lorentz transformations**. Important examples of Lorentz transformations include **time reversal**, $\Lambda^0{}_0 = -1$, $\Lambda^i{}_j = \delta^i{}_j$, with all other elements zero, i.e. the reflection of the time coordinate; **space reflection**, $\Lambda^0{}_0 = 1$, $\Lambda^i{}_j = -1$; and **rotations of space**, $\Lambda^0{}_0 = 1$, $\Lambda^i{}_j = A^i{}_j$, where A is a rotation (i.e. orthogonal) matrix. However, the most interesting Lorentz transformations are the **Lorentz boosts**, transformations that mix space and time coordinates. By way of example, we consider a transformation that does not affect the coordinates x^2 and x^3. It is then straightforward to verify that the condition (V200) requires Λ to have the form

$$\Lambda = \begin{pmatrix} \cosh\lambda & \sinh\lambda & & \\ \sinh\lambda & \cosh\lambda & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \tag{V201}$$

where λ is a free parameter. The Lorentz boost describes the transformation between two coordinate systems moving relative to each other in x^1 direction with relative velocity v. The boost velocity is related to the boost parameter λ as $\tanh\lambda = -v/c$. For velocities $|v| \ll c$ much smaller than the speed of light, $|\lambda| \ll 1$, hence $\cosh\lambda \simeq 1$ and $\sinh\lambda \simeq -v/c$. The transformed coordinates are then given by $x'^1 \simeq x^1 + \lambda x^0 = x^1 - vt$ and $x'^0 \simeq x^0 + \lambda x^1$ which is equivalent to $t' = t + \mathcal{O}(x^1 v/c^2)$. This shows how for small velocities the Lorentz transformation leaves time approximately invariant, $t' \simeq t$, and just describes the change of coordinates $x'^1 = x^1 - vt$ between two moving coordinate frames. (These 'non-relativistic' transformations are called Galilei transformations.) However, for relativistic velocities, $|v| \sim c$, the Lorentz transformation mixes space and time coordinates inseparably and leads to the principal effects of special relativity, the dilation of time, length contraction, the non-invariance of mass, etc. For a physical discussion of these effects we refer to courses in special relativity.

[2] In the literature one often finds the alternative definition $\eta = -\mathrm{d}x^0 \otimes \mathrm{d}x^0 + \sum_i \mathrm{d}x^i \otimes \mathrm{d}x^i$. The overall sign difference between the two conventions, $\eta \leftrightarrow -\eta$, does not have any significant consequences.

V6.3 Metric and integration

A metric provides the means to determine the 'volume' of d-dimensional manifolds, i.e. the length of curves, the area of surfaces, the volume of three-dimensional structures, etc. Recall that the good objects to integrate on a d-dimensional manifold are d-forms. For a coordinate transformation $y \mapsto y'(y)$, the y- and y'-coordinate representations of a d-form have weight functions related by $\omega(y) = \omega(y'(y)) \det(\frac{\partial y'}{\partial y})$, cf. Eq. (V169). On a general manifold, the Jacobian of the coordinate transformation can be an arbitrary invertible matrix, hence the weight can change arbitrarily: there does not exist a 'canonical' choice for the top-form.

The situation is different on (orientable) manifolds with a metric If we choose the weight function for the y'-system as $\omega(y') = \sqrt{g(y')}$,[3] that of the y-system turns out to have the *same* form, $\omega(y) = \sqrt{g(y'(y)} \det\left(\frac{\partial y'}{\partial y}\right) = \sqrt{g(y)}$, where the second step follows from Eq. (V196). Therefore the form

$$\boxed{\omega = \sqrt{g(y')}\, \mathrm{d}y'^1 \wedge \cdots \wedge \mathrm{d}y'^d = \sqrt{g(y)}\, \mathrm{d}y^1 \wedge \cdots \wedge \mathrm{d}y^d,} \tag{V202}$$

called the **canonical volume form** on the manifold, has the distinguishing property of being invariant under coordinate transformations.

The **volume of a manifold** is now defined as the integral over the volume form,

$$\boxed{\mathrm{vol}(M) \equiv \int_M \omega.} \tag{V203}$$

For a standard scalar product and Cartesian coordinates, $g = 1$, and $\omega = \mathrm{d}x^1 \wedge \ldots \mathrm{d}x^d$, the integral reduces to the standard 'volume integral' discussed in chapter C4. In cases where the integral does not exist – think of the two-dimensional plane, $M = \mathbb{R}^2$ – we speak of a manifold of undetermined or infinite volume. For a general coordinate system, the volume integral becomes

$$\mathrm{vol}(M) = \int_M \sqrt{g(y)}\, \mathrm{d}y^1 \wedge \ldots \wedge \mathrm{d}y^d = \int_U \sqrt{g(y)}\, \mathrm{d}y^1 \ldots \mathrm{d}y^d, \tag{V204}$$

where the second representation emphasizes that it may be interpreted as the integral of the pullback of the volume form over the y-coordinate domain (cf. discussion on p. 468).

EXAMPLE In a Cartesian basis, the standard metric in $\mathbb{R}^3$ is given by (V190), i.e. it has $\det g = 1$. Therefore the volume form is $\omega = \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3$. If we switch to spherical coordinates, the metric tensor is given by (V197). We now have $\sqrt{g} = r^2 \sin\theta$, hence the **spherical representation of the volume form** reads $\omega = r^2 \sin\theta\, \mathrm{d}r \wedge \mathrm{d}\theta \wedge \mathrm{d}\phi$. Of course, this result was to be expected from our discussion of integration in spherical coordinates in section C4.3.

[3] On a manifold with indefinite metric, this needs to be replaced by $\sqrt{|g(y')|}$, however we will drop the modulus symbol for better readability.

The **two sphere** can be locally identified with the coordinate domain $U(\theta,\phi)$ with the spherical metric $g_{\theta\theta}=1, g_{\phi\phi}=\sin^2\theta$. This means that its volume form, or in view of the two-dimensionality better to say its **spherical area form**, is given by $\omega=\sin\theta \mathrm{d}\theta\wedge\mathrm{d}\phi$. We had considered this form before (cf. Eq.Eq. (V163)) and saw that its full integration indeed yields the area of the sphere, 4π.

V6.4 Hodge star

The spaces of p forms and $(d-p)$-forms, $\Lambda^p(M)$ and $\Lambda^{d-p}(M)$, both have the same dimensionality $\binom{d}{p}$. This suggests that there might be a linear bijection $\Lambda^p(M)\to\Lambda^{d-p}(M)$, assigning p-forms to $(d-p)$-forms. For a given basis, it is indeed straightforward to construct a map uniquely assigning to the basis p-forms of $\Lambda^p(M)$ corresponding basis $(d-p)$-forms of $\Lambda^{d-p}(M)$, hence implementing a bijection (think how!). For example, in $d=3$ one might assign the basis 1-forms of a coordinate system to $(3-1=2)$-forms as $\mathrm{d}y^1\leftrightarrow \mathrm{d}y^2\wedge\mathrm{d}y^3, \mathrm{d}y^2\leftrightarrow \mathrm{d}y^3\wedge\mathrm{d}y^1$, and $\mathrm{d}y^3\leftrightarrow\mathrm{d}y^1\wedge\mathrm{d}y^2$, or the 0 form 1 to the $(3-0=3)$-form $\mathrm{d}y^1\wedge\mathrm{d}y^2\wedge\mathrm{d}y^3$. However, much as with maps between vectors and dual vectors, the dependence of this map on a basis makes it not canonical.

In the following we will show how a metric can be engaged to modify the assignment above to a canonical bijection, $*:\Lambda^p(M)\to\Lambda^{d-p}(M)$, known as the **Hodge star**. Only then will we be in a position to motivate the importance of this map and discuss its applications in mathematics and physics.

Definition of the Hodge star

REMARK Once more the notation assumes a positive metric, so that we are entitled to write square roots of determinants as $\sqrt{g}$. For an indefinite metric, this needs to be replaced by $\sqrt{|g|}$.

Let us begin by considering $d=3$ and writing the above prototypical assignment as $\mathrm{d}y^i\mapsto\frac{1}{2}\epsilon_{ijk}\mathrm{d}y^j\wedge\mathrm{d}y^k$. The non-canonical nature of this map shows in that it will change form under a change of coordinates, $y\mapsto y'(y)$. At the same time, we notice that the index structure of the expression does not look nice: the index i appears upstairs on the left but downstairs on the right. Both these deficiencies can be removed in one go via the definition

$$\mathrm{d}y^i\mapsto *\mathrm{d}y^i=\tfrac{1}{2}\sqrt{g}g^{ij}\epsilon_{jkl}\mathrm{d}y^k\wedge\mathrm{d}y^l. \tag{V205}$$

Here, the index raising operation via the matrix elements g^{ij} of the *inverse* metric (cf. Eq. (L55)) fixes the index positioning, and the presence of the factor $\sqrt{g}$ makes the map invariant under transformations $y\mapsto y'(y)$. While the latter statement requires proof, it can be made plausible as follows. Assume Eq. (V205) to hold in the primed system and then transcribe it to unprimed coordinates as $\sqrt{g(y'(y))}\overset{(V194)}{=}\sqrt{g(y)}\det J^{-1}$ where $\mathrm{d}y'^i=\frac{\partial y'^i}{\partial y^m}\mathrm{d}y^m\equiv J^i{}_m\mathrm{d}y^m$.

This leads to the appearance of a product of 3 matrix elements of the Jacobi matrix, fully antisymmetric in the matrix indices, i.e. the *determinant* $\det J$, which cancels the factor $\det J^{-1}$. As a result, the Hodge start operation in the unprimed system looks the same as in the primed one. For a full formulation of the proof we refer to the info section below.

Before turning to the discussion of this map, we note that the above definition generalizes to forms of arbitrary degree as

$$*(\mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p}) = \frac{\sqrt{g}}{(d-p)!} g^{i_1 j_1} \ldots g^{i_p j_p} \epsilon_{j_1 \ldots j_p j_{p+1} \ldots j_d} \mathrm{d}y^{j_{p+1}} \wedge \cdots \wedge \mathrm{d}y^{j_d}. \tag{V206}$$

The **Hodge star** is thus defined as a linear map acting on generic p-forms as

$$\begin{aligned} &* : \Lambda^p(M) \to \Lambda^{(d-p)}(M), \qquad \phi \mapsto *\phi, \\ &*\phi = *\left(\frac{1}{p!} \phi_{i_1,\ldots,i_p} \mathrm{d}y^{i_1} \wedge \mathrm{d}y^{i_p} \right) = \frac{\sqrt{g}}{p!(d-p)!} \phi^{j_1,\ldots,j_p} \epsilon_{j_1 \ldots j_p j_{p+1} \ldots j_d} \mathrm{d}y^{j_{p+1}} \wedge \cdots \wedge \mathrm{d}y^{j_d}, \end{aligned} \tag{V207}$$

where $\phi^{j_1,\ldots,j_p} = \phi_{i_1,\ldots,i_p} g^{i_1 j_1} \ldots g^{i_p j_p}$. This definition states that a p-form with components $\phi_{i_1,\ldots,i_p}$ gets mapped to a $(d-p)$-form with components $(*\phi)_{j_{p+1},\ldots,j_d} = \frac{1}{p!} \sqrt{g} \phi^{j_1,\ldots,j_p} \epsilon_{j_1,\ldots,j_d}$. A second application of the star maps this $(d-p)$-form back to a p-form (since $d-(d-p)=p$). Indeed it is straightforward to verify that the Hodge star operation is almost self-involutory,

$$** \phi = \mathrm{sgn}(g)(-)^{p(d-p)} \phi, \tag{V208}$$

i.e. up to a sign factor, the two-fold application of $*$ leaves forms invariant.

EXERCISE Check this property for $d=3$, or perhaps even for general d.

INFO The proof of the **coordinate invariance of the Hodge star operation** is somewhat technical but nevertheless instructive.[4] There are different ways of verifying the invariance. One is to start from the definition (V206) and (i) transform the argument, i.e. the wedge product of basis forms $\mathrm{d}y^i$, to the $\mathrm{d}y'^j$-basis. Using the yet–to–be–established invariance, one then (ii) applies $*$ to the product of $\mathrm{d}y'^j$ basis forms according to the y'-version of Eq. (V206). The invariance property is established if the result coincides with the application of the original y-version of the definition to the original form.

Before testing this feature, we note that we will need to painstakingly discriminate between $g^{ij}(y(y'))$, i.e. the functions $g^{ij}(y)$ expressed in new coordinates and $g^{kl}(y')$, i.e. the matrix elements of the inverse metric in new coordinates. The two quantities are related by (cf. Eq. (V191)) $g^{kl}(y') = (J^{-1})^k{}_i (J^{-1})^l{}_j g^{ij}(y(y'))$, or (iii) $(J^{-1})^l{}_j g^{ij}(y(y')) = J^i{}_k g^{kl}(y')$, where we noted that the contravariant tensor g^{kl} transforms with the inverse of the Jacobi matrix (recapitulate why, if

[4] There exist alternative definitions of the Hodge star which do not utilize coordinate representations. While the coordinate invariance of these is manifest, they require some more conceptual overhead and are therefore not discussed here.

necessary). Finally, it will be expedient to write wedge products of forms as $\mathrm{d}y^{i_1} \wedge \cdots \wedge \mathrm{d}y^{i_p} \equiv \bigwedge_{a=1}^{p} \mathrm{d}y^{i_a}$.

If we now apply the $*$-operation (V206) (defined for the y'-coordinate system) to the transformed basis we obtain

$$
\begin{aligned}
*\bigwedge_{a=1}^{p} \mathrm{d}y^{i_a} &\overset{\text{(i)}}{=} * \bigwedge_{a=1}^{p} (J^{-1})^{i_a}{}_{k_a} \mathrm{d}y'^{k_a} = \bigwedge_{a=1}^{p} (J^{-1})^{i_a}{}_{k_a} * \mathrm{d}y'^{k_a} = \\
&\overset{\text{(ii)}}{=} \frac{\sqrt{g(y')}}{(d-p)!} \prod_{a=1}^{p} (J^{-1})^{i_a}{}_{k_a} g^{k_a l_a}(y') \epsilon_{l_1 \ldots l_d} \bigwedge_{b=p+1}^{d} \mathrm{d}y'^{l_b} = \\
&\overset{\text{(iii)}}{=} \frac{\sqrt{g(y')}}{(d-p)!} \prod_{a=1}^{p} J^{l_a}{}_{j_a} g^{i_a j_a}(y(y')) \epsilon_{l_1 \ldots l_d} \bigwedge_{b=p+1}^{d} \mathrm{d}y'^{l_b} = \\
&= \frac{\sqrt{g(y')}}{(d-p)!} \prod_{a=1}^{p} J^{l_a}{}_{j_a} g^{i_a j_a}(y(y')) \epsilon_{l_1 \ldots l_d} \bigwedge_{b=p+1}^{d} J^{l_b}{}_{j_b} \mathrm{d}y^{j_b} = \\
&= \frac{\sqrt{g(y')}}{(d-p)!} \epsilon_{l_1 \ldots l_d} \prod_{c=1}^{d} J^{l_c}{}_{j_c} \prod_{a=1}^{p} g^{i_a j_a}(y(y')) \bigwedge_{b=p+1}^{d} \mathrm{d}y^{j_b} = \\
&= \frac{\sqrt{g(y')}}{(d-p)!} \det J \epsilon_{j_1 \ldots j_d} \prod_{a=1}^{p} g^{i_a j_a}(y(y')) \bigwedge_{b=p+1}^{d} \mathrm{d}y^{j_b} = \\
&= \frac{\sqrt{g(y') \det J^2}}{(d-p)!} \prod_{a=1}^{p} g^{i_a j_a}(y(y')) \epsilon_{j_1 \ldots j_d} \bigwedge_{b=p+1}^{d} \mathrm{d}y^{j_b} = \\
&= \frac{\sqrt{g(y)}}{(d-p)!} g^{i_1 j_1}(y) \ldots g^{i_p j_p}(y) \epsilon_{j_1 \ldots j_d} \mathrm{d}y^{j_{p+1}} \wedge \cdots \wedge \mathrm{d}y^{j_d}.
\end{aligned}
$$

where in the last step we expressed $g^{ij}(y(y')) = g^{ij}(y)$ as functions of the y-coordinates. Comparing the outermost parts of this chain of equalities we observe that consistency with Eq. (V206) is established *using* the y'-version of the definition. This establishes its invariance, although it has to be admitted that the proof lacks elegance.

EXAMPLE Consider three-dimensional space parameterized in terms of spherical coordinates. The components of the inverse of the diagonal metric are given by $g^{rr} = 1$, $g^{\theta\theta} = r^{-2}$, $g^{\phi\phi} = (r \sin\theta)^{-2}$. With $\sqrt{g} = r^2 \sin\theta$, Eq. (V205) yields

$$
\begin{aligned}
*\mathrm{d}r &= \tfrac{1}{2}\sqrt{g}\, g^{rr} \epsilon_{rjk}\, \mathrm{d}y^j \wedge \mathrm{d}y^k = r^2 \sin\theta\, \mathrm{d}\theta \wedge \mathrm{d}\phi, \\
*\mathrm{d}\theta &= \tfrac{1}{2}\sqrt{g}\, g^{\theta\theta} \epsilon_{\theta jk} \mathrm{d}y^j \wedge \mathrm{d}y^k = \sin\theta\, \mathrm{d}\phi \wedge \mathrm{d}r, \\
*\mathrm{d}\theta &= \tfrac{1}{2}\sqrt{g}\, g^{\phi\phi} \epsilon_{\phi jk} \mathrm{d}y^j \wedge \mathrm{d}y^k = \sin\theta^{-1}\, \mathrm{d}r \wedge \mathrm{d}\theta.
\end{aligned}
\tag{V209}
$$

V6.5 Vectors vs. one-forms vs. two-forms in $\mathbb{R}^3$

REMARK To simplify the notation we consider positive metrics for which $\sqrt{|g|} = \sqrt{g}$ throughout. For an indefinite metric, all formulas remain unchanged, except that the modulus under the square root has to be put pack in place.

In $\mathbb{R}^3$, there are three distinct categories of tensors[5] involving three coefficient functions:

$$\begin{aligned} \text{vectors:} \quad & \partial_v = v^1\partial_1 + v^2\partial_2 + v^3\partial_3, \\ \text{one-forms:} \quad & \phi = \phi_1 \mathrm{d}y^1 + \phi_2 \mathrm{d}y^2 + \phi_3 \mathrm{d}y^3, \\ \text{two-forms:} \quad & \omega = \omega_{12}\mathrm{d}y^1 \wedge \mathrm{d}y^2 + \omega_{23}\mathrm{d}y^2 \wedge \mathrm{d}y^3 + \omega_{31}\mathrm{d}y^3 \wedge \mathrm{d}y^1. \end{aligned} \tag{V210}$$

All of these play a role in physics, since as we saw above, various physical quantities (forces, currents, densities, etc.) are best described as differential forms. In contrast, the traditional physics approach uniformly treats all three-component objects in $\mathbb{R}^3$ (and analogously in spaces of different dimension) as vector fields. This is possible since forms and vectors can be mapped to each other using 'translation rules', which in turn depend on a metric.

However, there is a price to be paid for turning from the more natural form-representation of observables to the monotonicity of vector fields. For example, in its differential form version the all-important Stokes' theorem Eq. (V184) assumes a simple and coordinate invariant form. The one-, two- and three-dimensional versions of the theorem may be recast in a vector language to obtain the traditional Stokes' and Gauss' theorems for vector field integration. In general coordinates the vector differential operators $\nabla, \nabla\times, \nabla\cdot$ appearing in these relations assume a complicated form and this is because the procedure needed to translate them to vector fields turns something simple to something more complicated.

In view of the importance of the traditional approach to the formulation of physical theories, this section discusses the translation between forms and vectors and its ramifications in the operations of vector calculus. We will return to the subject from a physical perspective in chapter V7 where we compare the traditional and the form-oriented approach to the formulation of electrodynamics.

If we want to pass between forms and vectors in three-dimensional spaces we need to know how to convert one-forms to vectors, and one-forms to two-forms. The conversion of vectors to two-forms is then achieved by a composition of these two elementary operations. The **passage between forms and vectors** is achieved via the general isomorphism, $J : V \to V^*$,[6] between vector spaces and their dual spaces discussed in section L3.3. Recall that to a vector $v \in V$ one may assign a dual vector $J(v) \in V^*$ by requiring that

$$g(v, w) = J(v)w, \qquad \forall w \in V. \tag{V211}$$

[5] All operations discussed in this section are defined 'locally', i.e. they work for the vectors and forms of a vector space, and equally for the vector fields and differential forms of a manifold.

[6] The same symbol J is frequently used for both the isomorphism $V \to V^*$ and the Jacobian of smooth maps. The two quantities are unrelated and no confusion should arise.

operation	invariant	components
vector $\to$ 1-form	$\phi = J(\partial_v)$	$\phi_i = v^j g_{ji}$
1-form $\to$ vector	$\partial_v = J^{-1}(\phi)$	$v^j = \phi_i g^{ij}$
1-form $\to$ 2-form	$\omega = *\phi$	$\omega_{ij} = \sqrt{g} g^{kl} \phi_l \epsilon_{kij}$
2-form $\to$ 1-form	$\phi = *\omega$	$\phi_i = \frac{1}{2\sqrt{g}} g_{ij} \epsilon^{jkl} \omega_{kl}$
2-form $\to$ vector	$\partial_v = J^{-1}(*\omega)$	$v^i = \frac{1}{2\sqrt{g}} \epsilon^{ijk} \omega_{jk}$
vector $\to$ 2-form	$\omega = *J(\partial_v)$	$\omega_{ij} = \sqrt{g} v^k \epsilon_{kij}$

Table V6.1: Passing between vectors, 1-forms and 2-forms in three-dimensional metric space.

In a component language this condition is written as $(J(v))_i \equiv v_i = g_{ij} v^j$, and $J^{-1}(J(v))^i = v^i = g^{ij} v_j$ for the inverse map, where the dual vector and the vector are distinguished by the co- and contravariant positioning of the indices, respectively. In the same way a vector *field*, $\partial_v = v^j \partial_{y^j}$, defines a differential one-form, $J(\partial_v)$, with components $J(\partial_v)_i \equiv v_i = v^j g_{ji}$. The action of the inverse map on a differential form, $\phi = \phi_i \mathrm{d}y^i$, yields a vector, $J^{-1}(\phi)$, with components $J^{-1}(\phi)^j \equiv \phi^j = \phi_i g^{ij}$. Again, the distinction is solely indicated by the positioning of indices; if the symbol for a differential form appears with indices upstairs, a *vector* is at hand, etc. The action of J on one-forms and vectors is summarized by

$$J(v^j \partial_j) = v^j g_{ji} \mathrm{d}y^i, \qquad J^{-1}(\phi_i \mathrm{d}y^i) = \phi_i g^{ij} \partial_j. \tag{V212}$$

The **passage between one-forms and two-forms** is defined by the $d = 3$ version of the Hodge star. To a one-form, ϕ, the Hodge star assigns a two-form, $\omega \equiv *\phi$, with component representation (cf. Eq. (V207)) $\omega_{ij} = \sqrt{g} \phi^k \epsilon_{kij} = \sqrt{g} g^{kl} \phi_l \epsilon_{kij}$. From a two-form, ω, we may pass back to a one-form by applying the Hodge star once more, $\phi = *\omega$. In components, $\phi_i = \frac{\sqrt{g}}{2} \omega^{no} \epsilon_{noi} = \frac{\sqrt{g}}{2} g_{ij} g^{jm} g^{kn} g^{lo} \epsilon_{mno} \omega_{kl} = \frac{1}{2\sqrt{g}} g_{ij} \epsilon^{jkl} \omega_{kl}$, where we used $\epsilon_{noi} = g_{ij} g^{jm} \epsilon_{mno}$ and in the second step Eq. (L168) to convert the antisymmetrized product of three metric coefficients in to a determinant. Finally, we may pass **from two-forms to vectors** in a two-step transformation, which first maps a two-form, ω, to a one form, $*\omega$, and that to a vector, $J^{-1}(*\omega)$. The component representation of this mapping is given by $v^i = g^{il} (*\omega)_l = \frac{1}{2\sqrt{g}} g^{il} g_{lm} \epsilon^{mjk} \omega_{jk} = \frac{1}{2\sqrt{g}} \epsilon^{ijk} \omega_{jk}$. The inverse operation, $\omega = *J(\partial_v)$, has the component representation $\omega_{ij} = \sqrt{g} v^k \epsilon_{kij}$. An overview of all these operations is given in table V6.1.

These operations may now be applied to translate the form-representations of various differential and integral operations to their traditional formulations in vector analysis.

EXERCISE Formulate the general formulas derived below for the example of spherical coordinates (r, θ, ϕ) with diagonal metric $g_{rr} = 1$, $g_{\theta\theta} = r^2$, $g_{\phi\phi} = r^2 \sin^2 \theta$. Check that the previously derived relations (V76), (V94), and (V108) are reproduced.

Gradient: The gradient of a function f is the vector field associated with the one-form $\mathrm{d}f$,

the exterior derivative of f. It is defined as

$$\nabla f = J^{-1}(\mathrm{d}f) \tag{V213}$$

and its components are given by

$$\boxed{\nabla f^i = g^{ij}\partial_i f.} \tag{V214}$$

This representation is equivalent to the earlier definition of the gradient of a function in curvilinear coordinates, Eq. (V69). As discussed in section **??**, the gradient vector field points in the direction of the steepest ascent of the function f, and to describe this geometric orientation a metric is required. Within the framework of forms, the variation of f variation is described without metric by the exterior derivative $\mathrm{d}f$.

Divergence: The divergence is an operation assigning to a vector field a scalar function through a first-oder derivative operation. This is reminiscent of the action of the exterior derivative on a two-form which, likewise, converts a three-component object (the form) to a scalar quantity (the single weight function characterizing the resulting three-form) via a first-order derivative. To make the correspondence concrete, we start from a vector field and map it to a two-form through the relation, $\omega = *J(\partial_v)$. An exterior derivative converts the two- to a three-form, $\mathrm{d}\omega = \mathrm{d}(*J\partial_v)$. Finally, the (non-derivative) Hodge star operation is applied to map the 3-form to a $(3-3)$ zero form, i.e. a function. The succession of the three operations,

$$\nabla \cdot \partial_v \equiv (*\,\mathrm{d}\,*\,J)\partial_v, \tag{V215}$$

thus assigns functions to vector fields in a coordinate invariant manner via a single derivative and may be considered a *definition* of the **divergence** of the vector field.

To confirm the equivalence to the previous definition (V93), which was motivated by a geometric analysis of the sources of a vector field, we apply the succession of operations to a vector field with components v^i according to the prescriptions summarized in table V6.1. This leads to the coordinate representation (verify!)

$$\boxed{\nabla \cdot \partial_v = \frac{1}{\sqrt{g}}\partial_i\left(\sqrt{g}v^i\right).} \tag{V216}$$

The expression on the r.h.s. is indeed equivalent to Eq. (V93).

Curl: The curl is an operation assigning to a vector field (a three-component object) another vector field via a first-order derivative operation. In form-language a similar assignment may be achieved by starting from a one-form (three components), acting with d to obtain a two-form (again three components). This suggests to *define* the curl as

$$\nabla \times \partial_v = (J^{-1} * \mathrm{d}\,J)\partial_v, \tag{V217}$$

i.e. we first pass from a vector field ∂_v a one-form, $J(\partial_v)$, act by d to obtain a two-form, convert that one to a one-form, to finally map back to a vector field. The equivalence of

this operation to the previous construction, Eq. (V107), i.e. a geometric description of the circulation content of a vector field, is shown by application of the coordinate representation of the operations summarized in table V6.1 to a vector field with components v^i. This leads to (check it!)

$$\boxed{(\nabla \times \partial_v)^i = \frac{1}{\sqrt{g}} \epsilon^{ijk} \partial_j \left(g_{kl} v^l \right),} \tag{V218}$$

which is equivalent to Eq. (V107).

Laplacian: The Laplacian is a second-order derivative operation turning functions into functions.[7] The invariant succession of steps achieving this operation reads

$$(\text{0-form}) \xrightarrow{\mathrm{d}} (\text{1-form}) \xrightarrow{*} (\text{2-form}) \xrightarrow{\mathrm{d}} (\text{3-form}) \xrightarrow{*} (\text{0-form}),$$

or $\Delta \equiv * \mathrm{d} * \mathrm{d}$. This can be written as

$$\Delta = (* \mathrm{d} * J)(J^{-1} \mathrm{d}) = \nabla \cdot \nabla, \tag{V219}$$

i.e. as the divergence of the gradient as defined above. In this way contact with the conventional definition of the Laplace operator (V97) is established. The coordinate representation, obtained by straightforward composition of Eqs. (V214) and (V216), reads

$$\boxed{\Delta = \frac{1}{\sqrt{g}} \partial_i \left(\sqrt{g} g^{ij} \partial_j \right).} \tag{V220}$$

For the the example of the Laplacian in spherical coordinates, see Eq. (V115).

INFO The usefulness of the Hodge star $*$ and the metric isomorphism J is not limited to three-dimensional situations. As an example, consider **physical force** which, regardless of dimension, the present approach describes by a one-form, f, cf. discussion on p. 462. In physics, the same quantity is represented by a vector ∂_f. The translation between the two quantities is achieved by the metric isomorphism, $\partial_f = J^{-1} f$. This relationship follows directly from their respective definitions: in form language, the energy difference corresponding to a small displacement vector, ∂_Δ, is described by the (negative of the) force form acting on the vector, $-f(\partial_\Delta)$. Within the traditional approach, the same quantity is given by the scalar product of the force vector and the displacement vector, $-g(\partial_f, \partial_\Delta)$. Comparing the two expressions, $f_j (\partial_\Delta)^j = (\partial_f)^i g_{ij} (\partial_f)^j$, we realize that $f_j = (\partial_f)^i g_{ij}$, i.e. ∂_f and f are related by the isomorphism J. For a conservative force, there exists a **potential function**, φ, such that $-f = \mathrm{d}\varphi$. In this case, $-f(\partial_\Delta) = \mathrm{d}\varphi(\partial_\Delta) = \partial_\Delta(\varphi)$, i.e. energy differences between nearby points are described by the changes of a potential function φ. The force *vector*, $-\partial_f$, corresponding to $\mathrm{d}\varphi$ is given by $J^{-1}(\mathrm{d}\varphi) \overset{(V213)}{=} \nabla\varphi$ and so we re-discover the statement that conservative forces are the gradients of functions. However, one may argue that the description of forces in terms of forms

[7] There exists a generalized variant of the Laplacian acting on forms of arbitrary degree. However, we will not discuss this extension here.

is more natural and direct: physical forces are *measured* (cf. discussion on p. 148) by monitoring the work required to move a test particle between nearby points in space, that is via linear assignments (separation in space) $\to$ (number). This is precisely what a differential form does, i.e. one-forms are the 'natural' mathematical objects describing forces. The construction of a vector 'pointing in the direction of the force' requires a metric and complicates affairs. For example, in form language the exterior derivatives of conservative force potentials assume a simple form $f = -\mathrm{d}\varphi = \partial_i\varphi \mathrm{d}y^i$ in any coordinate system. By contrast, gradient vector fields, $\partial_f = -\partial_i\varphi g^{ij}\partial_i$ contain derivatives mixed with elements of the metric and this combination of objects complicates the mathematics. (This reflects in the empirical fact that the discussion of the gradient in spherical coordinates in introductory lecture courses is a subject generally unpopular with students.)

As a four-dimensional example consider the current three-form defined in the info section on p. 472. In physics, current is described by a **four-component current vector field**, ∂_j (here, the subscript refers to current, j, and is not an index). Its zeroth component, $j^0 = \rho$, and spatial components, j^i, are the particle density, $\rho(x)$, and the components, $j^i(x)$, of a spatial current density vector 'pointing in the direction of current flow', respectively. The dependence of $j^\mu(x)$ on the space time argument $x = (x^0, x^1, x^2, x^3) = (t, x^1, x^2, x^3)$ describes spatio-temporal fluctuations of these quantities.

One may guess on formal grounds how the connection between the current three-form (V161) and the current vector, ∂_j, is established: an application of the Hodge star transforms the 3-form into a $4 - 3 = 1$ form, and a subsequent application of J^{-1} maps the latter to a vector. For the space-time manifold with its signature $(1, -3)$ metric, g, these operations are given by

$$\begin{aligned}\partial_j \equiv J^{-1}(*\,j) &\overset{(V207)}{=} J^{-1}\left(\frac{1}{3!}j^{\mu\nu\sigma}\epsilon_{\mu\nu\sigma\rho}\mathrm{d}y^\rho\right) \overset{(V212)}{=} \frac{1}{3!}j^{\mu\nu\sigma}\epsilon_{\mu\nu\sigma\rho}g^{\rho\tau}\partial_\tau = \\ &= \frac{1}{3!}j_{\lambda\kappa\delta}g^{\lambda\mu}g^{\kappa\nu}g^{\delta\sigma}g^{\rho\tau}\epsilon_{\mu\nu\sigma\rho}\partial_\tau \overset{(L168)}{=} -\frac{1}{3!}j_{\lambda\kappa\delta}\epsilon^{\lambda\kappa\delta\tau}\partial_\tau, \end{aligned} \tag{V221}$$

where in the last step we used $\det(g) = -1$. Using that $\epsilon^{\lambda\kappa\delta\tau} = -\epsilon^{\tau\lambda\kappa\delta}$ we identify the components of the current vector field through the r.h.s. of the equation as

$$j^\tau = \frac{1}{3!}\epsilon^{\tau\lambda\kappa\delta}j_{\lambda\kappa\delta}. \tag{V222}$$

This construction confirms the physical expectation that the current vector and the current form are closely related to each other. Specifically, the zeroth component, $j^0 = \rho = -\frac{1}{3!}j_{\lambda\kappa\delta}\epsilon^{\lambda\kappa\delta 0} = +\frac{1}{3!}j_{\lambda\kappa\delta}\epsilon^{0\lambda\kappa\delta} = j_{123}\epsilon^{0123} = j_{123}$, is given by the weight function of the density form, Eq. (**??**), which we argued describes the particle density. Turning to the spatial components, $j^3 = -\frac{1}{3!}j_{\lambda\kappa\delta}\epsilon^{\lambda\kappa\delta 3} = -j_{012}\epsilon^{0123} = -j_{012}$ quantifies the current flow in 3-direction. Up to a sign, the above construction identifies it with the weight function j_{012} of the three-form (**??**) measuring the time dependent flow of particles through area elements in the 12-plane. In a similar manner, we obtain $j^2 = -j_{031}\epsilon^{0312} = -j_{031}$ and $j^1 = -j_{023}\epsilon^{0231} = -j_{023}$. This shows how the current flow in a certain direction (vector language) is related to the current flow through area elements perpendicular to that direction (form language).

As with the physical force discussed above, one may reason that the definition of current in terms of 'the number of particles flowing through an area per unit time' is more natural than that in terms of a 'vector pointing in the direction of current flow'. This is because *any* detector measures

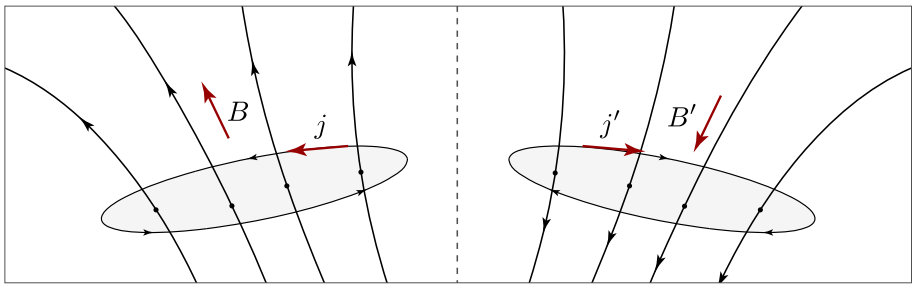


Figure V30: The magnetic field ('vector') $B \propto \operatorname{curl} j$ generated by a current density ('vector') j is not in fact a vector, since it does not transform in a contravariant manner. For example, under space reflection at a plane (indicated by the dashed line), the current vector reflects properly, but the magnetic field vector (computed according to the right hand rule familiar from introductory physics courses) reflects *and* changes sign. No contravariant vector would behave in this way. This is why the magnetic field is sometimes called an axial vector or a pseudovector.

flow by counting the number of particles per unit area. The form-definition of the current quantifies just this and therefore directly connects to experiment. On the other hand, the translation between experiment and the more traditional current=vector approach requires the excess baggage of a metric. We will return to this point in the next chapter when we discuss current flow in the context of electrodynamics.

V7 Case study: Differential forms and electrodynamics

REMARK This is not an introduction to electrodynamics. However, readers familiar with the subject at the level of an undergraduate experimental physics course should be able to follow the discussion. Starting from a summary of essential phenomenological facts, we will sketch the construction of differential equations (the Maxwell equations) encapsulating the laws of electrodynamics in the language of differential forms. For the benefit of readers familiar with the theory of electrodynamics, we will also compare to the standard vector field representation of Maxwell theory. In doing so, we will point out a number of advantages, both methodological and conceptual, of the differential form approach.

In this chapter, we will frequently compare vectors with their associated one- or two-forms. For example, the electric field, E, is described as a one-form or a vector, respectively. We will discriminate between the two objects by denoting differential forms by plain symbols (E) and the corresponding vectors by underlined symbols, $(\underline{E})$. As usual, the components of vectors and forms, E_i and E^i, respectively, are discriminated by the positioning of indices.

Throughout this chapter, the signature $(1,3)$ metric of space-time will play an important role. For convenience, we will work in a representation in which the metric assumes the form of the Minkovski metric, $\eta = \mathrm{diag}(1,-1,-1,-1)$, and we will denote coordinates by the symbols x^μ to highlight that an orthonormalized basis is used. (The usage of orthonormal coordinates facilitates the comparison of the vector and the form representation of the theory. The latter is manifestly coordinate invariant and the choice of coordinates is of secondary importance.)

James Clerk Maxwell 1831–79

Scottish theoretical physicist and mathematician. Amongst many other achievements, he is credited with the formulation of the theory of electromagnetism, synthesizing all previous unrelated experiments and equations of electricity, magnetism and optics into a consistent theory. (He is also known for creating the first true color photograph in 1861.)

In this chapter we will illustrate the power of exterior calculus in physics on the example of electromagnetism. The modern theory of electromagnetism was formulated in the nineteenth century by Maxwell, then in the language of vectors. Below, we will review the physical principles underlying these equations and then formulate them in the language of forms. Importantly, this is more than a change of language. The theory of electromagnetism is intimately related to that of relativity. In fact, it was the first 'relativistically invariant' theory, i.e. a theory compatible with transformations between coordinate systems moving relative to each other with velocities comparable to that of the speed of light. Central to Einstein's theory of relativity is the *metric* of space-time. Within special relativity, the Lorentz transformations stabilizing the Minkovski metric in the sense of Eq. (V200) describe how coordinates change between different systems, and in the later extension of general relativity the metric describes how space time acquires curvature due to the presence of masses. It is, therefore, evident that attention should be payed to the proper treatment of the metric in relativistic theories, and this is where the traditional description of electromagnetism fails.

Within the traditional approach, all physical quantities relevant to electromagnetism — electric and magnetic fields, and currents — are treated as vectors. However, the true identity of a physical quantity ultimately follows from a measurement protocol and in the case of electromagnetic fields and currents this means that they are all differential forms in space-time, not vectors. As discussed in previous chapters the translation to vectors requires the metric, and it only helps to complicate the mathematical formulation of the theory. Even more serious is the fact that the vectorial formulation obscures the role of the metric in a relativistically invariant context — one can never be sure if the appearance of a metric tensor is required for 'physical reasons' or only serves as a translational tool. That this way of teaching electrodynamics has not changed in the last 100 years likely is due to social inertia. At any rate, we hope that the exposition below helps to convince the reader that an alternative formulation, more in line with various modern developments in physics, is possible and certainly not more difficult than the traditional one.

V7.1 The ingredients of electrodynamics

In this section we introduce the essential ingredients of the theory of electromagnetism — space-time, charges and currents, and electromagnetic fields — both from a physical and a mathematical perspective. This will prepare the discussion of the next section where these building blocks are put in relation to each other.

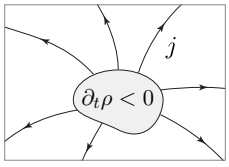
Space-time

The 'arena' in which classical electrodynamics is defined is flat space-time, i.e. the manifold $M = \mathbb{R}^4$ equipped with the signature $(1,3)$ Minkovski metric $\eta = \mathrm{diag}(1,-1,-1,-1)$. The arrangement of indices in this representation corresponds to a coordinate system $x = x^\mu = (x^0, x^1, x^2, x^3) \equiv (ct, x^1, x^2, x^3)$, where $x^0 = ct$, t is time, and c the speed of light, and x^i, $i = 1,2,3$ an orthonormal system of spatial coordinates. The theory defined on this manifold describes electromagnetism in the context of special relativity. As a side remark we note that the the extension to general relativity and the presence of gravitation requires the generalization of M to a curved space-time with a non-constant signature $(1,3)$ metric. While this represents a major complication, both physically and mathematically, the concept of Riemannian manifolds introduced above defines the proper mathematical framework to handle the situation.

Both, within the traditional and the exterior calculus approach we discriminate between a **relativistically invariant and a non-invariant representation of electrodynamics**. These standard denotations are not ideal because electrodynamics is compatible with the laws of relativity no matter how it is represented. The difference is that the 'invariant' formulation treats space and time on equal footings and is formulated on $(\mathbb{R}^4, \eta)$, i.e. space-time with Minkovski metric. The 'non-invariant formulation' splits $\mathbb{R}^4 = \mathbb{R} \times \mathbb{R}^3$ into a one-dimensional time-axis, and three-dimensional space. In this reading, $\mathbb{R}^3$ assumes the role of the relevant manifold, while time is a parameter. For example, the electric field, $\underline{E}(t,x)$ is a three-dimensional vector field on $\mathbb{R}^3$, depending on time, t, as a parameter, and the now *three-dimensional* spatial coordinate vectors $x = \{x^i\}$. (Within the invariant formulation, the electric field gets absorbed into an 'invariant' object, the field-strength tensor to be discussed below.) Keep in mind that when the non-invariant notation (t,x) appears, x is three-dimensional, while the coordinate $x = \{x^\mu\}$ of the invariant formulation contains time as $x^0 = ct$ and is four-dimensional.

Following the historical sequence of developments, we will first introduce the theory in its non-invariant version. Later in the section, we will then pass to the invariant reformulation.

Charges and currents



Charges and currents are the sources of electromagnetic fields. Within the current framework, the presence of charges and currents is described by the current three-form introduced on page 472. The three-form j and various of its descendants to be discussed momentarily are sometimes called **matter fields** because both charge densities and currents are tied to the presence of matter. (An electron carrying a negative unit-charge, for example.) The denotation stresses the difference to the electromagnetic fields, E, D, B, H which are immaterial.

An important feature of electromagnetism is the **conservation of charge**. This means that temporal changes in the charge density, $\partial_t \rho \neq 0$ must be compensated by the flow of currents. For example, if in a certain region of space, the charge density decreases this implies the presence of a net outward current, see the figure. Within the traditional approach,

this statement is made quantitative by the non-invariant form of the **current conservation relation**

$$-\frac{1}{c}\partial_t \rho = \nabla \cdot \underline{j},$$

i.e. a diminishing of charge is equivalent to the presence of sources in the three-component current vector field.

EXERCISE Gauss' theorem may be applied to transform the the differential relation above into a more intuitive integral relation. To this end, define the charge contained in a region of space as $Q = \int_V \mathrm{d}V\, \rho$, where we are using the syntax of standard vector analysis. If $\rho(t, x)$ depends on time then $Q = Q(t)$ becomes time dependent, i.e. the charge inside the volume is allowed to fluctuate. Apply the continuity relation and Gauss' theorem (V91) to verify that the rate of changes in Q is given by

$$\mathrm{d}_t Q = -\int_{\partial V} \mathrm{d}S \cdot \underline{j}, \tag{V223}$$

i.e. by the integral of the current over the surface ∂V of V. This shows how the loss of charge in the interior of the volume goes along with current flow through its surface.

Expressed in terms of the four-component current vector field $j = \{j^\mu\} = (\rho, j^1, j^2, j^3)$ introduced in the info section on p. 500 the continuity relation assumes the now relativistically invariant form $\partial_0 j^0 + \partial_i j^i = \partial_\mu j^\mu = 0$, where we noted $\partial_0 \rho = \partial_{x_0} \rho = \frac{1}{c}\partial_t \rho$.

To translate to the form language, we use the relation between the current vector and the current three-form Eq. (V222):

$$\partial_\mu j^\mu = \frac{1}{3!}\partial_\mu \epsilon^{\mu\nu\rho\sigma} j_{\nu\rho\sigma}.$$

Comparison with the component representation of the exterior derivative, Eq. (V175) shows that this equals the single component of the four-form, $\mathrm{d}j$. Within the exterior calculus approach, current the continuity relation thus assumes the compact form

$$\boxed{\mathrm{d}j = 0,} \tag{V224}$$

where j is the current three form Eq. (V161).

Within the non-invariant approach, charge density and current are described by a **density three form**, ρ' and a **current two-form**, j', respectively. These quantities are introduced via their relation to the invariant current three form, viz.

$$j = \rho' + j' \wedge \mathrm{d}t, \tag{V225}$$

where the r.h.s. *defines* ρ' and j'. The definition is made more explicit by writing the invariant j as $j = \sum_{\mu<\nu<\sigma} j_{\mu\nu\sigma} \mathrm{d}x^\mu \wedge \mathrm{d}x^\mu \wedge \mathrm{d}x^\sigma = \sum_{i<j} j_{0ij} \mathrm{d}x^0 \wedge \mathrm{d}x^i \wedge \mathrm{d}x^j + j_{123} \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3$. Comparison with the definition (V225) leads to the identification

$$\rho' \equiv \rho\, \mathrm{d}x^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}x^3, \qquad\qquad \rho = j_{123}$$

$$j' \equiv \frac{1}{2} j_{ij}\, \mathrm{d}x^i \wedge \mathrm{d}x^j, \qquad\qquad j_{ij} = j_{0ij}. \tag{V226}$$

The coefficients j_{ij} of the current two-form describe current flow through surface elements in the ij-plane in the same way as the coefficients $j_{0ij} = j_{ij}$ of the three-form. The splitting off of a factor $\mathrm{d}t$ in $j \wedge \mathrm{d}t$ merely is a matter of convenience that helps to formulate the non-invariant theory. To keep the notation simple we will write $j' = j$ and $\rho' = \rho$ when no confusion is possible, i.e. within the non-invariant approach, the density form is denoted by ρ and the current *two*-form by j. As an exercise verify that the current three-form continuity relation $\mathrm{d}j = 0$ assumes the form

$$\partial_t \rho + \mathrm{d}j = 0, \tag{V227}$$

when expressed in the density-current form decomposition.

We finally note that integration over the density and current density form yields form-language expressions for macroscopic charges and currents, respectively. Specifically, the **charge contained in a volume** V is defined as

$$\int_V \rho = Q, \tag{V228}$$

i.e. the integral of the current three-form over the volume. In cases where $\rho(t,x)$ is time dependent, $Q = Q(t)$ will depend on time as well. Similarly, the **current flowing through a two-dimensional surface** S is defined as

$$\int_S j = I, \tag{V229}$$

i.e. the integral of the two-form j over the surface. For time dependent current densities, $j(t,x)$, the current $I(t)$ becomes a function of time. The **macroscopic law of current conservation** now assumes the form

$$d_t Q = \int_V \partial_t \rho \overset{(V227)}{=} -\int_V \mathrm{d}j \overset{(V184)}{=} -\int_{\partial V} j = -I. \tag{V230}$$

This formula is the form-analog of the traditional relation Eq. (V223).

Electromagnetic fields

Electromagnetism is about the the mutual influence of charged matter — as described by the current three form — and electromagnetic fields. The non-invariant formulation of the traditional approach discriminates four fields, $\underline{E}, \underline{D}, \underline{B}, \underline{H}$, all three-component vector fields in space-time. Conceptually, these are vector fields defined on (the tangent bundle) of space, $\mathbb{R}^3$. Following the conventions of the present section, they should, therefore, be denoted as ∂_E, etc. However, this notation would be so alien to the traditional approach, that we prefer to use the more conventional $\underline{E}$. Likewise, we will write $\underline{E} = E^i \underline{e}_i$ (instead of $\partial_E = E^i \partial_{x^i}$) for the expansion of these fields in the coordinate basis. However, keep in mind that $\underline{E}$ keeps being a vector field in the sense of section **??**.

field	name	nature	degree	sector
E	electric field	electric	1	homogeneous
B	magnetic induction	magnetic	2	
D	displacement field	electric	2	inhomogeneous
H	magnetic field	magnetic	1	

Table V7.1: The four differential forms describing the electromagnetic fields within the framework of exterior calculus.

Within the exterior calculus approach, the same four objects are described by differential forms of degree one (E, H) and two (D, B). Both the physical meaning of these forms and their relation to the vector fields of the traditional approach will be discussed in section **??** after the fundamental laws of electromagnetism have been introduced. For the moment we just refer to table V7.1 where a number of essential features characterizing these forms are anticipated. Note that the fields can be organized in groups of two as indicated in the table. Specifically, the fields E, D are electric in nature, while D, H are magnetic. The fields E, B describe the influence of electromagnetic fields on matter, as discussed in section **??** while D, H are created via the reciprocal influence of charged matter on fields as discussed in section **??**. (In the table, this distinction is indicated by the labels homogeneous vs. inhomogeneous which emphasize that D, H will ber described by inhomogeneous differential equations in which matter-sources appear as inhomogeneities.)

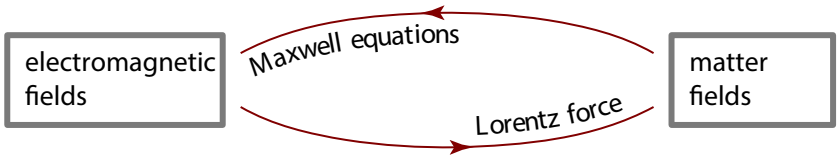


Figure V31: Maxwell theory describes the creation of fields by given distributions of charges and currents. Conversely, the Lorentz force describes the mechanical feedback of fields on charges via forces.

Having defined the basic constituents of the theory, we next discuss their interconnections via the the laws of electromagnetism. These laws describe how charged matter is affected by electromagnetic fields through a force called the Lorentz force. A second group of laws, known as the *inhomogeneous* Maxwell equations, describes the inverse influence, viz. the creation of fields by charges and currents (see Fig. V31). Third, the *homogeneous* Maxwell equations describe intrinsic relations between the fields. In the following we discuss these three groups of laws in turn.

V7.2 Laws of electrodynamics I: Lorentz force

Consider a point particle carrying charge q. If that particle is exposed to electric and/or magnetic field it will experience mechanical forces. In the following, we discuss these forces and

show how they *define* the electric and magnetic fields as one- and two-forms, respectively. We will then establish the connection to the traditional language where the fields are understood as vectors.

Electric and magnetic field forms

In the presence of an electric field the test particle experiences an **electrostatic force** whose magnitude is proportional to both the charge and the field strength. In form-language, this force is described by a one-form, $F_{\mathrm{E}} \in \Lambda^1(\mathbb{R}^3)$. The force *defines* the **electric field one-form** as $E = F/q \in \Lambda^1(\mathbb{R}^3)$, i.e. the electric field equals the acting force per charge. We may consider this statement a *definition* of the electric field.

If a magnetic field is present and the particle is in motion, it experiences a second force, the **magnetic force**, F_{M}. The magnitude of this force is proportional to the particle's charge and velocity, and to the magnetic field. As with the electric field, the magnetic field is defined through the work done against the Lorentz force in a displacement process. To this end, assume that the particle with its velocity vector $\partial_v = \underline{v}$ is displaced in motion by a vector $\partial_\Delta = \underline{\Delta}$.[1] Empirically, one finds that the work W required for this process is proportional to q, linear in $\underline{v}$ and $\underline{\Delta}$, and that it is antisymmetric under exchange of these arguments. This means that the work is described by the application of a two-form B to these arguments, $W = qB(\partial_v, \partial_\Delta)$. This work relation defines the **magnetic field two form**, B. Recalling the definition of the inner derivative, Eq. (L283), the work relation may be written as $W = q(i_{\partial_v} B)(\partial_\Delta)$, where the one form $i_{\partial_v} B$ is obtained by substitution of the argument ∂_v into the two form B. The ensuing one form $F_{\mathrm{M}} \equiv q i_{\partial_v} B$ defines the (velocity dependent) magnetic force, and its application to a displacement vector $F_{\mathrm{M}}(\partial_\Delta) = q(i_{\partial_v} B)(\partial_\Delta) = qB(\partial_v, \partial_\Delta)$ defines the magnetic work.

The total force acting on a particle in the presence of an electric and a magnetic field, $F_{\mathrm{E}} + F_{\mathrm{M}}$ is called the **Lorentz force**, and given by

$$\boxed{F = q\,(E + i_v B)\,.} \tag{V231}$$

INFO It can be instructive to **visualize the electric and magnetic field forms**. Following the conventions defined in Fig. L21(d)), the electric field, E, and the force form, F_{E}, can be represented through a pattern of parallel planes, as in Fig. V32. The work $E(\partial_\Delta)$ done along the displacement of a charge along a vector $\partial_\Delta = \underline{\Delta}$, is represented through the number of planes intersected by the (Cartesian representation of) the vector.

Similarly, the two-form B is represented by a pattern of parallel lines (cf. the rules defined in Fig. L21(c)). As indicated in Fig. **??**(b), the readout $B(\partial_v, \partial_\Delta)$ of the form on a pair of vectors, $\partial_v = \underline{v}$ and $\partial_\Delta = \underline{\Delta}$ is proportional to the number of flux lines penetrating the area defined by the vectors (cf. the indicated parallelogram). In line with this picture, the magnetic force one-form, F_M, is represented by a pattern of planes spanned by the vector $\underline{v}$ and the flux lines. This yields the work

[1] In experimental reality one would consider a thin current carrying wire such whose microscopic charge carriers move with drift velocity $\underline{v}$ along the wire axis. One would then study the work required to displace the wire by $\underline{\Delta}$.

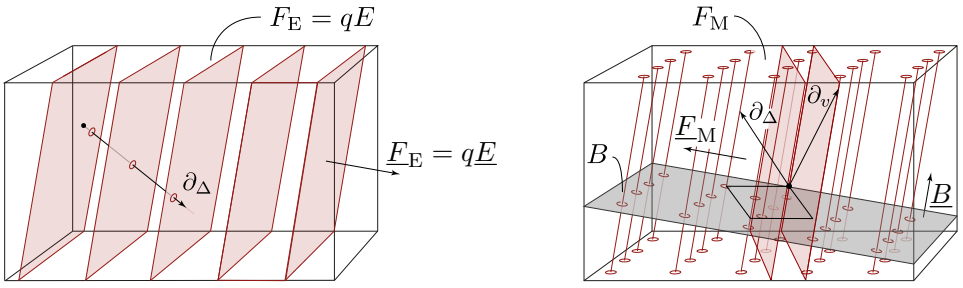


Figure V32: On the visualization of the electric field one-form, E, the two-form, B, and of the corresponding force forms $F_{\mathrm{E}}, F_{\mathrm{M}}$. The figure also indicates the orientation of the corresponding vectors of the traditional approach. Further discussion, see text.

to be done against the force under a displacement, $F_{\mathrm{M}}(\partial_\Delta) = B(\partial_v, \partial_\Delta)$, as the number of planes intersected by ∂_Δ.

Generally speaking, visualizations of this type can facilitate the qualitative understanding of a situation. However, they usually appear as doodle sketches and are not used as elements of quantitative constructions.

Vectorial definition of electric and magnetic forces

In traditional language, both the electric and the magnetic field are described by three-component vector fields $\underline{E}$ and $\underline{B}$ in the tangent bundle $T\mathbb{R}^3$. The **electric field** $\underline{E}$ is dual to the one-form E under the metric isomorphism $\underline{F}_{\mathrm{E}} = J^{-1}(F_{\mathrm{E}})$ and $\underline{E} = J^{-1}(E)$. Notice that the (Minkovski) metric enters the translation. This is important inasmuch as the measurement of forces defines a form, not a vector, i.e. physically, the form is more 'fundamental' than its vector dual, cf. discussion on p. 500. We thus encounter the first case where the vectorial language obscures the role of the metric. (Later in our discussion of the Maxwell equations we will see that there is only one instance where the metric is truly needed for physical reasons, viz. in the definition of the relation between the fields (E, B) and (D, H).)

In a **component language**, the electric field form and its associated vector are represented as

$$E = E_i \mathrm{d}x^i, \qquad \underline{E} = E^i \underline{e}_i, \qquad E^i = \eta^{ij} E_j = -E_i,$$

where $\underline{e}_i \equiv \partial_{x^i}$ are orthonormal coordinate basis vectors, and $E_i(t,x)$ and $E_i(t,x)$ are coefficients generally depending on space and time. The translation between vector and form coefficients, $E^i = \eta^{ij} E_j = -E_i$, follows from table V6.1 applied to the case $g_{ij} = \eta_{ij} = (-1)\delta_{ij}$. Here, the global sign change is of secondary importance.[2] By definition, the readout of the form on a displacement vector is then represented as $E_i \Delta^i = E^i \eta_{ij} \Delta^j$, i.e. as the scalar

[2] As some authors do, we might have redefined the metric as as $-\eta = \mathrm{diag}(-1,1,1,1)$. This would not affect the physics and make the relative sign go away. (Sign factors would then appear in the temporal sector of the theory.)

product $g(\underline{E}, \underline{\Delta}) = \eta(\underline{E}, \underline{\Delta})$ of the vectors $\underline{E}$ and $\underline{\Delta}$. This is equivalent to the statement that the vector $\underline{E}$ stands perpendicular on the planes representing the form E. (Make sure you understand this statement graphically.)

According to our discussion of section V6.4, the vector $\underline{B}$ canonically assigned to the two-form B is given by $\underline{B} = \partial_B = J^{-1}(*B)$. In a component representation we have (cf. table V6.1[3])

$$B = \frac{1}{2} B_{ij} \mathrm{d}x^i \wedge \mathrm{d}x^j, \qquad \underline{B} = B^i \underline{e}_i, \qquad B^i = \frac{1}{2} \epsilon^{ijk} B_{jk}. \tag{V232}$$

The vector corresponding to the magnetic force form, $F_{\mathrm{M}} = q i_{\partial_v} B = q B_{ij} v^i \mathrm{d}x^j$ is given by $\underline{F}_{\mathrm{M}} = J^{-1}(F_{\mathrm{M}}) = q B_{ij} v^i \eta^{jk} \underline{e}_k$. Using that (check!) $B_{ij} = \epsilon_{ijl} B^l$, this can be written as $\underline{F}_{\mathrm{M}} = -q \epsilon_{ijl} B^l v^i \underline{e}_j = q \underline{v} \times \underline{B}$. We thus conclude that the **Lorentz force in conventional language** is given by

$$\underline{F} = q(\underline{E} + \underline{v} \times \underline{B}).$$

V7.3 Laws of electrodynamics II: Maxwell equations

The Lorentz force describes the influence of electric and magnetic fields on charged particles (more generally, charged 'matter'). Conversely, the Maxwell equations describe the creation of electric and magnetic fields by charges and currents. Maxwell's equations are a set of four first-order linear partial differential equations for the fields E, D, B, H. They can be grouped into two sets of two, where the first group, the *homogeneous* Maxwell equations describe intrinsic connections between the fields E and B. The second group, the *inhomogeneous* equations describe how the fields D and H are created by charges and currents as represented by the forms ρ and j. At this level the two groups are independent, and they do not depend on the metric (as long as they are formulated in form–, rather than vector–language). The metric enters the stage, when the connections between the fields E and D (B and H) are considered. These fields are coupled through (non-differential) equations which need to be included into the framework on top of the Maxwell equations. In vacuum, the connection between the one form E (H) and the two-form D (B) is provided by the Hodge star, and it assumes a trivial form if an orthonormal system is used. The situation becomes more complicated in extended media, where microscopic properties of the host medium affect the coupling relations. This complication, which is the subject of **macroscopic electrodynamics**, will not be addressed in this text, i.e. we consider vacuum electrodynamics throughout.

In the next section we will substantiate this synopsis and construct Maxwell's equations out of experimental observations of electrodynamics.

INFO For later reference, we state **Maxwell's equation in their traditional form**, as taught in standard courses of electromagnetism. Here, the theory is formulated in terms of four vector fields,

[3] The formulas of the table apply to a positive metric, $g > 0$. For an indefinite metric such as the Minkovski metric we need to replace $\sqrt{g} \to \sqrt{|g|} = \sqrt{|\eta|} = 1$.

the electric field $\underline{E}$, the magnetic induction $\underline{B}$, the electric displacement field $\underline{D}$, and the magnetic field $\underline{H}$. These fields are created by electric charge densities, ρ and/or current densities $\underline{j}$. All constituents of the theory are functions of space and time, i.e. $\underline{X} = \underline{E}, \underline{D}, \underline{B}, \underline{H}, \underline{j}$ are vector fields $\underline{X} : \mathbb{R} \otimes \mathbb{R}^3 \to \mathbb{R}^3$, $(t, x) \mapsto \underline{X}(t, x)$, and $\rho : \mathbb{R} \otimes \mathbb{R}^3 \to \mathbb{R}$, $(t, x) \mapsto \rho(t, x)$ is a scalar field.

The connection between matter fields $(\rho, \underline{j})$ and electromagnetic fields is established by the Maxwell equations,[4]

$$\begin{aligned} \nabla \cdot \underline{D} &= 4\pi\rho, \\ \nabla \times \underline{H} - \frac{1}{c}\partial_t \underline{D} &= \frac{4\pi}{c}\underline{j}, \\ \nabla \cdot \underline{B} &= 0, \\ \nabla \times \underline{E} + \frac{1}{c}\partial_t \underline{B} &= 0, \end{aligned} \tag{V233}$$

where c is the speed of light. Here, the first two are the inhomogeneous equations and the second two the homogeneous ones. These equations need to be augmented with relations connecting the sets (E, B) and (D, H). In vacuum, these are the simple identifications, $\underline{E} = \underline{D}$, $\underline{B} = \underline{H}$.[5]

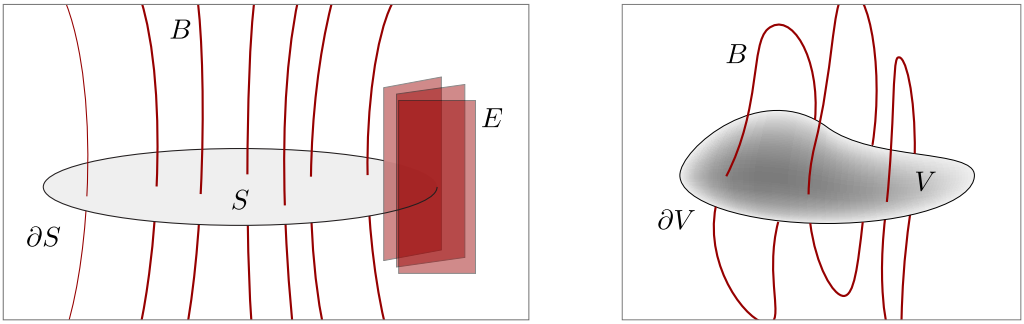


Figure V33: The 'homogeneous' laws of electromagnetism. Left – the law of induction: integration of the electric one form E (indicated by shaded planes) over a closed curve ∂S bounding a surface S equals the integral of the negative time derivative, $-\partial_t B$, of the magnetic induction-two form over S. Right – the absence of magnetic charges: integration of the magnetic induction two-form B over a closed surface equals zero; lines characterizing the form are closed, indicating that the field has no sources.

[4] We here use so called CGS units. In other systems of units, for example the SI system, the equations assume a form which differs from the present one regarding constant prefactors for some terms.

[5] The constants appearing in the Maxwell equations depend on the used system of units. The absence of proportionality constants between $\underline{E}$ ($\underline{B}$) and $\underline{D}$ ($\underline{H}$) is a specialty of the so-called CGS units used here. For a discussion of the situation in other systems of units we refer to physics texts.

Homogeneous Maxwell equations

Empirically, we know that there are no 'magnetic charges'. In form language, the **absence of magnetic charges** means that the integration of the field two-form B over the surface ∂V of any region in space V yields zero,

$$\int_{\partial V} B = 0, \tag{V234}$$

i.e. there is no net outward magnetic flux. The situation is illustrated in the right panel of Fig. V33 where the two-form B is represented through *closed* field lines

By Stokes' theorem, this can be written as as a volume integral, $\int_{\partial V} B = \int_V \mathrm{d}B.$. The vanishing of this integral for any volume requires the closedness of the magnetic field form,

$$\boxed{\mathrm{d}B = 0.} \tag{V235}$$

This is the first of the two homogeneous Maxwell equations. Translated to vector language, it states that the magnetic induction $\underline{B}$ is a vector field without sources, cf. the third of Eqs. (V233).

EXERCISE Apply the relations of table (V6.1) to express the magnetic field two-form through its corresponding vector components. Then use the expression for the divergence of a vector field, Eq. (V216) to derive the third of the the traditional Maxwell equations.

The second homogeneous Maxwell equation expresses the **law of induction**: if a surface is threaded by a time-dependent magnetic field, B, an electric field winding around the surface is induced (see Fig. V33 left). Experiment shows that the integral of the field around the curve bounding the surface, $\int_{\partial S} E$, (i.e. the mechanical work required to drag a unit charge, $q = 1$, around the curve) equals the negative of the time derivative of the 'magnetic flux', $\int_S B$, through the surface,

$$\int_{\partial S} E + \frac{1}{c}\frac{\mathrm{d}}{\mathrm{d}t}\int_S B = 0. \tag{V236}$$

Applying Stokes' law to the first integral, and pulling the time derivative into the integral (the surface itself is static), we obtain $\int_S (\mathrm{d}E + c^{-1}\partial_t B) = 0$.[6] Once more, the validity of this relation for any integration domain implies the vanishing of the integrand,

$$\boxed{\mathrm{d}E + \frac{1}{c}\partial_t B = 0.} \tag{V237}$$

This is the second homogeneous Maxwell equation.

[6] We repeat that $\partial_t B = \partial_t \frac{1}{2} B_{ij}(x,t)\mathrm{d}x^i \wedge \mathrm{d}x^j$ acts on the time dependence of the form-coefficients as an ordinary partial derivative.

EXERCISE Using the vector representations of B and E, and the coordinate representation of the curl, Eq. (V218), show the that this equation translates to the fourth Maxwell equation in vector language.

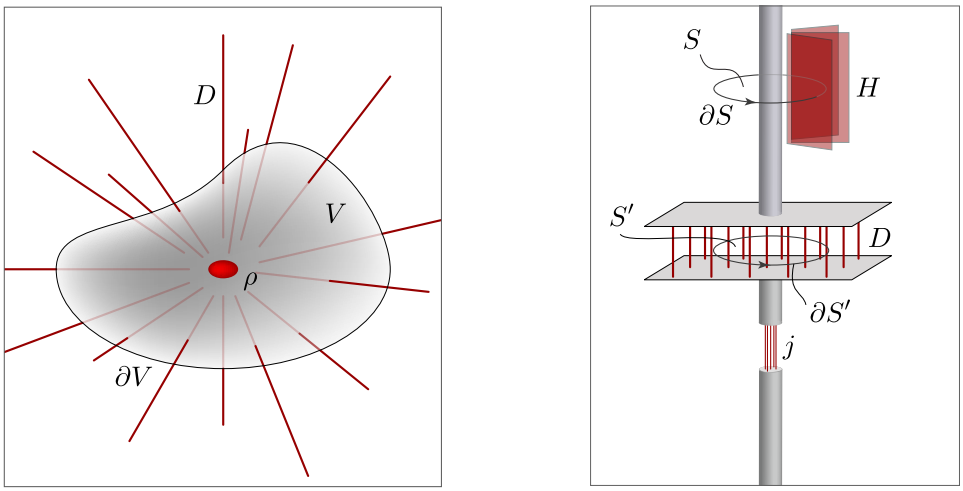


Figure V34: The 'inhomogeneous' laws of electromagnetism. Left – the law of Gauß: an electric charge density three-form, ρ, generates an electric displacement field, D. Integration of D over any closed surface equals the integral of ρ over the volume enclosed by the surface. Right – the law of Ampère-Maxwell: current flow described by a non-vanishing two-form, j, generates a magnetic field one-form, H, and/or a electric displacement field one-form, D. Empirically it is found tht the integral of the sum $H - \frac{1}{c}\partial_t D$ over a closed curve bounding a surface (such as S or S' in the figure) equals the integral of j over that surface.

Inhomogeneous Maxwell equations

The inhomogeneous equations describe the creation of the fields D, H by charges and currents. **Gauss' law**[7] states that electric charge is the source of the electric displacement field (see Fig. V34 right): The integral $\int_{\partial V} D$ of D over the surface ∂V of a volume V equals (4π) times the total charge $Q = \int_V \rho$ included in V, i.e.

$$\int_{\partial V} D = 4\pi \int_V \rho.$$

Once more we apply Stokes' theorem, $\int_V (\mathrm{d}D - 4\pi\rho) = 0$, to conclude that

$$\boxed{\mathrm{d}D = 4\pi\rho.} \tag{V238}$$

Finally, the law of **Ampère-Maxwell** states that electric current flow creates a magnetic field H and/or a time varying electric displacement field D. The relation is such that (see Fig. V34

[7] This is Gauss' law of physics which must not be confused with Gauss' theorem of mathematics Eq. (V91).

left) the integral $\int_{\partial S} H$ of the one-form H over the curve ∂S bounding a surface S is equal to the sum of $4\pi/c$ times the current flow through that surface, $4\pi I/c = \frac{4\pi}{c}\int_S j$, and c^{-1} times the time derivative $\frac{1}{c}\mathrm{d}_t \int_S D$ of the integral of the two-form D over the same surface:[8]

$$\int_{\partial S} H = \frac{4\pi}{c}\int_S j + \frac{1}{c}\int_S \partial_t D.$$

Once more, we apply Stokes' theorem to conclude that

$$\boxed{\mathrm{d}H - \frac{1}{c}\partial_t D = \frac{4\pi}{c} j.} \tag{V239}$$

EXERCISE Apply the same steps as in the context of the homogeneous Maxwell equations to translate the form-representation of Maxwell's equations to the inhomogeneous equations of the vectorial formulation, Eq. (V233).

Invariant formulation

Above, we have formulated Maxwell's equation in terms of forms defined in three-dimensional space $\mathbb{R}^3$. Time entered through the time dependence of the coefficient functions. To proceed towards a more 'invariant' formulation defined in space time, $\mathbb{R}^4 = \mathbb{R}\otimes\mathbb{R}^3$, we now introduce the two-forms

$$\begin{aligned} F &\equiv E\wedge \mathrm{d}x^0 + B, \\ G &\equiv -H\wedge \mathrm{d}x^0 + D. \end{aligned} \tag{V240}$$

The form F is called the **field strength tensor**, and G is called the **dual field strength tensor**. Note that F and G contain the forms appearing in the homogeneous and inhomogeneous Maxwell equations, respectively. At this point, these structures remain decoupled.

Specifically, we may rewrite the homogeneous Maxwell equations Eqs. (V235) and (V237) as $\mathrm{d}^s B = 0$ and $\mathrm{d}^s E + \partial_{x^0} B = 0$, where we temporarily use the symbol $\mathrm{d}^s(\dots) = \partial_i(\dots)\,\mathrm{d}x^i$ for the exterior derivative in three-dimensional space, i.e. in the space-like sector of the theory. The partial derivative $c^{-1}\partial_t = \partial_{x^0}$ differentiates w.r.t. the time-like coordinate. We now consider the full space-time exterior derivative which acts as $\mathrm{d}(\dots) = \mathrm{d}^s(\dots) + \partial_{x^0}(\dots)\mathrm{d}x^0$. With these conventions we obtain $\mathrm{d}F = (\mathrm{d}^s E\wedge \mathrm{d}x^0 + \mathrm{d}^s B + \partial_t B\wedge \mathrm{d}x^0 = (\mathrm{d}^s E + \partial_t B)\wedge \mathrm{d}x^0 + \mathrm{d}^s B = 0$, i.e. the two homogeneous Maxwell equations are equivalent to the **closedness of the field strength form**, $\mathrm{d}F = 0$.

[8] To understand the conspiracy of current and displacement field, recall that a time-varying current in a wire may be 'interrupted' by the insertion of capacitor plates, as shown in the figure. No electric current flows between the plates of the capacitor. Instead, we observe a time-varying field of electric origin between the plates, the displacement field. Both the displacement field and the electric current create a magnetic field winding around the wire/capacitor setup.

Likewise, we recall the definition of the full **current-three form** Eq. (V225), $j \equiv \rho' + \frac{1}{c} j' \wedge \mathrm{d}x^0$, in terms of the current two-form j' and the density form ρ', where we re-introduced primes to discriminate the non-invariant quantities from the invariant three form. . The two inhomogeneous Maxwell equations can now be combined to the relation $\mathrm{d}G = (-\mathrm{d}^s H + \partial_t D) \wedge \mathrm{d}x^0 + \mathrm{d}^s D = \frac{4\pi}{c} j' \wedge \mathrm{d}x^0 + 4\pi\rho' = 4\pi j$. Summarizing, we have managed to represent Maxwell's equations in the compact, and manifestly space-time invariant form

$$\boxed{\begin{aligned} \mathrm{d}F &= 0, \\ \mathrm{d}G &= 4\pi j, \end{aligned}} \tag{V241}$$

It is remarkable that the Maxwell equations, which describe such a diverse range of physical phenomena, can be represented in a form of this degree of compactness.

Electrodynamics and Minkovski metric

So far, the fields E, B and D, H entering the homogeneous and the inhomogeneous Maxwell equations, respectively, remained completely decoupled. The connection between these fields follows from the empirical observation that in vacuum and in an orthonormal coordinate system,

$$E_i = \frac{1}{2}\epsilon_{ijk} D_{jk}, \qquad H_i = \frac{1}{2}\epsilon_{ijk} B_{jk}, \tag{V242}$$

i.e. the components of the electric field equal those of the displacement field, and the components of the magnetic field equal those of the magnetic induction. The structure of these equations suggests that a *Hodge star* is at work.

To better understand this point, note that the application of Eq. (V206) to the wedge product of coordinate forms $\mathrm{d}x^\mu$ with diagonal metric $g_{\mu\nu} = \eta_{\mu\nu}$ yields $*(\mathrm{d}x^\mu \wedge \mathrm{d}x^\nu) = \frac{1}{2}\eta^{\mu\alpha}\eta^{\nu\beta}\epsilon_{\alpha\beta\gamma\delta}\mathrm{d}x^\gamma \wedge \mathrm{d}x^\delta$. Specifically, for $\mu = i$ and $\nu = 0$ we obtain

$$*(\mathrm{d}x^i \wedge \mathrm{d}x^0) = \tfrac{1}{2}\eta^{ii}\eta^{00}\epsilon_{i0jk}\,\mathrm{d}x^j \wedge \mathrm{d}x^k = -\tfrac{1}{2}\epsilon_{i0jk}\,\mathrm{d}x^j \wedge \mathrm{d}x^k = \tfrac{1}{2}\epsilon_{ijk}\,\mathrm{d}x^j \wedge \mathrm{d}x^k,$$

where $-\varepsilon_{i0jk} = \varepsilon_{0ijk} = \varepsilon_{ijk}$ was used. In a similar manner we find $*(\mathrm{d}x^i \wedge \mathrm{d}x^j) = -\epsilon_{ijk}\mathrm{d}x^k \wedge \mathrm{d}x^0$. Using these relations, the Hodge star may be applied to $F \overset{(V240)}{=} E_i \mathrm{d}x^i \wedge \mathrm{d}x^0 + \frac{1}{2}B_{ij}\mathrm{d}x^i \wedge \mathrm{d}x^j$ to obtain $*F = \frac{1}{2}E_i\epsilon_{ijk}\mathrm{d}x^j \wedge \mathrm{d}x^k - \frac{1}{2}B_{ij}\epsilon_{ijk}\mathrm{d}x^k \wedge \mathrm{d}x^0 \overset{(V242)}{=} \frac{1}{2}D_{jk}\mathrm{d}x^j \wedge \mathrm{d}x^k - H_k \mathrm{d}x^k \wedge \mathrm{d}x^0 \overset{(V240)}{=} G$. In this way the important identification

$$\boxed{*F = G,} \tag{V243}$$

is established. Eqs. (V241) and (V243) provide a complete description of the laws of classical electromagnetism. Although these equations are coordinate independent, the connections between the components of F and G assume a simple form only in systems with orthonormal metric, $g = \eta$. The coordinate transformations preserving this form of the metric are the Lorentz transformations (V200).[9]

[9] More generally, shifts of the coordinate origin, $x \to x + a$, $a \in \mathbb{R}^4$ also preserve the form of the equations. The generalized set of coordinate transformations, $x' = \Lambda x + a$, $\Lambda \in \mathrm{O}(1,3)$ defines the **Poincaré group**.

V7.4 Summary and Outlook

This concludes our survey of electrodynamics in form language. Given the scope of this text, our discussion had to focus on fundamental structures, rather than applications (but see the exercises xx). Starting with a survey of experimental observations, we have discussed the laws of electrodynamics first in the original non-invariant formulation and finally in a manifestly Lorentz invariant form. Incidentally, one may wonder how the '**traditional formulation**' of the invariant approach to electrodynamics looks like. The answer is that it does not really exist. The description of the theory in terms of four three-component vector fields $\underline{E}, \underline{B}, \underline{D}, \underline{H}$ is tailored to the separate treatment of space and time and has no good invariant extension. Even in traditional teaching it is standard to formulate the invariant approach in terms of tensor components $F_{\mu\nu}$, $G_{\mu\nu}$. These tensors are introduced as 4×4-matrices (but notice that they are contravariant tensors of degree $(0, 2)$, rather than proper 'matrices' which have degree $(1, 1)$ and one index upstairs) containing the components of $\underline{E}$ and $\underline{B}$ or $\underline{D}$ and $\underline{H}$ as entries. This, and all other operations are generally carried out in a coordinate heavy way. For example, the homogeneous Maxwell equation is written as $\partial_\sigma F_{\mu\nu} + \partial_\mu F_{\nu\sigma} + \partial_\nu F_{\sigma\mu}$ instead of $\mathrm{d}F = 0$. In this way, differential forms are effectively introduced but not discussed as such. Put differently, the proper Lorentz invariant formulation requires the introduction of forms and the abandoning of the all–is–vector dogma.

There remains the intersting difference that in physics texts theories such as electrodynamics (or special and general relativity) are almost categorically discussed in coordinates $(F_{\mu\nu})$ rather than in invariant language (F). The longevity of this tradition surely has to do with the fact that practical computations are generally done in coordinates. It is then tempting 'not to pay the price' to learn what a differential form is and to work with the formally introduced objects $F_{\mu\nu}$ from the outset. At the same time, one may argue that the invariant formulation is much stronger where it comes to understanding the basic structures of the theory, its connections to other disciplines, or its mathematical foundations.

Which language to prefer ultimately remains a matter of taste and personal inclination. The reason why an introduction to differential forms has been included in this text is the empirical observation that their application in physics is on the rise and that future generations of physicists may likely need this concept as part of their standard portfolio.

PV Problems: Vector Calculus

The solutions to odd-numbered problems are given in part S, section SV. Lecturers can obtain the solutions to even-numbered problems from the publishers by request.

P.V1 Curves

P.V1.2 Curve velocity

EV1.2.1 Velocity and acceleration

Consider the curve $\gamma = \{\mathbf{r}(t)\,|\,t \in (0, 2\pi/\omega)\}$, $\mathbf{r}(t) = (aC(t), S(t))^T \in \mathbb{R}^2$, with $C(t) = \cos[\pi\,(1 - \cos\omega t)]$, $S(t) = \sin[\pi((1 - \cos\omega t)]$, and $0 < a, \omega \in \mathbb{R}$.

(a) Calculate the curve's velocity vector, $\dot{\mathbf{r}}(t)$ and it's acceleration vector $\ddot{\mathbf{r}}(t)$. Can $\mathbf{r}(t)$ be expressed in terms of $\dot{\mathbf{r}}(t)$ and $\ddot{\mathbf{r}}(t)$?

(b) Can you represent the curve without the parameter t using an equation? Do you recognize the curve? Sketch the curve for the case $a = 2$.

(c) Calculate $\mathbf{r}(t) \cdot \dot{\mathbf{r}}(t)$. For which values of a is $\mathbf{r}(t) \cdot \dot{\mathbf{r}}(t) = 0$ true for all t?

PV1.2.2 Velocity and acceleration

Consider the curve $\gamma = \{\mathbf{r}(t)\,|\,t \in (-\infty, \infty)\}$, $\mathbf{r}(t) = (\mathrm{e}^{-t^2}, a\mathrm{e}^{t^2})^T \in \mathbb{R}^2$, with $0 < a \in \mathbb{R}$ ($0 < a < 1$ for (c)).

(a) Calculate the curve's velocity vector, $\dot{\mathbf{r}}(t)$, and it's acceleration vector $\ddot{\mathbf{r}}(t)$. Can $\mathbf{r}(t)$ be expressed in terms of $\dot{\mathbf{r}}(t)$ and $\ddot{\mathbf{r}}(t)$?

(b) Can you represent the curve without the parameter t using an equation? Do you recognize the curve? Sketch the curve for the case $a = 2$.

(c) Calculate $\mathbf{r}(t) \cdot \dot{\mathbf{r}}(t)$. Find the time $t(a)$, for which $\mathbf{r}(t) \cdot \dot{\mathbf{r}}(t) = 0$ holds. [Check your result: $t(\mathrm{e}^{-2}) = \pm 1$.]

P.V1.3 Curve length

EV1.3.1 Natural parametrization of a curve

Consider the curve $\mathbf{r}(t) = (t - \sin t, 1 - \cos t)^T \in \mathbb{R}^2$ for $t \in (0, 2\pi)$.

(a) Sketch the curve qualitatively.

(b) Determine it's arc length $s(t)$ in the time interval $(0, t)$. [Check your answer: $s(2\pi) = 8$.]

(c) Find the natural parametrization $\mathbf{r}_L(s)$. [Check your answer: $\mathbf{r}_L(4) = (\pi, 2)^T$.]

PV1.3.2 Natural parametrization of a curve

Consider the curve $\gamma = \{\mathbf{r}(t) \,|\, t \in (0, \tau)\}$, $\mathbf{r}(t) = \mathrm{e}^{ct}(\cos\omega t, \sin\omega t)^T \in \mathbb{R}^2$, with $c \in \mathbb{R}$.

(a) Sketch the curve for the case of $\tau = 8\pi/\omega$ and $c = 1/\tau$. [This information only applies to part (a), not for parts (b-f).]

(b) Calculate the magnitude of the velocity curve, $\|\dot{\mathbf{r}}(t)\|$.

(c) Calculate the arc length $s(t)$ in the time interval $(0, t)$.

(d) Determine the natural parametrization $\mathbf{r}_L(s)$.

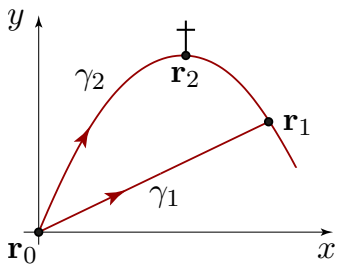
(e) Check explicitly that $\left\| \frac{\mathrm{d}\mathbf{r}_L}{\mathrm{d}s} \right\| = 1$.

[Check your answer: for $c = \omega = \tau = 1$: (b) $\sqrt{2}\mathrm{e}^t$, (c) $\sqrt{2}(\mathrm{e}^t - 1)$, (d) $\mathbf{r}_L(s) = [s/\sqrt{2} + 1]\left(\cos[\ln(s/\sqrt{2} + 1)], \sin[\ln(s/\sqrt{2} + 1)]\right)^T$.]

P.V1.4 Line integral

EV1.4.1 Line integral: mountain hike

Two hikers want to hike from the point $\mathbf{r}_0 = (0, 0)^T$ in the valley to a hut at the point $\mathbf{r}_1 = (3, 3a)^T$. Hiker 1 chooses the straight path from valley to hut, γ_1. Hiker 2 chooses a parabolic path, γ_2, via the mountain top at the apex of the parabola, at $\mathbf{r}_2 = (2, 4a)^T$ (see figure). They are acted on by the force of gravity $\mathbf{F}_g = -10\,\mathbf{e}_y$, and a height-dependent wind force, $\mathbf{F}_w = -y^2\,\mathbf{e}_x$.



Find the work, $W[\gamma_i] = -\int_{\gamma_i} \mathrm{d}\mathbf{r} \cdot \mathbf{F}$, performed by the hikers along γ_1 and γ_2, as function of the parameter a. [Check your results: for $a = 1$ one finds $W[\gamma_1] = 39$, $W[\gamma_2] = 303/5$.]

PV1.4.2 Line integrals in Cartesian coordinates

Let $\mathbf{F}(\mathbf{r}) = (x^2, z, y)^T$ be a three-dimensional vector field in Cartesian coordinates, with $\mathbf{r} = (x, y, z)^T$. Calculate the line integral $\int_\gamma \mathrm{d}\mathbf{r} \cdot \mathbf{F}$ along the following paths from $\mathbf{r}_0 \equiv (0, 0, 0)^T$ to $\mathbf{r}_1 \equiv (0, -2, 1)^T$:

(a) $\gamma_a = \gamma_1 \cup \gamma_2$ is the composite path consisting of γ_1, the straight line from $\mathbf{r}_0$ to $\mathbf{r}_2 \equiv (1, 1, 1)^T$, and γ_2, the straight line from $\mathbf{r}_2$ to $\mathbf{r}_1$.

(b) γ_b is parametrized by $\mathbf{r}(t) = (\sin(\pi t), -2t^{1/2}, t^2)^T$, with $0 < t < 1$.

(c) γ_c is a parabola in the y-z-plane with the form $z(y) = y^2 + \frac{3}{2}y$.

[Check your results: the sum of the answers from (a), (b) and (c) is -6.]

P.V2 Curvilinear Coordinates

P.V2.1 Polar coordinates

EV2.1.1 Coordinate transformations

Consider three points whose Cartesian coordinates (x, y, z) are P_1: $(3, -2, 4)$, P_2: $(1, 1, 1)$ and P_3: $(-3, 0, -2)$. What is the representation of these three points in cylindrical coordinates, (ρ, ϕ, z), and in spherical coordinates, (r, θ, ϕ)? (Give the angles in radians.)

PV2.1.2 Coordinate transformations

The point P_1 has spherical coordinates $(r, \theta, \phi) = (2, \pi/6, 2\pi/3)$. What are its Cartesian and cylindrical coordinates, (x, y, z) and (ρ, ϕ, z), respectively? The point P_2 has cylindrical coordinates $(\rho, \phi, z) = (4, \pi/4, 2)$. What are its Cartesian and spherical coordinates? (Give the angles in radians.)

P.V2.2 Coordinate transformations

P.V2.3 Coordinate basis and local basis

P.V2.4 Cylindrical and spherical coordinates

EV2.4.1 Cylindrical coordinates: velocity, kinetic energy, angular momentum

The relation between Cartesian and cylindrical coordinates is given by: $x = \rho\cos\phi$, $y = \rho\sin\phi$, $z = z$, with $\rho \in (0, \infty)$, $\phi \in (0, 2\pi)$, $z \in (-\infty, \infty)$.
Basis vectors: Construct the basis vectors for cylindrical coordinates, $\{\mathbf{e}_{y_i}\} = \{\mathbf{e}_\rho, \mathbf{e}_\phi, \mathbf{e}_z\}$, and show explicitly that they have the following properties:
(a) $\mathbf{e}_{y_i} \cdot \mathbf{e}_{y_j} = \delta_{ij}$ and (b) $\mathbf{e}_{y_i} \times \mathbf{e}_{y_j} = \varepsilon_{ijk}\mathbf{e}_{y_k}$.
Physical quantities: Show that in cylindrical coordinates (c) the velocity vector $\mathbf{v} = \frac{d}{dt}\mathbf{r}$,

(d) the kinetic energy $T = \frac{1}{2}m\mathbf{v}^2$ and (e) the angular momentum $\mathbf{L} = m(\mathbf{r} \times \mathbf{v})$ have the following forms:

$$\begin{aligned} \mathbf{v} &= \dot\rho\,\mathbf{e}_\rho + \rho\dot\phi\,\mathbf{e}_\phi + \dot z\,\mathbf{e}_z, \qquad T = \tfrac{1}{2}m\big[\dot\rho^2 + \rho^2\dot\phi^2 + \dot z^2\big], \\ \mathbf{L} &= m\big[-z\rho\dot\phi\,\mathbf{e}_\rho + (z\dot\rho - \rho\dot z)\,\mathbf{e}_\phi + \rho^2\dot\phi\,\mathbf{e}_z\big]. \end{aligned}$$

PV2.4.2 Cylindrical coordinates: velocity, kinetic energy, angular momentum

The relationship between Cartesian and spherical coordinates is given by: $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$, with $r \in (0,\infty)$, $\phi \in (0, 2\pi)$, $\theta \in (0,\pi)$.
Basis vectors: Construct the basis vectors for spherical coordinates, $\{\mathbf{e}_{y_i}\} = \{\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\phi\}$, and show explicitly that
(a) $\mathbf{e}_{y_i} \cdot \mathbf{e}_{y_j} = \delta_{ij}$ and (b) $\mathbf{e}_{y_i} \times \mathbf{e}_{y_j} = \varepsilon_{ijk}\,\mathbf{e}_{y_k}$.
Physical quantities: Show that in spherical coordinates (c) the velocity vector $\mathbf{v} = \frac{d}{dt}\mathbf{r}$, (d) the kinetic energy $T = \frac{1}{2}m\mathbf{v}^2$ and (e) the angular momentum $\mathbf{L} = m(\mathbf{r} \times \mathbf{v})$ are as follows:

$$\mathbf{v} = \dot r\,\mathbf{e}_r + r\,\dot\theta\mathbf{e}_\theta + r\dot\phi\sin\theta\,\mathbf{e}_\phi, \quad T = \tfrac{1}{2}m\big[\dot r^2 + r^2\dot\theta^2 + r^2\dot\phi^2\sin^2\theta\big], \quad \mathbf{L} = mr^2\big[\dot\theta\,\mathbf{e}_\phi - \dot\phi\sin\theta\,\mathbf{e}_\theta\big].$$

EV2.4.3 Line integral in polar coordinates: spiral

The curve $\gamma_S = \{\mathbf{r}(\rho,\phi) \in \mathbb{R}^2 |\ \rho = R + \frac{1}{2\pi}\phi\Delta,\ \phi \in (0, 2\pi)\}$, with $0 < R, \Delta \in \mathbb{R}$, describes a spiral path in two dimensions, parametrized using polar coordinates.

(a) Sketch the spiral path γ_S and calculate the line integral $W_1[\gamma_S] = \int_{\gamma_S} \mathrm{d}\mathbf{r}\cdot\mathbf{F}_1$ of the field $\mathbf{F}_1 = \mathbf{e}_\phi$ along γ_S. [Check your result: if $R = \Delta = 1$, then $W_1[\gamma] = 3\pi$.]

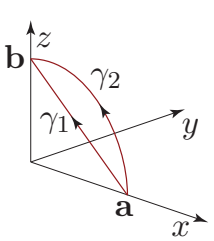
(b) Calculate the line integral $W_2[\gamma] = \int_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{F}_2$ of the field $\mathbf{F}_2 = \mathbf{e}_x$ along the straight path γ_G from the point $(R, 0)^T$ to the point $(R + \Delta, 0)^T$, and also along the spiral path γ_S. Are the results related? Explain!

PV2.4.4 Line integral in Cartesian and spherical coordinates

Consider the vector field $\mathbf{F} = (0, 0, fz)^{\mathrm{T}}$, with $f \in \mathbb{R}$. Compute the line integral $W[\gamma] = \int_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{F}$ from $\mathbf{a} = (1,0,0)^T$ to $\mathbf{b} = (0,0,1)^T$ explicitly along the following two paths:

(a) γ_1: a straight line. [Check your result: if $f = 2$, then $W[\gamma_1] = 1$.]

(b) γ_2: a segment of a circle with radius $R = 1$ centered at the origin. Use spherical coordinates. [Check your result: for $f = 3$, we have $W[\gamma_2] = \frac{3}{2}$.]



ɛV2.4.5 Line integral in spherical coordinates: satellite in orbit

A satellite travels along an unusual trajectory γ that circles the north-south-axis of the earth as it travels from a point high above the north pole to a point high above the south pole. In spherical coordinates the trajectory is given by $r(t) = r_0$, $\theta(t) = \omega_1 t$, $\phi(t) = \omega_2 t$, with $t \in (0, \pi/\omega_1)$. Due to the rotation of the earth, there is a wind in the upper atmosphere which exerts a force $\mathbf{F} = -F_0 \sin\theta\, \mathbf{e}_\phi$ on the satellite.

(a) Make a qualitative sketch of the orbit, for $\omega_2 = 20\omega_1$. How many times does the path wind around the north-south axis?

(b) What is the velocity vector $\dot{\mathbf{r}}$ written in spherical coordinates?

(c) Give the length $L[\gamma]$ of the orbit in terms of an integral. (You are not required to solve it.)

(d) Calculate, using the line integral $W[\gamma] = \int_\gamma d\mathbf{r} \cdot \mathbf{F}$, the work performed against the wind by the satellite along its orbit. [Check your result: if $F_0 = r_0 = \omega_1 = \omega_2 = 1$, then $W[\gamma] = -\frac{\pi}{2}$.]

ƿV2.4.6 Line integrals in cylindrical coordinates: bathtub drain

A soap bubble travels along a spiral-shaped path γ towards the drain of a bathtub. In cylindrical coordinates the path is given by $\rho(t) = \rho_0 \mathrm{e}^{-t/\tau}$, $\phi(t) = \omega t$, $z(t) = z_0 \mathrm{e}^{-t/\tau}$, with $\rho_0 > \rho_\mathrm{d}$ and $t \in [0, t_\mathrm{d}]$, where ρ_d is the drain radius and $t_\mathrm{d} = \tau \ln(\rho_0/\rho_\mathrm{d})$ the time at which the bubble reaches the drain.

(a) Make a qualitative sketch of the path (e.g. for $\omega = 6\pi/\tau$ in $\rho_0 = 10\rho_\mathrm{A}$).

(b) What is the velocity vector $\mathbf{v} = \dot{\mathbf{r}}$ in cylindrical coordinates? What is the magnitude of the final velocity, i.e $v_\mathrm{d} = \|\mathbf{v}(t_\mathrm{d})\|$?

(c) Show that the length of the path is given by $L[\gamma] = \tau v_\mathrm{d}\,(\rho_0/\rho_\mathrm{d} - 1)$.

(d) Using the line integral $W[\gamma] = \int_\gamma d\mathbf{r} \cdot \mathbf{F}$, find the work done by gravity $\mathbf{F} = -mg\mathbf{e}_z$ along the path of the soap bubble. Give a physical interpretation for this result!

[Check your results: if $\tau = 2/\omega$, $z_0 = 2\rho_0$ and $\rho_\mathrm{d} = \rho_0/3$, then: (b) $v_\mathrm{d} = \rho_0/\tau$, (c) $L = 2\rho_0$, (d) $W[\gamma] = mg\rho_0 4/3$.]

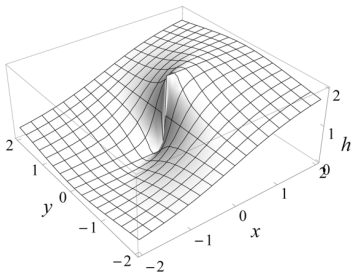
P.V2.5 Local coordinate bases and linear algebra

P.V3 Fields

P.V3.1 Scalar fields

EV3.1.1 Gradient of a mountain slope

A hiker encounters a mountain slope (as shown in the figure) whose height is given by the function $h(\mathbf{r}) = \frac{x}{r} + 1$ with $\mathbf{r} = (x, y)^T$ and $r = \sqrt{x^2 + y^2}$. Describe the topography of the slope by answering the following questions. Make use of the properties of the gradient vector $\boldsymbol{\nabla} h_{\mathbf{r}}$.



(a) Calculate the gradient $\boldsymbol{\nabla} h_{\mathbf{r}}$, and the total differential $\mathrm{d}h_{\mathbf{r}}(\mathbf{n})$ for the vector $\mathbf{n} = (n_x, n_y)^T$.

(b) The hiker is at the point $\mathbf{r} = (x, y)^T$. In which direction does the mountain slope increase most steeply?

(c) In which direction do the contour lines run at this point?

(d) Sketch a contour plot of the slope. Also draw the gradient vectors $\boldsymbol{\nabla} h_{\mathbf{r}}$ at the points $\mathbf{r}_1 = (-1, 1)^T$, $\mathbf{r}_2 = (0, \sqrt{2})^T$ and $\mathbf{r}_3 = (1, 1)^T$.

(e) Is there a contour line in the positive quadrant $(x, y \geq 0)$ such that $x = y$? If so, at what height does it occur?

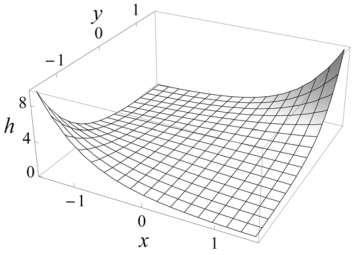
(f) Find an equation describing the contour line at height $h(\mathbf{r}) = H$ in the positive quadrant $(x, y \geq 0)$.

(g) Where is the slope at its shallowest? What is its height at that position?

(h) Where is the slope at its steepest? Describe, in detail, how its topography close to that point depends on x and y.

PV3.1.2 Gradient of a valley

A hiker encounters a valley as shown in the figure. The height of the valley is described by the equation $h(\mathbf{r}) = \mathrm{e}^{xy}$, with $\mathbf{r} = (x, y)^T$. Describe the topography of the valley by answering the following questions. Make use of the properties of the gradient vector $\boldsymbol{\nabla} h_{\mathbf{r}}$.



(a) Calculate the gradient $\boldsymbol{\nabla} h_{\mathbf{r}}$ and the total differential $\mathrm{d}h_{\mathbf{r}}(\mathbf{n})$ for the vector $\mathbf{n} = (n_x, n_y)^T$.

(b) The hiker stands at the point $\mathbf{r} = (x, y)^T$. In which direction does the slope of the valley increase most steeply?

(c) In which direction do the contour lines run at this point?

(d) Sketch a figure containing the contour plot of the side of the valley. Also draw the gradient vectors $\boldsymbol{\nabla} h_{\mathbf{r}}$ at the points $\mathbf{r}_1 = \frac{1}{\sqrt{2}}(-1, 1)^T$, $\mathbf{r}_2 = (0, 1)^T$ and $\mathbf{r}_3 = \frac{1}{\sqrt{2}}(1, 1)^T$.

(e) Obtain the equation for the contour line at a height $h(\mathbf{r}) = H(> 0)$.

(f) At what point is the valley at its flattest? What is its height at this point?

(g) At a distance of $r = \|\mathbf{r}\|$ from the origin, where is the valley slope at its steepest?

EV3.1.3 Gradient of $\mathrm{e}^{1/r}$

Consider the scalar field $\phi(\mathbf{r}) = \ln(r^{-1})$, where $r = \sqrt{x^2 + y^2 + z^2}$. At which spatial points does $|\boldsymbol{\nabla}\phi| = 1$ hold?

PV3.1.4 Gradient of $f(r)$

(a) For $\mathbf{r} \in \mathbb{R}^3$ and $r = \sqrt{x^2 + y^2 + z^2} = \|\mathbf{r}\|$, compute $\boldsymbol{\nabla} r$ and $\boldsymbol{\nabla} r^2$.

(b) Let $f(r)$ be a general, twice differentiable function of r. Calculate $\boldsymbol{\nabla} f(r)$ in terms of $f'(r)$, the first derivative of f with respect to r.

P.V3.2 Gradient fields

EV3.2.1 Scetching a vector field

Sketch the following vector fields in two dimensions, with $\mathbf{r} = (x, y)^T$:

(a) $\mathbf{A} : \mathbb{R}^2 \to \mathbb{R}^2, \qquad \mathbf{r} \mapsto \mathbf{A}(\mathbf{r}) = (\cos y, 0)^T.$

(b) $\mathbf{B} : \mathbb{R}^2 \to \mathbb{R}^2, \qquad \mathbf{r} \mapsto \mathbf{B}(\mathbf{r}) = \dfrac{1}{\sqrt{x^2 + y^2}}(x, -y)^T.$

For several vectors $\mathbf{r}$ in the domain of the vector field map [e.g. $\mathbf{A}$], the sketch should depict the corresponding vectors $\mathbf{A}(\mathbf{r})$ from the codomain of the map. For a chosen point $\mathbf{r}$ one draws an arrow with midpoint at $\mathbf{r}$, whose direction and length represents the vector $\mathbf{A}(\mathbf{r})$. The unit of length may be chosen differently for $\mathbf{r}$ vectors from the domain and $\mathbf{A}(\mathbf{r})$ vectors from the codomain, in order to avoid arrows from overlapping and to obtain an uncluttered figure (e.g. by drawing $\hat{\mathbf{A}}(\mathbf{r})$ unit vectors shorter than $\hat{\mathbf{r}}$ unit vectors). Indeed, for the visual depiction of codomain vectors usually only their directions and *relative* lengths are of interest, not their absolute lengths.

PV3.2.2 Scetching a vector field

Sketch the following vector fields in two dimensions:

(a) $\mathbf{A}(x, y) = (\cos x, 0)^T$, (b) $\mathbf{B}(x, y) = (2y, -x)^T$.

EV3.2.3 Potential of a vector field

Given a vector field $\mathbf{A}(\mathbf{r}) = (2xy + z^3, x^2, 3xz^2)^T$.

(a) Calculate the line integral $I_1 = \int_{\gamma_1} \mathrm{d}\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')$ from $\mathbf{0} = (0,0,0)^T$ to $\mathbf{b} = (1,1,1)^T$, along the path $\gamma_1 = \{\mathbf{r}(t) = (t,t,t)^T \mid 0 < t < 1\}$.

(b) Does the line integral depend on the shape of the path?

(c) Calculate the potential $\phi(\mathbf{r})$ of the vector field $\boldsymbol{A}(\mathbf{r})$ over the line integral $\phi(\mathbf{r}) = \int_{\gamma_\mathbf{r}} \mathrm{d}\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')$ along a suitably parametrized path $\gamma_\mathbf{r}$ from $\mathbf{0}$ to $\mathbf{r} = (x,y,z)^T$.

(d) Consistency check: Verify by explicit calculation that your result for $\phi(\mathbf{r})$ satisfies the equation $\nabla\phi(\mathbf{r}) = \mathbf{A}(\mathbf{r})$.

(e) Calculate the integral I_1 from part (a) over the vector field by considering the difference in potential $\phi(\mathbf{r})$ (the antiderivative!) at the integration limits $\mathbf{b}$ and $\mathbf{0}$. Consistency check: Do you obtain the same result as in part (a) of the exercise?

PV3.2.4 Line integral of a vector field

Calculate the line integral $W[\gamma] = \int_\gamma \mathrm{d}\mathbf{r} \cdot \mathbf{F}$ of the vector field $\mathbf{F}(\mathbf{r}) = (x\mathrm{e}^{yz}, y\mathrm{e}^{xz}, z\mathrm{e}^{xy})^T$ along the straight line γ from the point $\mathbf{0} = (0,0,0)^T$ to the point $\mathbf{b} = b(1,2,1)^T$, with $b \in \mathbb{R}$. [Check your result: for $b^2 = \ln 2$, $W[\gamma] = 7/2$.] Does the line integral depend on the path taken?

EV3.2.5 Line of magnetic field of a current-carrying conductor

This problem illustrates that $\partial_i B_j - \partial_j B_i = 0$ does not necessarily imply $\oint \mathrm{d}\mathbf{r} \cdot \mathbf{B} = 0$.
The magnetic field of an infinitely long current-carrying conductor has the form

$$\mathbf{B}(\mathbf{r}) = \frac{c}{x^2 + y^2} \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix}.$$

(a) Show that $\partial_i B_j - \partial_j B_i = 0$ holds if $\sqrt{x^2 + y^2} \neq 0$.

(b) Compute the line integral $W[\gamma_K] = \int_{\gamma_K} \mathrm{d}\mathbf{r} \cdot \mathbf{B}$ for the closed path along the circle with radius R around the origin, $\gamma_K = \{\mathbf{r}(t) = R(\cos t, \sin t, 0)^T | t \in [0, 2\pi]\}$.

(c) Compute the line integral $W[\gamma_R] = \int_{\gamma_R} \mathrm{d}\mathbf{r} \cdot \mathbf{B}$ for the closed path γ_R along the edges of the rectangle with corners $(1,0,0)^T$, $(2,0,0)^T$, $(2,3,0)^T$ and $(1,3,0)^T$.

(d) Are your results from (a) to (c) consistent with each other? Explain!

PV3.2.6 Line integral of vector field on non-simply connected domain

Consider the vector field

$$\mathbf{B}(\mathbf{r}) = \frac{1}{(x^2+y^2)^2}\begin{pmatrix} -yx^n \\ x^{n+1} \\ 0 \end{pmatrix}.$$

(a) For what value of the exponent n does $\partial_i B_j - \partial_j B_i = 0$ hold, if $\sqrt{x^2+y^2} \neq 0$?

In the following questions, use the value of n found in (a).

(b) Compute the line integral $W[\gamma_C] = \oint_{\gamma_C} \mathrm{d}\mathbf{r} \cdot \mathbf{B}$ for the closed path along the circle with radius R around the origin, $\gamma_C = \{\mathbf{r}(t) = R(\cos t, \sin t, 0)^T | t \in [0, 2\pi]\}$.

(c) What is the value of the line integral $W[\gamma_T] = \oint_{\gamma_T} \mathrm{d}\mathbf{r} \cdot \mathbf{B}$ for the closed path γ_T along the edges of the triangle with corners $(-1,-1,0)^T$, $(1,-1,0)^T$ and $(a,1,0)^T$, with $a \in \mathbb{R}$? Sketch the result as function of $a \in [-2,2]$. *Hint:* You may write down the result without a calculation, but should offer a justification for it.

P.V3.3 Sources of vector fields

EV3.3.1 Gauss' theorem – cube (Cartesian coordinates)

Consider the cube C, defined by $0 < x < a$, $0 < y < a$, $0 < z < a$, and the vector field $\mathbf{v}(\mathbf{r}) = (x^2, y^2, z^2)^T$. Calculate its outward flux through the surface of the cube, $\Phi = \int_{\partial C} \mathrm{d}\mathbf{S} \cdot \mathbf{v}$, in two ways:

(a) directly as a surface integral; and

(b) as a volume integral via Gauss's theorem.

[Check your result: if $a = 2$, then $\Phi = 48$.]

PV3.3.2 Gauss' theorem – cuboid (Cartesian coordinates)

Consider the cube C, defined by $0 < x < a$, $0 < y < a$, $0 < z < a$, and the vector field $\mathbf{w}(\mathbf{r}) = (-y^2, x^2, 0)^T$. Calculate its outward flux through all surfaces of the cube except the top (at $z = a$), $\Phi = \int_{\partial C \setminus \mathrm{top}} \mathrm{d}\mathbf{S} \cdot \mathbf{w}$, in two ways:

(a) directly as a surface integral;

(b) as a line integral via Stoke's theorem.

[Check your result: if $a = 2$, then $\Phi = -16$.]

EV3.3.3 Calculating volume of cylinder using Gauss' theorem

Calculate the volume of a cylinder with height h and radius R via a surface integral using Gauss's theorem and a vector field with the property that $\boldsymbol{\nabla} \cdot \mathbf{v} = 1$. One may choose $\mathbf{v} = z\mathbf{e}_z$, for example.

PV3.3.4 Calculating volume of sphere using Gauss' theorem

Calculate the volume of a sphere with radius R via a surface integral using Gauss's theorem and a vector field with the property that $\boldsymbol{\nabla} \cdot \mathbf{v} = 1$. One may choose $\mathbf{v} = \frac{1}{3}\mathbf{r}$, for example.

EV3.3.5 Flux integral: flux of vector field through surface with cylindrical symmetry

Consider a cylinder with midpoint at the origin, length $2h$ and radius R. A point charge Q sits at the origin, which emits an electric field of the form $\mathbf{E}(\mathbf{r}) = E_0\mathbf{r}/r^3$, with $E_0 = Q$. Find the outward flux $\Phi_Z = \Phi_T + \Phi_B + \Phi_S$ of this field through the entire surface of the cylinder, by first calculating the flux through (a) the top Φ_T and bottom Φ_B, as well as (b), the side Φ_S. [Check your results: $\Phi_Z = Q/\varepsilon_0$.]

PV3.3.6 Flux integral: flux of vector field through surface with cylindrical symmetry

Given the surface of revolution $S = S_{\text{Side}} + S_{\text{Bottom}} + S_{\text{Top}}$, with

$$\begin{aligned} S_{\text{Side}} &= \{(x,y,z) \in \mathbb{R}^3 : x^2 + y^2 = e^{-2az}, z \geq 0\} \\ S_{\text{Top}} &= \{(x,y,z) \in \mathbb{R}^3 : x^2 + y^2 \leq 1, z = 0\} \\ S_{\text{Bottom}} &= \{(x,y,z) \in \mathbb{R}^3 : x^2 + y^2 \leq e^{-2a}, z = 1\}. \end{aligned}$$

Sketch S and calculate, for the vector field $\mathbf{v}(x,y,z) = (x,y,-2z)$, the flux, $\Phi = \int \mathrm{d}\mathbf{S} \cdot \mathbf{v}$, (directed outwards) through each of the three individual surfaces, as well as through the whole surface S. [Check your results: if $a = 1$, then $\Phi_{\text{Side}} = -\Phi_{\text{Top}} = 2\pi\mathrm{e}^{-2}$.]

EV3.3.7 Gauss' theorem – cylinder (cylindrical coordinates)

Let the vector field $\mathbf{v}$ defined in cylindrical coordinates by

$$\mathbf{v} = z\rho\mathbf{e}_\rho$$

be given, as well as a cylindrical volume V defined by $\rho \in [0,R]$, $\phi \in [0, 2\pi[$, $z \in [0,H]$.

(a) Calculate the divergence of the vector field $\mathbf{v}$.
Note: The divergence of a vector field $A = A_\rho\mathbf{e}_\rho + A_\phi\mathbf{e}_\phi + A_z\mathbf{e}_z$ in cylindrical coordinates is given by:

$$\nabla \cdot \mathbf{A} = \frac{1}{\rho}\partial_\rho(\rho A_\rho) + \frac{1}{\rho}\partial_\phi A_\phi + \partial_z A_z$$

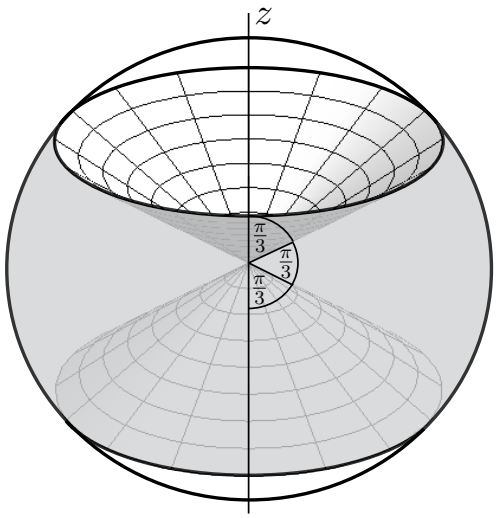
Calculate the flux Φ of the vector field $\mathbf{v}$ through the surface S of the cylindrical volume V via two methods:

(b) By calculating the surface integral $\Phi = \int_S \mathrm{d}\mathbf{S} \cdot \mathbf{v}$ explicitly.

(c) By using Gauss's theorem to convert to a volume integral of $\nabla \cdot \mathbf{v}$ and then calculate this integral explicitly.

PV3.3.8 Gauss' theorem – wedge ring (spherical coordinates)

Consider the "wedge-ring", K, which is shaded grey in the sketch. This shape can be expressed in spherical coordinates by the conditions $0 \leq r \leq R$ and $\pi/3 \leq \theta \leq 2\pi/3$ (Such a ring-like object, with wedge-shaped inner profile and rounded outer profile is constructed from a sphere with radius R, by removing a double cone centred on the z-axis with apex angle $\pi/3$.).
Calculate the outward flux Φ_K of the vector field $\mathbf{F}(\mathbf{r}) = r^2 \mathbf{e}_r$ through the surface ∂K of the wedge-ring, in two different ways:



(a) Calculate the surface integral $\Phi_K = \int_{\partial K} \mathrm{d}\mathbf{S} \cdot \mathbf{F}$ explicitly.

(b) Convert the surface integral into a volume integral of the divergence $\nabla \cdot \mathbf{F}$ using Gauss's theorem, and calculate the volume integral explicitly.
Hint: In Spherical coordinates:

$$\boldsymbol{\nabla} \cdot \mathbf{F} = \frac{1}{r^2}\partial_r \left(r^2 F_r\right) + \frac{1}{r \sin\theta}\partial_\theta \left(\sin\theta F_\theta\right) + \frac{1}{r \sin\theta}\partial_\phi F_\phi \, .$$

(c) For the vector field $\mathbf{G}(\mathbf{r}) = -\cos\theta \ \mathbf{e}_\theta$, calculate the outward flux $\tilde{\Phi}_K = \int_{\partial K} \mathrm{d}\mathbf{S} \cdot \mathbf{G}$ through the surface of the wedge-ring, either directly or by using Gauss's theorem.

P.V3.4 Circulation of vector fields

EV3.4.1 Gradient, divergence, curl

Consider the real function $f(x, y, z) = x^2 y + y^2 z$ and the vector field $\mathbf{v} = (xyz, y^2, z^2)^T$. Calculate ∇f, $\nabla \cdot \mathbf{v}$ and $\nabla \times \mathbf{v}$.

PV3.4.2 Gradient, divergence, curl

Given a scalar field $\phi(\mathbf{r}) = \sin x \cos y \, \mathrm{e}^z$ and a vector field $\mathbf{v}(\mathbf{r}) = (xyz, z^2y^2, z^3y)^T$. Calculate $\nabla\varphi$, $\nabla \cdot \mathbf{v}$ and $\nabla \times \mathbf{v}$. [Check your answer: At the points $\mathbf{r}_1 = (\pi/2, \pi/2, 0)^T$ and $\mathbf{r}_2 = (1,1,1)^T$, the results $\nabla\phi(\mathbf{r}_1) = (0,-1,0)^T$, $\nabla \cdot \mathbf{v}(\mathbf{r}_2) = 6$, $\nabla \times \mathbf{v}(\mathbf{r}_2) = (-1,1,-1)^T$ are valid.]

EV3.4.3 Source fields have no curl

Let $\varphi : \mathbb{R}^3 \to \mathbb{R}$ be a twice differentiable and continuous scalar field. Show that $\boldsymbol{\nabla} \times (\boldsymbol{\nabla}\varphi) = \mathbf{0}$.

PV3.4.4 Rotation fields have no divergence

Let $\mathbf{v} : \mathbb{R}^3 \to \mathbb{R}^3$ be a twice differentiable and continuous vector field. Show that $\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla} \times \mathbf{v}) = 0$.

EV3.4.5 Nabla identities

(a) Consider the scalar fields $f(x,y,z) = z\mathrm{e}^{-x^2}$ and $g(x,y,z) = yz^{-1}$, and the vector fields $\mathbf{A}(x,y,z) = x^2y\mathbf{e}_x$ and $\mathbf{B}(x,y,z) = \mathbf{e}_x$. Compute $\boldsymbol{\nabla}f$, $\boldsymbol{\nabla}g$, $\boldsymbol{\nabla} \cdot \mathbf{A}$, $\boldsymbol{\nabla} \times \mathbf{A}$, $\boldsymbol{\nabla} \cdot \mathbf{B}$, $\boldsymbol{\nabla} \times \mathbf{B}$. [Check your results: at the point $(x,y,z)^T = (1,1,1)^T$, $\boldsymbol{\nabla}f = (-2\mathrm{e}^{-1}, 0, \mathrm{e}^{-1})^T$, $\boldsymbol{\nabla}g = (0,1,-1)^T$, $\boldsymbol{\nabla} \cdot \mathbf{A} = 2$, $\boldsymbol{\nabla} \times \mathbf{A} = -\mathbf{e}_z$, $\boldsymbol{\nabla} \cdot \mathbf{B} = 0$, $\boldsymbol{\nabla} \times \mathbf{B} = 0$.]

(b) Prove the following identities for *general* scalar fields $f(x,y,z)$ and $g(x,y,z)$ and *general* vector fields $\mathbf{A}(x,y,z)$ and $\mathbf{B}(x,y,z)$ (using index notation, i.e. without representing $\mathbf{A}$, $\mathbf{B}$ and $\boldsymbol{\nabla}$ as column vectors):

(i) $\boldsymbol{\nabla}(fg) = f(\boldsymbol{\nabla}g) + g(\boldsymbol{\nabla}f)$

(ii) $\boldsymbol{\nabla}(\mathbf{A} \cdot \mathbf{B}) = \mathbf{A} \times (\boldsymbol{\nabla} \times \mathbf{B}) + \mathbf{B} \times (\boldsymbol{\nabla} \times \mathbf{A}) + (\mathbf{A} \cdot \nabla)\mathbf{B} + (\mathbf{B} \cdot \boldsymbol{\nabla})\mathbf{A}$

(iii) $\boldsymbol{\nabla} \cdot (f\mathbf{A}) = f(\boldsymbol{\nabla} \cdot \mathbf{A}) + \mathbf{A} \cdot (\boldsymbol{\nabla}f)$

Remark: For each identity the fields are assumed to be sufficiently differentiable.

(c) Check the identities from (b) explicitly for the fields given in (a).

PV3.4.6 Nabla identities

(a) Consider the scalar field $f(x,y,z) = y^{-1}\cos(z)$ and the vector fields $\mathbf{A}(x,y,z) = (-y, x, z^2)^T$ and $\mathbf{B}(x,y,z) = (x,0,1)^T$. Compute $\boldsymbol{\nabla}f$, $\boldsymbol{\nabla} \cdot \mathbf{A}$, $\boldsymbol{\nabla} \times \mathbf{A}$, $\boldsymbol{\nabla} \cdot \mathbf{B}$, $\boldsymbol{\nabla} \times \mathbf{B}$.

(b) Prove the following identities for a *general* scalar field $f(x,y,z)$ and *general* vector fields $\mathbf{A}(x,y,z)$ and $\mathbf{B}(x,y,z)$ (using index notation, i.e. without representing $\mathbf{A}$, $\mathbf{B}$ and $\boldsymbol{\nabla}$ as column vectors):

(i) $\boldsymbol{\nabla} \cdot (\mathbf{A} \times \mathbf{B}) = \mathbf{B} \cdot (\boldsymbol{\nabla} \times \mathbf{A}) - \mathbf{A} \cdot (\boldsymbol{\nabla} \times \mathbf{B})$

(ii) $\boldsymbol{\nabla} \times (f\mathbf{A}) = f\,(\boldsymbol{\nabla} \times \mathbf{A}) - \mathbf{A} \times (\boldsymbol{\nabla} f)$

(iii) $\boldsymbol{\nabla} \times (\mathbf{A} \times \mathbf{B}) = (\mathbf{B} \cdot \boldsymbol{\nabla})\,\mathbf{A} - (\mathbf{A} \cdot \boldsymbol{\nabla})\,\mathbf{B} + \mathbf{A}\,(\boldsymbol{\nabla} \cdot \mathbf{B}) - \mathbf{B}\,(\boldsymbol{\nabla} \cdot \mathbf{A})$

(iv) $\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \mathbf{A}) = \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \mathbf{A}) - \boldsymbol{\nabla}^2\mathbf{A}$ wobei $\boldsymbol{\nabla}^2 = (\boldsymbol{\nabla} \cdot \boldsymbol{\nabla})$

Remark: For each identity the fields are assumed to be sufficiently differentiable.

(c) Check the identities from (b) explixitly for the fields given in (a). [Check your results: at the point $(x, y, z)^T = (1, 1, 0)^T$: $\boldsymbol{\nabla} \cdot (\mathbf{A} \times \mathbf{B}) = 2$, $\boldsymbol{\nabla} \times (f\mathbf{A}) = (0, 0, 1)^T$, $\boldsymbol{\nabla} \times (\mathbf{A} \times \mathbf{B}) = (0, 2, 0)^T$, $\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \mathbf{A}) = 0$.]

E V3.4.7 Stokes' theorem – cube (Cartesian coordinates)

Consider the cuboid C, defined by $0 < x < a$, $0 < y < b$, $0 < z < c$, and the vector field $\mathbf{v}(\mathbf{r}) = (\frac{1}{2}x^2 + x^2 y, \frac{1}{2}x^2 y^2, 0)^T$. Calculate its outward flux through the surface of the cuboid, $\Phi = \int_{\partial C} \mathrm{d}\mathbf{S} \cdot \mathbf{v}$, in two ways:

(a) directly as a surface integral; and

(b) as a volume integral via Gauss's theorem.

[Check your results: if $a = 2$, $b = 3$, $c = \frac{1}{2}$, then $\Phi = 18$.]

P V3.4.8 Stokes' theorem – cuboid (Cartesian coordinates)

Consider the cuboid C, defined by $0 < x < a$, $0 < y < b$, $0 < z < c$, and the vector field $\mathbf{w}(\mathbf{r}) = \frac{1}{2}(yz^2, -xz^2, 0)^T$. Calculate its outward flux through all surfaces of the cuboid except the top (at $z = c$), $\Phi = \int_{\partial C \setminus \mathrm{top}} \mathrm{d}\mathbf{S} \cdot \mathbf{w}$, in two ways:

(a) directly as a surface integral;

(b) as a line integral via Stoke's theorem.

[Check your results: if $a = 2$, $b = 3$, $c = \frac{1}{2}$, then $\Phi = \frac{3}{2}$.]

E V3.4.9 Gradient, divergence, curl, Laplace in cylindrical coordinates

Let $f(\mathbf{r})$ be a scalar field and $\mathbf{B}(\mathbf{r}) = \mathbf{e}_u B_u + \mathbf{e}_v B_v + \mathbf{e}_w B_w$ be a vector field in a curvilinear orthogonal coordinate system with $\mathbf{r} = \mathbf{r}(u, v, w)$ and $\partial_u \mathbf{r} = b_u \mathbf{e}_u$, $\partial_v \mathbf{r} = b_v \mathbf{e}_v$, $\partial_v \mathbf{r} = b_v \mathbf{e}_v$. Then the gradient, divergence, curl and Laplace operator are given by

$$\boldsymbol{\nabla} f = \mathbf{e}_u \frac{1}{b_u} \partial_u f \; + \; \circlearrowright_{u\,v\,w} \; + \; \circlearrowright_{u\,v\,w} \quad ,$$

$$\boldsymbol{\nabla} \cdot \mathbf{B} = \frac{1}{b_u b_v b_w} \partial_u \left(b_v b_w B_u\right) \; + \; \circlearrowright_{u\,v\,w} \; + \; \circlearrowright_{u\,v\,w} \quad ,$$

$$\boldsymbol{\nabla} \times \mathbf{B} = \mathbf{e}_u \frac{1}{b_v b_w} \Big[\partial_v \left(b_w B_w\right) - \partial_w \left(b_v B_v\right)\Big] \; + \; \circlearrowright_{u\,v\,w} \; + \; \circlearrowright_{u\,v\,w} \quad ,$$

$$\boldsymbol{\nabla}^2 f = \boldsymbol{\nabla}\cdot(\boldsymbol{\nabla} f) = \frac{1}{b_u b_v b_w}\partial_u\left(\frac{b_v b_w}{b_u}\partial_u f\right) + \circlearrowright_{u,v,w} + \circlearrowright_{u,v,w} \quad .$$

Consider the cylindrical coordinates defined by $\mathbf{r} = (\rho\cos\phi, \rho\sin\phi, z)^T$.

(a) Find expressions for $\mathbf{e}_\rho$, $\mathbf{e}_\phi$, $\mathbf{e}_z$ and b_ρ, b_ϕ, b_z.

Starting from the formulae given above, find explicit formulas for

(b) $\boldsymbol{\nabla} f$, (c) $\boldsymbol{\nabla}\cdot\mathbf{B}$, (d) $\boldsymbol{\nabla}\times\mathbf{B}$, (e) $\boldsymbol{\nabla}^2 f$.

(f) Verify explicitly that $\boldsymbol{\nabla}\times(\boldsymbol{\nabla} f) = \mathbf{0}$, using the given formulae for the gradient and curl in general curvilinear coordinates u, v, w (i.e. not specifically cylindrical coordinates).

PV3.4.10 Gradient, divergence, curl, Laplace in spherical coordinates

We consider a curvilinear orthogonal coordinate system with coordinate $\mathbf{y} = (y^1, y^2, y^3) \equiv (u, v, w)$, position vector $\mathbf{r}(\mathbf{y}) = \mathbf{r}(u, v, w)$ and velocity vector $\partial_u\mathbf{r} = b_u\mathbf{e}_u$, $\partial_v\mathbf{r} = b_v\mathbf{e}_v$, $\partial_w\mathbf{r} = b_w\mathbf{e}_w$. Furthermore, $f(\mathbf{r})$ is a scalar field and $\mathbf{B}(\mathbf{r}) = \mathbf{e}_u B^u + \mathbf{e}_v B^v + \mathbf{e}_w B^w$ is a vector field. Then, the gradient, divergence, curl and Laplace operator are given by

$$\begin{aligned}
\boldsymbol{\nabla} f &= \mathbf{e}_u\frac{1}{b_u}\partial_u f + \circlearrowright_{u,v,w} + \circlearrowright_{u,v,w} \quad , \\
\boldsymbol{\nabla}\cdot\mathbf{B} &= \frac{1}{b_u b_v b_w}\partial_u\left(b_v b_w B^u\right) + \circlearrowright_{u,v,w} + \circlearrowright_{u,v,w} \quad , \\
\boldsymbol{\nabla}\times\mathbf{B} &= \mathbf{e}_u\frac{1}{b_v b_w}\left[\partial_v\left(b_w B^w\right) - \partial_w\left(b_v B^v\right)\right] + \circlearrowright_{u,v,w} + \circlearrowright_{u,v,w} \quad , \\
\boldsymbol{\nabla}^2 f &= \boldsymbol{\nabla}\cdot(\boldsymbol{\nabla} f) = \frac{1}{b_u b_v b_w}\partial_u\left(\frac{b_v b_w}{b_u}\partial_u f\right) + \circlearrowright_{u,v,w} + \circlearrowright_{u,v,w} \quad .
\end{aligned}$$

Consider the spherical coordinates defined by $\mathbf{r}(r,\theta,\phi) = (r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta)^T$.

(a) What do $\mathbf{e}_r$, $\mathbf{e}_\theta$, $\mathbf{e}_\phi$ and b_r, b_θ, b_ϕ look like? Based on the formulae given above, find an explicit formula for

(b) $\boldsymbol{\nabla} f$, (c) $\boldsymbol{\nabla}\cdot\mathbf{B}$, (d) $\boldsymbol{\nabla}\times\mathbf{B}$, (e) $\boldsymbol{\nabla}^2 f$.

(f) Verify explicitly, using the given formulae for the divergence and the curl for general curvilinear coordinates u, v, w (i.e. not specifically spherical coordinates), that $\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}\times\mathbf{B}) = 0$.

(g) Calculate $\boldsymbol{\nabla} f$, $\boldsymbol{\nabla}\cdot\mathbf{B}$, $\boldsymbol{\nabla}\times\mathbf{B}$ and $\boldsymbol{\nabla}^2 f$ for the fields $f(\mathbf{r}) = \|\mathbf{r}\|^2$ and $\mathbf{B}(\mathbf{r}) = (0,0,z)^T$. [Check your results: if $\mathbf{r} = (1,1,1)^T$, then $\boldsymbol{\nabla} f = (2,2,2)^T$, $\boldsymbol{\nabla}\cdot\mathbf{B} = 1$, $\boldsymbol{\nabla}\times\mathbf{B} = 0$ and $\boldsymbol{\nabla}^2 f = 6$.]

EV3.4.11 Gradient, divergence, curl (spherical coordinates)

Let $f(\mathbf{r}) = \frac{1}{r}$ be a given scalar field and a let $\mathbf{v}(\mathbf{r}) = (\mathrm{e}^{-r/a}/r)\mathbf{r}$ be a vector field with $\mathbf{r} = (x, y, z)^T$ and $r = \sqrt{x^2 + y^2 + z^2}$. Calculate $\boldsymbol{\nabla} f$, $\boldsymbol{\nabla} \cdot \mathbf{v}$, $\boldsymbol{\nabla} \times \mathbf{v}$ and $\boldsymbol{\nabla}^2 f$ explicitly for $r > 0$,

(a) in Cartesian coordinates;

(b) in spherical coordinates.

Show that your results from (a) and (b) are consistent with one another.

PV3.4.12 Gradient, divergence, curl (cylindrical coordinates)

Let $f(\mathbf{r}) = z(x^2 + y^2)$ be a given scalar field and let $\mathbf{v}(\mathbf{r}) = (zx, zy, 0)^T$ be a vector field. Calculate $\boldsymbol{\nabla} f$, $\boldsymbol{\nabla} \cdot \mathbf{v}$, $\boldsymbol{\nabla} \times \mathbf{v}$ and $\boldsymbol{\nabla}^2 f$ explicitly in

(a) Cartesian coordinates;

(b) cylindrical coordinates.

[Compare the results obtained in (a) and (b)!]

EV3.4.13 Stokes' theorem – magnetic dipole (spherical coordinates)

Every magnetic field can be represented as $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$, where the vector field $\mathbf{A}$ is known as the 'vector potential' of the field. For a magnetic dipole,

$$\mathbf{A} = \frac{1}{c}\frac{\mathbf{m} \times \mathbf{r}}{r^3}, \qquad \mathbf{B} = \frac{1}{c}\frac{3\mathbf{r}(\mathbf{m} \cdot \mathbf{r}) - \mathbf{m}r^2}{r^5},$$

where c is the speed of light. Let the constant dipole moment $\mathbf{m}$ be oriented in the z-direction, $\mathbf{m} = m\mathbf{e}_z$. Let H be a hemisphere with radius R, oriented with base surface in the xy-plane, symmetry axis along the positive z-axis and pole on the latter. Compute the flux integral of the magnetic field through this hemisphere, $\Phi_H = \int_H \mathrm{d}\mathbf{S} \cdot \mathbf{B}$, in two different ways:

(a) Directly, using spherical coordinates.

(b) Express Φ, using $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$ and Stokes' theorem, as a line integral of $\mathbf{A}$ over the boundary of the surface of H. Calculate the latter.

PV3.4.14 Stokes' theorem – cylinder (cylindrical coordinates)

Let Z be a cylinder with radius R and height aR^2, centred on the z-axis, with base in the xy-plane. For the vector field $\mathbf{v} = \frac{x^2+y^2}{z}(-y, x, 0)^T$, calculate the flux $\Phi_D = \int_D \mathrm{d}\mathbf{S} \cdot (\boldsymbol{\nabla} \times \mathbf{v})$ through the top D of the cylinder in two different ways:

(a) Directly, using cylindrical coordinates.

(b) By converting the problem to a line integral of $\mathbf{v}$ over the boundary ∂D of the top of the cylinder via Stoke's theorem, and then calculating the integral.

EV3.4.15 Stokes' theorem – magnetic field of infinite current-carrying wire (cylindrical coordinates)

Let an infinitely long, infinitesimally thin conductor be oriented along the z-axis and carry a current I. It generates a magnetic field of the following form:

$$\mathbf{B}(\mathbf{r}) = \frac{2I}{c}\frac{1}{x^2+y^2}\begin{pmatrix} -y \\ x \\ 0 \end{pmatrix} = \frac{2I}{c}\frac{1}{\rho}\mathbf{e}_\varphi, \qquad \text{for} \quad \rho = \sqrt{x^2+y^2} > 0.$$

Calculate the divergence and rotation of $\mathbf{B}(\mathbf{r})$ explicitly for $\rho > 0$ in

(a) Cartesian coordinates.

(b) Cylindrical coordinates [Compare your results from (a) and (b)!].

(c) Calculate, using cylindrical coordinates, the line integral $\oint_{\gamma_D} \mathbf{r}\cdot\mathbf{B}$ of the magnetic field along the edge γ_D of a circular disk, D, with radius $R > 0$, centred on the z-axis, and oriented parallel to the xy-plane.

(d) Calculate, using Stokes' theorem and the result from (c), the flux integral $\int_{D_A} \mathrm{d}\mathbf{S}\cdot(\boldsymbol{\nabla}\times\mathbf{B})$ of the curl of the magnetic field over the disk D prescribed in (c).

(e) From your results for $\boldsymbol{\nabla}\times\mathbf{B}$ from (a) and (d), conclude that the curl of the field is proportional to a two dimensional δ-function, i.e. it has the form $\boldsymbol{\nabla}\times\mathbf{B} = \mathbf{e}_z\, C\delta(x)\delta(y)$. Find the constant C. [Hint: The normalization of the two dimensional δ-function is given by the surface integral $\int_D \mathrm{d}S\,\delta(x)\delta(y) = 1$ for an arbitrary surface D that is parallel to the xy-plane and encloses the point $x = y = 0$.]

(f) Write the result obtained in (e) in the form $\boldsymbol{\nabla}\times\mathbf{B} = 4\pi\,\mathbf{j}(\mathbf{r})/c$ and determine $\mathbf{j}(\mathbf{r})$. This equation is Ampere's law (one of the Maxwell equations), where $\mathbf{j}(\mathbf{r})$ is the current density. Can you give a physical interpretation of your result for $\mathbf{j}(\mathbf{r})$?

PV3.4.16 Gauss' theorem – electrical field of a point charge (spherical coordinates)

The electric field of a point charge Q at the origin has the form

$$\mathbf{E}(\mathbf{r}) = Q\frac{1}{r^3}\mathbf{r} = Q\frac{1}{r^3}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = Q\frac{\mathbf{e}_r}{r^2}\,, \qquad \text{with} \quad r > 0, \qquad r = \sqrt{x^2+y^2+z^2}\,.$$

(ε_0 is the-so called dielectric constant). Calculate the divergence and the curl of $\mathbf{E}(\mathbf{r})$ explicitly for $r > 0$, in

(a) Cartesian coordinates.

(b) spherical coordinates. [Compare your results from (a) and (b)!]

(c) Calculate, using spherical coordinates, the flux $\Phi_K = \int_{O_K} \mathrm{d}\mathbf{S} \cdot \mathbf{E}$ of the electric field through the surface O_K of a sphere K with radius $R > 0$ centred at the origin.

(d) Calculate, using Gauss' theorem and the result from (c), the volume integral $\int_{V_K} \mathrm{d}V(\boldsymbol{\nabla} \cdot E)$ over the volume V_K of the sphere K described in (c).

(e) Conclude from your results for $\boldsymbol{\nabla} \cdot \mathbf{E}$ from (a) and (d), that the divergence of the field is proportional to a three dimensional δ-function, i.e. it has the form $\boldsymbol{\nabla} \cdot \mathbf{E} = C\,\delta^{(3)}(\mathbf{r})$. Find the constant C. [Hint: The normalization of $\delta^{(3)}(\mathbf{r}) = \delta(x)\delta(y)\delta(z)$ is given by the volume integral $\int_V \mathrm{d}V\,\delta^{(3)}(\mathbf{r}) = 1$, for any volume V that contains the origin.]

(f) Write your result from (a) in the form $\boldsymbol{\nabla} \cdot \mathbf{E} = 4\pi\rho(\mathbf{r})$, and determine $\rho(\mathbf{r})$. This equation is the (physical) Gauss' law (one of the Maxwell equations), where $\rho(\mathbf{r})$ is the charge density. Can you interpret your result in terms of $\rho(\mathbf{r})$?

E V3.4.17 Gauss' theorem – electrical dipole potential (spherical coordinates)

The potential of an electric dipole with dipole moment $\mathbf{p} = p\mathbf{e}_z$ is given by

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\frac{\mathbf{p}\cdot\mathbf{r}}{r^3} = \frac{1}{4\pi\varepsilon_0}\frac{pz}{r^3}$$

(a) Calculate the electric field $\mathbf{E} = -\nabla\Phi(\mathbf{r})$ explicitly in Cartesian coordinates.

(b) Represent $\Phi(\mathbf{r})$ in spherical coordinates and calculate the electric field explicitly in spherical coordinates. Compare this result with the result obtained in (a).
Hint: $\mathbf{e}_z = \cos\theta\mathbf{e}_r - \sin\theta\mathbf{e}_\theta$

(c) Calculate the divergence and the curl of the electric field explicitly in Cartesian coordinates.

(d) Calculate the divergence and the curl of the electric field explicitly in spherical coordinates. [Compare the results obtained in (b) and (c)!]

(e) According to the (physical) Gauss' law, we have $\int_S \mathrm{d}\mathbf{S} \cdot \mathbf{E} = Q/\varepsilon_0$, where Q is the total charge contained within the volume of S and ε_0 is the dielectric constant. Now let S be a surface on sphere centred on the origin with radius R. Calculate Q/ε_0 by converting the flux integral into a volume integral over $\nabla \cdot \mathbf{E}$ using the (mathematical) Gauss' theorem. Evaluate this integral using the result from (d). Is your result for Q/ε_0 sensible? Explain!

P V3.4.18 Stokes' theorem – magnetic field of opposite currents in parallel wires (cylindrical coordinates)

P.V4 Basic concepts of differential geometry

P.V4.1 Differentiable manifolds

S

Solutions

The fourth part of this book, labelled S, contains detailed solutions to all odd-numbered problems and to all case studies presented in the preceding three parts. Lecturers can obtain the solutions to even-numbered problems from the publishers by request.

SL Problems: Linear Algebra

S.L1 Mathematics before numbers

S.L1.1 Sets and Maps

ᴇL1.1.1 Composition of maps

(a) Since A maps $\mathbb{Z}$ to $\mathbb{Z}$ and B maps $\mathbb{Z}$ to $\mathbb{N}_0$, it follows that $C = B \circ A$ maps $\mathbb{Z}$ to $\mathbb{N}_0$. The image of n is $C(n) = B(A(n)) = B(n+1) = |n+1|$. To summarize:

$$C : \mathbb{Z} \to \mathbb{N}_0, \quad n \mapsto C(n) = |n+1|.$$

(b) A, B and C are all surjective. A is also injective and bijective. B is not injective, because any positive $n \in \mathbb{N}_0$ is the image of *two* points in $\mathbb{Z}$, $B(n) = B(-n) = n$. Consequently, B is not bijective either. It follows that C, too, is not injective and thus not bijective.

S.L1.2 Groups

ᴇL1.2.1 The group $\mathbb{Z}_2$

(a) The composition table implies the following properties:

+	0	1
0	0	1
1	1	0

(i) Closure: the result of any possible addition is listed in the table and belongs to the set $\{0, 1\}$. ✓

(i) Associativity:

$(1+0)+0 = 1+0 = 1 \stackrel{?}{=} 1+(0+0) = 1+0 = 1$ ✓
$(0+1)+0 = 1+0 = 1 \stackrel{?}{=} 0+(1+0) = 0+1 = 1$ ✓
$(1+1)+0 = 0+0 = 0 \stackrel{?}{=} 1+(1+0) = 1+1 = 0$ ✓
$(1+0)+1 = 1+1 = 0 \stackrel{?}{=} 1+(0+1) = 1+1 = 0$ ✓
$(0+1)+1 = 1+1 = 0 \stackrel{?}{=} 0+(1+1) = 0+0 = 0$ ✓
$(0+0)+1 = 0+1 = 1 \stackrel{?}{=} 0+(0+1) = 0+1 = 1$ ✓

(ii) The neutral element is 0, since adding it yields no change: $0+0 = 0$, $0+1 = 1$.

(iii) For every element in the group, there is exactly one inverse, since every row of the table contains exactly one 0.

(iv) The group is abelian since the table is symmetric with respect to the diagonal.

(b) The group $(\{+1,-1\},\bullet)$, with standard multiplication as group operation, is isomorphic to $\mathbb{Z}_2$, since their composition tables have the same structure if we identify $+1$ with 0 and -1 with 1.

$\bullet$	$+1$	-1
$+1$	$+1$	-1
-1	-1	$+1$

ᴇL1.2.3 Group of discrete translations in one dimension

(a) Consider the group axioms:

(i) Closure: The integers are closed under usual addition: $m,n\in\mathbb{Z}\Rightarrow m+n\in\mathbb{Z}$. All $x,y\in\mathbb{G}$ are integer multiples of λ, hence there exist integers $n_x,n_y\in\mathbb{Z}$ such that $x=\lambda n_x, y=\lambda n_y$. It follows that $T(x,y)=x+y=\lambda\cdot n_x+\lambda\cdot n_y=\lambda\cdot(n_x+n_y)\in\lambda\cdot\mathbb{Z}=\mathbb{G}$. ✓

(ii) Associativity: The usual addition rule for real numbers is associative: $a,b,c\in\mathbb{R}\Rightarrow(a+b)+c=a+(b+c)$. For $x,y,z\in\mathbb{G}$ we therefore have $T(T(x,y),z)=T(x+y,z)=(x+y)+z=x+(y+z)=T(x,y+z)=T(x,T(y,z))$. ✓

(iii) Neutral element: The neutral element is $0=\lambda\cdot 0\in\mathbb{G}$: For all $x\in\mathbb{G}$ we have: $T(x,0)=x+0=x$. ✓

(iv) Inverse element: The inverse element of $n\in\mathbb{Z}$ is $-n\in\mathbb{Z}$. Thus the inverse of $x=\lambda\cdot n\in\mathbb{G}$ is $-x\equiv\lambda\cdot(-n)\in\mathbb{G}$, since $T(x,-x)=\lambda\cdot n+\lambda\cdot(-n)=\lambda\cdot(n+(-n))=\lambda\cdot 0=0$. ✓

(v) Commutativity (for the group to be abelian): For all $x,y\in\mathbb{G}$ we have $T(x,y)=x+y=y+x=T(y,x)$, since the usual addition of real numbers is commutative. ✓

Since $(\mathbb{G},T)$ satisfies properties (i)-(v), it is an abelian group. ✓
Remark: For $\lambda=1$, the group $(\mathbb{G},T)$ is identical to $(\mathbb{Z},+)$.

(b) The group axioms of $(\mathbb{T},\boldsymbol{+})$ follow directly from those of $(\mathbb{G},T)$:

(i) Closure: $\mathcal{T}_x,\mathcal{T}_y\in\mathbb{T}\Rightarrow\mathcal{T}_x\boldsymbol{+}\mathcal{T}_y=\mathcal{T}_{T(x,y)}\in\mathbb{T}$, since if $x,y\in\mathbb{G}$, then $T(x,y)\in\mathbb{G}$ [see (a)]. ✓

(ii) Associativity: For $\mathcal{T}_x,\mathcal{T}_y,\mathcal{T}_z\in\mathbb{T}$ we have: $(\mathcal{T}_x\boldsymbol{+}\mathcal{T}_y)\boldsymbol{+}\mathcal{T}_z=\mathcal{T}_{T(x,y)}\boldsymbol{+}\mathcal{T}_z=\mathcal{T}_{T(T(x,y),z)}\overset{(a)}{=}\mathcal{T}_{T(x,T(y,z))}=\mathcal{T}_x\boldsymbol{+}\mathcal{T}_{T(y,z)}=\mathcal{T}_x\boldsymbol{+}(\mathcal{T}_y\boldsymbol{+}\mathcal{T}_z)$. ✓

(iii) Neutral element: The neutral element is $\mathcal{T}_0\in\mathbb{T}$: For all $\mathcal{T}_x\in\mathbb{T}$ we have: $\mathcal{T}_x\boldsymbol{+}\mathcal{T}_0=\mathcal{T}_{T(x,0)}=\mathcal{T}_{x+0}=\mathcal{T}_x$. ✓

(iv) Inverse element: The inverse element of $\mathcal{T}_x\in\mathbb{T}$ is $\mathcal{T}_{-x}\in\mathbb{T}$, where $-x$ is the inverse element of $x\in\mathbb{G}$ with respect to T, since $\mathcal{T}_x\boldsymbol{+}\mathcal{T}_{-x}=\mathcal{T}_{T(x,-x)}=\mathcal{T}_{x+(-x)}=\mathcal{T}_0$. ✓

(v) Commutativity (for the group to be abelian): For all $x,y\in\mathbb{G}$ we have $\mathcal{T}_x\boldsymbol{+}\mathcal{T}_y=\mathcal{T}_{T(x,y)}=\mathcal{T}_{T(y,x)}=\mathcal{T}_y\boldsymbol{+}\mathcal{T}_x$, since the composition rule T in $\mathbb{G}$ is commutative. ✓

Since $(\mathbb{T}, +)$ satisfies properties (i)-(v), it is an abelian group. ✓

ᴇL1.2.5 The permutation group

(a) The entries of the composition table can found by evaluating the image of 123 under P followed by P'. For example $123 \overset{[213]}{\longmapsto} 213 \overset{[321]}{\longmapsto} 231$, hence $[321] \circ [213] = [231]$.

$P' \circ P$	$[123]$	$[231]$	$[312]$	$[213]$	$[321]$	$[132]$
$[123]$	$[123]$	$[231]$	$[312]$	$[213]$	$[321]$	$[132]$
$[231]$	$[231]$	$[312]$	$[123]$	$[321]$	$[132]$	$[213]$
$[312]$	$[312]$	$[123]$	$[231]$	$[132]$	$[213]$	$[321]$
$[213]$	$[213]$	$[132]$	$[321]$	$[123]$	$[312]$	$[231]$
$[321]$	$[321]$	$[213]$	$[132]$	$[231]$	$[123]$	$[312]$
$[132]$	$[132]$	$[321]$	$[213]$	$[312]$	$[231]$	$[123]$

(b) The neutral element is the permutation that 'does nothing', $[123]$. Each element has a unique inverse, since every row and column contains the neutral element exactly once.

(c) The composition table is not symmetric, $P' \circ P \neq P \circ P'$, hence S_3 is *not* an abelian group. For example, $[312] \circ [213] = [132]$, whereas $[213] \circ [312] = [321]$.

S.L1.3 Fields

ᴇL1.3.1 Complex numbers – elementary computations

For $z_1 = 12 + 5\mathrm{i}$, $z_2 = -3 + 2\mathrm{i}$ and $z_3 = a - \mathrm{i}b$ $(a, b \in \mathbb{R})$ we find:

(a) $\bar{z}_1 = 12 - 5\mathrm{i}$

(b) $z_1 + z_2 = 12 + (-3) + (5 + 2)\mathrm{i} = 9 + 7\mathrm{i}$

(c) $z_1 + \bar{z}_3 = 12 + a + (5 + b)\mathrm{i}$

(d) $z_1 z_2 = 12 \cdot (-3) - 5 \cdot 2 + \mathrm{i}\,[5 \cdot (-3) + 12 \cdot 2] = -46 + 9\mathrm{i}$

(e) $\bar{z}_1 z_3 = 12 \cdot a - (-5) \cdot (-b) + \mathrm{i}\,[(-5) \cdot a + 12 \cdot (-b)] = 12a - 5b - \mathrm{i}(5a + 12b)$

(f) $\dfrac{z_1}{z_2} = \dfrac{12 + 5\mathrm{i}}{-3 + 2\mathrm{i}} = \dfrac{(12 + 5\mathrm{i})(-3 - 2\mathrm{i})}{(-3 + 2\mathrm{i})(-3 - 2\mathrm{i})} = \dfrac{-36 + 10 + \mathrm{i}(-15 - 24)}{9 + 4} = -2 - 3\mathrm{i}$

(g) $|z_1| = \sqrt{z_1 \bar{z}_1} = \sqrt{144 + 25} = 13$

(h) $|z_1 + z_2| = \sqrt{9^2 + 7^2} = \sqrt{130}$

(i) $az_2 + 3z_3 = (-3a + 2a\mathrm{i}) + (3a - 3b\mathrm{i}) = \mathrm{i}(2a - 3b)$

$|az_2 + 3z_3| = \sqrt{\mathrm{i}(2a - 3b) \cdot (-\mathrm{i})(2a - 3b)} = \sqrt{(2a - 3b)^2} = |2a - 3b|$

EL1.3.3 Algebraic manipulations with complex numbers

(a) $z + \bar{z} = x + \mathrm{i}y + x - \mathrm{i}y = 2x = 2\mathrm{Re}(z)\,,$

(b) $z - \bar{z} = x + \mathrm{i}y - (x - \mathrm{i}y) = \mathrm{i}2y = \mathrm{i}2\mathrm{Im}(z)\,,$

(c) $z \cdot \bar{z} = (x + \mathrm{i}y)(x - \mathrm{i}y) = x^2 + y^2\,,$

(d) $$\frac{z}{\bar{z}} \overset{\text{(c)}}{=} \frac{z \cdot z}{\bar{z} \cdot z} = \frac{(x + \mathrm{i}y)^2}{x^2 + y^2} = \frac{x^2 - y^2}{x^2 + y^2} + \mathrm{i}\frac{2xy}{x^2 + y^2}\,,$$

(e) $$\frac{1}{z} + \frac{1}{\bar{z}} = \frac{\bar{z} + z}{z \cdot \bar{z}} \overset{\text{(a),(c)}}{=} \frac{2x}{x^2 + y^2}\,,$$

(f) $$\frac{1}{z} - \frac{1}{\bar{z}} = \frac{\bar{z} - z}{z \cdot \bar{z}} \overset{\text{(b),(c)}}{=} \mathrm{i}\frac{(-2y)}{x^2 + y^2}\,,$$

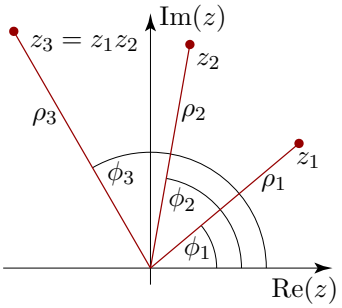
(g) $z^2 + z = (x + \mathrm{i}y)^2 + (x + \mathrm{i}y) = (x^2 - y^2 + x) + \mathrm{i}(2xy + y)\,,$

(h) $z^3 = (x + \mathrm{i}y)^3 = (x^3 + 3x^2\mathrm{i}y + 3x(\mathrm{i}y)^2 + (\mathrm{i}y)^3 = (x^3 - 3xy^2) + \mathrm{i}(3x^2y - y^3)\,.$

EL1.3.5 Multiplying complex numbers – geometrical interpretation

(a) With $z_j = (\rho_j \cos\phi_j, \rho_j \sin\phi_j)$ and the given trigonometric identities, we have

$$\begin{aligned} z_3 = z_1 z_2 &= \rho_1(\cos\phi_1 + \mathrm{i}\sin\phi_1)\rho_2(\cos\phi_2 + \mathrm{i}\sin\phi_2) \\ &= \rho_1\rho_2\left[(\cos\phi_1\cos\phi_2 - \sin\phi_1\sin\phi_2)\right. \\ &\quad \left. +\mathrm{i}\,(\sin\phi_1\cos\phi_2 + \cos\phi_1\sin\phi_2)\right] \\ &= \rho_1\rho_2\left[\cos(\phi_1 + \phi_2) + \mathrm{i}\sin(\phi_1 + \phi_2)\right] \\ &\equiv \rho_3\left[\cos\phi_3 + \mathrm{i}\sin\phi_3\right] \end{aligned}$$



We read off: $\rho_3 = \rho_1\rho_2$, $\phi_3 = (\phi_1 + \phi_2)\,\mathrm{mod}(2\pi)$. ✓

(b) The complex number $z = x + \mathrm{i}y$ is represented in the complex plane by the Cartesian coordinates $z \mapsto (x, y)$, or the polar coordinates $\rho = |z| = \sqrt{x^2 + y^2}$, $\phi = \arg(z) = \arctan\left(\frac{y}{x}\right)$. The latter formula determines ϕ only modulo π; to uniquely fix $\phi \in [0, 2\pi)$, we identify the quadrant containing the point (x, y).

$z_1 = \sqrt{3} + \mathrm{i} \mapsto (\sqrt{3}, 1)$ $\quad \rho_1 = \sqrt{3+1} = 2$ $\quad \phi_1 = \arctan\left(\frac{1}{\sqrt{3}}\right) = \frac{\pi}{6}$

$z_2 = -2 + 2\sqrt{3}\mathrm{i} \mapsto (-2, 2\sqrt{3})$ $\quad \rho_2 = \sqrt{12+4} = 4$ $\quad \phi_2 = \arctan\left(\frac{-2\sqrt{3}}{2}\right) = \frac{2\pi}{3}$

$z_3 = z_1 z_2 = (\sqrt{3} + \mathrm{i})(-2 + 2\sqrt{3}\mathrm{i})$ $\quad \rho_3 = \sqrt{16 \cdot 3 + 16} = 8$ $\quad \phi_3 = \arctan\left(\frac{4}{-4\sqrt{3}}\right) = \frac{5\pi}{6}$

$= -4\sqrt{3} + 4\mathrm{i} \mapsto (-4\sqrt{3}, 4)$

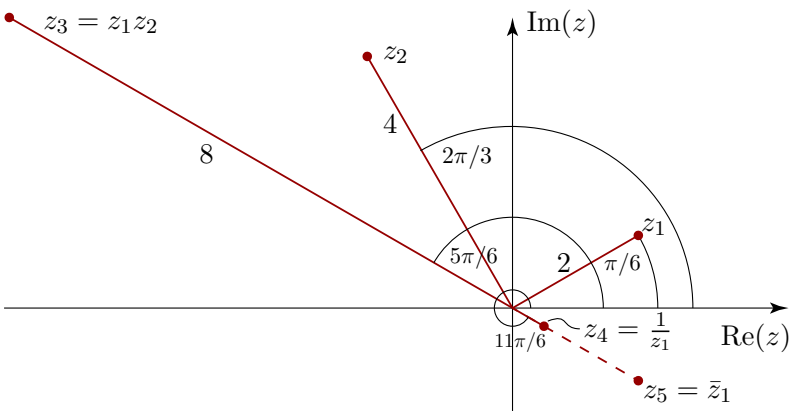
$z_4 = \frac{1}{z_1} = \frac{1}{\sqrt{3}+\mathrm{i}} = \frac{(\sqrt{3}-\mathrm{i})}{(\sqrt{3}+\mathrm{i})(\sqrt{3}-\mathrm{i})}$ $\quad \rho_4 = \frac{1}{4}\sqrt{3+1} = \frac{1}{2}$ $\quad \phi_4 = \arctan\left(\frac{-1/4}{\sqrt{3}/4}\right) = \frac{11\pi}{6}$

$= \frac{\sqrt{3}}{4} - \frac{1}{4}\mathrm{i} \mapsto \left(\frac{\sqrt{3}}{4}, -\frac{1}{4}\right)$

$z_5 = \bar{z}_1 = \sqrt{3} - \mathrm{i} \mapsto (\sqrt{3}, -1)$ $\quad \rho_5 = \sqrt{3+1} = 2$ $\quad \phi_5 = \arctan\left(\frac{-1}{\sqrt{3}}\right) = \frac{11\pi}{6}$

As expected, we find:

$\rho_3 = \rho_1\rho_2$
$\phi_3 = \phi_1 + \phi_2$
$\rho_4 = 1/\rho_1$
$\phi_4 = -\phi_1 \mathrm{mod}(2\pi)$
$\rho_5 = \rho_1$
$\phi_5 = -\phi_1 \mathrm{mod}(2\pi)$



ᴇL1.3.7 Field axioms for $\mathbb{F}_4$

Multiplication table: The first row and column must contain only zeroes, since $x \cdot 0 = 0 \cdot x = 0$ for each element x in the field. (Reason: $x \cdot y = x \cdot (y + 0) = x \cdot y + x \cdot 0$, hence $x \cdot 0 = 0$.) The second row and column follow from $1 \cdot x = x$. The remaining four entries must be arranged symmetrically to ensure commutativity. Let us begin by specifying the inverses of a and b, by entering a 1 in each of their columns.

$\cdot$	0	1	a	b
0	0	0	0	0
1	0	1	a	b
a	0	a		
b	0	b		

Suppose that in each column the 1 appears *on* the diagonal; then the table's symmetry requires the remaining off-diagonal entries to contain the same element x, i.e. $a \cdot b = x = b \cdot a$. This implies the relations

$$a \cdot x = a \cdot (a \cdot b) \overset{\text{assoc.}}{=} (a \cdot a) \cdot b = 1 \cdot b = b \quad \Leftrightarrow \quad a \cdot x = b$$
$$b \cdot x = b \cdot (b \cdot a) \overset{\text{assoc.}}{=} (b \cdot b) \cdot a = 1 \cdot a = a \quad \Leftrightarrow \quad b \cdot x = a$$

$\cdot$	0	1	a	b
0	0	0	0	0
1	0	1	a	b
a	0	a	1	x
b	0	b	x	1

(contradiction)

which lead to a contradiction, since it is easily verified that no element $x \in \{0, 1, a, b\}$ can satisfy both equations.

Therefore the 1 must appear as off-diagonal entry in each column, $a \cdot b = 1 = b \cdot a$. Finally, the two remaining diagonal entries need to be filled with a or b. If $a \cdot a = a$, then associativity would again lead to a contraction: $1 = b \cdot a = b \cdot (a \cdot a) \overset{\text{assoc.}}{=} (b \cdot a) \cdot a = 1 \cdot a = a$. Thus $a \cdot a = b$ must hold, and analogously, $b \cdot b = a$.

$\cdot$	0	1	a	b
0	0	0	0	0
1	0	1	a	b
a	0	a	b	1
b	0	b	1	a

Addition table: To ensure commutativity, the table must be symmetric. Each element has an additive inverse, hence and each row and column must contain exactly one 0. Consider the option $a + 1 = 0$. Then distributivity would yield $0 = b \cdot 0 = b \cdot (a + 1) \overset{\text{distr.}}{=} b \cdot a + b \cdot 1 = 1 + b$, hence 1 would have two additive inverses (a *and* b), contradicting the field axioms. Analogously, the option $b + 1 = 0$ would likewise lead to a contradiction. Thus, the only remaining option, $1 + 1 = 0$, must hold. The rest of the addition table follows from analogous arguments.

$+$	0	1	a	b
0	0	1	a	b
1	1	0	b	a
a	a	b	0	1
b	b	a	1	0

S.L2 Vector spaces

S.L2.4 Vector spaces: examples

ᴇL2.4.1 Vector space axioms: rational numbers

(a) First, we show that $(\mathbb{Q}^2, +)$ forms an abelian group.

(i) Closure holds by definition. ✓

(ii) Associativity:
$$\left[\begin{pmatrix} x^1 \\ x^2 \end{pmatrix} + \begin{pmatrix} y^1 \\ y^2 \end{pmatrix}\right] + \begin{pmatrix} z^1 \\ z^2 \end{pmatrix} = \begin{pmatrix} x^1 + y^1 \\ x^2 + y^2 \end{pmatrix} + \begin{pmatrix} z^1 \\ z^2 \end{pmatrix} = \begin{pmatrix} x^1 + y^1 + z^1 \\ x^2 + y^2 + z^2 \end{pmatrix}$$
$$= \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} + \begin{pmatrix} y^1 + z^1 \\ y^2 + z^2 \end{pmatrix} = \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} + \left[\begin{pmatrix} y^1 \\ y^2 \end{pmatrix} + \begin{pmatrix} z^1 \\ z^2 \end{pmatrix}\right]. \checkmark$$

(iii) Neutral element: $\begin{pmatrix} 0 \\ 0 \end{pmatrix}$ is the neutral element. ✓

(iv) Additive inverse: $\begin{pmatrix} -x^1 \\ -x^2 \end{pmatrix} \in \mathbb{Q}^2$ is the additive inverse of $\begin{pmatrix} x^1 \\ x^2 \end{pmatrix} \in \mathbb{Q}^2$. ✓

(v) Commutativity: follows (component-wise) from the commutativity of $\mathbb{Q}$. ✓

Second, we show that scalar multiplication, $\cdot$, likewise has the properties required for $(\mathbb{Q}^2, +, \cdot)$ to form a vector space. Since the product of two rational numbers is always rational $\left(\frac{p_1}{q_1} \cdot \frac{p_2}{q_2} = \frac{(p_1 p_2)}{(q_1 q_2)}\right)$, closure holds by definition. Moreover:

(vi) Multiplication of a sum of scalars and a vector is distributive:
$$(\lambda + \mu) \cdot \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} = \begin{pmatrix} (\lambda + \mu)x^1 \\ (\lambda + \mu)x^2 \end{pmatrix} = \begin{pmatrix} \lambda x^1 + \mu x^1 \\ \lambda x^2 + \mu x^2 \end{pmatrix} = \lambda \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} + \mu \begin{pmatrix} x^1 \\ x^2 \end{pmatrix}. \checkmark$$

(vii) Multiplication of a scalar and a sum of vectors is distributive:
$$\lambda \cdot \left[\begin{pmatrix} x^1 \\ x^2 \end{pmatrix} + \begin{pmatrix} y^1 \\ y^2 \end{pmatrix}\right] = \begin{pmatrix} \lambda x^1 + \lambda y^1 \\ \lambda x^2 + \lambda y^2 \end{pmatrix} = \lambda \begin{pmatrix} x^1 \\ x^2 \end{pmatrix} + \lambda \begin{pmatrix} y^1 \\ y^2 \end{pmatrix}. \checkmark$$

(viii) Multiplication of a product of scalars and a vector is associative:

$$(\lambda\mu)\cdot\begin{pmatrix}x^1\\x^2\end{pmatrix}=\begin{pmatrix}\lambda\mu x^1\\\lambda\mu x^2\end{pmatrix}=\lambda\left[\mu\cdot\begin{pmatrix}x^1\\x^2\end{pmatrix}\right]\,.\;\checkmark$$

(ix) Neutral element: $1\cdot\begin{pmatrix}x^1\\x^2\end{pmatrix}=\begin{pmatrix}x^1\\x^2\end{pmatrix}\,.\;\checkmark$

Therefore, the triple $(\mathbb{Q}^2,+,\cdot)$ represents a $\mathbb{Q}$-vector space.

(b) The set of integers $\mathbb{Z}$ does not form a field, since not for each $a\in\mathbb{Z}\setminus\{0\}$ a multiplicative inverse $a^{-1}\in\mathbb{Z}$ exists (e.g. the equation $2\cdot a=1$ has no solution within the integers). Hence, it is also *not* possible to construct any vector space over the integers.

EL2.4.3 Vector space of real functions

We have to verify that all the axioms for a vector space are satisfied. First, $(F,\,\boldsymbol{+}\,)$ indeed has all the properties of an abelian group:

(i) Closure holds by definition: adding two functions from F again yields a function in F. ✓

(ii,v) Associativity and commutativity follow trivially from the corresponding properties of $\mathbb{R}$. For example associativity:

$$\Big[f\boldsymbol{+}\big[g\boldsymbol{+}h\big]\Big](x)=f(x)+\big[g\boldsymbol{+}h\big](x)=f(x)+\Big(g(x)+h(x)\Big)$$
$$=\Big(f(x)+g(x)\Big)+h(x)=\big[f\boldsymbol{+}g\big](x)+h(x)=\Big[\big[f\boldsymbol{+}g\big]\boldsymbol{+}h\Big](x)\,.\;\checkmark$$

(iii) The neutral element is the null function, defined by $f_e:x\mapsto f_e(x)\equiv 0$, since $f\boldsymbol{+}f_e:x\mapsto f(x)+f_e(x)=f(x)+0=f(x)$. ✓

(iv) The additive inverse of f is $-f$, defined by $-f:x\mapsto(-f)(x)\equiv -f(x)$, since $f\boldsymbol{+}(-f):x\mapsto f(x)+(-f(x))=0$. ✓

Moreover, multiplication of any function with a scalar also has all the properties required for $(F,\,\boldsymbol{+}\,,\cdot)$ to be a vector space. Closure holds per definition. Furthermore:

(vi) Multiplication of a sum of scalars and a function is distributive:

$$\big[(\gamma+\lambda)\cdot f\big](x)=(\gamma+\lambda)f(x)=\gamma f(x)+\lambda f(x)=\big[\gamma\cdot f\big](x)+\big[\lambda\cdot f\big](x)$$
$$=\big[\gamma\cdot f\boldsymbol{+}\lambda\cdot f\big](x)\,.\;\checkmark$$

(vii) Multiplication of a scalar and a sum of functions is distributive:

$$\big[\lambda\cdot(f+g)\big](x)=\lambda\Big(\big[f\boldsymbol{+}g\big](x)\Big)=\lambda\Big(f(x)+g(x)\Big)=\lambda f(x)+\lambda g(x)$$

$$= \big[\lambda \cdot f\big](x) + \big[\lambda \cdot g\big](x) = \big[\lambda \cdot f + \lambda \cdot g\big](x)\,. \checkmark$$

(viii) Multiplication of a product of scalars and a function is associative:

$$\big[(\gamma\lambda) \cdot f\big](x) = (\gamma\lambda) f(x) = \gamma\Big(\lambda f(x)\Big) = \gamma\big[\lambda \cdot f\big](x) = \big[\gamma \cdot (\lambda \cdot f)\big](x)\,. \checkmark$$

(ix) Neutral element: $\big[1 \cdot f\big](x) = 1 f(x) = f(x)$. ✓

Therefore, the triple $(F, +, \cdot)$ is an $\mathbb{R}$ vector space.

EL2.4.5 E: Vector space with unusual composition rule – addition

First, we show that $(V_a, +)$ forms an abelian group.

(i) Closure holds by definition. ✓

(ii) Associativity:
$$\begin{aligned}(\mathbf{v}_x + \mathbf{v}_y) + \mathbf{v}_z &= \mathbf{v}_{x+y+a} + \mathbf{v}_z = \mathbf{v}_{(x+y+a)+z+a} = \mathbf{v}_{x+y+z+2a} \\ &= \mathbf{v}_{x+(y+z+a)+a} = \mathbf{v}_x + \mathbf{v}_{y+z+a} = \mathbf{v}_x + (\mathbf{v}_y + \mathbf{v}_z)\,. \checkmark\end{aligned}$$

(iii) Neutral element:
$$\mathbf{v}_x + \mathbf{v}_{-a} = \mathbf{v}_{x+(-a)+a} = \mathbf{v}_x\,, \quad \Rightarrow \quad \mathbf{0} = \mathbf{v}_{-a}\,. \checkmark$$

(iv) Additive inverse:
$$\mathbf{v}_x + \mathbf{v}_{-x-2a} = \mathbf{v}_{x+(-x-2a)+a} = \mathbf{v}_{-a} = \mathbf{0}\,, \quad \Rightarrow \quad -\mathbf{v}_x = \mathbf{v}_{-x-2a}\,. \checkmark$$

(v) Commutativity :
$$\mathbf{v}_x + \mathbf{v}_y = \mathbf{v}_{x+y+a} = \mathbf{v}_{y+x+a} = \mathbf{v}_y + \mathbf{v}_x\,. \checkmark$$

Second, we show that scalar multiplication, $\cdot$, likewise has the properties required for $(V_a, +, \cdot)$ to form a vector space. Closure holds by definition. Moreover:

(vi) Multiplication of a sum of scalars and a vector is distributive:

$$\begin{aligned}(\gamma + \lambda) \cdot \mathbf{v}_x &= \mathbf{v}_{(\gamma+\lambda)x+a(\gamma+\lambda-1)} = \mathbf{v}_{\gamma x+a(\gamma-1)+\lambda x+a(\lambda-1)+a} \\ &= \mathbf{v}_{\gamma x+a(\gamma-1)} + \mathbf{v}_{\lambda x+a(\lambda-1)} = \gamma \cdot \mathbf{v}_x + \lambda \cdot \mathbf{v}_x\,. \checkmark\end{aligned}$$

(vii) Multiplication of a scalar and a sum of vectors is distributive:

$$\begin{aligned}\lambda \cdot (\mathbf{v}_x + \mathbf{v}_y) &= \lambda \cdot \mathbf{v}_{x+y+a} = \mathbf{v}_{\lambda(x+y+a)+a(\lambda-1)} = \mathbf{v}_{\lambda x+a(\lambda-1)+\lambda y+a(\lambda-1)+a} \\ &= \mathbf{v}_{\lambda x+a(\lambda-1)} + \mathbf{v}_{\lambda y+a(\lambda-1)} = \lambda \cdot \mathbf{v}_x + \lambda \cdot \mathbf{v}_y\,. \checkmark\end{aligned}$$

(viii) Multiplication of a product of scalars and a vector is associative:

$$(\gamma\lambda) \cdot \mathbf{v}_x = \mathbf{v}_{(\gamma\lambda)x+a(\gamma\lambda-1)} = \mathbf{v}_{\gamma(\lambda x+a(\lambda-1))+a(\gamma-1)} = \gamma \cdot \mathbf{v}_{\lambda x+a(\lambda-1)} = \gamma \cdot (\lambda \cdot \mathbf{v}_x)\,. \checkmark$$

(ix) Neutral element: $1 \cdot \mathbf{v}_x = \mathbf{v}_{x+a(1-1)} = \mathbf{v}_x\,. \checkmark$

Therefore, the triple $(V_a, +, \cdot)$ represents an $\mathbb{R}$-vector space.

S.L2.5 Basis and dimension

ᴇL2.5.1 Linear independence

(a) The three vectors are linearly independent if and only if the only solution to the equation

$$\mathbf{0} = a^1\mathbf{v}_1 + a^2\mathbf{v}_2 + a^3\mathbf{v}_3 = a^1\begin{pmatrix}0\\1\\2\end{pmatrix} + a^2\begin{pmatrix}1\\-1\\1\end{pmatrix} + a^3\begin{pmatrix}2\\-1\\4\end{pmatrix}, \quad \text{with} \quad a^j \in \mathbb{R}, \qquad (1)$$

is the trivial one, $a^1 = a^2 = a^3 = 0$. The vector equation (1) yields a system of three equations, (i)-(iii), one for each of the three components of (1), which we solve as follows:

(i)	$0a^1 + 1a^2 + 2a^3 = 0$	$\overset{\text{(i)}}{\Rightarrow}$	(iv)	$a^2 = -2a^3$
(ii)	$1a^1 - 1a^2 - 1a^3 = 0$	$\overset{\text{(iv) in (ii)}}{\Rightarrow}$	(v)	$a^1 = -a^3$
(iii)	$2a^1 + 1a^2 + 4a^3 = 0$	$\overset{\text{(iv,v) in (iii)}}{\Rightarrow}$	(vi)	$0 = 0$

(i) yields (iv): $a^2 = -2a^3$. (iv) inserted into (ii) yields (v): $a^1 = -a^3$. Inserting (iv) and (v) into (iii) yields no new information. There are thus infinitely many non-trivial solutions (one for every value of $a^3 \in \mathbb{R}$), hence $\mathbf{v}_1$, $\mathbf{v}_2$ and $\mathbf{v}_3$ are not linearly independent.

(b) The desired vector $\mathbf{v}_2' = (x, y, z)^T$ should be linearly independent from $\mathbf{v}_1$ and $\mathbf{v}_3$, i.e. its components x, y and z should be chosen such that the equation $\mathbf{0} = a^1\mathbf{v}_1 + a^2\mathbf{v}_2' + a^3\mathbf{v}_3$ has no non-trivial solution, i.e. that it implies $a^1 = a^2 = a^3 = 0$:

(i)	$0a^1 + xa^2 + 2a^3 = 0$	$\overset{\text{(i)}}{\Rightarrow}$	(iv)	choose $x = 0$, then $a^3 = 0$.
(ii)	$1a^1 + ya^2 - 1a^3 = 0$	$\overset{\text{(iv) in (ii)}}{\Rightarrow}$	(v)	choose $y = 0$, then $a^1 = 0$.
(iii)	$2a^1 + za^2 + 4a^3 = 0$	$\overset{\text{(iv),(v) in (iii)}}{\Rightarrow}$	(vi)	choose $z = 1$, then $a^2 = 0$.

(i) yields (iv): $2a^3 = -xa^2$; to enforce $a^3 = 0$ we choose $x = 0$. (iv) inserted into (ii) yields (v): $a^1 = -ya^2$; to enforce $a^1 = 0$ we choose $y = 0$. (iv,v) inserted into (iii) yields $za^2 = 0$; to enforce $a^2 = 0$ we choose $z = 1$. Thus $\mathbf{v}_2' = (0, 0, 1)^T$ is a choice for which $\mathbf{v}_1$, $\mathbf{v}_2'$ are $\mathbf{v}_3$ linearly indepedent. This choice is not unique – there are infinitely many alternatives; one of them, e.g. is $\mathbf{v}_2' = (0, 1, 0)^T$.

ᴇL2.5.3 Einstein summation convention

(a) $a_i b^i = b^j a_j$ is true, since i and j are dummy variables which are summed over, hence we may rename as we please:

$$a_i b^i = \sum_{i=1}^{2} a_i b^i = a_1 b^1 + a_2 b^2 = b^1 a_1 + b^2 a_2 = \sum_{j=1}^{2} b^j a_j = b^j a_j \,. \checkmark$$

(b) $a_i\delta^i{}_j b^j = a_k b^k$ is true, since $\delta^i{}_j$ is nonzero only for $i=j$, in which case it equals 1:

$$a_i\delta^i{}_j b^j = a_1\underbrace{(\delta^1{}_1)}_{=1}b^1 + a_1\underbrace{(\delta^1{}_2)}_{=0}b^2 + a_2\underbrace{(\delta^2{}_1)}_{=0}b^1 + a_2\underbrace{(\delta^2{}_2)}_{=1}b^2 = a_1b^1 + a_2b^2 = a_kb^k\,. \checkmark$$

(c) $a_ib^ja_jb^k \stackrel{?}{=} a_kb^la_lb^i$ is false, since the indices i and k are *not* repeated, i.e. they are not summed over and hence may not renamed. For example, for $i=1$ and $k=2$ the left-hand side, $a_1(b^1a_1+b^2a_2)b^2$, clearly differs from right-hand side, $a_2(b^1a_1+b^2a_2)b^1$.

(d) $a_1a_ib^1b^i + b^2a_ja_2b^j = (a_ib^i)^2$ is true, since multiplication is associative and commutative and we may rename dummy indices as we please:

$$a_1a_ib^1b^i + b^2a_ja_2b^j = a_1b^1a_ib^i + a_2b^2a_ib^i = (a_1b^1+a_2b^2)(a_ib^i) = (a_jb^j)(a_ib^i) = (a_ib^i)^2\,. \checkmark$$

In practice, the arguments illustrated above need not be written out explicitly. Relations such as (a), (b) and (d) may be simply written down without further discussion.

S.L3 Euclidean geometry

S.L3.1 Scalar product of $\mathbb{R}^n$

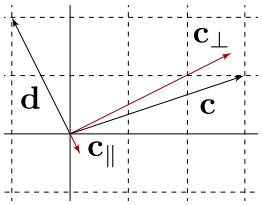
S.L3.2 Normalization and orthogonality

ᴇL3.2.1 Angle, orthogonal decomposition

(a) $$\cos(\angle(\mathbf{a},\mathbf{b})) = \frac{\mathbf{a}\cdot\mathbf{b}}{\|\mathbf{a}\|\|\mathbf{b}\|} = \frac{3\cdot 7+4\cdot 1}{\sqrt{9+16}\cdot\sqrt{49+1}} = \frac{1}{\sqrt{2}} \quad\Rightarrow\quad \angle(\mathbf{a},\mathbf{b}) = \frac{\pi}{4}$$

(b) $$\mathbf{c}_\parallel = \frac{(\mathbf{c}\cdot\mathbf{d})\mathbf{d}}{\|\mathbf{d}\|^2} = \frac{3\cdot(-1)+1\cdot 2}{1+4}\begin{pmatrix}-1\\2\end{pmatrix} = \frac{1}{5}\begin{pmatrix}1\\-2\end{pmatrix}$$

$$\mathbf{c}_\perp = \mathbf{c}-\mathbf{c}_\parallel = \begin{pmatrix}3\\1\end{pmatrix} - \frac{1}{5}\begin{pmatrix}1\\-2\end{pmatrix} = \frac{7}{5}\begin{pmatrix}2\\1\end{pmatrix}$$



Consistency check: $\mathbf{c}_\perp\cdot\mathbf{c}_\parallel = \frac{1}{25}\big(1\cdot 14 - 2\cdot 7\big) = 0$. ✓

S.L3.3 Inner product spaces

ᴇL3.3.2 Unconvential inner product

All the defining properties of an inner product are satisfied:

(i) Symmetric:

$$\langle \mathbf{x}, \mathbf{y} \rangle = x_1 y_1 + x_1 y_2 + x_2 y_1 + 3 x_2 y_2 = y_1 x_1 + y_1 x_2 + y_2 x_1 + 3 y_2 x_2 = \langle \mathbf{y}, \mathbf{x} \rangle \,. \checkmark$$

(ii,iii) Linear:

$$\begin{aligned} \langle \lambda \mathbf{x} + \mathbf{y}, \mathbf{z} \rangle &= (\lambda x_1 + y_1) z_1 + (\lambda x_1 + y_1) z_2 + (\lambda x_2 + y_2) z_1 + 3(\lambda x_2 + y_2) z_2 \\ &= (\lambda x_1 z_1 + \lambda x_1 z_2 + \lambda x_2 z_1 + 3 \lambda x_2 z_2) + (y_1 z_1 + y_1 z_2 + y_2 z_1 + 3 y_2 z_2) \\ &= \lambda \langle \mathbf{x}, \mathbf{z} \rangle + \langle \mathbf{y}, \mathbf{z} \rangle \,. \checkmark \end{aligned}$$

(iii) Positive semi-definite:

$$\langle \mathbf{x}, \mathbf{x} \rangle = x_1 x_1 + x_1 x_2 + x_2 x_1 + 3 x_2 x_2 = (x_1 + x_2)^2 + 2 x_2^2 \;\geq\; 0 \,. \checkmark$$

If $\langle \mathbf{x}, \mathbf{x} \rangle$, then $\mathbf{x} = (0, 0)^T$. ✓

ᴇL3.3.3 Projection onto an orthonormal basis

(a) $\langle \mathbf{e}'_1, \mathbf{e}'_1 \rangle = \frac{1}{2}\big[1 \cdot 1 + 1 \cdot 1\big] = 1 \,,$ $\qquad \langle \mathbf{e}'_1, \mathbf{e}'_2 \rangle = \frac{1}{2}\big[1 \cdot 1 + (-1) \cdot 1\big] = 0 \,.$
$\langle \mathbf{e}'_2, \mathbf{e}'_2 \rangle = \frac{1}{2}\big[1 \cdot 1 + (-1) \cdot (-1)\big] = 1$

The two vectors are normalized and orthogonal to each other, $\langle \mathbf{e}'_i, \mathbf{e}'_j \rangle = \delta_{ij}$, therefore they form an orthonormal basis of $\mathbb{R}^2$. ✓

(b) Since the vectors $\{\mathbf{e}'_1, \mathbf{e}'_2\}$ form an orthonormal basis, the component w^i of the vector $\mathbf{w} = (-2, 3)^T = \mathbf{e}'_i w^i$ with respect to this basis is given by the projection $w^i = \langle \mathbf{e}'^i, \mathbf{w} \rangle$:

$$\begin{aligned} w^1 &= \langle \mathbf{e}'^1, \mathbf{w} \rangle = \tfrac{1}{\sqrt{2}}\big[1 \cdot (-2) + 1 \cdot 3\big] = \tfrac{1}{\sqrt{2}} \,, \\ w^2 &= \langle \mathbf{e}'^2, \mathbf{w} \rangle = \tfrac{1}{\sqrt{2}}\big[1 \cdot (-2) - 1 \cdot 3\big] = -\tfrac{5}{\sqrt{2}} \,. \end{aligned}$$

ᴇL3.3.5 Non-orthonormal basis vectors and metric

(a) $\hat{\mathbf{v}}_1 = \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \quad \hat{\mathbf{v}}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}; \qquad \Rightarrow \qquad \hat{\mathbf{e}}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \tfrac{1}{2}\hat{\mathbf{v}}_1 \,, \; \hat{\mathbf{e}}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\tfrac{1}{2}\hat{\mathbf{v}}_1 + \hat{\mathbf{v}}_2 \,.$

The vectors $\hat{\mathbf{v}}_1$ and $\hat{\mathbf{v}}_2$ form a basis, because both standard basis vectors $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ can be written in terms of them.

(b) A representation of the vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ as column vectors in the standard basis of $\mathbb{R}^2$ can be found as follows:

$$\hat{\mathbf{x}} = \hat{\mathbf{v}}_1 x^1 + \hat{\mathbf{v}}_2 x^2, \quad x^1 = 3,\ x^2 = -4 \quad \Rightarrow \hat{\mathbf{x}} = \begin{pmatrix}2\\0\end{pmatrix}3 + \begin{pmatrix}1\\1\end{pmatrix}(-4) = \begin{pmatrix}2\\-4\end{pmatrix}.$$

$$\hat{\mathbf{y}} = \hat{\mathbf{v}}_1 y^1 + \hat{\mathbf{v}}_2 y^2, \quad y^1 = -1,\ y^2 = 3 \quad \Rightarrow \hat{\mathbf{y}} = \begin{pmatrix}2\\0\end{pmatrix}(-1) + \begin{pmatrix}1\\1\end{pmatrix}3 = \begin{pmatrix}1\\3\end{pmatrix}.$$

Scalar product: $\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_{\mathbb{R}^2} = \begin{pmatrix}2\\-4\end{pmatrix} \cdot \begin{pmatrix}1\\3\end{pmatrix} = 2 \cdot 1 + (-4) \cdot 3 = -10\,.$

(c)
$$g_{11} = \langle \hat{\mathbf{v}}_1, \hat{\mathbf{v}}_1 \rangle_{\mathbb{R}^2} = 4\,, \qquad g_{12} = \langle \hat{\mathbf{v}}_1, \hat{\mathbf{v}}_2 \rangle_{\mathbb{R}^2} = 2\,,$$
$$g_{21} = \langle \hat{\mathbf{v}}_2, \hat{\mathbf{v}}_1 \rangle_{\mathbb{R}^2} = 2\,, \qquad g_{22} = \langle \hat{\mathbf{v}}_2, \hat{\mathbf{v}}_2 \rangle_{\mathbb{R}^2} = 2\,.$$

(d)
$$\langle \hat{\mathbf{x}}, \hat{\mathbf{y}} \rangle_{\mathbb{R}^2} = \langle \mathbf{x}, \mathbf{y} \rangle_g = x^i g_{ij} y^j$$
$$= 3 \cdot 4 \cdot (-1) + 3 \cdot 2 \cdot 3 + (-4) \cdot 2 \cdot (-1) + (-4) \cdot 2 \cdot 3 = -10\,. \checkmark \quad [= \text{(b)}]$$

ᴇL3.3.7 Gram-Schmidt orthonormalization

Strategy: iterative orthogonalization and normalization, starting from $\mathbf{v}_{1,\perp} = \mathbf{v}_1$:

Starting vector: $\mathbf{v}_{1,\perp} = \mathbf{v}_1 = (1,-2,1)^T$

Normalizing $\mathbf{v}_{1,\perp}$: $\mathbf{e}'_1 = \dfrac{\mathbf{v}_{1,\perp}}{\|\mathbf{v}_{1,\perp}\|} = \frac{1}{\sqrt{6}}(1,-2,1)^T = \mathbf{e}'^1\,.$

Orthogonalizing $\mathbf{v}_2$: $\mathbf{v}_{2,\perp} = \mathbf{v}_2 - \mathbf{e}'_1\langle \mathbf{e}'^1, \mathbf{v}_2 \rangle = (1,1,1)^T - \mathbf{e}'_1(0)$

Normalizing $\mathbf{v}_{2,\perp}$: $\mathbf{e}'_2 = \dfrac{\mathbf{v}_{2,\perp}}{\|\mathbf{v}_{2,\perp}\|} = \frac{1}{\sqrt{3}}(1,1,1)^T = \mathbf{e}'^2\,.$

Orthogonalizing $\mathbf{v}_3$: $\mathbf{v}_{3,\perp} = \mathbf{v}_3 - \mathbf{e}'_1\langle \mathbf{e}'^1, \mathbf{v}_3 \rangle - \mathbf{e}'_2\langle \mathbf{e}'^2, \mathbf{v}_3 \rangle$

$= (0,1,2)^T - \mathbf{e}'_1(0) - \frac{1}{\sqrt{3}}(1,1,1)^T \left(3\frac{1}{\sqrt{3}}\right) = (-1,0,1)^T$

Normalizing $\mathbf{v}_{3,\perp}$: $\mathbf{e}'_3 = \dfrac{\mathbf{v}_{3,\perp}}{\|\mathbf{v}_{3,\perp}\|} = \frac{1}{\sqrt{2}}(-1,0,1)^T = \mathbf{e}'^3\,.$

S.L3.4 Complex scalar product

S.L4 Vector product

S.L4.2 Algebraic formulation

ᴇL4.2.1 Elementary computations with vectors

Using $\mathbf{a} = (4,3,1)^T$ and $\mathbf{b} = (1,-1,1)^T$ gives:

(a)
$$\|\mathbf{b}\| = \sqrt{1+1+1} = \sqrt{3}$$
$$\mathbf{a}-\mathbf{b} = (4-1, 3-(-1), 1-1)^T = (3,4,0)^T$$
$$\mathbf{a}\cdot\mathbf{b} = 4\cdot 1 + 3\cdot(-1) + 1\cdot 1 = 2$$
$$\mathbf{a}\times\mathbf{b} = \begin{pmatrix}4\\3\\1\end{pmatrix}\times\begin{pmatrix}1\\-1\\1\end{pmatrix} = \begin{pmatrix}3\cdot 1 - 1\cdot(-1)\\ 1\cdot 1 - 4\cdot 1\\ 4\cdot(-1) - 3\cdot 1\end{pmatrix} = \begin{pmatrix}4\\-3\\-7\end{pmatrix}$$

(b)
$$\mathbf{a}_\parallel = \frac{\mathbf{a}\cdot\mathbf{b}}{\|\mathbf{b}\|^2}\mathbf{b} = \frac{2}{3}\mathbf{b} = \frac{2}{3}(1,-1,1)^T$$
$$\mathbf{a}_\perp = \mathbf{a} - \mathbf{a}_\parallel = (4,3,1)^T - (2/3,-2/3,2/3)^T = (10/3, 11/3, 1/3)^T$$

(c)
$$\mathbf{a}_\parallel\cdot\mathbf{b} = \frac{2}{3}\mathbf{b}\cdot\mathbf{b} = \frac{2}{3}\cdot 3 = 2 = \mathbf{a}\cdot\mathbf{b}\ \checkmark$$
$$\mathbf{a}_\perp\cdot\mathbf{b} = \frac{10}{3} - \frac{11}{3} + \frac{1}{3} = 0\ \checkmark$$
$$\mathbf{a}_\parallel\times\mathbf{b} = \frac{2}{3}\begin{pmatrix}1\\-1\\1\end{pmatrix}\times\begin{pmatrix}1\\-1\\1\end{pmatrix} = \frac{2}{3}\begin{pmatrix}(-1)\cdot 1 - 1\cdot(-1)\\ 1\cdot 1 - 1\cdot 1\\ 1\cdot(-1) - (-1)\cdot 1\end{pmatrix} = \begin{pmatrix}0\\0\\0\end{pmatrix}\ \checkmark$$
$$\mathbf{a}_\perp\times\mathbf{b} = \frac{1}{3}\begin{pmatrix}10\\11\\1\end{pmatrix}\times\begin{pmatrix}1\\-1\\1\end{pmatrix} = \frac{1}{3}\begin{pmatrix}11+1\\1-10\\-10-11\end{pmatrix} = \begin{pmatrix}4\\-3\\-7\end{pmatrix} = \mathbf{a}\times\mathbf{b}\ \checkmark$$

As expected, we have: $\mathbf{a}_\parallel\cdot\mathbf{b} = \mathbf{a}\cdot\mathbf{b}$, $\mathbf{a}_\perp\cdot\mathbf{b} = 0$, $\mathbf{a}_\parallel\times\mathbf{b} = \mathbf{0}$ and $\mathbf{a}_\perp\times\mathbf{b} = \mathbf{a}\times\mathbf{b}$. ✓

ᴇL4.2.3 Levi-Civita tensor

(a) $a^i b^j \epsilon_{ij2} = -a^k \epsilon_{k2l} b^l$ is true. Indeed, writing out both sides explicitly, we find:

$$a^i b^j \epsilon_{ij2} = a^1 b^3 \epsilon_{132} + a^3 b^1 \epsilon_{312} = a^3 b^1 - a^1 b^3,$$
$$-a^k \epsilon_{k2l} b^l = -a^1 \epsilon_{123} b^3 - a^3 \epsilon_{321} b^1 = a^3 b^1 - a^1 b^3.$$

More compactly, we can bring the r.h.s into the form of the l.h.s by relabeling summation indices and using the antisymmetry of the ϵ tensor: $-a^k \epsilon_{k2l} b^l = -a^i b^j \epsilon_{i2j} = a^i b^j \epsilon_{ij2}$.

For the next two problems, we use the identity $\epsilon_{ijk}\epsilon_{mnk} = \delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}$. To be able to apply it, it might be necessary to cyclicly rearrange indices on one of the Levi-Civita factors.

(b)
$$\epsilon_{1ik}\epsilon_{kj1} = \epsilon_{1ik}\epsilon_{j1k} = \delta_{1j}\delta_{i1} - \delta_{11}\delta_{ij} = \begin{cases} -1 & \text{if } i = j \in \{2,3\},\\ 0 & \text{otherwise.}\end{cases}$$

Note: for $i = j = 1$, the delta functions yield $\delta_{1j}\delta_{i1} - \delta_{11}\delta_{ij} = 1\cdot 1 - 1\cdot 1 = 0$.

As a check, we write out the k-sum explicitly: $\epsilon_{1ik}\epsilon_{kj1} = \epsilon_{1i1}\epsilon_{1j1} + \epsilon_{1i2}\epsilon_{2j1} + \epsilon_{1i3}\epsilon_{3j1}$. The first term vanishes, because two indices on ϵ are equal. The second term is nonzero only for $i = j = 3$, in which case it yields $\epsilon_{132}\epsilon_{231} = (-1)\cdot(+1) = -1$. The third term is nonzero only for $i = j = 2$ in which case it yields $\epsilon_{123}\epsilon_{321} = (+1)\cdot(-1) = -1$.

(c) $$\epsilon_{1ik}\epsilon_{kj2} = \epsilon_{1ik}\epsilon_{j2k} = \delta_{1j}\delta_{i2} - \delta_{12}\delta_{ij} = \delta_{1j}\delta_{i2} = \begin{cases} 1 & \text{if } i = 2 \text{ and } j = 1, \\ 0 & \text{otherwise.} \end{cases}$$

As a check, we write out the k-sum explicitly: $\epsilon_{1ik}\epsilon_{2kj} = \epsilon_{1i1}\epsilon_{21j} + \epsilon_{1i2}\epsilon_{22j} + \epsilon_{1i3}\epsilon_{23j}$. The first and second terms vanish, since they contain ϵ-factors on which two indices are equal. The third term is nonzero only if $i = 2$ and $j = 1$, in which case it yields $\epsilon_{123}\epsilon_{231} = 1$.

S.L4.3 Further properties of the vector product

ɛL4.3.1 Grassmann identity (BAC-CAB) and Jacobi identity

(a) Consider the k-th component of $\mathbf{a}\times(\mathbf{b}\times\mathbf{c})$ in an orthonormal basis, for $k \in \{1,2,3\}$:

$$[\mathbf{a}\times(\mathbf{b}\times\mathbf{c})]^k \overset{\text{(i)}}{=} a^i[\mathbf{b}\times\mathbf{c}]^j\epsilon_{ijk} \overset{\text{(ii)}}{=} a^i b^m c^n \epsilon_{mnj}\epsilon_{kij} \overset{\text{(iii)}}{=} a^i b^m c^n(\delta_{mk}\delta_{ni} - \delta_{mi}\delta_{nk})$$
$$\overset{\text{(iv)}}{=} a^i b^k c^i - a^i b^i c^k \overset{\text{(v)}}{=} b^k(\mathbf{a}\cdot\mathbf{c}) - c^k(\mathbf{a}\cdot\mathbf{b})$$

Explanation: We (i,ii) employed the Levi-Civita representation of the cross product; (iii) used the identity from the hint to perform the sum over the repeated index j in the product of two Levi-Civita tensors; (iv) performed the sums on the repeated indices m and n, exploiting the Kronecker-δs; and (v) identified the remaining sums on i as scalar products. As a guide for the eye, we used horizontal brackets ('contractions') to indicate which repeated indices will be summed over in the next step.

(b) $$\mathbf{a}\times(\mathbf{b}\times\mathbf{c}) + \mathbf{b}\times(\mathbf{c}\times\mathbf{a}) + \mathbf{c}\times(\mathbf{a}\times\mathbf{b})$$
$$\overset{\text{Grassmann}}{=} \big[\mathbf{b}(\mathbf{a}\cdot\mathbf{c}) - \mathbf{c}(\mathbf{a}\cdot\mathbf{b})\big] + \big[\mathbf{c}(\mathbf{b}\cdot\mathbf{a}) - \mathbf{a}(\mathbf{b}\cdot\mathbf{c})\big] + \big[\mathbf{a}(\mathbf{c}\cdot\mathbf{b}) - \mathbf{b}(\mathbf{c}\cdot\mathbf{a})\big] = \mathbf{0}\,.\checkmark$$

(c) $\mathbf{a} = (1,1,2)^T$, $\mathbf{b} = (3,2,0)^T$, $\mathbf{c} = (2,1,1)^T$. $\quad \mathbf{a}\cdot\mathbf{c} = 5\,, \quad \mathbf{a}\cdot\mathbf{b} = 5\,.$

$$\mathbf{b}\times\mathbf{c} = \begin{pmatrix}3\\2\\0\end{pmatrix}\times\begin{pmatrix}2\\1\\1\end{pmatrix} = \begin{pmatrix}2\\-3\\-1\end{pmatrix}, \qquad \mathbf{a}\times(\mathbf{b}\times\mathbf{c}) = \begin{pmatrix}1\\1\\2\end{pmatrix}\times\begin{pmatrix}2\\-3\\-1\end{pmatrix} = \begin{pmatrix}5\\5\\-5\end{pmatrix}.$$
$$\mathbf{a}\times\mathbf{b} = \begin{pmatrix}1\\1\\2\end{pmatrix}\times\begin{pmatrix}3\\2\\0\end{pmatrix} = \begin{pmatrix}-4\\6\\-1\end{pmatrix}, \qquad \mathbf{c}\times(\mathbf{a}\times\mathbf{b}) = \begin{pmatrix}2\\1\\1\end{pmatrix}\times\begin{pmatrix}-4\\6\\-1\end{pmatrix} = \begin{pmatrix}-7\\-2\\-16\end{pmatrix}.$$
$$\mathbf{c}\times\mathbf{a} = \begin{pmatrix}2\\1\\1\end{pmatrix}\times\begin{pmatrix}1\\1\\2\end{pmatrix} = \begin{pmatrix}1\\-3\\1\end{pmatrix}, \qquad \mathbf{b}\times(\mathbf{c}\times\mathbf{a}) = \begin{pmatrix}3\\2\\0\end{pmatrix}\times\begin{pmatrix}1\\-3\\1\end{pmatrix} = \begin{pmatrix}2\\-3\\-11\end{pmatrix}.$$

$$\mathbf{b}(\mathbf{a}\cdot\mathbf{c}) - \mathbf{c}(\mathbf{a}\cdot\mathbf{b}) = 5\begin{pmatrix}3\\2\\0\end{pmatrix} - 5\begin{pmatrix}2\\1\\1\end{pmatrix} = \begin{pmatrix}5\\5\\-5\end{pmatrix} = \mathbf{a}\times(\mathbf{b}\times\mathbf{c})\,.\checkmark$$

$$\mathbf{a}\times(\mathbf{b}\times\mathbf{c})+\mathbf{b}\times(\mathbf{c}\times\mathbf{a})+\mathbf{c}\times(\mathbf{a}\times\mathbf{b})=\begin{pmatrix}5\\5\\-5\end{pmatrix}+\begin{pmatrix}-7\\-2\\16\end{pmatrix}+\begin{pmatrix}2\\-3\\-11\end{pmatrix}=\mathbf{0}\,.\checkmark$$

ᴇL4.3.3 Scalar triple product

(a) $$S(y)=\mathbf{v}_1\cdot(\mathbf{v}_2\times\mathbf{v}_3)=\begin{pmatrix}1\\0\\2\end{pmatrix}\cdot\left(\begin{pmatrix}3\\2\\1\end{pmatrix}\times\begin{pmatrix}-1\\-2\\y\end{pmatrix}\right)=$$

$$=\begin{pmatrix}1\\0\\2\end{pmatrix}\cdot\begin{pmatrix}2y+2\\-1-3y\\-4\end{pmatrix}=(2y+2)+0-8=2y-6$$

(b) $$\mathbf{0}=a^1\mathbf{v}_1+a^2\mathbf{v}_2+a^3\mathbf{v}_3=a^1\begin{pmatrix}1\\0\\2\end{pmatrix}+a^2\begin{pmatrix}3\\2\\1\end{pmatrix}+a^3\begin{pmatrix}-1\\-2\\y\end{pmatrix},\quad\text{with}\quad a^j\in\mathbb{R}.$$

This vector equation yields a system of three equations which we solve as follows:

(i)	$1a^1+3a^2-1a^3=0$	$\overset{\text{(ii)}}{\Rightarrow}$	(iv)	$a^3=a^2$
(ii)	$0a^1+2a^2-2a^3=0$	$\overset{\text{(iv) in (i)}}{\Rightarrow}$	(v)	$a^1=-2a^2$
(iii)	$2a^1+1a^2+ya^3=0$	$\overset{\text{(iv),(v) in (iii)}}{\Rightarrow}$	(vi)	$a^2(-4+1+y)=0$

(ii) yields (iv): $a^3=a^2$. Inserting (iv) into (i) yields (v): $a^1=-2a^2$. Inserting (iv) and (v) into (iii) yields (vi): $a^2(y-3)=0$. For $y\neq 3$ we have $0\overset{\text{(vi)}}{=}a^2\overset{\text{(v)}}{=}a^1\overset{\text{(iv)}}{=}a^3$, thus the vectors are linearly independent. For $y=3$, however, (vi) yields $0=0$, hence it does not fix the value of a^2. There are then infinitely many non-trivial solutions (one for every value of $a^2\in\mathbb{R}$), hence $\mathbf{v}_1$, $\mathbf{v}_2$ and $\mathbf{v}_3$ are linearly dependent.

(c) For $y=3$ we have $S(3)\overset{\text{(a)}}{=}2\cdot 3-6=0$, hence the volume of the parallelepiped spanned by the three vectors vanishes. Therefore they all lie in the same plane in $\mathbb{R}^3$ and thus are linearly dependent, as found in (b).

Remark: This example illustrates the following general fact: three vectors in $\mathbb{R}^3$ are linearly dependent if and only if their scalar triple product vanishes.

S.L5 Matrices I: general theory

S.L5.1 Linear maps

S.L5.2 Matrices

S.L5.3 Matrix multiplication

ᴇL5.3.1 Matrix multiplication

The matrix product AB is defined only when A has the same number of columns as B has rows. The possible products of two of the matrices P, Q and R therefore are:

$$PQ = \begin{pmatrix} 4 & -3 & 1 \\ 2 & 2 & -4 \end{pmatrix} \begin{pmatrix} 3 & 0 & 1 \\ 1 & 2 & 5 \\ 1 & -6 & -1 \end{pmatrix} = \begin{pmatrix} 10 & -12 & -12 \\ 4 & 28 & 16 \end{pmatrix}, \quad PR = \begin{pmatrix} 4 & -3 & 1 \\ 2 & 2 & -4 \end{pmatrix} \begin{pmatrix} 3 & 0 \\ 1 & 2 \\ 1 & -6 \end{pmatrix} = \begin{pmatrix} 10 & -12 \\ 4 & 28 \end{pmatrix}.$$

$$QR = \begin{pmatrix} 3 & 0 & 1 \\ 1 & 2 & 5 \\ 1 & -6 & -1 \end{pmatrix} \begin{pmatrix} 3 & 0 \\ 1 & 2 \\ 1 & -6 \end{pmatrix} = \begin{pmatrix} 10 & -6 \\ 10 & -26 \\ -4 & -6 \end{pmatrix}, \quad RP = \begin{pmatrix} 3 & 0 \\ 1 & 2 \\ 1 & -6 \end{pmatrix} \begin{pmatrix} 4 & -3 & 1 \\ 2 & 2 & -4 \end{pmatrix} = \begin{pmatrix} 12 & -9 & 3 \\ 8 & 1 & -7 \\ -8 & -15 & 25 \end{pmatrix}.$$

$$QQ = \begin{pmatrix} 3 & 0 & 1 \\ 1 & 2 & 5 \\ 1 & -6 & -1 \end{pmatrix} \begin{pmatrix} 3 & 0 & 1 \\ 1 & 2 & 5 \\ 1 & -6 & -1 \end{pmatrix} = \begin{pmatrix} 10 & -6 & 2 \\ 10 & -26 & 6 \\ -4 & -6 & -28 \end{pmatrix}.$$

ᴇL5.3.3 Spin $\frac{1}{2}$ matrices

(a)
$$\begin{aligned} \mathbf{S}^2 &= \tfrac{1}{4} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \tfrac{1}{4} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} + \tfrac{1}{4} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &= \tfrac{1}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \tfrac{1}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \tfrac{3}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \tfrac{3}{4} \cdot \mathbb{1}. \end{aligned}$$

(b)
$$\begin{aligned} [S_x, S_y] &= \tfrac{1}{4} \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} - \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right] \\ &= \tfrac{1}{4} \left[\begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix} - \begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix} \right] = \tfrac{1}{2} \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix} = \mathrm{i} S_z. \\ [S_y, S_z] &= \tfrac{1}{4} \left[\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \right] \\ &= \tfrac{1}{4} \left[\begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} - \begin{pmatrix} 0 & -\mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix} \right] = \tfrac{1}{2} \begin{pmatrix} 0 & \mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} = \mathrm{i} S_x. \\ [S_z, S_x] &= \tfrac{1}{4} \left[\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \\ &= \tfrac{1}{4} \left[\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \right] = \tfrac{1}{2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \mathrm{i} S_y. \end{aligned}$$

(c) Commutators are antisymmetric, $[A, B] = -[B, A]$, and $[A, A] = 0$. From (b) we thus conclude that the spin $\frac{1}{2}$ matrices satisfy the commutation relation $[S_i, S_j] = \mathrm{i}\epsilon_{ijk} S_k$, where ϵ_{ijk} is the anti-symmetric Levi-Civita tensor. Thus $a_{ijk} = \mathrm{i}\epsilon_{ijk}$.

Remark: The 'spin' of a quantum mechanical particle is a type of internal angular momentum. The description of quantum mechanical spins in general requires three matrices, S_x, S_y and S_z, whose commutators satisfy the relation $[S_i, S_j] = \epsilon_{ijk} S_k$. These are the defining relations of the so-called SU(2) algebra, which underlies the quantum mechanical description of rotations. The spin $\frac{1}{2}$ matrices form a representation of this algebra in terms of 2×2 matrices. The description of quantum mechanical particles with spin d, with $2d \in \mathbb{Z}$, utilizes a representation of the SU(2) algebra in terms of $(2d+1) \times (2d+1)$ matrices.

ᴇL5.3.5 Matrix multiplication

(a) $$A = \begin{pmatrix} 0 & 0 & 0 \\ A_1 & A_2 & A_3 \\ 0 & 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} B_1 & 0 & 0 \\ 0 & B_2 & 0 \\ 0 & 0 & B_3 \end{pmatrix}, \quad AB = \begin{pmatrix} 0 & 0 & 0 \\ A_1B_1 & A_2B_2 & A_3B_3 \\ 0 & 0 & 0 \end{pmatrix}$$

(b) $$(AB)^i{}_j = \sum_k a^i{}_k b^k{}_j = \sum_k A_k \delta^i{}_m B_k \delta^k{}_j = \delta^i{}_m A_j B_j$$

$$AB \overset{\text{m-th row}}{=\!=\!\rightarrow} \begin{pmatrix} 0 & \dots & 0 \\ \vdots & & \vdots \\ A_1 & \dots & A_N \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{pmatrix} \begin{pmatrix} B_1 & 0 & \dots & 0 \\ 0 & B_2 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \dots & \dots & B_N \end{pmatrix} = \begin{pmatrix} 0 & \dots & 0 \\ \vdots & & \vdots \\ A_1B_1 & \dots & A_NB_N \\ \vdots & & \vdots \\ 0 & \dots & 0 \end{pmatrix}$$

S.L5.4 The inverse of a matrix

ᴇL5.4.1 Gaussian elimination and matrix inversion

(a) We express the system of equations in the form of an augmented matrix, and then bring the left side of the matrix into diagonal form. To do this, we successively replace each row by a suitable linear combination of rows [indicated by square brackets] of the previous extended matrix, i.e in the first step $[1] \to [1]$, $[2] \to \frac{1}{2}(3[2] - 2[1])$ and $[3] \to 6[3] + 2[1]$. It is advisable to keep the mental arithmetic simple by avoiding the occurrence of fractions until the left side has been brought into row echelon form (only zeros on one side of the diagonal).

$$\begin{array}{rcccc|c|} & x^1 & x^2 & x^3 & & & x^1 & x^2 & x^3 & \\ [1]: & 3 & 2 & -1 & 1 & & [1]: & 3 & 2 & -1 & 1 \\ [2]: & 2 & -2 & 4 & -2 & \longrightarrow & \frac{1}{2}(3[2]-2[1]): & 0 & -5 & 7 & -4 \\ [3]: & -1 & \frac{1}{2} & -1 & 0 & & 6[3]+2[1]: & 0 & 7 & -8 & 2 \end{array}$$

$$\swarrow$$

$$\begin{array}{rcccc|c|} \frac{1}{3}(5[1]+2[2]): & 5 & 0 & 3 & -1 & & \frac{1}{5}([1]-3[3]): & 1 & 0 & 0 & 1 \\ -[2]: & 0 & 5 & -7 & 4 & \longrightarrow & \frac{1}{5}([2]+7[3]): & 0 & 1 & 0 & -2 \\ \frac{1}{9}(7[2]+5[3]): & 0 & 0 & 1 & -2 & & [3]: & 0 & 0 & 1 & -2 \end{array}$$

Hence the solution to the system of equation is: $\mathbf{x} = (x^1, x^2, x^3)^T = (1, -2, -2)^T$.

(b) If the last equation is taken out of the system, we obtain after the second step (see above):

$$\begin{array}{rcccc|c|} & x^1 & x^2 & x^3 & & \\ [1]: & 3 & 2 & -1 & 1 & \\ \frac{1}{2}(3[2]-2[1]): & 0 & -5 & 7 & -4 & \end{array}$$

The system is now underdetermined, since there are more unknowns than equations. The solution thus depends on a free parameter, which we call $x^3 = \lambda$. We now complete the system with a corresponding third line and then bring the left side into a diagonal form:

$$\begin{array}{rcccc|c} & x^1 & x^2 & x^3 & & \\ [1]: & 3 & 2 & -1 & | & 1 \\ [2]: & 0 & -5 & 7 & | & -4 \\ [3]: & 0 & 0 & 1 & | & \lambda \end{array} \quad \longrightarrow \quad \begin{array}{rcccc|c} & x^1 & x^2 & x^3 & & \\ \frac{1}{5}\big[\frac{1}{3}(5[1]+2[2])-3[3]\big]: & 1 & 0 & 0 & | & -\frac{1}{5}(1+3\lambda) \\ -\frac{1}{5}([2]-7[3]): & 0 & 1 & 0 & | & \frac{1}{5}(4+7\lambda) \\ [3]: & 0 & 0 & 1 & | & \lambda \end{array}$$

There are evidently infinitely many solutions, $\mathbf{x} = (-\frac{1}{5} - \frac{3}{5}\lambda, \frac{4}{5} + \frac{7}{5}\lambda, \lambda)^T$. They lie along a straight line in R^3, parametrized by λ.

(c) By replacing the last equation by $-x^1 + \frac{2}{7}x^2 - x^3 = 0$, we obtain:

$$\begin{array}{rcccc|c} & x^1 & x^2 & x^3 & & \\ [1]: & 3 & 2 & -1 & | & 1 \\ [2]: & 2 & -2 & 4 & | & -2 \\ [3]: & -1 & \frac{2}{7} & -1 & | & 0 \end{array} \quad \longrightarrow \quad \begin{array}{rcccc|c} & x^1 & x^2 & x^3 & & \\ [1]: & 3 & 2 & -1 & | & 1 \\ \frac{1}{2}(3[2]-2[1]): & 0 & -5 & 7 & | & -4 \\ 6[3]+2[1]: & 0 & \frac{40}{7} & -8 & | & 2 \end{array}$$

$$\swarrow$$

$$\begin{array}{rcccc|c} \frac{1}{3}(5[1]+2[2]): & 5 & 0 & 3 & | & -1 \\ -[2]: & 0 & 5 & -7 & | & 4 \\ 8[2]+7[3]: & 0 & 0 & 0 & | & -18 \end{array}$$

The last equation reads $0x^1 + 0x^2 + 0x^3 = -18$, which is a logical contradiction. In this case, this system of equations thus has no solution.

(d) The equation $A\mathbf{x} = \mathbf{b}$ has the matrix $A = \begin{pmatrix} 3 & 2 & -1 \\ 2 & -2 & 4 \\ -1 & \frac{1}{2} & -1 \end{pmatrix}$. To calculate the inverse, A^{-1}, we start with an extended matrix, with the identity matrix placed on the right hand side. We then proceed by following exactly the same steps as in (a):

$$\begin{array}{rcccc|ccc} & x^1 & x^2 & x^3 & & & & \\ [1]: & 3 & 2 & -1 & | & 1 & 0 & 0 \\ [2]: & 2 & -2 & 4 & | & 0 & 1 & 0 \\ [3]: & -1 & \frac{1}{2} & -1 & | & 0 & 0 & 1 \end{array} \quad \longrightarrow \quad \begin{array}{rcccc|ccc} & x^1 & x^2 & x^3 & & & & \\ [1]: & 3 & 2 & -1 & | & 1 & 0 & 0 \\ \frac{1}{2}(3[2]-2[1]): & 0 & -5 & 7 & | & -1 & \frac{3}{2} & 0 \\ 6[3]+2[1]: & 0 & 7 & -8 & | & 2 & 0 & 6 \end{array}$$

$$\swarrow$$

$$\begin{array}{rcccc|ccc} \frac{1}{3}(5[1]+2[2]): & 5 & 0 & 3 & | & 1 & 1 & 0 \\ -[2]: & 0 & 5 & -7 & | & 1 & -\frac{3}{2} & 0 \\ \frac{1}{9}(7[2]+5[3]): & 0 & 0 & 1 & | & \frac{1}{3} & \frac{7}{6} & \frac{10}{3} \end{array} \quad \longrightarrow \quad \begin{array}{rcccc|ccc} & x^1 & x^2 & x^3 & & & & \\ \frac{1}{5}([1]-3[3]): & 1 & 0 & 0 & | & 0 & -\frac{1}{2} & -2 \\ \frac{1}{5}([2]+7[3]): & 0 & 1 & 0 & | & \frac{2}{3} & \frac{4}{3} & \frac{14}{3} \\ [3]: & 0 & 0 & 1 & | & \frac{1}{3} & \frac{7}{6} & \frac{10}{3} \end{array}$$

From this we can now identify the inverse matrix, and verify our answer from (a):

$$A^{-1} = \frac{1}{3}\begin{pmatrix} 0 & -\frac{3}{2} & -6 \\ 2 & 4 & 14 \\ 1 & \frac{7}{2} & 10 \end{pmatrix}, \qquad \mathbf{x} = A^{-1}\mathbf{b} = \frac{1}{3}\begin{pmatrix} 0 & -\frac{3}{2} & -6 \\ 2 & 4 & 14 \\ 1 & \frac{7}{2} & 10 \end{pmatrix}\begin{pmatrix} 1 \\ -2 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ -2 \\ -2 \end{pmatrix}. \checkmark$$

ᴇL5.4.3 Matrix inversion

(a) The inverse of $M_2 = \begin{pmatrix} 1+m & 0 \\ 1 & m \end{pmatrix}$ follows from the formula $\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$:

$$M_2^{-1} = \begin{pmatrix} \frac{1}{1+m} & 0 \\ -\frac{1}{m(1+m)} & \frac{1}{m} \end{pmatrix}. \quad \text{Check: } \begin{pmatrix} \frac{1}{1+m} & 0 \\ -\frac{1}{m(1+m)} & \frac{1}{m} \end{pmatrix} \cdot \begin{pmatrix} 1+m & 0 \\ 1 & m \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \checkmark$$

We compute the inverse of $M_3 = \begin{pmatrix} 1+m & 0 & 0 \\ 1 & m & 0 \\ 1 & 0 & m \end{pmatrix}$ using Gaussian elimination:

$$\begin{array}{lcccc|ccc} [1]: & 1+m & 0 & 0 & | & 1 & 0 & 0 \\ [2]: & 1 & m & 0 & | & 0 & 1 & 0 \\ [3]: & 1 & 0 & m & | & 0 & 0 & 1 \end{array} \longrightarrow \begin{array}{lcccc|ccc} \frac{1}{1+m}[1]: & 1 & 0 & 0 & | & \frac{1}{1+m} & 0 & 0 \\ \frac{1}{m}([2]-\frac{1}{1+m}[1]): & 0 & 1 & 0 & | & -\frac{1}{m(1+m)} & \frac{1}{m} & 0 \\ \frac{1}{m}([3]-\frac{1}{1+m}[1]): & 0 & 0 & 1 & | & -\frac{1}{m(1+m)} & 0 & \frac{1}{m} \end{array}$$

The right side of the augmented matrix gives the inverse matrix M_3^{-1}:

$$M_3^{-1} = \begin{pmatrix} \frac{1}{1+m} & 0 & 0 \\ -\frac{1}{m(1+m)} & \frac{1}{m} & 0 \\ -\frac{1}{m(1+m)} & 0 & \frac{1}{m} \end{pmatrix}. \text{ Check: } \begin{pmatrix} \frac{1}{1+m} & 0 & 0 \\ -\frac{1}{m(1+m)} & \frac{1}{m} & 0 \\ -\frac{1}{m(1+m)} & 0 & \frac{1}{m} \end{pmatrix} \begin{pmatrix} 1+m & 0 & 0 \\ 1 & m & 0 \\ 1 & 0 & m \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \checkmark$$

(b) The results for M_2^{-1} and M_3^{-1} have the following properties: the first diagonal element equals $\frac{1}{1+m}$, the remaining diagonal elements equal $\frac{1}{m}$, and the remaining elements of the first column equal $-\frac{1}{m(1+m)}$. The checks performed in (a) illustrate why these properties are needed. We thus formulate the following guess for the form of M_n^{-1} for a general n:

$$M_n^{-1} = \begin{pmatrix} \frac{1}{1+m} & 0 & 0 & \dots & 0 \\ -\frac{1}{m(1+m)} & \frac{1}{m} & 0 & \ddots & \vdots \\ -\frac{1}{m(1+m)} & 0 & \frac{1}{m} & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 \\ -\frac{1}{m(1+m)} & 0 & \dots & 0 & \frac{1}{m} \end{pmatrix}$$

Now let us check our guess explicitly: does $M_n^{-1} M_n = \mathbb{1}$ hold?

$$M_n^{-1} \cdot M_n = \begin{pmatrix} \frac{1}{1+m} & 0 & 0 & \dots & 0 \\ -\frac{1}{m(1+m)} & \frac{1}{m} & 0 & \ddots & \vdots \\ -\frac{1}{m(1+m)} & 0 & \frac{1}{m} & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 \\ -\frac{1}{m(1+m)} & 0 & \dots & 0 & \frac{1}{m} \end{pmatrix} \begin{pmatrix} 1+m & 0 & 0 & \dots & 0 \\ 1 & m & 0 & \ddots & \vdots \\ 1 & 0 & m & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 1 & 0 & \dots & 0 & m \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1+m}{1+m} & 0 & 0 & \dots & 0 \\ -\frac{1+m}{m(1+m)} + \frac{1}{m} + 0 + \dots & \frac{m}{m} & 0 & \ddots & \vdots \\ -\frac{1+m}{m(1+m)} + 0 + \frac{1}{m} + 0 + \dots & 0 & \frac{m}{m} & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 \\ -\frac{1+m}{m(1+m)} + 0 + \dots + 0 + \frac{1}{m} & 0 & \dots & 0 & \frac{m}{m} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \ddots & \vdots \\ 0 & 0 & \ddots & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix}. \checkmark$$

(c) Alternative formulation using index notation: $(M_n^{-1})^i{}_j = \frac{1}{m}\left(\delta^i{}_j - \frac{1}{1+m}\delta^1{}_j\right)$.

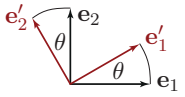
$$(M_n^{-1}\cdot M_n)^i{}_j = \sum_l (M_n^{-1})^i{}_l (M_n)^l{}_j = \sum_l \left(\tfrac{1}{m}\delta^i{}_l - \tfrac{1}{m(1+m)}\delta^1{}_l\right)\left(m\delta^l{}_j + \delta^1{}_j\right)$$
$$= \delta^i{}_j + \tfrac{1}{m}\delta^1{}_j - \tfrac{1}{1+m}\delta^1{}_j - \tfrac{1}{m(1+m)}\delta^1{}_j = \delta^i{}_j + \delta^1{}_j\tfrac{1+m-m-1}{m(1+m)} = \delta^i{}_j\,.\checkmark$$

S.L5.5 General linear maps and matrices

ᴇL5.5.1 Two-dimensional rotation matrices

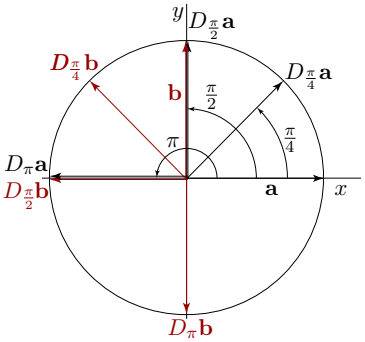
(a) For $R_\theta : \mathbf{e}_j \mapsto \mathbf{e}'_j = \mathbf{e}_i (R_\theta)^i{}_j$ the image vector $\mathbf{e}'_j$ yields column j of the rotation matrix:

$$R_\theta : \quad \begin{pmatrix}1\\0\end{pmatrix} \mapsto \begin{pmatrix}\cos\theta\\ \sin\theta\end{pmatrix}, \quad \begin{pmatrix}0\\1\end{pmatrix} \mapsto \begin{pmatrix}-\sin\theta\\ \cos\theta\end{pmatrix} \;\Rightarrow\; R_\theta = \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix}.$$



(b) For $\theta_1 = 0$, $\theta_2 = \frac{\pi}{4}$, $\theta_3 = \pi/2$ and $\theta_4 = \pi$ we have:

$$R_0 = \begin{pmatrix}1&0\\0&1\end{pmatrix}, \qquad R_0\mathbf{a} = \mathbf{a}, \qquad R_0\mathbf{b} = \mathbf{b}.$$
$$R_{\frac{\pi}{4}} = \tfrac{1}{\sqrt{2}}\begin{pmatrix}1&-1\\1&1\end{pmatrix}, \quad R_{\frac{\pi}{4}}\mathbf{a} = \tfrac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \quad R_{\frac{\pi}{4}}\mathbf{b} = \tfrac{1}{\sqrt{2}}\begin{pmatrix}-1\\1\end{pmatrix}.$$
$$R_{\frac{\pi}{2}} = \begin{pmatrix}0&-1\\1&0\end{pmatrix}, \qquad R_{\frac{\pi}{2}}\mathbf{a} = \begin{pmatrix}0\\1\end{pmatrix}, \qquad R_{\frac{\pi}{2}}\mathbf{b} = \begin{pmatrix}-1\\0\end{pmatrix}.$$
$$R_\pi = \begin{pmatrix}-1&0\\0&-1\end{pmatrix}, \qquad R_\pi\mathbf{a} = \begin{pmatrix}-1\\0\end{pmatrix}, \qquad R_\pi\mathbf{b} = \begin{pmatrix}0\\-1\end{pmatrix}.$$



(c) Using the addition theorems, we readily obtain:

$$R_\theta R_\phi = \begin{pmatrix}\cos\theta & -\sin\theta\\ \sin\theta & \cos\theta\end{pmatrix}\begin{pmatrix}\cos\phi & -\sin\phi\\ \sin\phi & \cos\phi\end{pmatrix} = \begin{pmatrix}\cos\theta\cos\phi - \sin\theta\sin\phi & -\cos\theta\sin\phi - \sin\theta\cos\phi\\ \sin\theta\cos\phi + \cos\theta\sin\phi & -\sin\theta\sin\phi + \cos\theta\cos\phi\end{pmatrix}$$
$$= \begin{pmatrix}\cos(\theta+\phi) & -\sin(\theta+\phi)\\ \sin(\theta+\phi) & \cos(\theta+\phi)\end{pmatrix} = R_{\theta+\phi}\,.\checkmark$$

(d) Rotating the vector $\mathbf{r} = (x, y)^T$ by the angle θ leaves its length unchanged:

$$R_\theta\mathbf{r} = \begin{pmatrix}x\cos\theta - y\sin\theta\\ x\sin\theta + y\cos\theta\end{pmatrix} \;\Rightarrow\; \|R_\theta\mathbf{r}\| = \sqrt{(x^2+y^2)(\cos^2\theta + \sin^2\theta) + (2\cos\theta\sin\theta)(xy - xy)}$$
$$= \sqrt{(x^2+y^2)} = \|\mathbf{r}\|\,.\checkmark$$

S.L5.6 Matrices describing coordinate changes

ᴇL5.6.1 Basistransformation und lineare Abbildung in $\mathbb{E}^2$

(a) The relation $\hat{\mathbf{e}}_j = \hat{\mathbf{e}}'_i T^i{}_j$ between old and new bases yields the transformation matrix T:

$$\begin{aligned} \hat{\mathbf{e}}_1 &= \tfrac{3}{4}\hat{\mathbf{e}}'_1 + \tfrac{1}{3}\hat{\mathbf{e}}'_2 \equiv \hat{\mathbf{e}}'_1 T^1{}_1 + \hat{\mathbf{e}}'_2 T^2{}_1 \\ \hat{\mathbf{e}}_2 &= -\tfrac{1}{8}\hat{\mathbf{e}}'_1 + \tfrac{1}{2}\hat{\mathbf{e}}'_2 \equiv \hat{\mathbf{e}}'_1 T^1{}_2 + \hat{\mathbf{e}}'_2 T^2{}_2 \end{aligned} \quad \Rightarrow \quad T = \begin{pmatrix} T^1{}_1 & T^1{}_2 \\ T^2{}_1 & T^2{}_2 \end{pmatrix} = \begin{pmatrix} \frac{3}{4} & -\frac{1}{8} \\ \frac{1}{3} & \frac{1}{2} \end{pmatrix} = \frac{1}{24}\begin{pmatrix} 18 & -3 \\ 8 & 12 \end{pmatrix}.$$

(b) Using T^{-1} and $\hat{\mathbf{e}}'_j = \hat{\mathbf{e}}_i (T^{-1})^i{}_j$ we can write the new basis in terms of the old:

$$T^{-1} = \frac{1}{\det T}\begin{pmatrix} T^2{}_2 & -T^1{}_2 \\ -T^2{}_1 & T^1{}_1 \end{pmatrix} = \frac{12}{5}\frac{1}{24}\begin{pmatrix} 12 & 3 \\ -8 & 18 \end{pmatrix} = \frac{1}{10}\begin{pmatrix} 12 & 3 \\ -8 & 18 \end{pmatrix} \equiv \begin{pmatrix} (T^{-1})^1{}_1 & (T^{-1})^1{}_2 \\ (T^{-1})^2{}_1 & (T^{-1})^2{}_2 \end{pmatrix}.$$

$$\begin{aligned} \hat{\mathbf{e}}'_1 &= \hat{\mathbf{e}}_1 (T^{-1})^1{}_1 + \hat{\mathbf{e}}_2 (T^{-1})^2{}_1 = \tfrac{6}{5}\hat{\mathbf{e}}_1 - \tfrac{4}{5}\hat{\mathbf{e}}_2 \,. \\ \hat{\mathbf{e}}'_2 &= \hat{\mathbf{e}}_1 (T^{-1})^1{}_2 + \hat{\mathbf{e}}_2 (T^{-1})^2{}_2 = \tfrac{3}{10}\hat{\mathbf{e}}_1 + \tfrac{9}{5}\hat{\mathbf{e}}_2 \,. \end{aligned}$$

Alternatively, these relations can be derived by solving the equations for $\hat{\mathbf{e}}_1$ and $\hat{\mathbf{e}}_2$ to give $\hat{\mathbf{e}}'_1$ and $\hat{\mathbf{e}}'_2$. (This is equivalent to finding T^{-1}.)

(c) The components of $\hat{\mathbf{x}} = \hat{\mathbf{e}}_j x^j = \hat{\mathbf{e}}'_i x'^i$ in the old and new bases, $\mathbf{x} = (x^1, x^2)^T$ and $\mathbf{x}' = (x'^1, x'^2)^T$ respectively, are related by $x'^i = T^i{}_j x^j$:

$$\mathbf{x} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \quad \mathbf{x}' = T\mathbf{x} = \frac{1}{24}\begin{pmatrix} 18 & -3 \\ 8 & 12 \end{pmatrix}\begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{4}{3} \end{pmatrix}, \Rightarrow \hat{\mathbf{x}} = \hat{\mathbf{e}}_1 + 2\hat{\mathbf{e}}_2 = \tfrac{1}{2}\hat{\mathbf{e}}'_1 + \tfrac{4}{3}\hat{\mathbf{e}}'_2 \,.$$

(d) The components of $\hat{\mathbf{y}} = \hat{\mathbf{e}}'_i y'^i = \hat{\mathbf{e}}_j y^j$ in the new and old bases, $\mathbf{y}' = (y'^1, y'^2)^T$ and $\mathbf{y} = (y^1, y^2)^T$ respectively, are related by $y^i = (T^{-1})^i{}_j y'^j$:

$$\mathbf{y}' = \begin{pmatrix} \frac{3}{4} \\ \frac{1}{3} \end{pmatrix}, \quad \mathbf{y} = T^{-1}\mathbf{y}' = \frac{1}{10}\begin{pmatrix} 12 & 3 \\ -8 & 18 \end{pmatrix}\begin{pmatrix} \frac{3}{4} \\ \frac{1}{3} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \Rightarrow \hat{\mathbf{y}} = \tfrac{3}{4}\hat{\mathbf{e}}'_1 + \tfrac{1}{3}\hat{\mathbf{e}}'_2 = \hat{\mathbf{e}}_1 \,.$$

(e) The matrix representation A' of the map $\hat{A}$ in the new basis describes its action on that basis: the image of basis vector j, written as $\hat{\mathbf{e}}'_j \overset{\hat{A}}{\mapsto} \hat{\mathbf{e}}'_i A'^i{}_j$, yields column j of A':

$$\begin{aligned} \hat{\mathbf{e}}'_1 &= 2\hat{\mathbf{e}}'_1 + 0\hat{\mathbf{e}}'_2 \equiv \hat{\mathbf{e}}'_1 A'^1{}_1 + \hat{\mathbf{e}}'_2 A'^2{}_1 \\ \hat{\mathbf{e}}'_2 &= 0\hat{\mathbf{e}}'_1 + 1\hat{\mathbf{e}}'_2 \equiv \hat{\mathbf{e}}'_1 A'^1{}_2 + \hat{\mathbf{e}}'_2 A'^2{}_2 \end{aligned} \quad \Rightarrow \quad A' = \begin{pmatrix} A'^1{}_1 & A'^1{}_2 \\ A'^2{}_1 & A'^2{}_2 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}.$$

The basis transformation T now yields the matrix representation A of $\hat{A}$ in the old basis:

$$A' = TAT^{-1} \;\Rightarrow\; A = T^{-1}A'T = \frac{1}{10}\begin{pmatrix} 12 & 3 \\ -8 & 18 \end{pmatrix}\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}\frac{1}{24}\begin{pmatrix} 18 & -3 \\ 8 & 12 \end{pmatrix} = \frac{1}{20}\begin{pmatrix} 38 & -3 \\ -12 & 22 \end{pmatrix}.$$

(f) For $\hat{\mathbf{x}} \overset{\hat{A}}{\mapsto} \hat{\mathbf{z}}$, the components $\hat{\mathbf{z}}$ are obtained by matrix multiplying the components of $\hat{\mathbf{x}}$ with the matrix representation of $\hat{A}$, in either the new or old basis:

$$\mathbf{z}' = A'\mathbf{x}' = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ \frac{4}{3} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{4}{3} \end{pmatrix}, \qquad \mathbf{z} = A\mathbf{x} = \frac{1}{20} \begin{pmatrix} 38 & -3 \\ -12 & 22 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \frac{8}{5} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

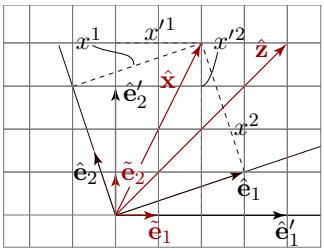
The results for $\mathbf{z}'$ and $\mathbf{z}$ are consistent, $T\mathbf{z} = \frac{1}{24} \begin{pmatrix} 18 & -3 \\ 8 & 12 \end{pmatrix} \frac{8}{5} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{4}{3} \end{pmatrix} = \mathbf{z}'$. ✓

(g) The component representation of the standard basis of $\mathbb{E}^2$ is $\tilde{\mathbf{e}}_1 = (1,0)^T$ and $\tilde{\mathbf{e}}_2 = (0,1)^T$. Once the old basis has been specified by making the choice $\hat{\mathbf{e}}_1 = 3\tilde{\mathbf{e}}_1 + \tilde{\mathbf{e}}_2 = (3,1)^T$ and $\hat{\mathbf{e}}_2 = -\frac{1}{2}\tilde{\mathbf{e}}_1 + \frac{3}{2}\tilde{\mathbf{e}}_2 = (-\frac{1}{2}, \frac{3}{2})^T$, that also fixes the new basis, as well as $\hat{\mathbf{x}}$ and $\hat{\mathbf{z}}$. The components of $\hat{\mathbf{x}}$ and $\hat{\mathbf{z}}$ in the standard basis of $\mathbb{E}^2$ can be computed via either the old or the new basis. In the standard basis we obtain the following representation:

$$\hat{\mathbf{e}}'_1 = \hat{\mathbf{e}}_i (T^{-1})^i{}_1 = \frac{6}{5} \begin{pmatrix} 3 \\ 1 \end{pmatrix} - \frac{4}{5} \begin{pmatrix} -\frac{1}{2} \\ \frac{3}{2} \end{pmatrix} = \begin{pmatrix} 4 \\ 0 \end{pmatrix}.$$

$$\hat{\mathbf{e}}'_2 = \hat{\mathbf{e}}_i (T^{-1})^i{}_2 = \frac{3}{10} \begin{pmatrix} 3 \\ 1 \end{pmatrix} + \frac{9}{5} \begin{pmatrix} -\frac{1}{2} \\ \frac{3}{2} \end{pmatrix} = \begin{pmatrix} 0 \\ 3 \end{pmatrix}.$$

(h)



$$\hat{\mathbf{x}} = \hat{\mathbf{e}}_i x^i = 1 \begin{pmatrix} 3 \\ 1 \end{pmatrix} + 2 \begin{pmatrix} -\frac{1}{2} \\ \frac{3}{2} \end{pmatrix} = \begin{pmatrix} 2 \\ 4 \end{pmatrix}, \qquad \hat{\mathbf{x}} = \hat{\mathbf{e}}'_i x'^i = \frac{1}{2} \begin{pmatrix} 4 \\ 0 \end{pmatrix} + \frac{4}{3} \begin{pmatrix} 0 \\ 3 \end{pmatrix} = \begin{pmatrix} 2 \\ 4 \end{pmatrix}. \checkmark$$

$$\hat{\mathbf{z}} = \hat{\mathbf{e}}_i z^i = \frac{8}{5} \begin{pmatrix} 3 \\ 1 \end{pmatrix} + \frac{8}{5} \begin{pmatrix} -\frac{1}{2} \\ \frac{3}{2} \end{pmatrix} = \begin{pmatrix} 4 \\ 4 \end{pmatrix}, \qquad \hat{\mathbf{z}} = \hat{\mathbf{e}}'_i z'^i = 1 \begin{pmatrix} 4 \\ 0 \end{pmatrix} + \frac{4}{3} \begin{pmatrix} 0 \\ 3 \end{pmatrix} = \begin{pmatrix} 4 \\ 4 \end{pmatrix}. \checkmark$$

By comparing $\hat{\mathbf{x}}$ and $\hat{\mathbf{z}}$ we see that $\hat{A}$ stretches the $\tilde{\mathbf{e}}_1$ direction by a factor 2.

ᴇL5.6.3 Basis transformations

(a) The effect of the map A on the standard basis, $\mathbf{e}_j \overset{A}{\mapsto} \mathbf{A}_j \equiv \mathbf{e}_i A^i{}_j$, gives the column vectors of the matrix representation $A = (\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3)$. In this case, we have:

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \overset{A}{\mapsto} \begin{pmatrix} \cos\theta_3 \\ \sin\theta_3 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \overset{A}{\mapsto} \begin{pmatrix} -\sin\theta_3 \\ \cos\theta_3 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \overset{A}{\mapsto} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

For the angle $\theta_3 = \pi$ we will use the compact notation $\cos\theta_3 = \sin\theta_3 = \frac{1}{\sqrt{2}} \equiv s$. Thus:

$$A = \begin{pmatrix} s & -s & 0 \\ s & s & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad B = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad C = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}.$$

(b)

$$\mathbf{y} = B\mathbf{x} = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \\ 1 \end{pmatrix}$$

(c)

$$D = CBA = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 3 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} A = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -3 & 0 & 1 \end{pmatrix} \begin{pmatrix} s & -s & 0 \\ s & s & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ s & s & 0 \\ -3s & 3s & 0 \end{pmatrix}$$

$$\mathbf{z} = D\mathbf{x} = \begin{pmatrix} 0 & 0 & 1 \\ s & s & 0 \\ -3s & 3s & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 2s \\ 0 \end{pmatrix}$$

(d) On one hand we have $\mathbf{e}_j \overset{A}{\mapsto} \mathbf{e}'_j$, with $\mathbf{e}v'_j = \mathbf{e}_i A^i{}_j$, because the image of the standard basis vector $\mathbf{e}_j$ under the mapping A, written in the standard basis, is given by the column vector j of the Matrix A, with components $A^i{}_j$. The inverse relationship is given by $\mathbf{e}_j = \mathbf{e}'_i (A^{-1})^i{}_j$. On the other hand however, we have that $\mathbf{e}_j = \mathbf{e}'_i T^i{}_j$, by the definition of the transformation matrix. It follows that $T = A^{-1}$. Using the fact that A is a rotation matrix, we know that: $A^{-1}(\theta_3) = A(-\theta_3)$. Therefore:

$$T = \begin{pmatrix} s & s & 0 \\ -s & s & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(e)

$$\mathbf{x}' = T\mathbf{x} = \begin{pmatrix} s & s & 0 \\ -s & s & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 2s \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{y}' = T\mathbf{y} = \begin{pmatrix} s & s & 0 \\ -s & s & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 3 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 4s \\ -2s \\ 1 \end{pmatrix}$$

(f)

$$B' = TBT^{-1} = A^{-1}BA = \begin{pmatrix} s & s & 0 \\ -s & s & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 3 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} A = \begin{pmatrix} 3s & s & 0 \\ -3s & s & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} s & -s & 0 \\ s & s & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} 4s^2 & -2s^2 & 0 \\ -2s^2 & 4s^2 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\mathbf{y}' = T\mathbf{y} = TB\mathbf{x} = \underbrace{TBT^{-1}}_{B'} \underbrace{T\mathbf{x}}_{\mathbf{x}'} = B'\mathbf{x}' = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 2s \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 4s \\ -2s \\ 1 \end{pmatrix} \qquad [= \text{(e)} \checkmark]$$

S.L6 Matrices II: determinants

S.L6.1 Determinant

ᴇL6.1.1 Calculating determinants

We expand the determinant along the indicated row or column:

$$\det A = \begin{vmatrix} 2 & 1 \\ 5 & -3 \end{vmatrix} = 2\cdot(-3) - 5\cdot 1 = -11\,.$$

$$\det B = \begin{vmatrix} 3 & 2 & 1 \\ 4 & -3 & 1 \\ 2 & -1 & 1 \end{vmatrix} \overset{\text{column 3}}{=} \begin{vmatrix} 4 & -3 \\ 2 & -1 \end{vmatrix} - \begin{vmatrix} 3 & 2 \\ 2 & -1 \end{vmatrix} + \begin{vmatrix} 3 & 2 \\ 4 & -3 \end{vmatrix} = -8\,.$$

$$\begin{aligned} \det C &= \begin{vmatrix} a & a & a & 0 \\ a & 0 & 0 & b \\ 0 & 0 & b & b \\ a & b & b & 0 \end{vmatrix} \overset{\text{row 2}}{=} -a \begin{vmatrix} a & a & 0 \\ 0 & b & b \\ b & b & 0 \end{vmatrix} + b \begin{vmatrix} a & a & a \\ 0 & 0 & b \\ a & b & b \end{vmatrix} \\ &= -a\left[a\begin{vmatrix} b & b \\ b & 0 \end{vmatrix} - a\begin{vmatrix} 0 & b \\ b & 0 \end{vmatrix}\right] + b\left[0 + 0 - b\begin{vmatrix} a & a \\ a & b \end{vmatrix}\right] \\ &= -a^2(-b^2) + a^2(-b^2) - b^2(ab - a^2) = a^2b^2 - ab^3\,. \end{aligned}$$

S.L7 Matrices III: diagonalizing a matrix

S.L7.3 Characteristic polynomial

S.L7.4 Matrix diagonalization

ᴇL7.4.1 Diagonalising real 2×2 matrices

(a) The zeros of the characteristic polynomial yield the eigenvalues:

Char. polynomial: $$0 \overset{!}{=} \det(A - \lambda\mathbb{1}) = \begin{vmatrix} -1-\lambda & 6 \\ -2 & 6-\lambda \end{vmatrix} = (-1-\lambda)(6-\lambda) + 12$$
$$= \lambda^2 - 5\lambda + 6 = (\lambda - 2)(\lambda - 3)$$

Eigenvalues: $\lambda_1 = 2, \quad \lambda_2 = 3\,.$

Eigenvectors:

$\lambda_1 = 2:$ $$\mathbf{0} \overset{!}{=} (A - \lambda_1\mathbb{1})\mathbf{v}_1 = \begin{pmatrix} -3 & 6 \\ -2 & 4 \end{pmatrix}\mathbf{v}_1 \quad \Rightarrow \quad \mathbf{v}_1 = \begin{pmatrix} 2 \\ 1 \end{pmatrix}.$$

$\lambda_2 = 3:$ $$\mathbf{0} \overset{!}{=} (A - \lambda_2\mathbb{1})\mathbf{v}_2 = \begin{pmatrix} -4 & 6 \\ -2 & 3 \end{pmatrix}\mathbf{v}_2 \quad \Rightarrow \quad \mathbf{v}_2 = \begin{pmatrix} 3 \\ 2 \end{pmatrix}.$$

Explicitly: The two rows of the matrix $(A - \lambda_j\mathbb{1})$ are proportional to each other (as expected, since the determinant of this matrix equals zero). Thus both rows yield the same

information about the eigenvector $\mathbf{v}_j$. For $\mathbf{v}_1 = (v^1{}_1, v^2{}_1)^T$ we have $-3v^1{}_1 + 6v^2{}_1 = 0$, thus it has the form $\mathbf{v}_1 = a_1(2,1)^T$. Similarly one finds $\mathbf{v}_2 = a_2(3,2)^T$. The prefactors a_1 and a_2 are *not* fixed by the eigenvalue equation, since if $\mathbf{v}_j$ satisfies $(A-\lambda_j\mathbb{1})\mathbf{v}_j = 0$, the same is true for $a_j\mathbf{v}_j$, with $a_j \in \mathbb{R}$. If one desires the eigenvectors to be normalized, the normalization condition $\|\mathbf{v}_j\| = 1$ fixes the absolute value of the prefactor, $|a_j|$. However, that is not the case here, hence we may choose the prefactor as we please – here we take $a_1 = a_2 = 1$.

The similarity transformation S contains the eigenvectors as columns; its inverse follows via the inversion formula for 2×2 matrices, $\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$:

Sim-Tr.: $$S = (\mathbf{v}_1, \mathbf{v}_2) = \begin{pmatrix} 2 & 3 \\ 1 & 2 \end{pmatrix}, \quad S^{-1} = \begin{pmatrix} 2 & -3 \\ -1 & 2 \end{pmatrix}.$$

Check: $$S^{-1}AS = \begin{pmatrix} 2 & -3 \\ -1 & 2 \end{pmatrix}\begin{pmatrix} -1 & 6 \\ -2 & 6 \end{pmatrix}\begin{pmatrix} 2 & 3 \\ 1 & 2 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix} \overset{\checkmark}{=} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}.$$

(b) The zeros of the characteristic polynomial yield the eigenvalues:

Char. polynomial: $$0 \overset{!}{=} \det(A-\lambda\mathbb{1}) = \begin{vmatrix} \frac{11}{5}-\lambda & -\frac{8}{5} \\ -\frac{8}{5} & -\frac{1}{5}-\lambda \end{vmatrix} = (\tfrac{11}{5}-\lambda)(-\tfrac{1}{5}-\lambda) - \tfrac{64}{25}$$
$$= \lambda^2 - 2\lambda - 3 = (\lambda-3)(\lambda+1)$$

Eigenvalues: $\lambda_1 = 3, \quad \lambda_2 = -1$.

Eigenvectors:

$$\lambda_1 = 3: \quad \mathbf{0} \overset{!}{=} (A-\lambda_1\mathbb{1})\mathbf{v}_1 = \frac{1}{5}\begin{pmatrix} -4 & -8 \\ -8 & -16 \end{pmatrix}\mathbf{v}_1 \quad \Rightarrow \quad \mathbf{v}_1 = a_1\begin{pmatrix} 2 \\ -1 \end{pmatrix}, \ |a_1| = \frac{1}{\sqrt{5}}.$$

$$\lambda_2 = -1: \quad \mathbf{0} \overset{!}{=} (A-\lambda_2\mathbb{1})\mathbf{v}_2 = \frac{1}{5}\begin{pmatrix} 16 & -8 \\ -8 & 4 \end{pmatrix}\mathbf{v}_2 \quad \Rightarrow \quad \mathbf{v}_2 = a_2\begin{pmatrix} 1 \\ 2 \end{pmatrix}, \ |a_2| = \frac{1}{\sqrt{5}}.$$

Explicitly: For the eigenvector $\mathbf{v}_1 = (v^1{}_1, v^2{}_1)^T$ we have $-4v^1{}_1 - 8v^2{}_1 = 0$, hence it has the form $\mathbf{v}_1 = a_1(2,-1)^T$. Analogously one finds $\mathbf{v}_2 = a_2(1,2)^T$. In the present case it is advisable to normalize the eigenvectors by $\|\mathbf{v}_j\| = 1$ (see below), which fixes the prefactors up to a sign: $a_1 = \pm\frac{1}{\sqrt{5}}$, $a_2 = \pm\frac{1}{\sqrt{5}}$. We here choose both prefactors positive (a different choice would be equally legitimate).

The similarity transformation S contains the eigenvectors as columns. Since the matrix A is *symmetric*, it is possible to choose S to be *orthogonal*, so that it satisfies $S^{-1} = S^T$. To achieve this, the eigenvectors must form an ortho*normal* system. They already are orthogonal (for a symmetric matrix, eigenvectors having different eigenvalues are always orthogonal); since we have normalized them above, they are also orthonormal.

Sim-Tr.: $$S = (\mathbf{v}_1, \mathbf{v}_2) = \frac{1}{\sqrt{5}}\begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix}, \quad S^{-1} = S^T = \begin{pmatrix} \mathbf{v}_1^T \\ \mathbf{v}_2^T \end{pmatrix} = \frac{1}{\sqrt{5}}\begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix}.$$

Check: $$S^{-1}AS = \frac{1}{\sqrt{5}}\begin{pmatrix} 2 & -1 \\ 1 & 2 \end{pmatrix}\frac{1}{5}\begin{pmatrix} 11 & -8 \\ -8 & -1 \end{pmatrix}\frac{1}{\sqrt{5}}\begin{pmatrix} 2 & 1 \\ -1 & 2 \end{pmatrix} = \begin{pmatrix} 3 & 0 \\ 0 & -1 \end{pmatrix} \overset{\checkmark}{=} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}.$$

Remark: Of course it is also possible to construct the similarity transformation S using eigenvectors that are *not* normalized. However then its inverse, $\tilde{S}^{-1}$, will not equal $\tilde{S}^T$, but will have to be found in an additional step using the appropriate inversion formula. For example, if we choose the prefactors above as $a_1 = 1$ and $a_2 = 2$, thus taking $\tilde{\mathbf{v}}_1 = (2,-1)^T$ and $\tilde{\mathbf{v}}_2 = (2,4)^T$ as eigenvectors, we obtain:

Sim.-Tr.: $$\tilde{S} = (\tilde{\mathbf{v}}_1, \tilde{\mathbf{v}}_2) = \begin{pmatrix} 2 & 2 \\ -1 & 4 \end{pmatrix}, \quad \tilde{S}^{-1} = \frac{1}{10}\begin{pmatrix} 4 & -2 \\ 1 & 2 \end{pmatrix}.$$

Since the columns of S and $\tilde{S}$, and the rows of S^{-1} and $\tilde{S}^{-1}$, only differ by prefactors, the check here works analogously to the one above:

Check: $$\tilde{S}^{-1}A\tilde{S} = \frac{1}{10}\begin{pmatrix} 4 & -2 \\ 1 & 2 \end{pmatrix}\frac{1}{5}\begin{pmatrix} 11 & -8 \\ -8 & -1 \end{pmatrix}\begin{pmatrix} 2 & 2 \\ -1 & 4 \end{pmatrix} = \begin{pmatrix} 3 & 0 \\ 0 & -1 \end{pmatrix} \overset{\checkmark}{=} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}.$$

ᴇL7.4.3 Diagonalising complex 2×2 matrices

(a) The zeros of the characteristic polynomial yield the eigenvalues:

Char. polynomial: $$0 \overset{!}{=} \det(A - \lambda\mathbb{1}) = \begin{vmatrix} -\mathrm{i} - \lambda & 0 \\ 2 & \mathrm{i} - \lambda \end{vmatrix} = (-\mathrm{i} - \lambda)(\mathrm{i} - \lambda)$$

Eigenvalues: $\lambda_1 = +\mathrm{i}, \quad \lambda_2 = -\mathrm{i}$.

Eigenvectors:

$$\lambda_1 = +\mathrm{i}: \quad \mathbf{0} \overset{!}{=} (A - \lambda_1\mathbb{1})\mathbf{v}_1 = \begin{pmatrix} -2\mathrm{i} & 0 \\ 2 & 0 \end{pmatrix}\mathbf{v}_1 \quad \Rightarrow \quad \mathbf{v}_1 = a_1\begin{pmatrix} 0 \\ 1 \end{pmatrix}, \ |a_1| = 1\,.$$

$$\lambda_2 = -\mathrm{i}: \quad \mathbf{0} \overset{!}{=} (A - \lambda_2\mathbb{1})\mathbf{v}_2 = \begin{pmatrix} 0 & 0 \\ 2 & 2\mathrm{i} \end{pmatrix}\mathbf{v}_2 \quad \Rightarrow \quad \mathbf{v}_2 = a_2\begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix}, \ |a_2| = \frac{1}{\sqrt{2}}\,.$$

Explicitly: For the eigenvector $\mathbf{v}_1 = (v^1{}_1, v^2{}_1)^T$ we have $-2\mathrm{i}v^1{}_1 + 0v^2{}_1 = 0$, thus it has the form $\mathbf{v}_1 = a_1(0,1)^T$. Similarly one finds $\mathbf{v}_2 = a_2(1,\mathrm{i})^T$. The prefactors are complex numbers and thus have the general form $a_j = |a_j|(\cos\phi_j + \mathrm{i}\sin\phi_j)$, with norm $|a_j|$ and phase ϕ_j. The statement of the problem requested normalized eigenvectors, satisfying $\|\mathbf{v}_j\| = 1$. This fixes the norm $|a_j|$ of each prefactor, but not its phase, which we may choose as we please. We here choose $\phi_j = 0$, hence $a_1 = 1$ and $a_2 = \frac{1}{\sqrt{2}}$.

The similarity transformation S contains the eigenvectors as columns; its inverse follows via the inversion formula for 2×2 matrices, which holds also for complex matrices:

Sim-Tr.: $$S = (\mathbf{v}_1, \mathbf{v}_2) = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ 1 & \frac{\mathrm{i}}{\sqrt{2}} \end{pmatrix}, \qquad S^{-1} = \begin{pmatrix} -\mathrm{i} & 1 \\ \sqrt{2} & 0 \end{pmatrix}.$$

Check: $$S^{-1}AS = \begin{pmatrix} -\mathrm{i} & 1 \\ \sqrt{2} & 0 \end{pmatrix}\begin{pmatrix} -\mathrm{i} & 0 \\ 2 & \mathrm{i} \end{pmatrix}\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ 1 & \frac{\mathrm{i}}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix} \overset{\checkmark}{=} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}.$$

(b) The zeros of the characteristic polynomial yield the eigenvalues:

Char. polynomial: $0 \stackrel{!}{=} \det(A-\lambda\mathbb{1}) = \begin{vmatrix} 1-\lambda & \mathrm{i} \\ -\mathrm{i} & 1-\lambda \end{vmatrix} = (1-\lambda)^2 - 1 = \lambda(\lambda-2)$

Eigenvalues: $\lambda_1 = 0, \quad \lambda_2 = 2$.

Eigenvectors:

$$\lambda_1 = 0: \quad \mathbf{0} \stackrel{!}{=} (A-\lambda_1\mathbb{1})\mathbf{v}_1 = \begin{pmatrix} 1 & \mathrm{i} \\ -\mathrm{i} & 1 \end{pmatrix}\mathbf{v}_1 \quad \Rightarrow \quad \mathbf{v}_1 = a_1\begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix}, \quad |a_1| = \frac{1}{\sqrt{2}}\,.$$

$$\lambda_2 = 2: \quad \mathbf{0} \stackrel{!}{=} (A-\lambda_2\mathbb{1})\mathbf{v}_2 = \begin{pmatrix} -1 & \mathrm{i} \\ -\mathrm{i} & -1 \end{pmatrix}\mathbf{v}_2 \quad \Rightarrow \quad \mathbf{v}_2 = a_2\begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix}, \quad |a_2| = \frac{1}{\sqrt{2}}\,.$$

Explicitly: For the Eigenvector $\mathbf{v}_1 = (v^1{}_1, v^2{}_1)^T$ we have $v^1{}_1 + \mathrm{i}v^2{}_1 = 0$, hence it has the form $\mathbf{v}_1 = a_1(1,\mathrm{i})^T$. Similarly one finds $\mathbf{v}_2 = a_2(1,-\mathrm{i})^T$. The normalization condition fixes the norm of both prefactors, but not their phases, which we can choose as we please. We here take the phases to be zero and use real prefactors: $a_1 = a_2 = \frac{1}{\sqrt{2}}$.

The similarity transformation S contains the eigenvectors as columns. Since the matrix A is *hermitian*, it is possible to choose S to be *unitary*, so that it satisfies $S^{-1} = S^\dagger$. To achieve this, the eigenvectors must form an ortho*normal* system (with respect to the *complex* scalar product). They already are orthogonal (for a hermitian matrix, eigenvectors having different eigenvalues are always orthogonal); since we have normalized them above, they are also orthonormal.

Sim-Tr.: $S = (\mathbf{v}_1, \mathbf{v}_2) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ \mathrm{i} & -\mathrm{i} \end{pmatrix}, \quad S^{-1} = S^\dagger = \begin{pmatrix} \mathbf{v}_1^\dagger \\ \mathbf{v}_2^\dagger \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -\mathrm{i} \\ 1 & \mathrm{i} \end{pmatrix}.$

Check: $S^{-1}AS = \frac{1}{2}\begin{pmatrix} 1 & -\mathrm{i} \\ 1 & \mathrm{i} \end{pmatrix}\begin{pmatrix} 1 & \mathrm{i} \\ -\mathrm{i} & 1 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ \mathrm{i} & -\mathrm{i} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 2 \end{pmatrix} \stackrel{\checkmark}{=} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}.$

ᴇL7.4.5 Diagonalising a matrix that depends on a variable

Char. Poly.:
$$\begin{aligned} 0 \stackrel{!}{=} \det(A-\lambda\mathbb{1}) &= \begin{vmatrix} x-\lambda & 1 & 0 \\ 1 & 2-\lambda & 1 \\ 3-x & -1 & 3-\lambda \end{vmatrix} \\ &= (x-\lambda)(2-\lambda)(3-\lambda) + (3-x) + (x-\lambda) - (3-\lambda) \\ &= (x-\lambda)(2-\lambda)(3-\lambda) \end{aligned}$$

Eigenvalues: $\lambda_1 = x, \quad \lambda_2 = 2, \quad \lambda_3 = 3$; Eigenvectors:

$$\mathbf{0} \stackrel{!}{=} (A-\lambda_1\mathbb{1})\mathbf{v}_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 2-x & 1 \\ 3-x & -1 & 3-x \end{pmatrix}\mathbf{v}_1 \stackrel{\text{Gauss}}{\longrightarrow} \mathbf{v}_1 = a_1\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad |a_1| = \frac{1}{\sqrt{2}}$$

$$\mathbf{0} \overset{!}{=} (A-\lambda_2\mathbb{1})\mathbf{v}_2 = \begin{pmatrix} x-2 & 1 & 0 \\ 1 & 0 & 1 \\ 3-x & -1 & 1 \end{pmatrix}\mathbf{v}_2 \quad \overset{\text{Gauss}}{\longrightarrow} \mathbf{v}_2 = a_2\begin{pmatrix} 1 \\ 2-x \\ -1 \end{pmatrix},\ |a_2| = \frac{1}{\sqrt{6-4x+x^2}}$$

$$\mathbf{0} \overset{!}{=} (A-\lambda_3\mathbb{1})\mathbf{v}_3 = \begin{pmatrix} x-3 & 1 & 0 \\ 1 & -1 & 1 \\ 3-x & -1 & 0 \end{pmatrix}\mathbf{v}_3 \quad \overset{\text{Gauss}}{\longrightarrow} \mathbf{v}_3 = a_3\begin{pmatrix} 1 \\ 3-x \\ 2-x \end{pmatrix},\ |a_3| = \frac{1}{\sqrt{14-10x+2x^2}}$$

ᴇL7.4.7 Inertia tensor

Point masses: $m_1=4$ at $\mathbf{r}_1=(1,0,0)^T$; $m_2=M$ at $\mathbf{r}_2=(0,1,2)^T$; $m_3=1$ at $\mathbf{r}_3=(0,4,1)^T$.

$$\widetilde{I}_{ij} = \sum_a m_a\left(\delta_{ij}\mathbf{r}_a^2 - r^i{}_a r^j{}_a\right) \quad\Rightarrow\quad \widetilde{I} = \sum_a m_a \begin{pmatrix} \mathbf{r}_a^2 - r^1{}_a r^1{}_a & -r^1{}_a r^2{}_a & -r^1{}_a r^3{}_a \\ -r^2{}_a r^1{}_a & \mathbf{r}_a^2 - r^2{}_a r^2{}_a & -r^2{}_a r^3{}_a \\ -r^3{}_a r^1{}_a & -r^3{}_a r^2{}_a & \mathbf{r}_a^2 - r^3{}_a r^3{}_a \end{pmatrix}$$

$$\widetilde{I} = 4\cdot\begin{pmatrix} 1-1 & 0 & 0 \\ 0 & 1-0 & 0 \\ 0 & 0 & 1-0 \end{pmatrix} + M\cdot\begin{pmatrix} 5-0 & 0 & 0 \\ 0 & 5-1 & -2 \\ 0 & -2 & 5-4 \end{pmatrix} + 1\cdot\begin{pmatrix} 17-0 & 0 & 0 \\ 0 & 17-16 & -4 \\ 0 & -4 & 17-1 \end{pmatrix}$$

$$= \begin{pmatrix} 5M+17 & 0 & 0 \\ 0 & 4M+5 & -2(M+2) \\ 0 & -2(M+2) & M+20 \end{pmatrix}.$$

The zeros of the characteristic polynomial yield the moments of inertia (eigenvalues):

$$\begin{aligned} 0 \overset{!}{=} \det(\widetilde{I}-\lambda\mathbb{1}) &= \begin{vmatrix} 5M+17-\lambda & 0 & 0 \\ 0 & 4M+5-\lambda & -2(M+2) \\ 0 & -2(M+2) & M+20-\lambda \end{vmatrix} \\ &= (5M+17-\lambda)\Big[(4M+5-\lambda)(M+20-\lambda) - 4(M+2)^2\Big] \\ &= (5M+17-\lambda)\Big[\lambda^2 - 5(M+5)\lambda + 69M + 84\Big] \end{aligned}$$

Moments of inertia:
$$\begin{aligned} \lambda_1 &= 5M+17\,, \\ \lambda_{2,3} &= \tfrac{1}{2}\Big[5(M+5) \pm \sqrt{25(M+5)^2 - 4(69M+84)}\Big] \\ &= \tfrac{1}{2}\Big[5(M+5) \pm \sqrt{25M^2 - 26M + 289}\Big]\,. \end{aligned}$$

For $M=5$: $\lambda_1 = 42$, $\lambda_{2,3} = \frac{1}{2}\big[50 \pm \sqrt{784}\big] = 25 \pm 14$, hence $\lambda_2 = 39$, $\lambda_3 = 11$.

ᴇL7.4.9 Degenerate eigenvalue problem

Characteristic polynomial:
$$0 \overset{!}{=} \det(A-\lambda\mathbb{1}) = \begin{vmatrix} 2-\lambda & -1 & 2 \\ -1 & 2-\lambda & -2 \\ 2 & -2 & 5-\lambda \end{vmatrix}$$

$$\begin{aligned}\det(A-\lambda\mathbb{1}) &\overset{\text{(i)}}{=} (2-\lambda)\big[(2-\lambda)(5-\lambda)-4\big]-(-1)\big[(-1)(5-\lambda)+4\big]+2\big[2-(2-\lambda)2\big]\\ &\overset{\text{(ii)}}{=} (2-\lambda)\big[\lambda^2-7\lambda+6\big]+5(\lambda-1) \overset{\text{(iii)}}{=} (2-\lambda)\big[(\lambda-1)(\lambda-6)\big]+5(\lambda-1)\\ &\overset{\text{(iv)}}{=} (\lambda-1)\big[(2-\lambda)(\lambda-6)+5\big] \overset{\text{(v)}}{=} -(\lambda-1)(\lambda-1)(\lambda-7)\,.\end{aligned}$$

Remarks: (i) We calculate the determinant using the Laplace expansion along the first column, and (ii) then simplify. (iii) From the hint that $\lambda=1$ is an eigenvalue, we know that $\det(A-\lambda\mathbb{1})$, and thus the square bracket, too, must contain a factor of $(\lambda-1)$. (iv) We evaluate this bracket and factorize (v) again, using the quadratic formula for example:

(v): $\quad(2-\lambda)(\lambda-6)+5=-\lambda^2+8\lambda-7=-(\lambda-1)(\lambda-7)$, since $\frac{-8\pm\sqrt{64-28}}{-2}=4\mp3=\begin{cases}1\\7\end{cases}$

Alternatively (if the factorization is not apparent): (iii′) completely multiply out $\det(A-\lambda\mathbb{1})$, (iv′) then use polynomial division to factorize out the factor $(\lambda-1)$, and (v′) factorize the residual quadratic polynomial as in step (v) above:

$$\begin{aligned}\det(A-\lambda\mathbb{1}) &\overset{\text{(iii′)}}{=} -\lambda^3+9\lambda^2-15\lambda+7 \overset{\text{(iv′)}}{=} (\lambda-1)(-\lambda^2+8\lambda-7)\\ &\overset{\text{(v′)}}{=} -(\lambda-1)(\lambda-1)(\lambda-7)\,.\end{aligned}$$

(ii′) Polynomial division:

$$\begin{array}{rl}(-\lambda^3+9\lambda^2-15\lambda+7)\,/\,(\lambda-1) = & -\lambda^2+8\lambda-7\\ \underline{\lambda^3-\lambda^2} & \\ 8\lambda^2-15\lambda & \\ \underline{-8\lambda^2+8\lambda} & \\ -7\lambda+7 & \\ \underline{7\lambda-7} & \\ 0 & \end{array}$$

Eigenvalue: $\lambda_1=1,\quad \lambda_2=1,\quad \lambda_3=7$. The eigenvalues λ_1 and λ_2 are degenerate.

Determination of the normalized eigenvector $\mathbf{v}_3$ of the non-degenerate eigenvalue λ_3:

$$\mathbf{0}\overset{!}{=}(A-\lambda_3\mathbb{1})\mathbf{v}_3=\begin{pmatrix}-5&-1&2\\-1&-5&-2\\2&-2&-2\end{pmatrix}\mathbf{v}_3 \quad\overset{\text{Gauss}}{\longrightarrow}\quad \mathbf{v}_3=a_3\begin{pmatrix}1\\-1\\2\end{pmatrix},\ a_3=\frac{1}{\sqrt{6}}\,.$$

Details of the Gauss method:

$$\left(\begin{array}{ccc|c} v^1{}_3 & v^2{}_3 & v^3{}_3 & \\ -5 & -1 & 2 & 0\\ -1 & -5 & -2 & 0\\ 2 & -2 & -2 & 0\end{array}\right)\longrightarrow\left(\begin{array}{ccc|c} v^1{}_3 & v^2{}_3 & v^3{}_3 & \\ & -[1]: & 5\ \ 1\ -2 & 0\\ & \frac{1}{12}([1]-5[2]): & 0\ \ 2\ \ 1 & 0\\ & -\frac{1}{6}([3]+2[2]): & 0\ \ 2\ \ 1 & 0\end{array}\right)\longrightarrow\left(\begin{array}{ccc|c} v^1{}_3 & v^2{}_3 & v^3{}_3 & \\ & \frac{1}{10}(2[1]-[2]): & 1\ \ 0\ -\frac{1}{2} & 0\\ & \frac{1}{2}[2]: & 0\ \ 1\ \ \frac{1}{2} & 0\\ & [2]-[3]: & 0\ \ 0\ \ 0 & 0\end{array}\right)$$

The system on the right gives two relations between the components of $\mathbf{v}_3=(v^1{}_3,v^2{}_3,v^3{}_3)^T$, viz. $v^1{}_3-\frac{1}{2}v^3{}_3=0$ and $v^2{}_3+\frac{1}{2}v^3{}_3=0$. Since the third row contains only zeros, the

eigenvector is determined (as expected) only up to a pre-factor $a_3 \in \mathbb{C}$, which can be freely chosen: $\mathbf{v}_3 = a_3(1,-1,2)^T$. The normalization condition $\|\mathbf{v}_3\| = 1$ implies that $a_3 = \pm\frac{1}{\sqrt{6}}$; here we select the positive sign (the negative sign would be equally legitimate).

Determination of the eigenvectors $\mathbf{v}_j$ of the degenerate eigenvalue $\lambda_j = 1$ (with $j = 1, 2$):

$$\mathbf{0} \stackrel{!}{=} (A - \lambda_j \mathbb{1})\mathbf{v}_j = \begin{pmatrix} 1 & -1 & 2 \\ -1 & 1 & -2 \\ 2 & -2 & 4 \end{pmatrix} \mathbf{v}_j .$$

All three rows are proportional to each other, $[3] = 2[1] = -2[2]$; therefore they yield only *one* relation between the components of $\mathbf{v}_j = ({v^1}_j, {v^2}_j, {v^3}_j)^T$, namely ${v^1}_j - {v^2}_j + 2{v^3}_j = 0$. Therefore, we can choose two components of $\mathbf{v}_j$ freely and thereby construct two linearly independent eigenvectors, e.g., $\mathbf{v}_1 = (1,1,0)^T$ and $\mathbf{v}_2 = (0,2,1)^T$.
We construct an orthonormal basis of eigenvectors: Since A is a real *symmetric* matrix, eigenvectors for different eigenvalues are orthogonal to each other, i.e. $\mathbf{v}_j \cdot \mathbf{v}_3 = 0$ for $j = 1, 2$, as can be verified easily. Thus we just have to orthogonalize the two degenerate eigenvectors, $\mathbf{v}_1$ and $\mathbf{v}_2$. We use the Gram-Schmidt process, for e.g. $\mathbf{v}'_1 = \mathbf{v}_1/|\mathbf{v}_1| = \frac{1}{\sqrt{2}}(1,1,0)^T$ and

$$\mathbf{v}'_{2,\perp} = \mathbf{v}_2 - \mathbf{v}'_1\,(\mathbf{v}'_1 \cdot \mathbf{v}_2) = \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix} - \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \frac{2}{\sqrt{2}} = \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}; \quad \mathbf{v}'_2 = \frac{\mathbf{v}'_{2,\perp}}{|\mathbf{v}'_{2,\perp}|} = \frac{1}{\sqrt{3}} \begin{pmatrix} -1 \\ 1 \\ 1 \end{pmatrix}.$$

$\{\mathbf{v}'_1, \mathbf{v}'_2, \mathbf{v}_3\}$ now form an orthonormal basis of $\mathbb{R}^3$.
Construction of the similarity transformation: Since A is symmetric, we have $S^{-1} = S^T$, where the transformation matrix S contains the orthonormalized eigenvectors as column vectors:

$$S = (\mathbf{v}'_1, \mathbf{v}'_2, \mathbf{v}_3) = \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3} & -\sqrt{2} & 1 \\ \sqrt{3} & \sqrt{2} & -1 \\ 0 & \sqrt{2} & 2 \end{pmatrix}, \quad S^{-1} = S^T = \begin{pmatrix} \mathbf{v}'^T_1 \\ \mathbf{v}'^T_2 \\ \mathbf{v}^T_3 \end{pmatrix} = \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3} & \sqrt{3} & 0 \\ -\sqrt{2} & \sqrt{2} & \sqrt{2} \\ 1 & -1 & 2 \end{pmatrix}.$$

Check: $S^{-1}AS = S^{-1} \begin{pmatrix} 2 & -1 & 2 \\ -1 & 2 & -2 \\ 2 & -2 & 5 \end{pmatrix} \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3} & -\sqrt{2} & 1 \\ \sqrt{3} & \sqrt{2} & -1 \\ 0 & \sqrt{2} & 2 \end{pmatrix}$

$$= \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3} & \sqrt{3} & 0 \\ -\sqrt{2} & \sqrt{2} & \sqrt{2} \\ 1 & -1 & 2 \end{pmatrix} \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{3} & -\sqrt{2} & 7 \\ \sqrt{3} & \sqrt{2} & -7 \\ 0 & \sqrt{2} & 14 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 7 \end{pmatrix} \stackrel{\checkmark}{=} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}.$$

ᴇL7.4.11 Determinant equals product of eigenvalues

If A is diagonalizable, then we have $S^{-1}AS = \Lambda$, where Λ is the diagonalized form of A. Using the multiplication rule for determinants we find:

$$\textstyle\prod_{j=1}^{n} \lambda_j = \det \Lambda = \det(S^{-1}AS) = \det S^{-1} \cdot \det A \cdot \det S = \det A\,. \checkmark$$

Remark: The above assertion also holds for non-diagonalizable matrices: The eigenvalues $\lambda_1, \ldots, \lambda_n$ of A are the zeros of the characteristic polynomial $\det(A - \lambda\mathbb{1})$, thus

$$\det(A - \lambda\mathbb{1}) = (\lambda_1 - \lambda) \cdot (\lambda_2 - \lambda) \cdot \ldots \cdot (\lambda_n - \lambda)\,.$$

We now set $\lambda = 0$ and immediately obtain $\det A = \prod_{j=1}^{n} \lambda_j$. ✓

S.L7.5 Functions of matrices

ᴇL7.5.1 Functions of matrices

(a) For $A = \begin{pmatrix} 0 & a \\ 0 & 0 \end{pmatrix}$ we have $A^2 = 0$, thus the Taylor series for e^A contains only two terms:

$$\mathrm{e}^A = A^0 + A = \mathbb{1} + A = \begin{pmatrix} 1 & a \\ 0 & 1 \end{pmatrix}.$$

(b) We seek e^A, with $A = \theta\tilde{\sigma}$, $\tilde{\sigma} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. The matrix $\tilde{\sigma}$ has the following properties:

$$\tilde{\sigma}^2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -\mathbb{1}, \quad \tilde{\sigma}^{2m} = (\tilde{\sigma}^2)^m = (-1)^m\mathbb{1}, \quad \tilde{\sigma}^{2m+1} = \tilde{\sigma}(\tilde{\sigma}^2)^m = (-1)^m\tilde{\sigma}.$$

Therefore:
$$e^A = \sum_{l=0}^{\infty} \frac{1}{l!}A^l = \sum_{m=0}^{\infty} \frac{1}{(2m)!}\theta^{2m} \underbrace{\tilde{\sigma}^{2n}}_{(-1)^m\mathbb{1}} + \sum_{m=0}^{\infty} \frac{1}{(2m+1)!}\theta^{2m+1} \underbrace{\tilde{\sigma}^{2m+1}}_{(-1)^m\tilde{\sigma}}$$
$$= \mathbb{1}\cos\theta + \tilde{\sigma}\sin\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

Remark: This matrix describes a rotation by the angle θ in $\mathbb{R}^2$. Evidently $\mathrm{e}^{\theta\tilde{\sigma}}$ is an exponential representation of such a rotation matrix.

(c) First equality:

$$f(A) = \sum_{l=0}^{\infty} c_l \big(\underbrace{SDS^{-1}}_{A}\big)^l \overset{\text{(i)}}{=} \sum_{l=0}^{\infty} c_l S D^l S^{-1} = S\Big(\sum_{l=0}^{\infty} c_l D^l\Big)S^{-1} = Sf(D)S^{-1}\,.$$

(i) For the third step we used the following relation:

$$\big(SAS^{-1}\big)^l = \big(SA\underbrace{S^{-1}}_{=\mathbb{1}}\big)\big(\underbrace{S}_{=\mathbb{1}}A\underbrace{S^{-1}}_{=\mathbb{1}}\big)\big(\underbrace{S}_{=\mathbb{1}}AS^{-1}\big)\cdots\big(SAS^{-1}\big) = SA^lS^{-1}\,.$$

Second equality:

$$\big[f(D)\big]_{ij} = \Big[\sum_{l=0}^{\infty} c_l D^l\Big]_{ij} = \sum_{l=0}^{\infty} c_l \big[D^l\big]_{ij} \overset{\text{(ii)}}{=} \sum_{l=0}^{\infty} c_l \lambda_i^l \delta_{ij} = \delta_{ij}\sum_{l=0}^{\infty} c_l\lambda_i^l = \delta_{ij} f(\lambda_i)\,.$$

(ii) For the third step we used the fact that the l-th power of a diagonal matrix D is diagonal too, with $D^l = \mathrm{diag}(\lambda_1^l, \ldots, \lambda_n^l)$.

(d) Given: e^A, with $A = \theta \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. We begin by diagonalizing A:

Char. Polynom: $0 \stackrel{!}{=} \det(A - \lambda\mathbb{1}) = \lambda^2 + \theta^2 \;\Rightarrow$ Eigenvalues: $\lambda_\pm = \pm\mathrm{i}\theta$.

Normalized eigenvectors: $\mathbf{0} \stackrel{!}{=} (A - \lambda_\pm\mathbb{1})\mathbf{v}_\pm \;\Rightarrow\; \mathbf{v}_\pm = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \mp\mathrm{i} \end{pmatrix}$.

Similarity transf.: $S = (\mathbf{v}_+, \mathbf{v}_-) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -\mathrm{i} & \mathrm{i} \end{pmatrix}, \qquad S^{-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & \mathrm{i} \\ 1 & -\mathrm{i} \end{pmatrix}$.

$\mathrm{e}^A = S\mathrm{e}^D S^{-1}$:
$$\mathrm{e}^A = S\begin{pmatrix} \mathrm{e}^{\mathrm{i}\theta} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\theta} \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & \mathrm{i} \\ 1 & -\mathrm{i} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ -\mathrm{i} & \mathrm{i} \end{pmatrix}\begin{pmatrix} \mathrm{e}^{\mathrm{i}\theta} & \mathrm{i}\mathrm{e}^{\mathrm{i}\theta} \\ \mathrm{e}^{-\mathrm{i}\theta} & -\mathrm{i}\mathrm{e}^{-\mathrm{i}\theta} \end{pmatrix}$$
$$= \frac{1}{2}\begin{pmatrix} \mathrm{e}^{\mathrm{i}\theta} + \mathrm{e}^{-\mathrm{i}\theta} & \mathrm{i}\mathrm{e}^{\mathrm{i}\theta} - \mathrm{i}\mathrm{e}^{-\mathrm{i}\theta} \\ -\mathrm{i}\mathrm{e}^{\mathrm{i}\theta} + \mathrm{i}\mathrm{e}^{-\mathrm{i}\theta} & \mathrm{e}^{\mathrm{i}\theta} + \mathrm{e}^{-\mathrm{i}\theta} \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

This agrees with the result from (b).

ᴇL7.5.3 Exponential representation of 2-dimensional rotation matrix

(a) We use the product decomposition $R_\theta = \big[R_{\theta/m}\big]^m$. For $m \gg 1$, $\theta/m \ll 1$ we have $\cos(\theta/m) = 1 + \mathcal{O}\big((\theta/m)^2\big)$ and $\sin(\theta/m) = \theta/m + \mathcal{O}\big((\theta/m)^3\big)$. Therefore

$$R_{\theta/m} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} 1 & -\frac{\theta}{m} \\ \frac{\theta}{m} & 1 \end{pmatrix} + \mathcal{O}\big((\tfrac{\theta}{m})^2\big) = \mathbb{1} + \tfrac{\theta}{m}\tilde{\sigma} + \mathcal{O}\big((\tfrac{\theta}{m})^2\big), \quad \tilde{\sigma} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

(b) The identity $\lim_{m\to\infty}[1 + x/m]^m = \mathrm{e}^x$ now yields an exponential representation of R_θ:

$$R_\theta = \lim_{m\to\infty}\big[R_{\theta/m}\big]^m = \lim_{m\to\infty}\big[\mathbb{1} + \tfrac{\theta}{m}\tilde{\sigma}\big]^m = \mathrm{e}^{\theta\tilde{\sigma}}.$$

S.L8 Orthogonality and unitarity

S.L8.1 Orthogonal and unitary maps

S.L8.2 Orthogonal and unitary matrices

ᴇL8.2.1 Orthogonal and unitary matrices

(a) The real matrix A is orthogonal, since

$$AA^T = \begin{pmatrix} \sin\theta & \cos\theta \\ -\cos\theta & \sin\theta \end{pmatrix}\begin{pmatrix} \sin\theta & -\cos\theta \\ \cos\theta & \sin\theta \end{pmatrix} = \mathbb{1}.$$

The complex matrix B is not unitary, since

$$BB^\dagger = \frac{1}{1-\mathrm{i}}\frac{1}{1+\mathrm{i}}\begin{pmatrix} 2 & 1+\mathrm{i} & 0 \\ 1+\mathrm{i} & -1 & 1 \\ 0 & 2 & \mathrm{i} \end{pmatrix}\begin{pmatrix} 2 & 1-\mathrm{i} & 0 \\ 1-\mathrm{i} & -1 & 2 \\ 0 & 1 & -\mathrm{i} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 6 & 1-3\mathrm{i} & 2+2\mathrm{i} \\ 1+3\mathrm{i} & 4 & -2-\mathrm{i} \\ 2-2\mathrm{i} & -2+\mathrm{i} & 5 \end{pmatrix} \neq \mathbb{1}.$$

(b) $$\mathbf{x} = (1,2)^T\,, \qquad \mathbf{a} = A\mathbf{x} = (\sin\theta + 2\cos\theta, -\cos\theta + 2\sin\theta)^T,$$
$$\|\mathbf{x}\| = \sqrt{5}\,, \qquad \|\mathbf{a}\| = \sqrt{5\sin^2\theta + 5\cos^2\theta + \sin\theta\cos\theta(4-4)} = \sqrt{5}\,.$$

Since A is orthogonal, the norm is conserved.

(c) $$\mathbf{y} = (1,2,\mathrm{i})^T\,, \qquad \mathbf{b} = B\mathbf{y} = \frac{1}{1-\mathrm{i}}(2 + 2(1+\mathrm{i}), (1+\mathrm{i}) - 2 + \mathrm{i}, 4+\mathrm{i}^2)^T$$
$$\|\mathbf{y}\| = \sqrt{1+4+1} = \sqrt{6}\,, \quad \|\mathbf{b}\| = \sqrt{\tfrac{1}{2}\big[(16+4) + (1+4) + (9)\big]} = \sqrt{17}\,.$$

Since B is not unitary, the norm is not conserved.

SC Solutions: Calculus

S.C1 Differentiation of one-dimensional functions

S.C1.3 Derivatives of selected functions

EC1.3.1 Derivatives

(a) $f'(x) = \frac{3}{4}x^2 - 6x + 9$

(b) $f'(x) = \dfrac{1}{2\sqrt{2x^3}}$

(c) $f'(x) = \mathrm{e}^x(2x-1)$

(d) $f'(x) = \sin\left[\pi\left(x+\frac{1}{6}\right)\right] + \pi x \cos\left[\pi\left(x+\frac{1}{6}\right)\right]$

(e) $f'(x) = 2\pi \sin(\pi x)\cos(\pi x)$

(f) $f'(x) = \dfrac{\cos x \cos x + \sin x \sin x}{\cos^2 x} = \dfrac{1}{\cos^2 x}$

(g) $f'(x) = \ln x + x\dfrac{1}{x} = \ln x + 1$

(h) $f'(x) = \ln(9x^2) + x\dfrac{1}{9x^2}18x = \ln(9x^2) + 2$

(i) $f'(x) = \frac{1}{2}(\mathrm{e}^x - \mathrm{e}^{-x}) = \sinh(x)$

(j) $f'(x) = \dfrac{(\mathrm{e}^x + \mathrm{e}^{-x})(\mathrm{e}^x + \mathrm{e}^{-x}) - (\mathrm{e}^x - \mathrm{e}^{-x})(\mathrm{e}^x - \mathrm{e}^{-x})}{(\mathrm{e}^x + \mathrm{e}^{-x})^2} = \dfrac{4}{(\mathrm{e}^x + \mathrm{e}^{-x})^2} = \dfrac{1}{\cosh^2 x}$

EC1.3.3 Derivatives of inverse functions

For each of the following cases, we have to restrict our attention to domains on which the function of interest is *bijective*, else its inverse is not defined.

(a) $\ln(y)$ is the inverse function of $\exp(x)$, with $\exp(\ln(y)) = y$. Since $\exp\colon \mathbb{R} \to (0,\infty)$ is monotonic with $\exp'(x)$ strictly positive for all $x \in \mathbb{R}$, its inverse, $\ln\colon (0,\infty) \to \mathbb{R}$, is monotic too, with $\ln'(y)$ strictly positive for all $y \in (0,\infty)$. Thus

$$\ln'(y) = \frac{1}{\exp'(x)|_{x=\ln y}} = \frac{1}{\exp(\ln y)} = \frac{1}{y}\,.$$

(b) $\arctan(y)$ is the inverse function of $\tan(x)$, with $\tan(\arctan(y)) = y$. Since $\tan$ is a periodic function, its inverse $\arctan$ has infinitely many branches, one for each x-domain

on which a bijection can be defined. We consider only the x-domain centered on zero, where $\tan\colon (-\frac{\pi}{2}, \frac{\pi}{2}) \to \mathbb{R}$ is monotonic, with $\tan'(x) = \sec^2 x$ strictly positive. Then its inverse, $\arctan\colon \mathbb{R} \to (-1, 1)$, likewise has strictly positive slope:

$$\arctan'(y) = \frac{1}{\tan'(x)|_{x=\arctan y}} = \frac{1}{\sec^2(\arctan y)} = \frac{1}{1+\tan^2(\arctan y)} = \frac{1}{1+y^2}\,.$$

(c) $\arccos(y)$ is the inverse function of $\cos(x)$, with $\cos(\arccos(y)) = y$. Since $\cos$ is a periodic function, its inverse $\arccos$ has infinitely many branches, one for each x-domain on which a bijection can be defined. We consider two branches where $\arccos$ has positive or negative slope, respectively. I: On the domain $x \in (0, \pi)$, the function $\cos\colon (0, \pi) \to (1, -1)$ has inverse $\arccos\colon (-1, 1) \to (\pi, 0)$, with $\cos'(x) = -\sin(x)$ strictly negative. II: On the domain $x \in (-\pi, 0)$, the function $\cos\colon (-\pi, \pi) \to (-1, 0)$ has inverse $\arccos\colon (-1, 1) \to (-\pi, 0)$, with $\cos'(x) = -\sin(x)$ strictly positive. Using upper/lower signs for branch I/II, we obtain

$$\arccos'(y) = \frac{1}{\cos'(x)|_{x=\arccos y}} = \frac{-1}{\sin(\arccos y)} = \frac{\mp 1}{\sqrt{1-\cos^2(\arccos y)}} = \frac{\mp 1}{\sqrt{1-y^2}}\,.$$

Unless stated otherways, the notation $\arccos$ usually refers to branch I.

S.C2 Integration of one-dimensional functions

EC2.3.1 Integration by parts

(a) $I(z) = \int_0^z \mathrm{d}x\, \overset{u}{x}\, \overset{v'}{\mathrm{e}^{2x}} = \Big[\overset{u}{x}\, \overset{v}{\tfrac{1}{2}\mathrm{e}^{2x}}\Big]_0^z - \int_0^z \mathrm{d}x\, \overset{u'}{1}\, \cdot \overset{v}{\tfrac{1}{2}\mathrm{e}^{2x}} = \tfrac{1}{2}z\mathrm{e}^{2z} - \tfrac{1}{4}\left[\mathrm{e}^{2z}-1\right]$

$I'(z) = \left[\tfrac{1}{2}(1+2z) - \tfrac{1}{4}2\right]\mathrm{e}^{2z} \overset{\checkmark}{=} z\mathrm{e}^{2z}$ $\qquad I(\tfrac{1}{2}) \overset{\checkmark}{=} \tfrac{1}{4}$

Note the cancellation pattern: $I' = u'v + uv' - u'v = uv'$. [Similarly for (c,d).]

(b) $I(z) = \int_0^z \mathrm{d}x\, \overset{u}{x^2}\, \overset{v'}{\mathrm{e}^{2x}} = \Big[\overset{u}{x^2}\, \overset{v}{\tfrac{1}{2}\mathrm{e}^{2x}}\Big]_0^z - \int_0^z \mathrm{d}x\, \overset{u'}{2x}\, \overset{v}{\tfrac{1}{2}\mathrm{e}^{2x}}$

The integral on the right can be done by integrating by parts a second time, see (a):

$I(z) \overset{\text{(a)}}{=} \tfrac{1}{2}z^2\mathrm{e}^{2z} - \tfrac{1}{2}z\mathrm{e}^{2z} + \tfrac{1}{4}\left[\mathrm{e}^{2z}-1\right]$

$I'(z) = \left[\tfrac{1}{2}(2z+2z^2) - \tfrac{1}{2}(1+2z) + \tfrac{1}{4}2\right]\mathrm{e}^{2z} \overset{\checkmark}{=} z^2\mathrm{e}^{2z}$ $\qquad I(\tfrac{1}{2}) \overset{\checkmark}{=} \tfrac{\mathrm{e}}{8} - \tfrac{1}{4}$

Since we integrated by parts twice, I' yields more involved cancellations than for (a).

(c) $I(z) = \int_0^z \mathrm{d}x\, \overset{u}{(\ln x)} \cdot \overset{v'}{1} = \Big[\overset{u}{(\ln x)}\, \overset{v}{x}\Big]_0^z - \int_0^z \mathrm{d}x\, \overset{u'}{\tfrac{1}{x}}\, \overset{v}{x} = (\ln z)z - z$

$$I'(z) = \tfrac{1}{z}z + \ln z - 1 \overset{\checkmark}{=} \ln z \qquad I(1) \overset{\checkmark}{=} -1$$

(d) $$I(z) = \int_0^z \mathrm{d}x\ \overset{u}{(\ln x)} \cdot \overset{v'}{\tfrac{1}{\sqrt{x}}} = \Big[\overset{u}{(\ln x)}\ \overset{v}{2\sqrt{x}}\Big]_0^z - \int_0^z \mathrm{d}x\ \overset{u'}{\tfrac{1}{x}}\ \overset{v}{2\sqrt{x}} = (\ln z)2\sqrt{z} - 4\sqrt{z}$$

To evaluate $[\ln(x)\sqrt{x}]_{x=0}$, we used the rule of l'Hopital:

$$\Big[(\ln x)\sqrt{x}\Big]_{x=0} = \lim_{x\to 0}\frac{\ln x}{x^{-1/2}} = \lim_{x\to 0}\frac{\frac{\mathrm{d}}{\mathrm{d}x}\ln x}{\frac{\mathrm{d}}{\mathrm{d}x}x^{-1/2}} = \lim_{x\to 0}\frac{x^{-1}}{-\frac{1}{2}x^{-3/2}} = \lim_{x\to 0}\big[-2x^{1/2}\big] = 0\,.$$

Thus the divergence of $\ln(x)$ for $x \to 0$ is so slow that $\sqrt{x}$ suppresses it.

$$I'(z) = 2\left[\tfrac{1}{z}\sqrt{z} + (\ln z)\tfrac{1}{2}\tfrac{1}{\sqrt{z}}\right] - 4\tfrac{1}{2}\tfrac{1}{\sqrt{z}} \overset{\checkmark}{=} (\ln z)\tfrac{1}{\sqrt{z}} \qquad I(1) \overset{\checkmark}{=} -4$$

(e) $$I(z) = \int_0^z \mathrm{d}x\ \overset{u}{\sin x}\ \overset{v'}{\sin x} = \Big[\overset{u}{\sin x}\ \overset{v}{(-\cos x)}\Big]_0^z - \int_0^z \mathrm{d}x\ \underbrace{\overset{u'}{\cos x}\ \overset{v}{(-\cos x)}}_{\sin^2 x - 1}$$

Reexpress the integral on the right in terms of $I(z)$,

$$I(z) = -\sin z\cos z - I(z) + \int_0^z \mathrm{d}x\ 1\ , \qquad \text{and solve for } I(z)\text{:}$$

$$I(z) = \tfrac{1}{2}(-\sin z\cos z + z)$$

$$I'(z) = \tfrac{1}{2}(-\cos^2 z + \sin^2 z + 1) \overset{\checkmark}{=} \sin^2 z \qquad I(\pi) \overset{\checkmark}{=} \tfrac{\pi}{2}$$

(f) $$I(z) = \int_0^z \mathrm{d}x\ \overset{u}{\sin^3 x}\ \overset{v'}{\sin x} = \Big[\overset{u}{\sin^3 x}\ \overset{v}{(-\cos x)}\Big]_0^z - \int_0^z \mathrm{d}x\ \big(3\sin^2 x\ \overset{u'}{\underbrace{\cos x}}\big)\ \overset{v}{(-\cos x)}$$

Reexpress the integral on the right in terms of $I(z)$,

$$I(z) = -\sin^3 z\cos z - 3\Big[I(z) - \int_0^z \mathrm{d}x\ \sin^2 x\Big]\ , \qquad \text{solve for } I(z)\text{, and use (e):}$$

$$I(z) \overset{\text{(e)}}{=} \tfrac{1}{4}\left[-\sin^3 z\cos z + \tfrac{3}{2}(-\sin z\cos z + z)\right]$$

$$I'(z) = \tfrac{1}{4}\Big[-3\sin^2 z\underbrace{\cos^2 z}_{1-\sin^2 z} + \sin^4 z + \tfrac{3}{2}(-\cos^2 z + \sin^2 z + 1)\Big] \overset{\checkmark}{=} \sin^4 z \quad I(\pi) \overset{\checkmark}{=} \tfrac{3\pi}{8}$$

EC2.3.3 Integration by substitution

(a) $$I(z) = \int_0^z \mathrm{d}x\ x\cos(x^2+\pi) \qquad [y(x) = x^2,\ \mathrm{d}y = 2x\ \mathrm{d}x]$$
$$= \tfrac{1}{2}\int_{y(0)}^{y(z)} \mathrm{d}y\ \cos(y+\pi) = \tfrac{1}{2}\sin(y+\pi)\Big|_0^{z^2} = \tfrac{1}{2}\sin(z^2+\pi)$$

$$I'(z) = \tfrac{1}{2}\cos(z^2+\pi)\ \tfrac{\mathrm{d}}{\mathrm{d}z}z^2 \overset{\checkmark}{=} \cos(z^2+\pi)\ z \qquad I(\sqrt{\tfrac{\pi}{2}}) \overset{\checkmark}{=} -\tfrac{1}{2}$$

(b)
$$I(z) = \int_0^z \mathrm{d}x\ \sin^3 x \cos x \qquad [y(x) = \sin x,\ \mathrm{d}y = \cos x\ \mathrm{d}x]$$
$$= \int_{y(0)}^{y(z)} \mathrm{d}y\ y^3 = \tfrac{1}{4}y^4\Big|_0^{\sin z} = \tfrac{1}{4}\sin^4 z$$
$$I'(z) = \sin^3 z\ \tfrac{\mathrm{d}}{\mathrm{d}z}\sin z \overset{\checkmark}{=} \sin^3 z\cos z \qquad I(\tfrac{\pi}{4}) \overset{\checkmark}{=} \tfrac{1}{16}$$

(c)
$$I(z) = \int_0^z \mathrm{d}x\ \sqrt{1+\ln(x+1)}\ \tfrac{1}{x+1} \qquad \big[y(x) = \ln(x+1),\ \mathrm{d}y = \tfrac{1}{1+x}\ \mathrm{d}x\big]$$
$$= \int_{y(0)}^{y(z)} \mathrm{d}y\ \sqrt{1+y} = \tfrac{2}{3}(1+y)^{3/2}\Big|_0^{\ln(z+1)} = \tfrac{2}{3}\Big[\big(1+\ln(z+1)\big)^{3/2} - 1\Big]$$
$$I'(z) = \big(1+\ln(z+1)\big)^{1/2}\tfrac{\mathrm{d}}{\mathrm{d}z}\ln(z+1) \overset{\checkmark}{=} \sqrt{1+\ln(z+1)}\ \tfrac{1}{z+1} \qquad I(\mathrm{e}^3-1) \overset{\checkmark}{=} \tfrac{14}{3}$$

(d)
$$I(z) = \int_0^z \mathrm{d}x\ x^3\mathrm{e}^{-x^4} \qquad [y(x) = x^4,\ \mathrm{d}y = 4x^3\ \mathrm{d}x]$$
$$= \tfrac{1}{4}\int_{y(0)}^{y(z)} \mathrm{d}y\ \mathrm{e}^{-y} = -\tfrac{1}{4}\mathrm{e}^{-y}\Big|_0^{z^4} = \tfrac{1}{4}\Big[1-\mathrm{e}^{-z^4}\Big]$$
$$I'(z) = \tfrac{1}{4}\mathrm{e}^{-z^4}\tfrac{\mathrm{d}}{\mathrm{d}z}z^4 \overset{\checkmark}{=} \mathrm{e}^{-z^4}z^3 \qquad I(\sqrt[4]{\ln 2}) \overset{\checkmark}{=} \tfrac{1}{8}$$

EC2.3.5 $\sqrt{1-x^2}$ Integrals by trigonometric substitution

(a) Substitution: $x = \sin(y)$, with inverse function $y = \arcsin(x)$. Express each occurrence of x in terms of y: $\frac{\mathrm{d}x}{\mathrm{d}y} = \cos(y)$, $\Rightarrow\ \mathrm{d}x = \mathrm{d}y\cos(y)$. Moreover: $1-\sin^2(y) = \cos^2(y)$.

$$I(z) = \int_0^z \mathrm{d}x\ \frac{1}{\sqrt{1-x^2}} = \int_{\arcsin 0}^{\arcsin(z)} \mathrm{d}y\ \cos y\frac{1}{\sqrt{1-\sin^2 y}} = \int_0^{\arcsin(z)} \mathrm{d}y\ \cos y\frac{1}{\sqrt{\cos^2 y}}$$
$$= \int_0^{\arcsin(z)} \mathrm{d}y = y\Big|_0^{\arcsin(z)} = \boxed{\arcsin(z)}$$

Check your result: $I\big(\frac{1}{\sqrt{2}}\big) = \arcsin\big(\frac{1}{\sqrt{2}}\big) = \frac{\pi}{4}$, since $\sin\big(\frac{\pi}{4}\big) = \frac{1}{\sqrt{2}}$. ✓

Check by differentiating; let $\arcsin(z) = u$, $\sin(u) = z$:

$$\frac{\mathrm{d}I(z)}{\mathrm{d}z} = \frac{\mathrm{d}\arcsin(z)}{\mathrm{d}z} = \frac{1}{\frac{\mathrm{d}\sin(u)}{\mathrm{d}u}\Big|_{u=\arcsin(z)}} = \frac{1}{\cos u\big|_{u=\arcsin(z)}}$$
$$= \frac{1}{\sqrt{1-\sin^2 u}\Big|_{u=\arcsin(z)}} = \frac{1}{\sqrt{1-\sin^2(\arcsin(z))}} = \boxed{\frac{1}{\sqrt{1-z^2}}}\ \checkmark$$

(b) Substitution: $x = \frac{1}{2}\sin(y)$, with inverse function $y = \arcsin(2x)$. Express each occurrence of x in terms of y: $\frac{\mathrm{d}x}{\mathrm{d}y} = \frac{1}{2}\cos(y)$, $\Rightarrow \quad \mathrm{d}x = \mathrm{d}y\,\frac{1}{2}\cos(y)$. Moreover: $1-\sin^2(y) = \cos^2(y)$.

$$I(z) = \int_0^z \mathrm{d}x\,\sqrt{1-4x^2} = \int_{\arcsin 0}^{\arcsin(2z)} \mathrm{d}y\,\tfrac{1}{2}\cos y\sqrt{1-\sin^2 y} = \tfrac{1}{2}\int_0^{\arcsin(2z)} \mathrm{d}y\,\cos^2 y$$

We compute the $\cos^2(y)$ integral by integrating by parts, with $u = \cos y$, $v = \sin y$, $u' = -\sin y$, $v' = \cos y$:

$$\tilde{I}(a) = \int_0^a \mathrm{d}y\,\overset{u}{\cos}(y)\overset{v'}{\cos}(y) \overset{uv-\int u'v}{=} \Big[\cos(y)\,\sin(y)\Big]_0^a - \int_0^a \mathrm{d}y\,\underbrace{[-\sin(y)]\sin(y)}_{\cos^2(y)-1}$$

$$= a + \cos(a)\sin(a) - \tilde{I}(a)$$

$$\Rightarrow \tilde{I}(a) = \tfrac{1}{2}\big[a + \cos(a)\sin(a)\big]$$

With $a = \arcsin(2z)$ and $I(z) = \frac{1}{2}\tilde{I}\big(\arcsin(2z)\big)$ we thus obtain:

$$I(z) = \tfrac{1}{4}\Big[a + \sin(a)\cos(a)\Big]_{a=\arcsin(2z)} = \tfrac{1}{4}\Big[a + \sin(a)\sqrt{1-\sin^2(a)}\Big]_{a=\arcsin(2z)}$$

$$= \tfrac{1}{4}\Big[\arcsin(2z) + 2z\sqrt{1-4z^2}\Big]$$

Check your result: $I\big(\frac{1}{2}\big) = \frac{1}{4}\Big[\arcsin(1) + 1\cdot\sqrt{1-4\cdot\big(\frac{1}{4}\big)^2}\Big] = \frac{\pi}{8}$ ✓

Check by differentiating:

$$\tfrac{\mathrm{d}I(z)}{\mathrm{d}z} \overset{(a)}{=} \tfrac{1}{4}\left[\tfrac{2}{\sqrt{1-(2z)^2}} + 2\sqrt{1-4z^2} + 2z\tfrac{-8z}{2\sqrt{1-4z^2}}\right] = \tfrac{1}{4}\left[\tfrac{2-8z^2}{\sqrt{1-4z^2}} + 2\sqrt{1-4z^2}\right] = \sqrt{1-4z^2}$$

✓

EC2.3.7 $1/(1-x^2)$ Integrals by hyperbolic substitution

(a) $$\tfrac{\mathrm{d}}{\mathrm{d}y}\tanh(y) = \tfrac{\mathrm{d}}{\mathrm{d}y}\tfrac{\sinh(y)}{\cosh(y)} = \tfrac{\cosh^2(y)-\sinh^2(y)}{\cosh^2(y)} = \tfrac{1}{\cosh^2(y)} = \operatorname{sech}^2(y)\,.\checkmark$$

$$1-\tanh^2(y) = \tfrac{\cosh^2(y)-\sinh^2(y)}{\cosh^2(y)} = \tfrac{1}{\cosh^2(y)} = \operatorname{sech}^2(y)\,.\checkmark$$

(b) Substitution: $x = \tanh(y)$, with inverse function $y = \operatorname{arctanh}(x)$. Express each occurrence of x in terms of y: $\frac{\mathrm{d}x}{\mathrm{d}y} = \operatorname{sech}^2(y)$, $\Rightarrow \quad \mathrm{d}x = \mathrm{d}y\,\operatorname{sech}^2(y)$. Moreover: $1-\tanh^2(y) = \operatorname{sech}^2(y)$.

$$I(z) = \int_0^z \mathrm{d}x\,\frac{1}{1-x^2} = \int_{\operatorname{arctanh} 0}^{\operatorname{arctanh}(z)} \mathrm{d}y\,\operatorname{sech}^2 y\,\frac{1}{\operatorname{sech}^2 y} = \int_0^{\operatorname{arctanh}(z)} \mathrm{d}y\,1 = \operatorname{arctanh}(z)$$

Check your result: $I\left(\frac{3}{5}\right) = \operatorname{arctanh}\left(\frac{2}{3}\right) = \ln 2$, since $\tanh\left(\ln 2\right) = \frac{e^{\ln 2} - e^{-\ln 2}}{e^{\ln 2} + e^{-\ln 2}} = \frac{2-1/2}{2+1/2} = \frac{3}{5}$. ✓

Check by differentiating; let $\operatorname{arctanh}(z) = u$, $\tanh(u) = z$:

$$\begin{aligned}\frac{\mathrm{d}I(z)}{\mathrm{d}z} &= \frac{\mathrm{d}\operatorname{arctanh}(z)}{\mathrm{d}z} = \frac{1}{\left.\frac{\mathrm{d}\tanh(u)}{\mathrm{d}u}\right|_{u=\operatorname{arctanh}(z)}} = \frac{1}{\left.\operatorname{sech}^2 u\right|_{u=\operatorname{arctanh}(z)}} \\ &= \cosh^2(\operatorname{arctanh}(z)) = \frac{1}{1-\tanh^2(\operatorname{arctanh}(z)} = \frac{1}{1-z^2}\checkmark\end{aligned}$$

EC2.3.9 $1/(1+x^2)$ Integral via partial fraction decomposition

(a) The integral has the form $I = \int_0^z \mathrm{d}x\, f(x)$, with

$$f(x) = \frac{1}{1+x^2} = \frac{1}{(1+\mathrm{i}x)(1-\mathrm{i}x)}\,, \tag{1}$$

and can be computed using a partial fraction decomposition. We make the ansatz

$$f(x) = \frac{A}{1+\mathrm{i}x} + \frac{B}{1-\mathrm{i}x}\,, \tag{2}$$

and determine the constants A and B, by bringing (2) into the form (1):

$$f(x) = \frac{A(1-\mathrm{i}x) + B(1+\mathrm{i}x)}{(1+\mathrm{i}x)(1-\mathrm{i}x)} = \frac{(A+B) + (B-A)\mathrm{i}x}{(1+\mathrm{i}x)(1-\mathrm{i}x)}\,. \tag{3}$$

Comparing coefficients of x^0 and x^1 in the numerators of (3) and (1) yields $A = B$ and $A = \frac{1}{2}$. We now insert these coefficients into (2) and integrate:

$$I(z) = \int_0^z \mathrm{d}x\, f(x) = \frac{1}{2}\int_0^z \mathrm{d}x \left[\frac{1}{1+\mathrm{i}x} + \frac{1}{1-\mathrm{i}x}\right] = \frac{1}{2\mathrm{i}} \ln\left(\frac{1+\mathrm{i}z}{1-\mathrm{i}z}\right).$$

(b) Computing the integral using the substitution $y = \tan(x)$ yields $I(z) = \arctan(z)$. To establish the equivalence of the latter with the result from (a), we explicitly compute $\arctan(x)$:

$$y = \arctan(x) \quad \Rightarrow \quad x = \tan(y) = \frac{\sin(y)}{\cos(y)} = \frac{e^{\mathrm{i}y} - e^{-\mathrm{i}y}}{\mathrm{i}(e^{\mathrm{i}y} + e^{-\mathrm{i}y})} = \frac{1 - e^{-\mathrm{i}2y}}{\mathrm{i}(1 + e^{-\mathrm{i}2y})}\,.$$

We now solve this equation for y:

$$\begin{aligned}\mathrm{i}x(1 + e^{-2\mathrm{i}y}) &= 1 - e^{-2\mathrm{i}y} \\ e^{-2\mathrm{i}y} &= \frac{1-\mathrm{i}x}{1+\mathrm{i}x}\,, \quad \Rightarrow \quad y = -\frac{1}{2\mathrm{i}} \ln\left(\frac{1-\mathrm{i}x}{1+\mathrm{i}x}\right) = \frac{1}{2\mathrm{i}} \ln\left(\frac{1+\mathrm{i}x}{1-\mathrm{i}x}\right).\end{aligned}$$

Thus $\arctan(z)$ is indeed equal to the expression obtained in (a). ✓

ᴇC2.3.11 Partial fraction decomposition

(a) The integral has the form $I(z) = \int_0^z \mathrm{d}x\, f(x)$, with

$$f(x) = \frac{3x+3}{(x+1)^2(x-2)} = \frac{3}{(x+1)(x-2)}\,, \tag{1}$$

and can be computed using a partial fraction decomposition. To this end, we make the ansatz

$$f(x) = \frac{A}{x+1} + \frac{B}{x-2}\,, \tag{2}$$

and determine the coefficients A and B by writing (2) in the form (1):

$$f(x) = \frac{A(x-2)+B(x+1)}{(x+1)(x-2)} = \frac{(A+B)x - 2A + B}{(x+1)(x-2)}\,. \tag{3}$$

Comparing coefficients in the numerators of (3) and (1) we obtain:

$$A + B = 0 \qquad \Rightarrow \qquad A = -B\,, \tag{4}$$

$$-2A + B = 3 \quad \overset{(4)}{\Rightarrow} \quad -3A = 3 \quad \Rightarrow \quad A = -1,\ B = 1\,. \tag{5}$$

Now we insert the coefficients from (5) into (2) and integrate:

$$I(z) = \int_0^z \mathrm{d}x\, f(x) = \int_0^z \mathrm{d}x \left[\frac{-1}{x+1} + \frac{1}{x-2}\right] = \Big[-\ln|x+1| + \ln|x-2|\Big]_0^z$$
$$= \ln\left|\frac{1-\frac{1}{2}z}{1+z}\right|.$$

Remark: The form of the ansatz (2), as well as the coefficients A and B, follow from the asymptotic behavior of the function $f(x)$ at its poles $x = -1$ and $x = 2$, respectively:

$$x = -1+\epsilon: \qquad f(-1+\varepsilon) = \frac{3}{(-1+\epsilon+1)(-1+\epsilon-2)} \overset{\epsilon\to 0}{\longrightarrow} -\frac{1}{\epsilon} + \mathcal{O}(\epsilon^0)\,. \tag{6}$$

$$x = 2+\epsilon: \qquad f(2+\varepsilon) = \frac{3}{(2+\epsilon+1)(2+\epsilon-2)} \overset{\epsilon\to 0}{\longrightarrow} \frac{1}{\epsilon} + \mathcal{O}(\epsilon^0)\,. \tag{7}$$

Eqs. (6) and (7) directly imply that $A = -1$ and $B = 1$, because these are the only values for which ansatz (2) shows the same asymptotic behavior as the function (1) at its poles.

(b) The integral has the form $I(z) = \int_0^z \mathrm{d}x\, f(x)$, with

$$f(x) = \frac{3x}{(x+1)^2(x-2)}\,, \tag{8}$$

and can be computed using a partial fraction decomposition. To this end, we make the ansatz

$$f(x) = \frac{A}{x+1} + \frac{B}{(x+1)^2} + \frac{C}{x-2}\,, \tag{9}$$

and determine the coefficients A, B and C by bringing (9) into the form (8):

$$\begin{aligned} f(x) &= \frac{A(x+1)(x-2) + B(x-2) + C(x+1)^2}{(x+1)^2(x-2)} \\ &= \frac{A(x^2-x-2) + Bx - 2B + C(x^2+2x+1)}{(x+1)^2(x-2)} \\ &= \frac{(A+C)x^2 + (-A+B+2C)x - 2A - 2B + C}{(x+1)^2(x-2)}\,. \end{aligned} \tag{10}$$

Comparing coefficients in the numerators of (10) and (8), we obtain:

$$A + C = 0 \quad \Rightarrow \quad A = -C\,, \tag{11}$$

$$-A + B + 2C = 3 \quad \overset{(11)}{\Rightarrow} \quad B + 3C = 3 \;\Rightarrow\; B = 3 - 3C\,, \tag{12}$$

$$-2A - 2B + C = 0 \quad \overset{(11)}{\Rightarrow} \quad 3C - 2B = 0 \tag{13}$$

$$\overset{(12,13)}{\Rightarrow} \quad 3C - 2(3-3C) = 0 \;\Rightarrow\; C = \tfrac{2}{3}, B = 1, A = -\tfrac{2}{3}\,. \tag{14}$$

Now we insert the coefficients from (12) into (9) and integrate:

$$\begin{aligned} I(z) &= \int_0^z f(x) = \int_0^z \mathrm{d}x \left[-\frac{2}{3}\frac{1}{x+1} + \frac{1}{(x+1)^2} + \frac{2}{3}\frac{1}{x-2} \right] \\ &= \left[-\frac{2}{3}\ln|x+1| - \frac{1}{x+1} + \frac{2}{3}\ln|x-2| \right]_0^z = \frac{2}{3}\ln\left|\frac{1-\frac{1}{2}z}{1+z}\right| + \frac{z}{z+1}\,. \end{aligned}$$

Remark: The form of the ansatz (9) as well as the coefficients A, B and C follow from the asymptotic behavior of the function $f(x)$ at its poles $x = -1$ and $x = 2$, respectively:

$$x = -1 + \epsilon: \qquad f(-1+\varepsilon) = \frac{3(-1+\epsilon)}{(-1+\epsilon+1)^2(-1+\epsilon-2)} = \frac{-3(1-\epsilon)}{\epsilon^2(-3)(1-\frac{1}{3}\epsilon)} \tag{15}$$

$$\xrightarrow{\epsilon\to 0} \frac{(1-\epsilon)(1+\frac{1}{3}\epsilon+\mathcal{O}(\epsilon^2))}{\epsilon^2} = \frac{1}{\epsilon^2} - \frac{2}{3\epsilon} + \mathcal{O}(\epsilon^0)\,. \tag{16}$$

$$x = 2 + \epsilon: \qquad f(2+\varepsilon) = \frac{3(2+\epsilon)}{(2+\epsilon+1)^2(2+\epsilon-2)} \tag{17}$$

$$\xrightarrow{\epsilon\to 0} \frac{6(1+\mathcal{O}(\epsilon^1))}{3^2\,\epsilon} = \frac{2}{3\epsilon} + \mathcal{O}(\epsilon^0)\,. \tag{18}$$

For the step from (15) to (16) we used the first two terms of the geometric series, $\frac{1}{1-y} \xrightarrow{y\to 0} 1 + y$, with $y = \frac{1}{3}\epsilon$. [For a discussion of the geometric series, see Sec. C5.2, cf. Eq. (**??**)]. Eqs. (16) and (17) directly imply that $A = -\frac{2}{3}$, $B = 1$ and $C = \frac{2}{3}$, because these are the only values for which ansatz (9) shows the same asymptotic behavior as the function (8) at its poles.

EC2.3.13 Elementary Gaussian integral

(a) We compute I using polar coordinates: $x = \rho\cos\phi$, $y = \rho\sin\phi$, $\mathrm{d}x\mathrm{d}y = \rho\,\mathrm{d}\rho\,\mathrm{d}\phi$.

$$I = \int_{-\infty}^{+\infty} \mathrm{d}x\mathrm{d}y\ \mathrm{e}^{-(x^2+y^2)} = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\infty} \mathrm{d}\rho\ \rho\ \mathrm{e}^{-\rho^2} = 2\pi\ \left[-\frac{1}{2}\mathrm{e}^{-\rho^2}\right]_0^{\infty} = \pi\,.$$

(b) In the two-dimensional integral I, the x and y integrals are independent and factorize:

$$I = \int_{-\infty}^{+\infty} \mathrm{d}x\mathrm{d}y\ \mathrm{e}^{-(x^2+y^2)} = \left[\int_{-\infty}^{\infty} \mathrm{d}x\ \mathrm{e}^{-x^2}\right]\left[\int_{-\infty}^{\infty} \mathrm{d}y\ \mathrm{e}^{-y^2}\right] = \underbrace{\left[\int_{-\infty}^{\infty} \mathrm{d}x\ \mathrm{e}^{-x^2}\right]}_{I_0(1)}{}^2 = [I_0(1)]^2$$

$I_0(1) = +\sqrt{I} = \sqrt{\pi}\,.$ (Sign: $I_0(1)$ is positive since the integrand $\mathrm{e}^{-x^2} > 0$.)

The required Gaussian integral $I_0(a)$ is obtained using the substitution method $\tilde{x} = \sqrt{a}x$:

$$I_0(a) = \int_{-\infty}^{\infty} \mathrm{d}x\,\mathrm{e}^{-ax^2} \overset{\tilde{x}=\sqrt{a}\,x}{=} \int_{-\infty}^{\infty} \frac{\mathrm{d}\tilde{x}}{\sqrt{a}}\,\mathrm{e}^{-\tilde{x}^2} = \sqrt{\frac{\pi}{a}}\,.$$

EC2.3.15 Definite exponential integrals of the form $\int_0^\infty \mathrm{d}x\, x^n e^{-ax}$

Below, I_n stands for $I_n(a)$, i.e. the a dependence of the integral will not be indicated explicitly.

(a) Repeated partial integration gives:

$$I_n = \int_0^{\infty} \mathrm{d}x\, x^n e^{-ax}$$

$$I_0 = \int_0^{\infty} \mathrm{d}x\,\mathrm{e}^{-ax} = -\frac{\mathrm{e}^{-ax}}{a}\bigg|_0^{\infty} = \frac{1}{a}$$

$$I_1 = \int_0^{\infty} \mathrm{d}x\ \overset{u}{x}\,\overset{v'}{\mathrm{e}^{-ax}} \overset{uv-\int u'v}{=} \left[x\left(-\frac{\mathrm{e}^{-ax}}{a}\right)\right]_0^{\infty} - \int_0^{\infty} \mathrm{d}x\,1\left(-\frac{\mathrm{e}^{-ax}}{a}\right) = 0 + \frac{1}{a}I_0 = \frac{1}{a^2}$$

$$I_2 = \int_0^{\infty} \mathrm{d}x\ \overset{u}{x^2}\overset{v'}{\mathrm{e}^{-ax}} \overset{uv-\int u'v}{=} \left[x^2\left(-\frac{\mathrm{e}^{-ax}}{a}\right)\right]_0^{\infty} - \int_0^{\infty} \mathrm{d}x\,2x\left(-\frac{\mathrm{e}^{-ax}}{a}\right) = 0 + \frac{2}{a}I_1 = \frac{2}{a^3}$$

$\ldots$

$$I_n = \int_0^{\infty} \mathrm{d}x\ \overset{u}{x^n}\overset{v'}{e^{-ax}} \overset{uv-\int u'v}{=} x^n\left[-\frac{1}{a}\mathrm{e}^{-ax}\right]_0^{\infty} - \int_0^{\infty} \mathrm{d}x\,nx^{n-1}\left(-\frac{1}{a}\mathrm{e}^{-ax}\right) = \frac{n}{a}I_{n-1}$$

The resulting pattern is:

$$I_n = \frac{n}{a}I_{n-1} = \frac{n}{a}\frac{n-1}{a}I_{n-2} = \frac{n}{a}\frac{n-1}{a}\frac{n-2}{a}I_{n-3} = \frac{n}{a}\frac{n-1}{a}\frac{n-2}{a}\cdots\frac{2}{a}\frac{1}{a}\frac{1}{a} = \frac{n!}{a^{n+1}}\,.$$

(b) Repeated differentiation gives:

$$
\begin{aligned}
I_0 &= \int_0^\infty \mathrm{d}x\, \mathrm{e}^{-ax} && \Rightarrow \quad I_0 = -\frac{\mathrm{e}^{-ax}}{a}\bigg|_0^\infty = \frac{1}{a} \\
\frac{\mathrm{d}I_0}{\mathrm{d}a} &= \int_0^\infty \mathrm{d}x\, (-x)\mathrm{e}^{-ax} = -I_1 && \Rightarrow \quad I_1 = (-)^1 \frac{\mathrm{d}}{\mathrm{d}a}\frac{1}{a} = \frac{1}{a^2} \\
\frac{\mathrm{d}^2 I_0}{\mathrm{d}a^2} &= \int_0^\infty \mathrm{d}x\, (-x)^2\mathrm{e}^{-ax} = (-)^2 I_2 && \Rightarrow \quad I_2 = (-)^2 \frac{\mathrm{d}^2}{\mathrm{d}a^2}\frac{1}{a} = -\frac{\mathrm{d}}{\mathrm{d}a}\left[\frac{1}{a^2}\right] = \frac{2\cdot 1}{a^3} \\
\frac{\mathrm{d}^3 I_0}{\mathrm{d}a^3} &= \int_0^\infty \mathrm{d}x\, (-x)^3\mathrm{e}^{-ax} = (-)^3 I_3 && \Rightarrow \quad I_3 = (-)^3 \frac{\mathrm{d}^3}{\mathrm{d}a^3}\frac{1}{a} = -\frac{\mathrm{d}}{\mathrm{d}a}\left[\frac{2\cdot 1}{a^3}\right] = \frac{3\cdot 2\cdot 1}{a^4}
\end{aligned}
$$

The resulting pattern is:

$$
\frac{\mathrm{d}^n I_0}{\mathrm{d}a^n} = \int_0^\infty \mathrm{d}x\, (-x)^n\mathrm{e}^{-an} = (-)^n I_n \quad \Rightarrow \quad I_n = (-)^n \frac{\mathrm{d}^n}{\mathrm{d}a^n}\frac{1}{a} = -\frac{\mathrm{d}}{\mathrm{d}a}\left[\frac{(n-1)!}{a^n}\right] = \frac{n!}{a^{n+1}}\,.
$$

S.C3 Partial differentiation

S.C3.1 Partial derivative

ᴇC3.1.1 Partial derivatives

(a) $f(x,y) = x^2y^3 - 2xy, \qquad \partial_x f(x,y) = 2xy^3 - 2y\,, \qquad \partial_y f(x,y) = 3x^2y^2 - 2x\,.$

(b) $f(x,y) = \sin\left[x\mathrm{e}^{2y}\right], \qquad \partial_x f(x,y) = \cos\left[x\mathrm{e}^{2y}\right]\mathrm{e}^{2y}\,, \qquad \partial_y f(x,y) = \cos\left[x\mathrm{e}^{2y}\right]2x\mathrm{e}^{2y}\,.$

S.C3.2 Multiple partial derivatives

ᴇC3.2.1 Partial derivates of first and second order

$$
\begin{aligned}
\partial_x r = \partial_x\sqrt{x^2+y^2} = \frac{1}{2}\frac{2x}{\sqrt{x^2+y^2}} = \frac{x}{r}, \qquad &\text{similarly:} \quad \partial_y r = \frac{y}{r} \\
\partial_x f(\mathbf{r}) = \partial_x \frac{x}{r} = \frac{1}{r} - x\cdot\frac{1}{r^2}\cdot\frac{x}{r} &= \frac{r^2-x^2}{r^3} = \frac{y^2}{r^3} \\
\partial_y f(\mathbf{r}) = \partial_y \frac{x}{r} = -x\cdot\frac{1}{r^2}\cdot\frac{y}{r} &= -\frac{xy}{r^3} \\
\partial^2_{y,x} f(\mathbf{r}) = \partial_y\left(\frac{y^2}{r^3}\right) = \frac{2y}{r^3} - y^2\cdot\frac{3}{r^4}\cdot\frac{y}{r} &= \frac{2yr^2-3y^3}{r^5} = \frac{2yx^2-y^3}{r^5} \\
\partial^2_{x,y} f(\mathbf{r}) = \partial_x\left(-\frac{xy}{r^3}\right) = -\frac{y}{r^3} + xy\cdot\frac{3}{r^4}\cdot\frac{x}{r} &= \frac{-yr^2+3x^2y}{r^5} = \frac{2yx^2-y^3}{r^5}
\end{aligned}
$$

$$\partial_x^2 f(\mathbf{r}) = \partial_x \left(\frac{y^2}{r^3}\right) = -y^2 \frac{3}{r^4} \cdot \frac{x}{r} = -\frac{3xy^2}{r^5}$$
$$\partial_y^2 f(\mathbf{r}) = \partial_y \left(-\frac{xy}{r^3}\right) = -\frac{x}{r^3} + xy \cdot \frac{3}{r^4} \cdot \frac{y}{r} = \frac{-xr^2 + 3xy^2}{r^5} = \frac{2xy^2 - x^3}{r^5}$$

S.C3.3 Chain rule for functions of several variables

ᴇC3.3.1 Chain rule for functions of two variables

(a) Direct computation of $f(\mathbf{g}(\mathbf{x}))$ and its partial derivatives yields:

$$f(\mathbf{g}(\mathbf{x})) = \|\mathbf{g}(\mathbf{x})\| = \left\|\left(\ln x^2, 3\ln x^1\right)^T\right\| = \ln^2 x^2 + 9\ln^2 x^1 \,.$$
$$\partial_{x^1} f(\mathbf{g}(\mathbf{x})) = \partial_{x^1}\left[\ln^2 x^2 + 9\ln^2 x^1\right] = \left[0 + 9(2\ln x^1)\,\partial_{x^1}\ln x^1\right] = \frac{18\ln x^1}{x^1}\,,$$
$$\partial_{x^2} f(\mathbf{g}(\mathbf{x})) = \partial_{x^2}\left[\ln^2 x^2 + 9\ln^2 x^1\right] = \left[(2\ln x^2)\,\partial_{x^2}\ln x^2 + 0\right] = \frac{2\ln x^2}{x^2}\,.$$

(b) The chain rule, $\partial_{x^k} f(\mathbf{g}(\mathbf{x})) = \sum_j \left[\partial_{y^j} f(\mathbf{y})\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})} \partial_{x^k} g^j(\mathbf{x})$, yields the same results:

$$\begin{aligned}\partial_{x^1} f(\mathbf{g}(\mathbf{x})) &= \left[\partial_{y^1} f(\mathbf{y})\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})}\cdot \partial_{x^1} g^1(\mathbf{x}) + \left[\partial_{y^2} f(\mathbf{y})\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})}\cdot \partial_{x^1} g^2(\mathbf{x}) \\ &= \left[\partial_{y^1}\left[(y^1)^2 + (y^2)^2\right]\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})}\cdot \partial_{x^1}\left[\ln x^2\right] + \left[\partial_{y^2}\left[(y^1)^2 + (y^2)^2\right]\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})}\cdot \partial_{x^1}\left[3\ln x^1\right] \\ &= 0 + \left[2y^2\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})}\cdot \frac{3}{x^1} = 2g^2(\mathbf{x})\,\frac{3}{x^1} = 2(3\ln x^1)\frac{3}{x^1} = \frac{18\ln x^1}{x^1} \overset{\checkmark}{=} \text{(a)}.\end{aligned}$$

$$\begin{aligned}\partial_{x^2} f(\mathbf{g}(\mathbf{x})) &= \left[\partial_{y^1} f(\mathbf{y})\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})}\cdot \partial_{x^2} g^1(\mathbf{x}) + \left[\partial_{y^2} f(\mathbf{y})\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})}\cdot \partial_{x^2} g^2(\mathbf{x}) \\ &= \left[\partial_{y^1}\left[(y^1)^2 + (y^2)^2\right]\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})}\cdot \partial_{x^2}\left[\ln x^2\right] + \left[\partial_{y^2}\left[(y^1)^2 + (y^2)^2\right]\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})}\cdot \partial_{x^2}\left[3\ln x^1\right] \\ &= \left[2y^1\right]_{\mathbf{y}=\mathbf{g}(\mathbf{x})}\cdot \frac{1}{x^2} + 0 = 2g^1(\mathbf{x})\cdot \frac{1}{x^2} = 2\ln x^2 \frac{1}{x^2} = \frac{2\ln x^2}{x^2} \overset{\checkmark}{=} \text{(a)}.\end{aligned}$$

In both (a) and (b), computing the partial derivatives involves first differentiating the sum of squares, then differenting logarithms. The chain rule route (b) simply makes this notationally somewhat more explicit than the direct route (a).

S.C4 Multi-dimensional integration

S.C4.1 Cartesian area and volume integrals

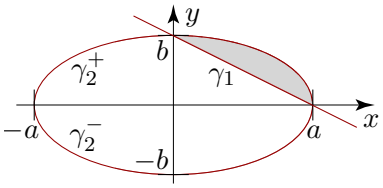
ᴇC4.1.1 Two-dimensional integration (Cartesian coordinates)

$$I(a) = \int_G \mathrm{d}x\mathrm{d}y f(x,y) = \int_0^1 \mathrm{d}y \int_1^{a-y} \mathrm{d}x\, xy = \int_0^1 \mathrm{d}y\; y\left[\tfrac{1}{2}x^2\right]_1^{a-y} = \tfrac{1}{2}\int_0^1 \mathrm{d}y\; y\left[(a-y)^2 - 1\right]$$

$$= \tfrac{1}{2}\int_0^1 \mathrm{d}y\,\Big[y^3 - ay^2 + (a^2-1)y\Big] = \big[\tfrac{1}{8}y^4 - \tfrac{1}{3}ay^3 + \tfrac{1}{4}(a^2-1)y^2\big]_0^1 = -\tfrac{1}{8} - \tfrac{1}{3}a + \tfrac{1}{4}a^2\,.$$

EC4.1.3 Area enclosed by curves (Cartesian coordinates)

(a) Along the curve γ_1, the components $x = t$ and $y = b(1 - t/a)$ satisfy the equation of a straight line, namely $y = b(1-x/a)$. Along the curve γ_2 the components $x = a\cos t$ and $y = b\sin t$ satisfy the equation of an ellipse with semi-axes a and b, namely $x^2/a^2 + y^2/b^2 = 1$.



(b) When computing areas it is useful to parametrize curves by one of the coordinates of $\mathbb{R}^2$. Here we use x as the curve parameter (y would work equally well) and parametrize the upper and lower branches of the ellipse, $\gamma_2^\pm$, by $y_2^\pm(x) = \pm b\sqrt{1 - x^2/a^2}$, with $|x| < a$. Its area is then described by $-a < x < a$ and $y_2^-(x) < y < y_2^+(x)$:

$$S(a,b) = \int_{-a}^{a}\mathrm{d}x\int_{y_2^-(x)}^{y_2^+(x)}\mathrm{d}y\,1 = \int_{-a}^{a}\mathrm{d}x\,\big[y_2^+(x) - y_2^-(x)\big] = 2\int_{-a}^{a}\mathrm{d}x\,b\sqrt{1-x^2/a^2}$$
$$\overset{x=a\sin u}{=} 2ab\int_{-\pi/2}^{\pi/2}\mathrm{d}u\cos^2 u \overset{\text{part. int.}}{=} 2ab\tfrac{1}{2}\Big[u + \sin u\cos u\Big]_{-\pi/2}^{\pi/2} = \pi ab\,.$$

(c) We parametrize the straight line γ_1 by $y_1(x) = b(1 - x/a)$. According to the figure, it intersects the ellipse γ_2 at the points $(a,0)^T$ and $(0,b)^T$. This is consistent with the following algebraic argument: Since $y_1(x) \geq 0$ for $x \leq a$, the straight line γ_1 intersects only the positive branch γ_2^+ of the ellipse, namely when

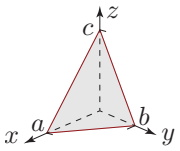
$$0 = y_1(x) - y_2^+(x) = b(1 - x/a) - b\sqrt{1 - \tfrac{x^2}{a^2}}\,, \quad \Rightarrow \quad x = a \;\text{ or }\; x = 0\,.$$

The desired area (shaded in sketch) is thus described by $0 < x < a$ and $y_1(x) < y < y_2^+(x)$:

$$A(a,b) = \int_0^a \mathrm{d}x\int_{y_1(x)}^{y_2^+(x)}\mathrm{d}y\,1 = \int_0^a \mathrm{d}x\,\big[y_2^+(x) - y_1(x)\big] = \int_0^a \mathrm{d}x\,b\left[\sqrt{1-\tfrac{x^2}{a^2}} - \big(1 - \tfrac{x}{a}\big)\right]$$
$$\overset{\text{(a)}}{=} \tfrac{1}{4}\pi ab - b\left[x - \tfrac{1}{2}\tfrac{x^2}{a}\right]_0^a = ab(\tfrac{1}{4}\pi - \tfrac{1}{2})\,.$$

Geometric consideration: the desired area is a quarter of the area of the ellipse, namely $\frac{1}{4}\pi ab$, minus the area of a triangle with base a and height b, namely $\frac{1}{2}ab$.

EC4.1.5 Area integral for volume of a pyramid (Cartesian coordinates)



(a) The plane E intersects the three axes at $x = a$, $y = b$ and $z = c$. Therefore the pyramid has base area $A = \frac{1}{2}ab$, height $h = c$ and volume $V = \frac{1}{3}Ah = \frac{1}{6}abc$.

(b) The diagonal of the pyramid's base area in the xy plane is described by $y_D(x) = b(1 - x/a)$, and the base area itself by $0 \le x \le a$ and $0 \le y \le y_D(x)$. The pyramid's height above the base are is $h(x, y) = c(1 - x/a - y/b)$. Thus the volume is:

$$V = \int_A \mathrm{d}x\mathrm{d}y\, h(x,y) = \int_0^a \mathrm{d}x \int_0^{y_D(x)} \mathrm{d}y\, c\left(1 - \tfrac{x}{a} - \tfrac{y}{b}\right) = c\int_0^a \mathrm{d}x \left[y\left(1 - \tfrac{x}{a}\right) - \tfrac{1}{2}\tfrac{y^2}{b}\right]_0^{y_D(x)}$$
$$= c\int_0^a \mathrm{d}x \left[b\left(1 - \tfrac{x}{a}\right)^2 - \tfrac{1}{2}b^2\left(1 - \tfrac{x}{a}\right)^2 \tfrac{1}{b}\right] = \tfrac{1}{2}cb\left(-\tfrac{1}{3}a\right)\left[(1 - \tfrac{x}{a})^3\right]_0^a = \tfrac{1}{6}abc\,. \checkmark$$

S.C4.2 Curvilinear area integrals

EC4.2.1 Area of an ellipse (elliptical polar coordinates)

(a) In elliptical polar coordinates, the area element is given by:

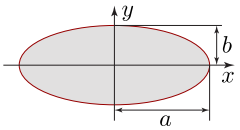
$$\mathrm{d}x\,\mathrm{d}y = \mathrm{d}\mu\,\mathrm{d}\phi\,||\partial_\mu \mathbf{r} \times \partial_\phi \mathbf{r}||.$$

The integration measure can be calculated by using $\mathbf{r} = \mu a\cos\phi\,\mathbf{e}_1 + \mu b\sin\phi\,\mathbf{e}_2$:

$$\|\partial_\mu \mathbf{r} \times \partial_\phi \mathbf{r}\| = \left\| \begin{pmatrix} a\cos\phi \\ b\sin\phi \\ 0 \end{pmatrix} \times \begin{pmatrix} -a\mu\sin\phi \\ b\mu\cos\phi \\ 0 \end{pmatrix} \right\| = ab\,\mu(\cos^2\phi + \sin^2\phi) = ab\,\mu\,.$$

The integration limits now correspond to $0 < \mu < \infty$, $0 < \phi < 2\pi$. Thus,

$$I = ab\int_0^\infty \mathrm{d}\mu\,\mu \int_0^{2\pi} \mathrm{d}\phi\, f(\mu^2) = 2\pi ab\int_0^\infty \mathrm{d}\mu\,\mu\, f(\mu^2)\,.$$



(b) In Cartesian coordinates, an ellipse is defined by $(x/a)^2 + (y/b)^2 = 1$, and in elliptical coordinates by $\mu^2 = 1$. Using elliptical coordinates, its area can be computed as follows:

$$A_E = \int_{(x/a)^2+(y/b)^2\le 1} \mathrm{d}x\,\mathrm{d}y = \int_{\mathbb{R}^2} \mathrm{d}x\,\mathrm{d}y\, f\left((x/a)^2 + (y/b)^2\right) \quad \text{with} \quad f(\mu^2) = \begin{cases} 1 & \text{for } 0 < \mu^2 \le 1, \\ 0 & \text{for } \mu^2 > 1, \end{cases}$$
$$= \int_0^{2\pi} \mathrm{d}\phi \int_0^\infty \mathrm{d}\mu\, ab\,\mu\, f(\mu^2) = 2\pi ab\int_0^1 \mathrm{d}\mu\,\mu\, = 2\pi ab\frac{1}{2} = \pi ab\,.$$

S.C4.3 Curvilinear volume integrals

ᴇC4.3.1 Volume and moment of inertia (cylindrical coordinates)

In cylindrical coordinates, $x = \rho\cos\phi$, $y = \rho\sin\phi$, z, the volume element is $\mathrm{d}V = \mathrm{d}\phi\,\mathrm{d}z\,\mathrm{d}\rho\,\rho$ and the perpendicular distance to the z axis is $d_\perp^2 = x^2 + y^2 = \rho^2$. The homogeneous body F has density $\rho_0 = M/V_F$. The integration region is $0 < \phi < 2\pi$, $H \le z \le 2H$, $0 < \rho \le az$, hence the integral over ρ has a z-dependent upper limit and must be computed before the integral over z:

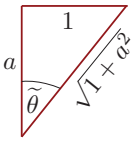
(a) $$V_F(a) = \int_K \mathrm{d}V = \int_0^{2\pi}\mathrm{d}\phi\int_H^{2H}\mathrm{d}z\int_0^{az}\mathrm{d}\rho\,\rho = 2\pi\int_H^{2H}\mathrm{d}z\left[\frac{\rho^2}{2}\right]_0^{az} = \pi a^2\int_H^{2H}\mathrm{d}z\,z^2$$
$$= \pi a^2\left[\frac{z^3}{3}\right]_H^{2H} = \frac{7\pi a^2}{3}H^3\,.$$

(b) $$I_F(a) = \int_K \mathrm{d}V\,\rho_0\,\rho^2 = \rho_0\int_0^{2\pi}\mathrm{d}\phi\int_H^{2H}\mathrm{d}z\int_0^{az}\mathrm{d}\rho\,\rho^3 = 2\pi\int_H^{2H}\mathrm{d}z\left[\frac{\rho^4}{4}\right]_0^{az}$$
$$= \rho_0\frac{\pi a^4}{2}\int_H^{2H}\mathrm{d}z\,z^4 = \rho_0\frac{\pi a^4}{2}\left[\frac{z^5}{5}\right]_H^{2H} = \rho_0\frac{31\pi a^4}{10}H^5 = \frac{93a^2}{70}MH^2\,.$$

ᴇC4.3.3 Volume of a buoy (spherical coordinates)

(a) In spherical coordinates, $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$, the volume element is $\mathrm{d}V = r^2\sin\theta\mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi$. The inequality for z can be written as $r\cos\theta \ge a\sqrt{r^2\sin^2\theta(\cos^2\phi+\sin^2\phi)} = ar\sin\theta$, or $1/a \ge \tan\theta \Rightarrow \theta \le \arctan(1/a) \equiv \widetilde{\theta}$.

(b) $$V(R,a) = \int_0^R \mathrm{d}r\,r^2\int_0^{\widetilde{\theta}}\mathrm{d}\theta\,\sin\theta\int_0^{2\pi}\mathrm{d}\phi = \left[\tfrac{1}{3}r^3\right]_0^R\Big[-\cos\theta\Big]_0^{\widetilde{\theta}}\cdot 2\pi$$
$$= \frac{2\pi}{3}R^3\left[1 - \frac{a}{\sqrt{1+a^2}}\right] \quad \text{since} \quad \cos\widetilde{\theta} = a/\sqrt{1+a^2}$$



ᴇC4.3.5 Wave functions of two-dimensional harmonic oscillator (polar coordinates)

(a) The area integral O factorizes into a radial integral P and an angular integral $\widetilde{P}$:

Area integral: $$O_{nn'}^{mm'} = \int_{\mathbb{R}^2}\mathrm{d}S\,\overline{\Psi}_{nm}(\mathbf{r})\Psi_{n'm'}(\mathbf{r})$$
$$= \int_0^\infty \mathrm{d}\rho\,\rho\int_0^{2\pi}\mathrm{d}\phi\big(\overline{R}_{n|m|}(\rho)\overline{Z}_m(\phi)\big)\big(R_{n'|m'|}(\rho)Z_{m'}(\phi)\big)$$
$$= P_{nn'}^{|m||m'|}\widetilde{P}^{mm'},$$

Radial integral: $P_{nn'}^{|m||m'|} = \int_0^\infty \mathrm{d}\rho\, \rho\, R_{n|m|}(\rho) R_{n'|m'|}(\rho) \quad (\text{since } \overline{R} = R),$

Angular integral: $\widetilde{P}^{mm'} = \int_0^{2\pi} \mathrm{d}\phi\, \overline{Z}_m(\phi) Z_{m'}(\rho)\,.$

(b) The angular integral over the functions $Z_m(\phi) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}m\phi}$ can be calculated easily for arbitrary m and m'. To evaluate the case $m \neq m'$ we use the Euler identity, $\mathrm{e}^{\mathrm{i}2\pi k} = 1$ if $k \in \mathbb{Z}$:

$$\widetilde{P}^{mm'} = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\phi\, \mathrm{e}^{\mathrm{i}(-m+m')\phi}$$
$$= \left\{ \begin{array}{lll} \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\phi\, \mathrm{e}^0 = 1 & \text{for} & m = m' \\ \frac{1}{2\pi} \frac{\mathrm{e}^{\mathrm{i}2\pi(m'-m)} - 1}{\mathrm{i}(m'-m)} \overset{\text{Euler}}{=} \frac{1}{2\pi} \frac{1-1}{\mathrm{i}(m'-m)} = 0 & \text{for} & m \neq m' \end{array} \right\} = \delta_{mm'}\,. \checkmark$$

(c) According to (b), $O_{nn'}^{mm'} \propto \delta_{mm'}$, hence only radial integrals of the form $P_{nn'}^{mm}$ are of interest here. We compute them using the substitution $x = \rho^2$, $\mathrm{d}x = 2\rho\,\mathrm{d}\rho$, and $\int_0^\infty \mathrm{d}x\, x^n \mathrm{e}^{-x} = n!$:

$$P_{00}^{00} = \int_0^\infty \mathrm{d}\rho\, \rho \left[\sqrt{2}\mathrm{e}^{-\rho^2/2}\right]^2 = \int_0^\infty \mathrm{d}x\, \mathrm{e}^{-x} = 1\,.$$
$$P_{11}^{11} = \int_0^\infty \mathrm{d}\rho\, \rho \left[\sqrt{2}\rho\mathrm{e}^{-\rho^2/2}\right]^2 = \int_0^\infty \mathrm{d}x\, x\, \mathrm{e}^{-x} = 1\,.$$
$$P_{22}^{22} = \int_0^\infty \mathrm{d}\rho\, \rho \left[\rho^2\mathrm{e}^{-\rho^2/2}\right]^2 = \int_0^\infty \mathrm{d}x\, \tfrac{1}{2}x^2\mathrm{e}^{-x} = \tfrac{1}{2}\cdot 2 = 1\,.$$
$$P_{22}^{00} = \int_0^\infty \mathrm{d}\rho\, \rho \left[\sqrt{2}(\rho^2-1)\mathrm{e}^{-\rho^2/2}\right]^2 = \int_0^\infty \mathrm{d}x\, (x^2-2x+1)\mathrm{e}^{-x} = (2-2\cdot 1+1) = 1\,.$$
$$P_{20}^{00} = \int_0^\infty \mathrm{d}\rho\, \rho\sqrt{2}(\rho^2-1)\mathrm{e}^{-\rho^2/2}\sqrt{2}\mathrm{e}^{-\rho^2/2} = \int_0^\infty \mathrm{d}x\, (x-1)\mathrm{e}^{-x} = 1-1 = 0\,.$$

It follows that $O_{00}^{00} = O_{11}^{11} = O_{22}^{22} = O_{22}^{00} = 1$ and $O_{20}^{00} = 0$. ✓

S.C4.4 Curvilinear integration in arbitrary dimensions

EC4.4.1 Surface integral: area of a sphere

(a) We use $\mathbf{r}(x,y) = (x, y, \sqrt{R^2-x^2-y^2})^T$ to parametrize the upper half-sphere by Cartesian coordinates on the disk D. Computing the coordinate basis vectors, we find

$$\partial_x \mathbf{r} = \left(1, 0, \tfrac{-x}{\sqrt{R^2-x^2-y^2}}\right)^T, \qquad \partial_y \mathbf{r} = \left(0, 1, \tfrac{-y}{\sqrt{R^2-x^2-y^2}}\right)^T.$$

$$\|\partial_x\mathbf{r}\times\partial_y\mathbf{r}\| = \Big[\|\partial_x\mathbf{r}\|^2\,\|\partial_x\mathbf{r}\|^2 - \|\partial_x\mathbf{r}\cdot\partial_y\mathbf{r}\|^2\Big]^{1/2}$$
$$= \left[\left(1+\tfrac{x^2}{R^2-x^2-y^2}\right)\left(1+\tfrac{y^2}{R^2-x^2-y^2}\right) - \tfrac{x^2y^2}{(R^2-x^2-y^2)^2}\right]^2 = \tfrac{R}{\sqrt{R^2-x^2-y^2}}\,.$$

To compute the area of the sphere, $A_S = 2A_{S_+} = 2\int_D \mathrm{d}x\mathrm{d}y\,\|\partial_x\mathbf{r}\times\partial_y\mathbf{r}\|$, we integrate over the disk D defined by the inequalities $|x|<R$ and $y\le\sqrt{R^2-x^2}$:

$$A_S = \int_{-R}^{R}\mathrm{d}x\int_{-\sqrt{R^2-x^2}}^{\sqrt{R^2-x^2}}\mathrm{d}y\,\tfrac{2R}{\sqrt{R^2-x^2-y^2}} = \int_{-R}^{R}\mathrm{d}x\int_{-\sqrt{R^2-x^2}}^{\sqrt{R^2-x^2}}\mathrm{d}y\,\tfrac{2R}{\sqrt{R^2-x^2}}\,\frac{1}{\sqrt{1-\frac{y^2}{R^2-x^2}}}.$$

Using the substitution $t=\frac{y}{\sqrt{R^2-x^2}}$, with $t\in(-1,1)$, we obtain

$$A_S = \int_{-R}^{R}\mathrm{d}x\int_{-1}^{1}\mathrm{d}t\,\tfrac{2R}{\sqrt{1-t^2}} = 2R\int_{-R}^{R}\mathrm{d}x\big[\arcsin t\big]_{-1}^{1} = 2R(2R)\left[\tfrac{\pi}{2}-\left(-\tfrac{\pi}{2}\right)\right] = 4\pi R^2\,.$$

(b) We use $\mathbf{r}(\theta,\phi) = R(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)^T$ to parametrize the sphere by spherical coordinates. Computing the coordinate basis vectors, we find

$$\partial_\theta\mathbf{r} = R(\cos\theta\cos\phi,\cos\theta\sin\phi,\cos\theta)^T,\quad \partial_\phi\mathbf{r} = R(-\sin\theta\sin\phi,\sin\theta\cos\phi,0)^T,$$
$$\|\partial_\theta\mathbf{r}\times\partial_\phi\mathbf{r}\|^2 = \|\partial_\theta\mathbf{r}\|^2\,\|\partial_\theta\mathbf{r}\|^2 - \|\partial_\theta\mathbf{r}\cdot\partial_\phi\mathbf{r}\|^2 = R^2-0=R^2\,.$$

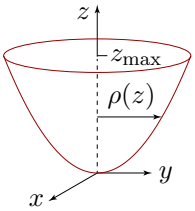
To compute the area of the sphere, we integrate over the full domain $U=(0,\pi)\times(0,2\pi)$:

$$A_S = \int_S \mathrm{d}S = \int_U \mathrm{d}\theta\mathrm{d}\phi\,\|\partial_\theta\mathbf{r}\times\partial_\phi\mathbf{r}\| = R^2\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi}\mathrm{d}\theta\sin\theta = -2\pi R^2\Big[\cos\theta\Big]_0^{\pi} = 4\pi R^2\,.$$

EC4.4.3 Volume and surface integral: parabolic solid of revolution

(a) In cylindrical coordinates the paraboloid P is defined by $z(\rho)=\rho^2$, or equivalently, $\rho(z)=\sqrt{z}$. It's volume is:

$$V = \int_K \mathrm{d}V = \int_0^{2\pi}\mathrm{d}\phi\int_0^{z_{\max}}\mathrm{d}z\int_0^{\rho(z)}\mathrm{d}\tilde\rho\,\tilde\rho = 2\pi\int_0^{z_{\max}}\mathrm{d}z\,\frac{z}{2} = \tfrac{\pi}{2}\,z_{\max}^2\,.$$



(b) The surface A of the parabolic part of the surface of K is calculated as follows:

Parametrization of P: $\mathbf{r}(\phi,z) = \rho\,\mathbf{e}_\rho + z\,\mathbf{e}_z$, with $\rho=\rho(z)=\sqrt{z}$.

Tangent vectors: $\partial_\phi\mathbf{r} = \rho\,\mathbf{e}_\phi$, $\partial_z\mathbf{r} = \rho'\,\mathbf{e}_\rho + \mathbf{e}_z$, with $\rho' = \partial_z\rho(z) = \frac{1}{2\sqrt{z}}$.

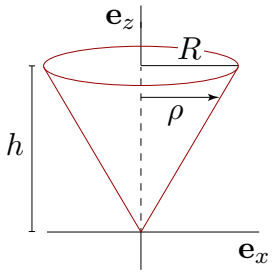
This gives: $\|\partial_\phi\mathbf{r}\times\partial_z\mathbf{r}\| = \big[(\partial_\phi\mathbf{r})^2(\partial_z\mathbf{r})^2 - \partial_\phi\mathbf{r}\cdot\partial_z\mathbf{r}\big]^{\frac12}$

$$= \big[\rho^2\left(\rho'^2+1\right)-0\big]^{\frac12} = \sqrt{z}\left[\tfrac{1}{(2\sqrt{z})^2}+1\right]^{\frac12} = \big[\tfrac14+z\big]^{\frac12}.$$

$$\text{Paraboloid surface: } A = \int_P \mathrm{d}S = \int_P \mathrm{d}\phi\,\mathrm{d}z\,\|\partial_\phi \mathbf{r} \times \partial_z \mathbf{r}\| = \int_0^{2\pi} \mathrm{d}\phi \int_0^{z_{\max}} \mathrm{d}z\,\left[\tfrac{1}{4} + z\right]^{\frac{1}{2}}$$
$$= 2\pi \tfrac{2}{3}\left[\tfrac{1}{4} + z\right]^{\frac{3}{2}}\Big|_0^{z_{\max}} = \tfrac{\pi}{6}\left[(1 + 4z_{\max})^{\frac{3}{2}} - 1\right].$$

EC4.4.5 Area of a circular cone

We place the tip of the cone at the origin, as shown in the sketch. We adopt polar coordinates, $(\rho, \phi)^T$, defined on the domain $U = (0, R) \times (0, 2\pi)$, such that $x = \rho\cos\phi$, $y = \rho\sin\phi$. On the conical surface $z = b\rho$ with $b = h/R$, hence it can be parametrized as



$$\mathbf{r} : U \to S_C, \quad (\rho, \phi)^T \mapsto \mathbf{r}(\rho, \phi) = \begin{pmatrix} \rho\cos\phi \\ \rho\sin\phi \\ \rho b \end{pmatrix}.$$

The conical area $A_C = \int_{S_C} \mathrm{d}S = \int_U \mathrm{d}\rho\,\mathrm{d}\phi\,\|\partial_\rho \mathbf{r} \times \partial_\phi \mathbf{r}\|$ can thus be computed as follows:

$$\|\partial_\rho \mathbf{r} \times \partial_\phi \mathbf{r}\| = \left\| \begin{pmatrix} \cos\phi \\ \sin\phi \\ b \end{pmatrix} \times \begin{pmatrix} -\rho\sin\phi \\ \rho\cos\phi \\ 0 \end{pmatrix} \right\| = \rho \left\| \begin{pmatrix} b\cos\phi \\ -b\sin\phi \\ 1 \end{pmatrix} \right\| = \rho\sqrt{b^2 + 1}.$$
$$A_C = \int_0^R \mathrm{d}\rho\,\rho \int_0^{2\pi} \mathrm{d}\phi\sqrt{b^2 + 1} = \tfrac{1}{2}R^2(2\pi)\sqrt{b^2 + 1} = \pi R\sqrt{h^2 + R^2}.$$

S.C4.5 Changes of variables in higher-dimensional integration

EC4.5.1 Jacobian determinant for cylindrical coordinates

Cylindrical coordinates: $x^1 = \rho\cos\phi$, $x^2 = \rho\sin\phi$, $x^3 = z$.

$$\left|\frac{\partial(x^1, x^2, x^3)}{\partial(\rho, \phi, z)}\right| = \begin{vmatrix} \frac{\partial x^1}{\partial\rho} & \frac{\partial x^1}{\partial\phi} & \frac{\partial x^1}{\partial z} \\ \frac{\partial x^2}{\partial\rho} & \frac{\partial x^2}{\partial\phi} & \frac{\partial x^2}{\partial z} \\ \frac{\partial 3^2}{\partial\rho} & \frac{\partial 3^2}{\partial\phi} & \frac{\partial 3^2}{\partial z} \end{vmatrix} = \begin{vmatrix} \cos\phi & -\rho\sin\phi & 0 \\ \sin\phi & \rho\cos\phi & 0 \\ 0 & 0 & 1 \end{vmatrix} = \rho(\cos\phi^2 + \sin^2\phi) = \rho$$

EC4.5.3 Three-dimensional Gaussian integral via linear transformation

Using the substitution $u = a(x + y)$, $v = b(z - y)$, $w = c(x - z)$ gives

$$I = \int_{\mathbb{R}^3} \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\mathrm{e}^{-\left[a^2(x+y)^2 + b^2(z-y)^2 + c^2(x-z)^2\right]} = \int_{\mathbb{R}^3} \mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w \left|\frac{\partial(x, y, z)}{\partial(u, v, w)}\right| \mathrm{e}^{-\left[u^2 + v^2 + x^2\right]}.$$

Because x, y and z are all integrated over $(-\infty,\infty)$, the same holds for u, v and w. Furthermore, because u, v and w are given as functions of x, y and z, the Jacobian determinant is calculated simply using the formula:

$$J = \left|\det\begin{pmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{pmatrix}\right|^{-1} = \left|\det\begin{pmatrix} a & a & 0 \\ 0 & b & -b \\ c & 0 & -c \end{pmatrix}\right|^{-1} = \Big|abc(-1-1+0)\Big|^{-1} = \frac{1}{2abc}.$$

Note: the Jacobian Determinant is always positive, because it is given by the *magnitude* of the determinant of the matrix of partial derivatives.
Note: alternatively the Jacobian determinant can also be calculated using $J = \left|\frac{\partial(x,y,z)}{\partial(u,v,w)}\right|$. For this, however, we must first invert the transformation (i.e. using Gaussian elimination), and determine x, y and z as functions of u, v and w. This gives $x = \frac{1}{2}(u/a + v/b + w/c)$, $y = \frac{1}{2}(u/a - v/b - w/c)$, $z = \frac{1}{2}(u/a + v/b - w/c)$, and

$$J = \left|\det\begin{pmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} & \frac{\partial x}{\partial w} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} & \frac{\partial y}{\partial w} \\ \frac{\partial z}{\partial u} & \frac{\partial z}{\partial v} & \frac{\partial z}{\partial w} \end{pmatrix}\right| = \frac{1}{2^3}\left|\det\begin{pmatrix} 1/a & 1/b & 1/c \\ 1/a & -1/b & -1/c \\ 1/a & 1/b & -1/c \end{pmatrix}\right| = \frac{1}{2^3 abc}\Big|2-(-2)+0\Big| = \frac{1}{2abc}.$$

Because in this case the Jacobian is independent of u, v and w, the integral $\int \mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w$ decomposes into three independent Gaussian integrals: $I = \sqrt{\pi^3}/(2abc)$.

EC4.5.5 General Gaussian integrals

(a) We write the exponent as $\mathbf{r}^T A\mathbf{r}$, with $\mathbf{r} = (x,y)^T$ and a symmetric matrix A, with $A_{12} = A_{21}$:

$$\begin{aligned}\mathbf{r}^T A\mathbf{r} &= \begin{pmatrix} x & y \end{pmatrix}\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = A_{11}\,x^2 + A_{12}\,xy + A_{21}\,yx + A_{22}\,y^2 \\ &\overset{!}{=} (a+3)x^2 + 2(a-3)xy + (a+3)y^2\end{aligned}$$

We therefore identify

$$A_{11} = A_{22} = a+3\,, \quad A_{12} = A_{21} = a-3\,, \quad \Rightarrow \quad A = \begin{pmatrix} a+3 & a-3 \\ a-3 & a+3 \end{pmatrix}.$$

Eigenvalues: $\quad 0 \overset{!}{=} \det(A - \lambda\mathbb{1}) = (2a-\lambda)(6-\lambda) \quad \Rightarrow \quad \lambda_1 = 2a\,, \quad \lambda_2 = 6\,.$

Normalized Eigenvectors:

$$\lambda_1 = 2a: \quad \mathbf{0} \overset{!}{=} (A - \lambda_1\mathbb{1})\,\mathbf{v}_1 = \begin{pmatrix} -a+3 & a-3 \\ a-3 & -a+3 \end{pmatrix}\mathbf{v}_1 \quad \Rightarrow \quad \mathbf{v}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

$$\lambda_2 = 6: \quad \mathbf{0} \overset{!}{=} (A - \lambda_2\mathbb{1})\,\mathbf{v}_2 = \begin{pmatrix} a-3 & a-3 \\ a-3 & a-3 \end{pmatrix}\mathbf{v}_2 \quad \Rightarrow \quad \mathbf{v}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

There therefore exists a transformation S such that $A = SDS^T$, with $D = \begin{pmatrix} 2a & 0 \\ 0 & 6 \end{pmatrix}$. The columns of this transformation S are the normalized Eigenvectors of A:

$$S = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

With $\tilde{\mathbf{r}} = (\tilde{x}, \tilde{y})^T = S^T \mathbf{r}$, the exponent thus takes the following form:

$$\begin{aligned}(a+3)x^2 + 2(a-3)xy + (a+3)y^2 = \mathbf{r}^T A \mathbf{r} = \mathbf{r}^T S D S^T \mathbf{r} = \tilde{\mathbf{r}}^T D \tilde{\mathbf{r}} \\ = \begin{pmatrix} \tilde{x} & \tilde{y} \end{pmatrix} \begin{pmatrix} 2a & 0 \\ 0 & 6 \end{pmatrix} \begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix} = 2a\tilde{x}^2 + 6\tilde{y}^2\end{aligned}$$

(b) Since $S^{-1} = S^T$, the inverse of the relation $\tilde{\mathbf{r}} = S^T \mathbf{r}$ is $\mathbf{r} = S\tilde{\mathbf{r}}$. Explicitly:

$$x = S_{11}\tilde{x} + S_{12}\tilde{y} = \frac{1}{\sqrt{2}}(\tilde{x} + \tilde{y}), \quad y = S_{21}\tilde{x} + S_{22}\tilde{y} = \frac{1}{\sqrt{2}}(\tilde{x} - \tilde{y})$$

The Jacobian determinant equals 1, since S is orthogonal. Explicitly:

$$J = \left| \det \begin{pmatrix} \frac{\partial x}{\partial \tilde{x}} & \frac{\partial x}{\partial \tilde{y}} \\ \frac{\partial y}{\partial \tilde{x}} & \frac{\partial y}{\partial \tilde{y}} \end{pmatrix} \right| = \left| \det \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \right| = \left| \det \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \right| = \left| \frac{1-(-1)}{\sqrt{2}^2} \right| = 1\,.$$

(c) We now compute $I(a)$, using the Gaussian integral $\int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-b^2x^2} = \frac{\sqrt{\pi}}{b}$ for the last step:

$$\begin{aligned}I(a) &= \int_{\mathbb{R}^2} \mathrm{d}x\, \mathrm{d}y\, \mathrm{e}^{-\left[(a+3)x^2 + 2(a-3)xy + (a+3)y^2\right]} = \int_{\mathbb{R}^2} \mathrm{d}x\, \mathrm{d}y\, \mathrm{e}^{-\mathbf{r}^T A \mathbf{r}} = \int_{\mathbb{R}^2} \mathrm{d}\tilde{x}\, \mathrm{d}\tilde{y}\, J\, \mathrm{e}^{-\tilde{\mathbf{r}}^T D \tilde{\mathbf{r}}} \\ &= \int_{\mathbb{R}^2} \mathrm{d}\tilde{x}\, \mathrm{d}\tilde{y}\, \mathrm{e}^{-\left(2a\tilde{x}^2 + 6\tilde{y}^2\right)} = \int_{-\infty}^{\infty} \mathrm{d}\tilde{x}\, \mathrm{e}^{-2a\tilde{x}^2} \int_{-\infty}^{\infty} \mathrm{d}\tilde{y}\, \mathrm{e}^{-6\tilde{y}^2} = \frac{\sqrt{\pi}}{\sqrt{2a}} \frac{\sqrt{\pi}}{\sqrt{6}} = \frac{\pi}{2\sqrt{3a}}\,.\end{aligned}$$

The result has the expected form: $I = \sqrt{\frac{\pi^n}{\det A}}$, with $n = 2$ and $\det A = \lambda_1 \lambda_2 = 12a$.

S.C5 Taylor series

S.C5.1 Approximating functions by polynomials

S.C5.2 Taylor expansion

ᴇC5.2.1 Addition theorems for sine and cosine

On the one hand: $\mathrm{e}^{\mathrm{i}(a+b)} = \cos(a+b) + \mathrm{i}\sin(a+b)$ (Euler-de Moivre identity). (1)

On the other hand: $\mathrm{e}^{\mathrm{i}(a+b)} = \mathrm{e}^{\mathrm{i}a}\mathrm{e}^{\mathrm{i}b} = (\cos a + \mathrm{i}\sin a)(\cos b + \mathrm{i}\sin b)$

$$= \cos a \cos b - \sin a \sin b + \mathrm{i}\,(\sin a \cos b + \cos a \sin b)\ . \qquad (2)$$

We compare the real and imaginary parts:

(a) $\mathrm{Re}\,(1) = \mathrm{Re}\,(2)$: $\Rightarrow$ $\cos(a+b) = \cos a \cos b - \sin a \sin b$.
(b) $\mathrm{Im}\,(1) = \mathrm{Im}\,(2)$: $\Rightarrow$ $\sin(a+b) = \sin a \cos b + \cos a \sin b$.

S.C5.3 Finite-order expansion

ɛC5.3.1 Taylor series

(a) Method 1: Use the known formula for the geometric series, $\frac{1}{1-x} = \sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$ (for $|x| < 1$), as well as the series expansion for sine, $\sin x = x - \frac{x^3}{6} + \mathcal{O}(x^5)$:

$$\begin{aligned} f(x) &= \frac{1}{1-\sin x} = \frac{1}{1-[x+\frac{1}{6}x^3+\mathcal{O}(x^5)]} \\ &= 1 + \left[x - \tfrac{1}{6}x^3\right] + \left[x - \tfrac{1}{6}x^3\right]^2 + \left[x - \tfrac{1}{6}x^3\right]^3 + \left[x - \tfrac{1}{6}x^3\right]^4 + \mathcal{O}(x^5) \\ &= 1 + x - \tfrac{1}{6}x^3 + x^2 - \tfrac{1}{3}x^4 + x^3 + x^4 + \mathcal{O}(x^5) \\ &= 1 + x + x^2 + \tfrac{5}{6}x^3 + \tfrac{2}{3}x^4 + \mathcal{O}(x^5)\,. \end{aligned}$$

Method 2: Determine the Taylor coefficients via successive derivatives:

$$\begin{aligned} f(x) &= \tfrac{1}{1-\sin x}, && \Rightarrow && f(0) = 1\,. \\ f^{(1)}(x) &= \tfrac{\cos(x)}{(1-\sin(x))^2} && \Rightarrow && f^{(1)}(0) = 1\,. \\ f^{(2)}(x) &= \tfrac{2\cos^2(x)}{(1-\sin(x))^3} - \tfrac{\sin(x)}{(1-\sin(x))^2} && \Rightarrow && f^{(2)}(0) = 2\,. \\ f^{(3)}(x) &= \tfrac{6\cos^3(x)}{(1-\sin(x))^4} - \tfrac{6\sin(x)\cos(x)}{(1-\sin(x))^3} - \tfrac{\cos(x)}{(1-\sin(x))^2} && \Rightarrow && f^{(3)}(0) = 5\,. \\ f^{(4)}(x) &= \tfrac{24\cos^4(x)}{(1-\sin(x))^5} - \tfrac{36\sin(x)\cos^2(x)}{(1-\sin(x))^4} + \tfrac{6\sin^2(x)}{(1-\sin(x))^3}\,. \\ &\quad - \tfrac{8\cos^2(x)}{(1-\sin(x))^3} + \tfrac{\sin(x)}{(1-\sin(x))^2} && \Rightarrow && f^{(4)}(0) = 16\,. \end{aligned}$$

$$\begin{aligned} \Rightarrow \quad f(x) &= f(0) + f^{(1)}(0)x + \tfrac{1}{2!}f^{(2)}(0)x^2 + \tfrac{1}{3!}f^{(3)}(0)x^3 + \tfrac{1}{4!}f^{(4)}(0)x^4 + \mathcal{O}\left(x^5\right) \\ &= 1 + x + x^2 + \tfrac{5}{6}x^3 + \tfrac{2}{3}x^4 + \mathcal{O}(x^5)\,. \end{aligned}$$

Remark: This example shows that taking successive derivatives of products or quotients is rather tedious, because each application of the product rule generates additional terms. If the series expansions of the involved factors are known, it is simpler to use these, as shown in Method 1.

(b) Method 1: Use the substitution $x = 1 + y$ and use the known series expansion of the logarithm, $\ln(1+y) = -\sum_{k=0}^{\infty} \frac{(-y)^{k+1}}{k+1}$, as well as the sine function [see (a)]:

$$g(x) = \sin(\ln(x)) = \sin(\ln(1+y)) = \sin\left(-\left(-y + \tfrac{1}{2}y^2 + \mathcal{O}(y^3)\right)\right)$$

$$= y - \tfrac{1}{2}y^2 + \mathcal{O}(y^3) \overset{y=x-1}{=} (x-1) - \tfrac{1}{2}(x-1)^2 + \mathcal{O}\left((x-1)^3\right).$$

Method 2: Determine the Taylor coefficients via successive derivatives:

$$\begin{aligned}
g(x) &= \sin(\ln(x)), && \Rightarrow \quad g(1) = \sin(\ln(1)) = 0\,.\\
g^{(1)}(x) &= \cos(\ln(x))\frac{1}{x}, && \Rightarrow \quad g^{(1)}(1) = \cos(0) = 1\,.\\
g^{(2)}(x) &= -\sin(\ln(x))\frac{1}{x^2} - \cos(\ln(x))\frac{1}{x^2}, && \Rightarrow \quad g^{(2)}(1) = -1\,.\\
\Rightarrow \quad g(x) &= g(1) + g^{(1)}(1)(x-1) + \tfrac{1}{2!}g^{(2)}(1)(x-1)^2 + \mathcal{O}\left((x-1)^3\right)\\
&= (x-1) - \tfrac{1}{2}(x-1)^2 + \mathcal{O}\left((x-1)^3\right).
\end{aligned}$$

(c) Method 1: Use the Taylor expansions for the exponential and cosine functions:

$$h(x) = \mathrm{e}^{\cos x} = \mathrm{e}^{\left[1-\frac{1}{2}x^2+\mathcal{O}(x^4)\right]} = \mathrm{e}^1\mathrm{e}^{-\left[\frac{1}{2}x^2+\mathcal{O}(x^4)\right]} = \mathrm{e}\left[1 - \tfrac{1}{2}x^2 + \mathcal{O}(x^4)\right].$$

Factoring out an e^1 before Taylor expanding is necessary in order to be able to use the well-known series expansion of the exponential function in a form (namely $\mathrm{e}^{-\frac{1}{2}x^2}$) in which its argument vanishes in the limit $x \to 0$, so that the series can be truncated after a few terms. If instead $\mathrm{e}^{1-\frac{1}{2}x^2}$ is expanded in powers of its full argument, $(1-\frac{1}{2}x^2)$, the complete Taylor series with infinitely many terms is needed to recover the correct result for $x \to 0$, namely e^1:

$$\mathrm{e}^{1-\frac{1}{2}x^2} = \sum_{l=0}^{\infty}\frac{1}{l!}(1-\tfrac{1}{2}x^2)^l \overset{x=0}{\longrightarrow} = \sum_{l=0}^{\infty}\frac{1}{l!} = \mathrm{e}^1\,.$$

To recover the second term in the Taylor expansion of $h(x)$ in this way, namely $-\frac{1}{2}x^2$, the binomial theorem has to be used: $(1+y)^l = \sum_{k=0}^{l}\frac{l!y^k}{k!(l-k)!}$:

$$\begin{aligned}
\mathrm{e}^{1-\frac{1}{2}x^2} &= \sum_{l=0}^{\infty}\frac{1}{l!}(1-\tfrac{1}{2}x^2)^l = \sum_{l=0}^{\infty}\frac{1}{l!}\sum_{k=0}^{l}\frac{l!(-\frac{1}{2}x^2)^k}{k!(l-k)!} = \sum_{l=0}^{\infty}\frac{1}{l!}\left[1 + l(-\tfrac{1}{2}x^2) + \mathcal{O}(x^4)\right]\\
&= \sum_{l=0}^{\infty}\frac{1}{l!} + \sum_{l=1}^{\infty}\frac{1}{(l-1)!}(-\tfrac{1}{2}x^2) + \mathcal{O}(x^4) = \mathrm{e}^1 - \mathrm{e}^1\tfrac{1}{2}x^2 + \mathcal{O}(x^4)\,.\checkmark
\end{aligned}$$

Clearly this approach is much more tedious than directly expanding $\mathrm{e}^{-\frac{1}{2}x^2}$!

Method 2: Determine the Taylor coefficients via successive derivatives:

$$\begin{aligned}
h(x) &= \mathrm{e}^{\cos x}, && \Rightarrow \quad h(0) = \mathrm{e}^1\,.\\
h^{(1)}(x) &= -\sin x\ \mathrm{e}^{\cos x}, && \Rightarrow \quad h^{(1)}(0) = 0\,.\\
h^{(2)}(x) &= -\cos x\ \mathrm{e}^{\cos x} + (-\sin x)^2\ \mathrm{e}^{\cos x}, && \Rightarrow \quad h^{(2)}(0) = -\mathrm{e}^1\,.\\
\Rightarrow \quad h(x) &= h(0) + h^{(1)}(0)x + \tfrac{1}{2}h^{(2)}(0)\ x^2 + \mathcal{O}\left(x^3\right) = \mathrm{e} - \mathrm{e}\tfrac{1}{2}x^2 + \mathcal{O}(x^3)\,.
\end{aligned}$$

The question whether or not to factor out an e^1, discussed above for Method 1, does not arise at all for Method 2. The strategy of iteratively taking derivatives and setting $x = 0$ automatically finds the right answer. In this sense Method 2 is in general easier to apply, since no subtleties need to be considered.

S.C5.4 Solving equations by Taylor expansion

ᴇC5.4.1 Series expansion for iteratively solving an equation

(a) Equation to be solved: $y^2 - 1 = 2\varepsilon y$. (1)

Wanted: the Taylor series $y(\epsilon) = y_0 + y_1\epsilon + \frac{1}{2!}y_2\epsilon^2 + \mathcal{O}(\epsilon^3)$, with $y_n \equiv y^{(n)}(0)$. (2)

Method 1: Determine the Taylor coefficients via successive derivatives:

$$\text{(1)}: \quad y^2 - 1 = 2\varepsilon y \quad \overset{\epsilon=0}{\Rightarrow} \quad y_0^2 - 1 = 0 \quad \Rightarrow \quad y_0 = y(0) = \pm 1\,. \tag{3}$$

$$d_\varepsilon(3): \quad 2yy' = 2\varepsilon y' + 2y \quad \overset{\epsilon=0}{\Rightarrow} \quad 2y_0y_1 = 2y_0 \quad \Rightarrow \quad y_1 = y'(0) = 1\,. \tag{4}$$

$$d_\varepsilon(4): \quad 2yy'' + 2y'^2 = 2\varepsilon y'' + 4y' \quad \overset{\epsilon=0}{\Rightarrow} \quad 2y_0y_2 + 2y_1^2 = 4y_1 \quad \Rightarrow \quad y_2 = y''(0) = \pm 1\,.$$

This gives two solutions, corresponding to the sign chosen for y_0:

$$y_\pm(\varepsilon) \overset{(2)}{=} \pm 1 + \varepsilon \pm \tfrac{1}{2}\varepsilon^2 + \mathcal{O}(\varepsilon^3)\,. \tag{5}$$

Method 2: Insert (2) in equation (1) and keep all terms up to order ε^2:

$$\begin{aligned} \left(y_0 + \varepsilon y_1 + \tfrac{1}{2}y_2\varepsilon^2 + \mathcal{O}(\varepsilon^3)\right)^2 - 1 &= 2\varepsilon\left(y_0 + \varepsilon y_1 + \mathcal{O}(\varepsilon^2)\right) \\ y_0^2 + 2\varepsilon y_0y_1 + \varepsilon^2 y_1^2 + \varepsilon^2 y_0y_2 - 1 + \mathcal{O}(\varepsilon^3) &= 2\varepsilon y_0 + 2\varepsilon^2 y_1 + \mathcal{O}(\varepsilon^3) \end{aligned}$$

Matching the coefficients on the left and right hand sides gives, for ε^0: $y_0^2 - 1 = 0$, hence $y_0 = \pm 1$; for ε^1: $2y_0y_1 = 2y_0$, hence $y_1 = 1$; for ε^2: $y_1^2 + y_0y_2 = 2y_1$, hence $y_2 = \pm 1$. Thus we have reproduced the result (5) obtained from method 1. ✓

(b) Exact solution of the quadratic equation: $y_\pm = \frac{1}{2}\left(2\varepsilon \pm \sqrt{4\varepsilon^2 + 4}\right) = \varepsilon \pm \sqrt{\varepsilon^2 + 1}$.

Is the Taylor series of the exact solution consistent with the answer from (a)?

$$\begin{aligned} \text{Check:} \quad y_\pm(\varepsilon) &= \varepsilon \pm \sqrt{1} + \left.\frac{2\varepsilon}{2\sqrt{\varepsilon^2+1}}\right|_{\varepsilon=0} \varepsilon + \left.\left(\frac{1}{\sqrt{\varepsilon^2+1}} - \frac{2\varepsilon^2}{(\varepsilon^2+1)^{\frac{3}{2}}}\right)\right|_{\varepsilon=0} \frac{\varepsilon^2}{2} + \mathcal{O}\left(\varepsilon^3\right) \\ &= \varepsilon \pm 1 \pm \tfrac{1}{2}\varepsilon^2 + \mathcal{O}\left(\varepsilon^3\right). \checkmark \end{aligned}$$

ᴇC5.4.3 Taylor series for inverse function

(a) $\ln(x)$ is the inverse of e^x. We are looking for the series expansion of $y(x) \equiv \ln(1+x)$ in powers of x. This function fulfills the defining equation:

$$\mathrm{e}^{y(x)} \;=\; 1+x\,. \tag{1}$$

Wanted: the Taylor series $y(x) = y_0 + y_1 x + \frac{1}{2!}y_2 x^2 + \mathcal{O}(x^3)$, with $y_n \equiv y^{(n)}(0)$. (2)

Method 1: Determine the coefficients by iteratively computing derivatives:

$$\text{(1)}: \quad \mathrm{e}^{y(x)} = 1+x \quad \overset{x=0}{\Rightarrow} \quad \mathrm{e}^{y_0} = 1 \quad \Rightarrow \quad y_0 = y(0) = 0\,. \tag{3}$$

$$d_x(3): \quad y'\mathrm{e}^{y} = 1 \quad \overset{x=0}{\Rightarrow} \quad y_1\mathrm{e}^{y_0} = 1 \quad \Rightarrow \quad y_1 = y'(0) = 1\,. \tag{4}$$

$$d_x(4): \quad \left[(y')^2 + y''\right]\mathrm{e}^{y(0)} = 0 \quad \overset{x=0}{\Rightarrow} \quad \left[1^2 + y_2\right]\mathrm{e}^{0} = 0 \quad \Rightarrow \quad y_2 = y''(0) = -1\,.$$

$$\text{Solution:} \qquad \ln(1+x) \equiv y(x) \overset{(2)}{=} x - \tfrac{1}{2}x^2 + \mathcal{O}(x^3)\,. \tag{5}$$

Method 2: Insert the ansatz (2) into equation (1) and expand up to order $\mathcal{O}(x^2)$, using $\mathrm{e}^z = 1 + z + \frac{1}{2!}z^2 + \mathcal{O}(z^3)$:

$$\mathrm{e}^{y_0+y_1x+\frac{1}{2}y_2x^2+\mathcal{O}(x^3)} = 1+x\,,$$
$$\mathrm{e}^{y_0}\left[1 + \left(y_1x + \tfrac{1}{2}y_2x^2\right) + \tfrac{1}{2!}(y_1x)^2 + \mathcal{O}(x^3)\right] = 1+x\,.$$

Comparing coefficients on the left and right hand sides gives, for x^0: $\mathrm{e}^{y_0} = 1$, hence $y_0 = 0$; for x^1: $\mathrm{e}^{y_0}y_1 = 1$, hence $y_1 = 1$; for x^2: $\mathrm{e}^{y_0}\frac{1}{2}(y_2 + y_1^2) = 0$, hence $y_2 = -1$. Thus we have reproduced the result (5) from method 1. ✓

(b) $\frac{\ln(x)}{\ln(2)}$ is the inverse of 2^x. We are looking for the series expansion of $y(x) \equiv 2^x$ in powers of x. This function fufills the defining equation:

$$\frac{\ln(y(x))}{\ln(2)} \;=\; x\,. \tag{6}$$

Wanted: the Taylor series $y(x) = y_0 + y_1 x + \frac{1}{2!}y_2 x^2 + \mathcal{O}(x^3)$, mit $y_n \equiv y^{(n)}(0)$. (7)

Method 1: Determine the coefficients by iteratively computing derivatives:

$$\text{(6)}: \quad \frac{\ln(y(x))}{\ln(2)} = x \quad \overset{x=0}{\Rightarrow} \quad \ln y_0 = 0 \quad \Rightarrow \quad y_0 = y(0) = 1\,. \tag{8}$$

$$d_x(8): \quad \frac{y'}{\ln(2)y} = 1 \quad \overset{x=0}{\Rightarrow} \quad \frac{y_1}{\ln(2)y_0} = 1 \quad \Rightarrow \quad y_1 = y'(0) = \ln(2)\,. \tag{9}$$

$$d_x(9): \quad \frac{1}{\ln(2)}\left[\frac{y''}{y} - \frac{(y')^2}{y^2}\right] = 0 \quad \overset{x=0}{\Rightarrow} \quad \frac{y_2}{y_0} - \frac{(y_1)^2}{y_0^2} = 0 \quad \Rightarrow \quad y_2 = y''(0) = \ln^2(2)\,.$$

Solution: $$2^x \equiv y(x) \overset{(6)}{=} 1 + \ln(2)x + \tfrac{1}{2}\ln^2(2)\,x^2 + \mathcal{O}(x^3)\,. \tag{10}$$

Method 2: insert the ansatz (7) into equation (6) and keep all terms up to order $\mathcal{O}(x^2)$, using $\ln(1+z) = z - \frac{1}{2}z^2 + \mathcal{O}(z^3)$:

$$\begin{aligned} x\ln(2) &= \ln\left(y_0 + y_1 x + \frac{1}{2}y_2 x^2 + \mathcal{O}(x^3)\right) \\ &= \ln(y_0) + \ln\left(1 + \frac{y_1}{y_0}x + \frac{1}{2}\frac{y_2}{y_0}x^2 + \mathcal{O}(x^3)\right) \\ &= \ln(y_0) + \left(\frac{y_1}{y_0}x + \frac{1}{2}\frac{y_2}{y_0}x^2 + \mathcal{O}(x^3)\right) - \frac{1}{2}\left(\frac{y_1}{y_0}x + \frac{1}{2}\frac{y_2}{y_0}x^2 + \mathcal{O}(x^3)\right)^2 \\ &= \ln(y_0) + \frac{y_1}{y_0}x + \frac{1}{2}\frac{y_2}{y_0}x^2 - \frac{y_1^2}{y_0^2}x^2 + \mathcal{O}(x^3)\,. \end{aligned}$$

Comparing coefficients on the left and right hand sides gives, for x^0: $\ln(y_0) = 0$, thus $y_0 = 1$; for x^1: $\frac{y_1}{y_0} = \ln(2)$, thus $y_1 = \ln(2)$; for x^2: $\mathrm{e}^{y_0}\frac{1}{2y_0^2}(y_1^2 - y_2) = 0$, thus $y_2 = \ln^2(2)$. We therefore recover the result (10) obtained via Method 1.

S.C5.5 Higher-dimensional Taylor expansion

ᴇC5.5.1 Taylor expansions in two dimensions

(a) Multiplication of the series expansion of the exponential and cosine functions:

$$\begin{aligned} g(x,y) &= e^x \cos(x+2y) \\ &= \left[1 + x + \tfrac{1}{2}x^2 + \mathcal{O}(x^3)\right]\left[1 - \tfrac{1}{2}(x+2y)^2 + \mathcal{O}(x^3, y^3, x^2y, xy^2)\right] \\ &= \left[1 + x + \tfrac{1}{2}x^2 + \mathcal{O}(x^3)\right]\left[1 - \tfrac{1}{2}x^2 - 2y^2 - 2xy + \mathcal{O}(x^3, y^3, x^2y, xy^2)\right] \\ &= 1 - \tfrac{1}{2}x^2 - 2y^2 - 2xy + x + \frac{1}{2}x^2 + \mathcal{O}(x^3, y^3, x^2y, xy^2) \\ &= 1 + x - 2y^2 - 2xy + \mathcal{O}(x^3, y^3, x^2y, xy^2)\,. \end{aligned}$$

(b) The Taylor series of a function of two variables (including up to second order) reads:

$$\begin{aligned} g(x,y) &= \Big[1 + (x\partial_{\tilde{x}} + y\partial_{\tilde{y}}) + \tfrac{1}{2}(x\partial_{\tilde{x}} + y\partial_{\tilde{y}})(x\partial_{\tilde{x}} + y\partial_{\tilde{y}})\Big] g(\tilde{x},\tilde{y})\Big|_{\tilde{x}=\tilde{y}=0} \\ &\quad + \mathcal{O}(x^3, y^3, x^2y, xy^2) \\ &= \Big[1 + x\partial_x + y\partial_y + \tfrac{1}{2}x^2\partial_x^2 + \tfrac{1}{2}y^2\partial_y^2 + xy\partial_x\partial_y\Big] g(0,0) + \mathcal{O}(x^3, y^3, x^2y, xy^2)\,. \end{aligned}$$

Notation: $\partial_i g(0,0) \equiv \partial_i g(x,y)|_{x=y=0}$, i.e. take the derivative first, then set $x = y = 0$.

$$g(x,y) = \mathrm{e}^x \cos(x+2y)\,, \qquad \Rightarrow \qquad g(0,0) = 1\,.$$

$$
\begin{aligned}
\partial_x g(x,y) &= \mathrm{e}^x\cos(x+2y) - \mathrm{e}^x\sin(x+2y)\,, && \Rightarrow \quad \partial_x g(0,0) = 1\,.\\
&= g(x,y) - \mathrm{e}^x\sin(x+2y)\,,\\
\partial_x^2 g(x,y) &= \partial_x g(x,y) - \mathrm{e}^x\sin(x+2y) - \mathrm{e}^x\cos(x+2y)\\
&= -2\mathrm{e}^x\sin(x+2y)\,, && \Rightarrow \quad \partial_x^2 g(0,0) = 0\,.\\
\partial_y g(x,y) &= -2\mathrm{e}^x\sin(x+2y)\,, && \Rightarrow \quad \partial_y g(0,0) = 0\,.\\
\partial_y^2 g(x,y) &= -4\mathrm{e}^x\cos(x+2y)\,, && \Rightarrow \quad \partial_y^2 g(0,0) = -4\,.\\
\partial_x\partial_y g(x,y) &= -2\mathrm{e}^x\sin(x+2y) - 2\mathrm{e}^x\cos(x+2y) && \Rightarrow \quad \partial_x\partial_y g(0,0) = -2\,.\\
\partial_y\partial_x g(x,y) &= \partial_x\partial_y g(x,y) && \Rightarrow \quad \partial_y\partial_x g(0,0) = -2\,.\\
\Rightarrow \quad g(x,y) &= 1 + x - 2y^2 - 2xy + \mathcal{O}(x^3, y^3, x^2y, xy^2)\,.
\end{aligned}
$$

ᴇC5.5.3 Lagrange multipliers

Wanted: the extremum of the function $j(\mathbf{r}) = x^2 + y^2 + z^2$, with constraints $g_1(\mathbf{r}) = x + y + z - 1 = 0$ and $g_2(\mathbf{r}) = x - y + 2z - 2 = 0$. We insert the Lagrange multipliers λ_1 and λ_2, and search for the extremum of the auxiliary function J:

$$
\begin{aligned}
J(\mathbf{r};\lambda_1,\lambda_2) &= j(\mathbf{r}) - \lambda_1 g_1(\mathbf{r}) - \lambda_2 g_2(\mathbf{r})\\
&= x^2 + y^2 + z^2 - \lambda_1 x - \lambda_1 y - \lambda_1 z + \lambda_1 - \lambda_2 x + \lambda_2 y - 2\lambda_2 z + 2\lambda_2\,.
\end{aligned}
$$

The conditions for obtaining an extremum, $\partial_{\lambda_1} J = 0$, $\partial_{\lambda_2} J = 0$ and $\boldsymbol{\nabla} J = 0$, yield:

$$
[1]: \quad x + y + z - 1 = 0\,, \qquad [2]: \quad x - y + 2z - 2 = 0\,,
$$

$$
\begin{aligned}
[\tilde{1}]: &\quad \partial_x J = 2x - \lambda_1 - \lambda_2 = 0\,,\\
[\tilde{2}]: &\quad \partial_y J = 2y - \lambda_1 + \lambda_2 = 0\,,\\
[\tilde{3}]: &\quad \partial_y J = 2z - \lambda_1 - 2\lambda_2 = 0\,.
\end{aligned}
$$

We now use Gaussian elimination to remove λ_1 and λ_2 from equations $[\tilde{1}]$ to $[\tilde{3}]$:

$$
\begin{array}{lccccc|c}
 & x & y & z & \lambda_1 & \lambda_2 & \\
[\tilde{1}]: & 2 & 0 & 0 & -1 & -1 & 0\\
[\tilde{2}]: & 0 & 2 & 0 & -1 & 1 & 0\\
[\tilde{3}]: & 0 & 0 & 2 & -1 & -2 & 0
\end{array}
\quad\longrightarrow\quad
\begin{array}{lccccc|c}
 & x & y & z & \lambda_1 & \lambda_2 & \\
[\tilde{1}'] = \frac{1}{2}([\tilde{1}] + [\tilde{2}]): & 1 & 1 & 0 & -1 & 0 & 0\\
[\tilde{2}'] = 2[\tilde{2}] + [\tilde{3}]: & 0 & 4 & 2 & -3 & 0 & 0\\
[\tilde{3}'] = 3[\tilde{1}'] - [\tilde{2}']: & 3 & -1 & -2 & 0 & 0 & 0
\end{array}
$$

$[\tilde{3}']$ implies $3x - y - 2z = 0$. We now solve this equation, together with the above equations [1] and [2], for x, y and z, again using Gaussian elimination:

$$
\begin{array}{lccc|c}
 & x & y & z & \\
[1]: & 1 & 1 & 1 & 1\\
[2]: & 1 & -1 & 2 & 2\\
[\tilde{3}']: & 3 & -1 & -2 & 0
\end{array}
\quad\longrightarrow\quad
\begin{array}{lccc|c}
 & x & y & z & \\
[1'] = [1] + [2]: & 2 & 0 & 3 & 3\\
[2'] = [1] - [2]: & 0 & 2 & -1 & -1\\
[3'] = \frac{1}{7}(3[1] - [\tilde{3}'] - 2[2']): & 0 & 0 & 1 & \frac{5}{7}
\end{array}
\quad\longrightarrow\quad
\begin{array}{lccc|c}
 & x & y & z & \\
\frac{1}{2}([1'] - 3[3']): & 1 & 0 & 0 & \frac{3}{7}\\
\frac{1}{2}([2'] + [3']): & 0 & 1 & 0 & -\frac{1}{7}\\
[3']: & 0 & 0 & 1 & \frac{5}{7}
\end{array}
$$

Thus the desired extremum occurs at $x = \frac{3}{7}$, $\quad y = -\frac{1}{7}$, $\quad z = \frac{5}{7}$.

S.C6 Fourier calculus

S.C6.1 δ-Function

ᴇC6.1.1 Integrals with δ function

(a) $I_1(a) = \int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x-\pi)\sin(ax) = \sin(a\pi)\,.$

(b) $I_2(a) = \int_{\mathbb{R}^3} \mathrm{d}^3x\, \delta(\mathbf{x}-\mathbf{y})\, \mathbf{x}^2 = \mathbf{y}^2 = a^2 + 1^2 + 2^2\,.$

(c) $I_3(a) = \int_0^a \mathrm{d}x\, \dfrac{\delta(x-\pi)}{a+\cos^2(x/2)} = \begin{cases} \frac{1}{a+\cos^2(\pi/2)} = \frac{1}{a} & \text{for } a > \pi \\ \frac{1}{2a} & \text{for } a = \pi \\ 0 & \text{for } a < \pi \end{cases}.$

The δ peak at $x = \pi$ lies inside the domain of integration $[0, a]$ if $a > \pi$, and outside if $a < \pi$. The case $a = \pi$ yields half the value of the case $a > \pi$. (The latter statement follows from representing the δ function as a series of ever sharper, symmetric, normalized peaks: if one does not integrate over the full peak, but only up to its maximum, only half its weight contributes, hence $\int_{-\infty}^{0} \mathrm{d}x\, \delta(x) = \frac{1}{2}$ and $\int_0^{\infty} \mathrm{d}x\, \delta(x) = \frac{1}{2}$.)

(d) $I_4(a) = \int_0^3 \mathrm{d}x\, \delta(x^2-6x+8)\sqrt{\mathrm{e}^{ax}} = \int_0^3 \mathrm{d}x \left[\frac{\delta(x-4)}{2} + \frac{\delta(x-2)}{2}\right]\sqrt{\mathrm{e}^{xa}} = \frac{\sqrt{\mathrm{e}^{2a}}}{2} = \frac{\mathrm{e}^a}{2}\,.$

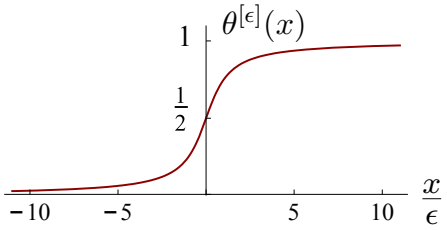
We use $\delta(g(x)) = \sum_i \frac{\delta(x-x_i)}{|g'(x_i)|}$, where x_i are the zeros of g. For $g(x) = x^2 - 6x + 8$ the zeros are $x_1 = 4$ and $x_2 = 2$. At these points the absolute value of $g'(x) = 2x - 6$ takes the values $|g'(x_1)| = 2$ and $|g'(x_2)| = 2$. Since x_1 lies outside the integration domain $[0, 3]$, only x_2 contributes to the integral.

ᴇC6.1.3 Lorentz representation of the Dirac delta function

We have to verify that in the limit $\epsilon \to 0$, $\delta^{[\epsilon]}(x)$ possesses the defining properties of the Dirac delta function, namely:

(i) $\delta(0) = \infty\,,$ (ii) $\delta(x \neq 0) = 0\,,$ (iii) $\int_{-\infty}^{\infty} \mathrm{d}x\, \delta(x) = 1\,.$

Lorentz peak: $\delta^{[\epsilon]}(x) = \delta^{[\epsilon]}(x) = \dfrac{\epsilon/\pi}{x^2+\epsilon^2}$.

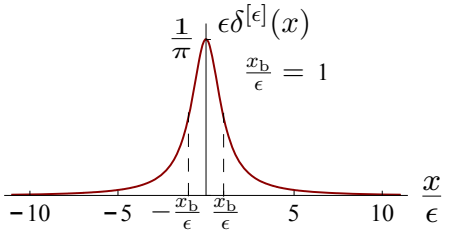


(i) Height: $\delta^{[\epsilon]}(0) = \dfrac{1}{\pi\epsilon} \overset{\epsilon\to 0}{\longrightarrow} \infty$. ✓

(ii) Width: $\dfrac{1}{2} = \dfrac{\delta^{[\epsilon]}(x_\mathrm{b})}{\delta^{[\epsilon]}(0)} = \dfrac{\epsilon^2}{x_\mathrm{b}^2+\epsilon^2}$

$\Rightarrow \quad x_\mathrm{b} = \epsilon \overset{\epsilon\to 0}{\longrightarrow} 0$. ✓

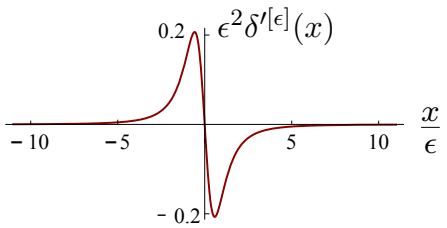
$\delta^{[\epsilon]}(x\neq 0) \overset{\epsilon\ll x}{\longrightarrow} \dfrac{\epsilon/\pi}{x^2}\left[1+\mathcal{O}(\epsilon^2/x^2)\right] \overset{\epsilon\to 0}{\longrightarrow} 0$. ✓



(iii) Weight, computed using by substitution:

$x = \epsilon\tan y = \epsilon\dfrac{\sin y}{\cos y}$,

$\dfrac{\mathrm{d}x}{\mathrm{d}y} = \dfrac{\epsilon}{\cos^2 y}$, $\quad x^2+\epsilon^2 = \dfrac{\epsilon^2}{\cos^2 y}$.



$$\int_{-\infty}^{\infty}\mathrm{d}x\,\delta^{[\epsilon]}(x) = \int_{-\infty}^{\infty}\mathrm{d}x\,\frac{\epsilon/\pi}{x^2+\epsilon^2} \overset{x=\epsilon\tan y}{=} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\mathrm{d}y\,\frac{\mathrm{d}x}{\mathrm{d}y}\frac{\epsilon/\pi}{\epsilon^2/\cos^2 y} = \frac{1}{\pi}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\mathrm{d}y = 1\,.\ \checkmark$$

Thus $\delta^{[\epsilon]}(x)$ does possess the defining properties (i)-(iii) of a Dirac δ function. ✓

(iv) Step: $\theta^{[\epsilon]}(x) = \displaystyle\int_{-\infty}^{x}\mathrm{d}x'\delta^{[\epsilon]}(x') = \frac{1}{\pi}\int_{-\frac{\pi}{2}}^{y(x)}\mathrm{d}y' = \frac{1}{\pi}y'\Big|_{-\frac{\pi}{2}}^{y(x)} = \frac{1}{\pi}\left[\arctan(x/\epsilon)+\frac{\pi}{2}\right]$

$$= \tfrac{1}{2}\left[\tfrac{2}{\pi}\arctan(x/\epsilon)+1\right] \quad \overset{\epsilon\to 0}{\longrightarrow} \begin{cases} 1 & \text{for} \quad x>0, \\ \frac{1}{2} & \text{for} \quad x=0, \\ 0 & \text{for} \quad x<0\,. \end{cases}$$

(v) Derivative: $\delta'^{[\epsilon]}(x) = \dfrac{\mathrm{d}}{\mathrm{d}x}\dfrac{\epsilon/\pi}{x^2+\epsilon^2} = -\dfrac{2x\epsilon/\pi}{(x^2+\epsilon^2)^2}$.

ᴇC6.1.5 Series representation of the coth function

$$\sum_{n\in\mathbb{Z}}\mathrm{e}^{-y|n|} = \sum_{n\geq 0}\mathrm{e}^{-yn} + \sum_{n\leq 0}\mathrm{e}^{yn} - 1 = 2\sum_{n\geq 0}\mathrm{e}^{-yn} - 1$$

$$= 2\sum_{n\geq 0} w^n - 1 \qquad (\text{with } w = e^{-y} < 1, \text{ thus this is a geometric series})$$

$$= 2\frac{1}{1-w} - 1 = \frac{1+w}{1-w} = \frac{1+\mathrm{e}^{-y}}{1-\mathrm{e}^{-y}} = \frac{\mathrm{e}^{-y/2}(\mathrm{e}^{y/2}+\mathrm{e}^{-y/2})}{\mathrm{e}^{-y/2}(\mathrm{e}^{y/2}-\mathrm{e}^{-y/2})} = \frac{\cosh(y/2)}{\sinh(y/2)} = \coth(y/2)\,.$$

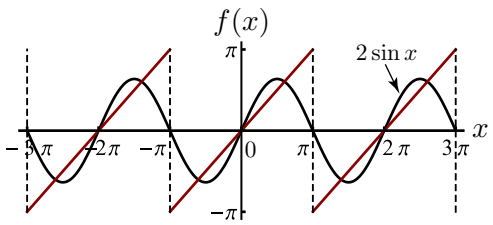
S.C6.2 Fourier series

EC6.2.1 Fourier series of the sawtooth function

Sawtooth function: $f(x) = x$ for $-\pi < x < \pi$, is periodic with period $L = 2\pi$. The Fourier series is defined by: $f(x) = \frac{1}{L}\sum_{k=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}kx}\tilde{f}_k$, with $k = 2\pi n/L = n$, for $n \in \mathbb{Z}$.

$$n \neq 0: \quad \tilde{f}_n = \int_{-\pi}^{\pi} \mathrm{d}x\, f(x)\mathrm{e}^{-\mathrm{i}nx} = \int_{-\pi}^{\pi} \mathrm{d}x\, x\mathrm{e}^{-\mathrm{i}nx} \overset{\text{part. int.}}{=} -\frac{x}{\mathrm{i}n}\mathrm{e}^{-\mathrm{i}nx}\Big|_{-\pi}^{\pi} + \int_{-\pi}^{\pi} \mathrm{d}x\, \frac{1}{\mathrm{i}n}\mathrm{e}^{-\mathrm{i}nx}$$
$$= \left[\frac{\mathrm{i}}{n}x\mathrm{e}^{-\mathrm{i}nx} + \frac{1}{n^2}\mathrm{e}^{-\mathrm{i}nx}\right]_{-\pi}^{\pi} = \frac{2\mathrm{i}\pi}{n}(-1)^n .$$

$$n = 0: \quad \tilde{f}_0 = \int_{-\pi}^{\pi} \mathrm{d}x\, x\mathrm{e}^0 = \int_{-\pi}^{\pi} \mathrm{d}x\, x = 0 .$$



Thus the Fourier series has the following form:

$$f(x) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}nx}\tilde{f}_n = \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \frac{\mathrm{i}}{n}(-1)^n\,\mathrm{e}^{\mathrm{i}nx} .$$

Remark: Evidently $\tilde{f}_n = -\tilde{f}_{-n}$ (a consequence of the fact that the function $f(x)$ is antisymmetric). The Fourier series can therefore also be rewritten as a sine series (not asked for here), by using $\mathrm{e}^{\mathrm{i}nx} - \mathrm{e}^{-\mathrm{i}nx} = 2\sin(nx)$:

$$f(x) = \sum_{n=1}^{\infty} \frac{2}{n}(-1)^{n+1}\sin(nx) .$$

EC6.2.3 Cosine Series

(a) Inserting the Fourier ansatz $f(x) = \frac{1}{L}\sum_{k'} \mathrm{e}^{\mathrm{i}k'x}\tilde{f}_{k'}$ into the formula for the Fourier coefficient yields:

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x) = \sum_{k'} \tilde{f}_{k'} \underbrace{\frac{1}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x\, \mathrm{e}^{\mathrm{i}(k'-k)x}}_{\equiv I_{kk'} = \delta_{kk'}} = \tilde{f}_k \;\checkmark \tag{1}$$

The orthonormality of the Fourier modes, $I_{kk'} = \delta_{kk'}$, is seen as follows:

$$I_{k=k'} = \frac{1}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x = 1 .$$

$$I_{k\neq k'} = \frac{1}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x\, \mathrm{e}^{\mathrm{i}(k'-k)x} = \frac{\mathrm{e}^{\mathrm{i}(k'-k)\frac{L}{2}} - \mathrm{e}^{-\mathrm{i}(k'-k)\frac{L}{2}}}{\mathrm{i}\,(k'-k)} = \frac{\mathrm{e}^{\mathrm{i}(k'-k)\frac{L}{2}}}{\mathrm{i}\,(k'-k)} \underbrace{\left(1 - \mathrm{e}^{-\mathrm{i}(k'-k)L}\right)}_{=1-\mathrm{e}^{-\mathrm{i}\frac{2\pi}{L}(n'-n)L}=0} = 0 .$$

(b) For an even function, we have $f(x) = f(-x)$. Therefore, we can write $\tilde{f}_k$ as follows using the substitution $x \to -x$ for the part of the integral where $x \in [-L/2, 0]$:

$$\begin{aligned}\tilde{f}_k &= \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x) = \int_0^{\frac{L}{2}} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x) + \int_{-\frac{L}{2}}^{0} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x) \\ &= \int_0^{\frac{L}{2}} \mathrm{d}x \left[\mathrm{e}^{-\mathrm{i}kx} f(x) + \mathrm{e}^{+\mathrm{i}kx} \underbrace{f(-x)}_{=f(x)}\right] = 2\int_0^{\frac{L}{2}} \mathrm{d}x\, \cos(kx) f(x)\,. \end{aligned} \tag{2}$$

Since $\cos(kx)$ is an even function in k, we have $\tilde{f}_k = \tilde{f}_{-k}$. It follows that:

$$f(x) = \frac{1}{L}\sum_k \mathrm{e}^{\mathrm{i}kx}\tilde{f}_k = \frac{\tilde{f}_0}{L} + \frac{1}{L}\sum_{k>0}\Big(\mathrm{e}^{\mathrm{i}kx}\tilde{f}_k + \mathrm{e}^{-\mathrm{i}kx}\underbrace{\tilde{f}_{-k}}_{=\tilde{f}_k}\Big) = \frac{1}{L}\tilde{f}_0 + \frac{1}{L}\sum_{k>0}\tilde{f}_k 2\cos(kx)$$

$$\equiv \frac{1}{2}a_0 + \sum_{k>0} a_k \cos(kx)\,, \qquad \text{with} \qquad a_k \equiv \frac{2}{L}\tilde{f}_k \overset{(2)}{=} \frac{4}{L}\int_0^{\frac{L}{2}} \mathrm{d}x\, \cos(kx) f(x)\,. \tag{3}$$

(c) Cosine coefficients via (3), where only terms with $k \geq 0$ occur:

$$k = 0: \qquad a_0 \overset{(3)}{=} \frac{4}{L}\int_0^{\frac{L}{2}} \mathrm{d}x\, \underbrace{\cos(0)}_{=1} f(x) = \frac{4}{L}\int_0^{\frac{L}{4}} \mathrm{d}x\, 1 + \frac{4}{L}\int_{\frac{L}{4}}^{\frac{L}{2}} \mathrm{d}x\, (-1) = 0 \tag{4}$$

$$\begin{aligned} k > 0: \qquad a_k &\overset{(3)}{=} \frac{4}{L}\int_0^{\frac{L}{2}} \mathrm{d}x\, \cos(kx) f(x) = \frac{4}{L}\int_0^{\frac{L}{4}} \mathrm{d}x\, \cos(kx) - \frac{4}{L}\int_{\frac{L}{4}}^{\frac{L}{2}} \mathrm{d}x\, \cos(kx) \\ &= \frac{4}{Lk}\left[2\sin(kL/4) - \sin(kL/2)\right]. \end{aligned} \tag{5}$$

In comparison, calculting the Fourier coefficients via (1) is a bit more cumbersome:

$$k = 0: \qquad \tilde{f}_0 \overset{(1)}{=} \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x\, \mathrm{e}^0 f(x) = \int_{-\frac{L}{4}}^{\frac{L}{4}} \mathrm{d}x - \int_{-\frac{L}{2}}^{-\frac{L}{4}} \mathrm{d}x - \int_{\frac{L}{4}}^{\frac{L}{2}} \mathrm{d}x = 0 \qquad [\overset{(4)}{=} \tfrac{L}{2}a_0 \checkmark] \tag{6}$$

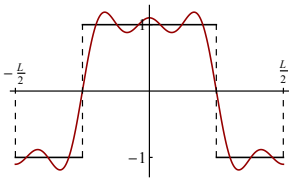
$$\begin{aligned} k \neq 0: \qquad \tilde{f}_k &\overset{(1)}{=} \int_{-\frac{L}{2}}^{\frac{L}{2}} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x) = \int_{-\frac{L}{4}}^{\frac{L}{4}} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} - \int_{-\frac{L}{2}}^{-\frac{L}{4}} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} - \int_{\frac{L}{4}}^{\frac{L}{2}} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} \\ &= \frac{1}{-\mathrm{i}k}\left[\left(\mathrm{e}^{-\mathrm{i}kL/4} - \mathrm{e}^{\mathrm{i}kL/4}\right) - \left(\mathrm{e}^{\mathrm{i}kL/4} - \mathrm{e}^{\mathrm{i}kL/2}\right) - \left(\mathrm{e}^{-\mathrm{i}kL/2} - \mathrm{e}^{-\mathrm{i}kL/4}\right)\right] \\ &= \frac{2}{k}\left[2\sin(kL/4) - \sin(kL/2)\right] \qquad [\overset{(5)}{=} \tfrac{L}{2}a_k \checkmark] \end{aligned} \tag{7}$$

Now set $0 \neq k = 2\pi n/L$ in (5), with $n \in \mathbb{Z}$:

$$a_k = \frac{2}{L}\tilde{f}_k \overset{(5)}{=} \frac{2}{\pi n}\left[2\sin(\pi n/2) - \underbrace{\sin(\pi n)}_{=0}\right] = \left\{ \begin{array}{ll} 0 & \text{for } 0 \neq n = 2m \\ \frac{4}{\pi(2m+1)}(-1)^m & \text{for } n = 2m+1 \end{array} \right\},$$

with $m \in \mathbb{N}_0$. Therefore the cosine representation (3) of $f(x)$ has the following form:

$$f(x) \overset{(3)}{=} \frac{4}{\pi} \sum_{m\geq 0} \frac{(-1)^m}{2m+1} \cos\left(\frac{2\pi(2m+1)x}{L}\right)$$
$$= \frac{4}{\pi}\left[\cos\left(\frac{2\pi x}{L}\right) - \frac{1}{3}\cos\left(\frac{6\pi x}{L}\right) + \frac{1}{5}\cos\left(\frac{10\pi x}{L}\right) + \dots\right]$$



The sketch shows the function $f(x)$ and the approximation thereof that arises from the first three terms of the cosine series.

ᴇC6.2.5 Parseval's identity and convolution

(a) Explicit computation of the integral:

$$\int_{-\pi}^{\pi} \mathrm{d}x\, \overline{f}\,(x)\, g\,(x) = \int_{-\pi}^{\pi} \mathrm{d}x\, x \sin\,(x) = \Big[-x\cos\,(x) + \sin\,(x)\Big]_{-\pi}^{\pi} = \pi + \pi = 2\pi\,. \quad (1)$$

Summation of Fourier coefficients: the saw-tooth function $f(x)$ has period $L = 2\pi$, hence its Fourier series has the form $f(x) = \frac{1}{L}\sum_k \mathrm{e}^{\mathrm{i}kx}\tilde{f}_k = \frac{1}{2\pi}\sum_n \mathrm{e}^{\mathrm{i}nx}\tilde{f}_n$, with $k = 2\pi n/L = n \in \mathbb{Z}$. The same is true for the sine function $g(x) = \sin(x)$. Their Fourier coefficients are known to have the following form:

$$\tilde{f}_n = \frac{2\pi\mathrm{i}\,(-1)^n}{n} \quad \text{for } n \neq 0\,, \quad \text{and} \quad \tilde{f}_0 = 0\,.$$
$$\tilde{g}_n = \frac{\pi}{\mathrm{i}}(\delta_{n,1} - \delta_{n,-1})\,, \quad \text{since} \quad g\,(x) = \sin\,(x) = \frac{1}{2\mathrm{i}}\left(\mathrm{e}^{\mathrm{i}x} - \mathrm{e}^{-\mathrm{i}x}\right) = \frac{1}{2\pi}\sum_n \mathrm{e}^{\mathrm{i}nx}\tilde{g}_n\,.$$

Parseval's identity yields:

$$\int_{-\pi}^{\pi} \mathrm{d}x\, \overline{f}\,(x)\, g\,(x) = \frac{1}{L}\sum_n \overline{\tilde{f}}_n\, \tilde{g}_n = \frac{1}{2\pi}\left[\overline{\tilde{f}}_1\tilde{g}_1 + \overline{\tilde{f}}_{-1}\tilde{g}_{-1}\right]$$
$$= \frac{1}{2\pi}\left[\frac{(-2\pi\mathrm{i})(-1)^{+1}}{(+1)}\cdot\frac{\pi}{\mathrm{i}} + \frac{(-2\pi\mathrm{i})(-1)^{-1}}{(-1)}\cdot\frac{(-\pi)}{\mathrm{i}}\right] = 2\pi \overset{\checkmark}{=} (1)\,.$$

(b) Special case of Parseval's identity : $\displaystyle\int_{-\pi}^{\pi} \mathrm{d}x\, |f(x)|^2 = \frac{1}{2\pi}\sum_n |\tilde{f}_n|^2.$

On the one hand:
$$\int_{-\pi}^{\pi} \mathrm{d}x\, |f(x)|^2 = \int_{-\pi}^{\pi} \mathrm{d}x\, x^2 = \frac{1}{3}x^3\Big|_{-\pi}^{\pi} = \frac{2\pi^3}{3}\,. \quad (2)$$

On the other hand:
$$\frac{1}{2\pi}\sum_{n=-\infty}^{\infty} |\tilde{f}_n|^2 = \frac{2}{2\pi}\sum_{n=1}^{\infty}\frac{(2\pi)^2}{n^2} = 4\pi\sum_{n=1}^{\infty}\frac{1}{n^2}\,. \quad (3)$$

Parseval: (2) = (3)
$$\sum_{n=1}^{\infty}\frac{1}{n^2} = \frac{\pi^2}{6}\,. \quad (4)$$

(c) Direct computation of the convolution integral: Since f and g are periodic, with the same period, the domain of integration can be chosen to be an arbitrary interval of length equal to this period. We here choose $(-\pi, \pi)$ and thus compute the following covolution integral:

$$(f * g)(x) = \int_{-\pi}^{\pi} \mathrm{d}x'\, f(x-x')g(x') = \int_{-\pi}^{\pi} \mathrm{d}x'\, g(x-x')f(x') = (g * f)(x)\,. \tag{5}$$

The formulas on the right express the fact that the convolution of two functions is commutative. (That can be seen, e.g., in Fourier space, since the convolution theorem gives $\widetilde{(f*g)}_k = \tilde{f}_k\,\tilde{g}_k = \tilde{g}_k\,\tilde{f}_k = \widetilde{(g*f)}_k$. Also see Eq. (7) below.) In the present case it is simplest to use the form on the right (the form on the left is discussed further below):

$$(g * f)(x) \overset{(5),\text{right}}{=} \int_{-\pi}^{\pi} \mathrm{d}x'\, \sin(x-x')\, x' = \Big[x'\cos(x-x') + \sin(x-x')\Big]_{-\pi}^{\pi} \tag{6a}$$

$$= \pi\cos(x-\pi) + \pi\cos(x+\pi) + \sin(x-\pi) - \sin(x+\pi) = -2\pi\cos x\,, \tag{6b}$$

since $\cos(x-\pi) = \cos(x+\pi) = -\cos(x)$ and $\sin(x-\pi) = \sin(x+\pi)$.

Alternative computation via summation of Fourier coefficients:

$$(f * g)(x) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} \tilde{f}_n\,\tilde{g}_n \mathrm{e}^{\mathrm{i}nx} = \frac{1}{2\pi}\sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \frac{2\pi\mathrm{i}\,(-1)^n}{n}\left(\frac{\pi}{\mathrm{i}}\right)\left[\delta_{n,1} - \delta_{n,-1}\right]\mathrm{e}^{\mathrm{i}nx}$$

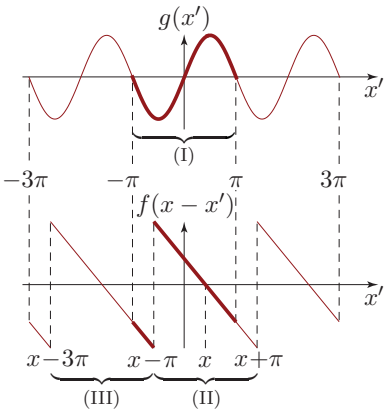
$$= \pi\left[\frac{(-1)^{+1}}{(+1)}\mathrm{e}^{-\mathrm{i}x} - \frac{(-1)^{-1}}{(-1)}\mathrm{e}^{-\mathrm{i}x}\right] = 2\pi\left[-\frac{1}{2}\mathrm{e}^{\mathrm{i}x} - \frac{1}{2}\mathrm{e}^{-\mathrm{i}x}\right] = -2\pi\cos(x) \overset{\checkmark}{=} (6b)\,.$$

Remark: It is instructive to perform the direct computation of the convolution integral also using the left expression in Eq. (5). The functions occurring therein are defined as follows, e.g. for $x \in (0, \pi)$ [an analogous discussion holds for $x \in (-\pi, 0)$]:

$$g(x') = \sin(x') \qquad \text{for} \qquad x' \in (-\pi, \pi) \quad \Rightarrow \quad -\pi < x' < \pi\,. \tag{I}$$

$$f(x-x') = \begin{cases} x-x' & \text{for} \quad x-x' \in (-\pi,\pi) \quad \Rightarrow \quad x-\pi < x' < x+\pi\,, \quad \text{(II)} \\ x-x'-2\pi & \text{for} \quad x-x' \in (\pi, 3\pi) \quad \Rightarrow \quad x-3\pi < x' < x-\pi\,. \quad \text{(III)} \end{cases}$$

When x' traverses the domain of integration $(-\pi, \pi)$, $g(x')$ is described by a single formula, (I), throughout the entire domain, whereas for $f(x-x')$ two cases have to be distinguished: since this function exhibits a discontinuity when its argument $x - x'$ passes the point π, we need formula (II) for $x - \pi < x' < \pi$, but formula (III) for $-\pi < x' < x - \pi$. [(III) is the 'periodic continuation' of (II), shifted by one period]. Two possible strategies for dealing with this situation are either (i) to shift the domain of integration, or (ii) to split it into two.



(i) Shifting the domain of integration: To avoid the discontinuity the domain of integration can be shifted from $(-\pi,\pi)$ to $(-\pi+x,\pi+x)$ (which is allowed, since the integrand is periodic). This yields (via the substitution $x''=x-x'$)

$$(f*g)(x)=\int_{x-\pi}^{x+\pi}\mathrm{d}x' f(x-x')g(x') \overset{x''=x-x'}{=} \int_{-\pi}^{\pi}\mathrm{d}x'' g(x-x'')f(x'')=(g*f)(x)\,, \quad (7)$$

thus reproducing Eq. $(5)_{\text{right}}$, which constitutes another proof of the fact that a convolution is commutative. For the current example, $(5)_{\text{right}}$ has the advantage compared to $(5)_{\text{left}}$ that not only g but also f are each described by only a *single* formula throughout the entire domain of integration, $g(x-x')=\sin(x-x')$ and $f(x')=x'$, so that in the above calculation from (6a) to (6b) it was not necessary to distinguish two cases separately.

(ii) Splitting the domain of integration: Alternatively, the discontinuity can be accounted for by accordingly splitting the domain $(-\pi,\pi)=(-\pi,x-\pi)\cup[x-\pi,\pi)$ into two:

$$\begin{aligned}
(f*g)(x) &\overset{(5)_{\text{left}}}{=} \int_{-\pi}^{\pi}\mathrm{d}x'\, f(x-x')g(x') = \int_{-\pi}^{x-\pi}\mathrm{d}x'\, f(x-x')g(x') + \int_{x-\pi}^{\pi}\mathrm{d}x'\, f(x-x')g(x') \\
&= \int_{-\pi}^{x-\pi}\mathrm{d}x'\, \underbrace{(x-x'-2\pi)}_{\text{(III)}}\underbrace{\sin(x')}_{\text{(I)}} + \int_{x-\pi}^{\pi}\mathrm{d}x'\, \underbrace{(x-x')}_{\text{(II)}}\underbrace{\sin(x')}_{\text{(I)}} \\
&= \int_{-\pi}^{\pi}\mathrm{d}x'\,(x-x')\sin(x') + (-2\pi)\int_{-\pi}^{x-\pi}\mathrm{d}x'\,\sin x' \\
&= \Big[-x\cos x' + x'\cos x' - \sin x'\Big]_{-\pi}^{\pi} + 2\pi\Big[\cos x'\Big]_{-\pi}^{x-\pi} \\
&= 0-2\pi+0+2\pi[\cos(x-\pi)+1] = -2\pi\cos x\,. \qquad (8)
\end{aligned}$$

For the current example the computation using strategy (i), shifting the domain of integration (or equivalently, exploiting the commutativity of convolutions), is simpler than using strategy (ii), splitting this domain. However, if *both* functions f and g are defined via periodic continuation and exhibit discontinuities, strategy (i) is not helpful: then the domain of integration will contain a discontinuity for both $(f*g)$ and $(g*f)$, so that splitting the domain of integration is unavoidable.

S.C6.3 Fourier transform

ɛC6.3.1 Properties of Fourier transformations

(a) Fourier transform of $f(x-a)$:

$$\int_{-\infty}^{\infty}\mathrm{d}x\,\mathrm{e}^{-\mathrm{i}kx}f(x-a) \overset{\bar{x}=x-a}{=} \int_{-\infty}^{\infty}\mathrm{d}\bar{x}\,\mathrm{e}^{-\mathrm{i}k(\bar{x}+a)}f(\bar{x}) = \mathrm{e}^{-\mathrm{i}ka}\int_{-\infty}^{\infty}\mathrm{d}\bar{x}\,\mathrm{e}^{-\mathrm{i}k\bar{x}}f(\bar{x}) = \mathrm{e}^{-\mathrm{i}ka}\tilde{f}_k\,.$$

(b) Fourier transform of $f(ax)$:

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(ax) \overset{\bar{x}=ax}{=} \int_{-\infty\cdot a}^{\infty\cdot a} \mathrm{d}\bar{x}\, \frac{1}{a}\, \mathrm{e}^{-\mathrm{i}\frac{k}{a}\bar{x}} f(\bar{x})$$

$$= \left\{ \begin{array}{ll} \dfrac{1}{a} \displaystyle\int_{-\infty}^{\infty} \mathrm{d}\bar{x}\, \mathrm{e}^{-\mathrm{i}\frac{k}{a}\bar{x}} f(\bar{x}) \;, & \text{falls } a > 0 \\ \dfrac{1}{a} \displaystyle\int_{\infty}^{-\infty} \mathrm{d}\bar{x}\, \mathrm{e}^{-\mathrm{i}\frac{k}{a}\bar{x}} f(\bar{x}) = -\dfrac{1}{a} \displaystyle\int_{-\infty}^{\infty} \mathrm{d}\bar{x}\, \mathrm{e}^{-\mathrm{i}\frac{k}{a}\bar{x}} f(\bar{x}) \;, & \text{falls } a < 0 \end{array} \right\} = \frac{1}{|a|}\, \tilde{f}_{k/a}$$

The change of the integration measure under the transformation $\bar{x} = ax$ can also be determined by considering the Jacobi determinant:

$$\int_{\mathbb{R}} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(ax) \overset{\bar{x}=ax}{=} \int_{\mathbb{R}} \mathrm{d}\bar{x}\, \frac{1}{|a|}\, \mathrm{e}^{-\mathrm{i}\frac{k}{a}\bar{x}} f(\bar{x}) = \frac{1}{|a|}\, \tilde{f}_{k/a}$$

ᴇC6.3.3 Fourier transformation of a Gauss peak

Normalized Gaussian: $$g^{[\sigma]}(x) = \frac{1}{\sqrt{2\pi}\sigma}\, \mathrm{e}^{-x^2/2\sigma^2} \;, \qquad \int_{-\infty}^{\infty} \mathrm{d}x\; g^{[\sigma]}(x) = 1 \;. \qquad (1)$$

Fourier transformation: $$\tilde{g}_k^{[\sigma]} = \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} g^{[\sigma]}(x) = \int_{-\infty}^{\infty} \mathrm{d}x\, \frac{1}{\sqrt{2\pi}\sigma}\, \mathrm{e}^{-\frac{1}{2\sigma^2}\left(x^2 + 2\sigma^2 \mathrm{i}kx\right)} \;.$$

Completing the square: $$\left(x^2 + 2\sigma^2 \mathrm{i}kx\right) = \left(x + \sigma^2 \mathrm{i}k\right)^2 + \sigma^4 k^2 \overset{\bar{x}=x+\sigma^2\mathrm{i}k}{=} \bar{x}^2 + \sigma^4 k^2 \;.$$

$$\tilde{g}_k^{[\sigma]} \overset{\mathrm{d}x=\mathrm{d}\bar{x}}{=} \int_{-\infty}^{\infty} \mathrm{d}\bar{x}\, \frac{1}{\sqrt{2\pi}\sigma}\, \mathrm{e}^{-\frac{\bar{x}^2}{2\sigma^2}} \mathrm{e}^{-\frac{\sigma^4 k^2}{2\sigma^2}} = \mathrm{e}^{-\sigma^2 k^2/2} \underbrace{\int_{-\infty}^{\infty} \mathrm{d}\bar{x}\, g^{[\sigma]}(\bar{x})}_{\overset{(1)}{=}1} = \mathrm{e}^{-\sigma^2 k^2/2} \;.$$

Remark: The Fourier transform of a Gaussian distribution with width σ is a Gaussian of width $1/\sigma$. This is a good example of Fourier reciprocity; the Fourier transform of a narrow distribution is a wide distribution and vice-versa.

ᴇC6.3.5 Poisson summation formulas

(a) We multiply the completeness relation with $f(y/L)$ and integrate over $x = y/L$:

Completeness: $$\frac{1}{L} \sum_{n\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}2\pi n y/L} = \sum_{m\in\mathbb{Z}} \delta(y - Lm) = \frac{1}{L} \sum_{m\in\mathbb{Z}} \delta\left(\tfrac{y}{L} - m\right) \qquad (1)$$

$\int \mathrm{d}x f(x)(1)$: $$\sum_{n\in\mathbb{Z}} \int_{-\infty}^{\infty} \mathrm{d}x\, f(x) \mathrm{e}^{-\mathrm{i}2\pi n x} = \sum_{m\in\mathbb{Z}} \int_{-\infty}^{\infty} \mathrm{d}x\, f(x) \delta(x - m) = \sum_{m\in\mathbb{Z}} f(m) \;.$$

The left integral corresponds to the Fourier transform, $\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{d}x\, f(x)\mathrm{e}^{-\mathrm{i}kx}$, with $k = 2\pi n$. Thus we obtain:

$$\sum_{n\in\mathbb{Z}} \tilde{f}(2\pi n) = \sum_{m\in\mathbb{Z}} f(m)\,. \tag{2}$$

(b) We set $f(x) = \mathrm{e}^{-a|x|}$, and then calculate the Fourier transform:

$$\tilde{f}(k) = \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x) = \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-(\mathrm{i}kx + a|x|)} = \frac{2a}{k^2 + a^2}\,.$$

The Poisson summation formula $\sum_n \tilde{f}(2\pi n) = \sum_m f(m)$ then gives:

$$\begin{aligned}\sum_{n\in\mathbb{Z}} \frac{2a}{(2\pi n^2 + a^2)} &= \sum_{m\in\mathbb{Z}} \mathrm{e}^{-a|m|} = 2\sum_{m=0}^{\infty} \mathrm{e}^{-am} - 1 \\ &= \frac{2}{1-\mathrm{e}^{-a}} - 1 = \frac{1+\mathrm{e}^{-a}}{1-\mathrm{e}^{-a}} = \frac{\mathrm{e}^{a/2}+\mathrm{e}^{-a/2}}{\mathrm{e}^{a/2}-\mathrm{e}^{-a/2}} = \coth\left(a/2\right).\end{aligned}$$

(c) We set $f(x) = \mathrm{e}^{-(ax^2+bx+c)}$, and then calculate the Fourier transform:

$$\begin{aligned}\tilde{f}(k) &= \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} f(x) = \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-a\left(x^2 + \frac{1}{a}(b+\mathrm{i}k)x\right) - c} \\ &= \int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-a\left(x+\frac{b+\mathrm{i}k}{2a}\right)^2} \mathrm{e}^{a\left(\frac{b+\mathrm{i}k}{2a}\right)^2 - c} = \sqrt{\tfrac{\pi}{a}}\,\mathrm{e}^{\frac{1}{4a}\left(b^2+2\mathrm{i}bk-k^2\right)-c}\,.\end{aligned}$$

The Poisson summation formula $\sum_m f(m) = \sum_n \tilde{f}(2\pi n)$ then gives:

$$\sum_{m\in\mathbb{Z}} \mathrm{e}^{-\left(am^2+bm+c\right)} = \sqrt{\frac{\pi}{a}}\,\mathrm{e}^{\left(\frac{b^2}{4a}-c\right)} \sum_{n\in\mathbb{Z}} \mathrm{e}^{-\frac{1}{a}\left(\pi^2 n^2 + \mathrm{i}\pi n b\right)}\,.$$

S.C6.4 Fourier transform applications

S.C6.5 Case Study: Frequency comb for high-precision measurements

A1: We insert the Fourier series for $p(t)$ into the formula for the Fourier transform of $p(t)$:

$$\tilde{p}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\, p(t) = \frac{1}{\tau}\sum_m \underbrace{\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{-\mathrm{i}\omega_m t}}_{2\pi\delta(\omega-\omega_m)} \tilde{p}_m = \omega_r \sum_m \tilde{p}_m \delta(\omega - \omega_m)\,,$$

with $\omega_r = 2\pi/\tau$. We now see that $\tilde{p}(\omega)$ is clearly a periodic frequency comb of δ functions, whose weights are fixed by the coefficients $\tilde{p}_m$ of the Fourier series.

A2: We insert $f(t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-\mathrm{i}\omega t} \tilde{f}(\omega)$ in $p(t)$ and perform the substitution $\omega = y\omega_r$ (and thus $\omega\tau = 2\pi y$):

$$p(t) = \sum_n f(t - n\tau) = \sum_n \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-\mathrm{i}\omega(t-n\tau)} \tilde{f}(\omega)$$
$$\overset{\omega = y\omega_r}{=} \sum_n \int_{-\infty}^{\infty} \mathrm{d}y\, \mathrm{e}^{\mathrm{i}2\pi y n} \underbrace{\left[\mathrm{e}^{-\mathrm{i}y\omega_r t} \tfrac{1}{\tau} \tilde{f}(y\omega_r)\right]}_{\equiv F(y)} = \sum_n \tilde{F}(2\pi n) \overset{\text{(Poisson)}}{=} \sum_m F(m)$$

Where we have defined the function $F(y) = \mathrm{e}^{-\mathrm{i}y\omega_r t} \frac{1}{\tau} \tilde{f}(y\omega_r)$, with Fourier transform $\tilde{F}(k)$, and used the Poisson summation formula. Using $\omega_m = m\omega_r = 2\pi m/\tau$, we thus obtain:

$$p(t) = \sum_m F(m) = \frac{1}{\tau} \sum_m \mathrm{e}^{-\mathrm{i}m\omega_r t} \underbrace{\tilde{f}(m\omega_r)}_{\equiv \tilde{p}_m} \overset{\omega_m = m\omega_r}{=} \frac{1}{\tau} \sum_m \mathrm{e}^{-\mathrm{i}\omega_m t} \tilde{p}_m \quad \text{with} \quad \tilde{p}_m = \tilde{f}(\omega_m)\,.$$

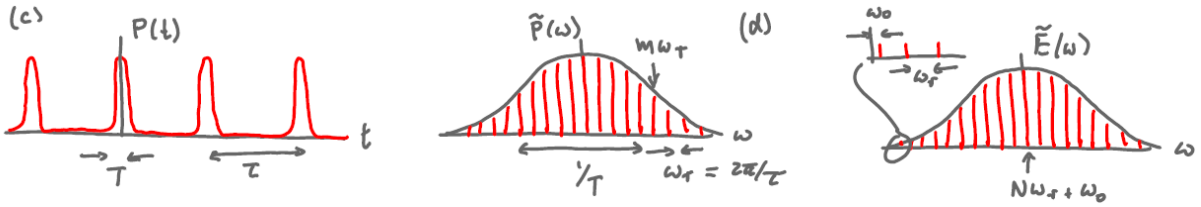
The middle term has the form of a discrete Fourier series, from which we can read off the discrete Fourier coefficients $\tilde{p}_m$ of $p(t)$. They are clearly given by $\tilde{p}_m = \tilde{f}(\omega_m)$, and correspond to the Fourier transform of $f(t)$ evaluated at the discrete frequencies ω_m.

A3: From (a) and (b) we directly obtain the following form for the Fourier transform of $p(t)$:

Fourier spectrum: $$\tilde{p}(\omega) \overset{\text{(a)}}{=} \omega_r \sum_m \tilde{p}_m \delta(\omega - \omega_m) \overset{\text{(b)}}{=} \omega_r \sum_m \tilde{f}(\omega_m) \delta(\omega - \omega_m)\,.$$

For a series of Gaussian functions, $p_G(t) = \sum_n f_G(t - n\tau)$, the envelope of the frequency comb, $\tilde{f}_G(\omega)$, also has the form of a Gaussian []:

Envelope: $$\tilde{f}_G(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} \frac{1}{\sqrt{2\pi T^2}} \mathrm{e}^{-\frac{t^2}{2T^2}} = \mathrm{e}^{-\frac{1}{2}T^2\omega^2}\,.$$



A4: The Fourier transform of $E(t) = \mathrm{e}^{-\mathrm{i}\omega_c t} p(t)$ is the same as that of $p(t)$, except shifted by a factor of ω_c:

$$\tilde{E}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} E(t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega'}{2\pi} \tilde{p}(\omega') \underbrace{\int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}(\omega - \omega_c - \omega')t}}_{2\pi\delta(\omega - \omega_c - \omega')} = \tilde{p}(\omega - \omega_c)$$

$$\overset{(c)}{=} \frac{2\pi}{\tau}\sum_m \tilde{f}(\omega_m)\delta(\omega-\omega_m-\omega_c) \overset{m=n-N}{=} \frac{2\pi}{\tau}\sum_n \tilde{f}(\omega_{n-N})\delta(\omega-\omega_n-\omega_0)\,.$$

In the last step we use $\omega_c = N\omega_r + \omega_0$ and a renaming of the summation indices, $m = n - N$, such that $\omega_m + \omega_c = \omega_n + \omega_0$. Thus $\tilde{E}(\omega)$ forms an 'offset-shifted' frequency comb, whose peaks relative to the Fourier frequencies ω_m are shifted by the offset frequency ω_0.

A5: We begin with the definition of the Fourier transform of $p_\gamma(t)$:

Definition:
$$\tilde{p}_\gamma(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} p_\gamma(t) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} \sum_n f(t-n\tau)\mathrm{e}^{-|n|\tau\gamma}$$

$t' = t - n\tau$:
$$= \underbrace{\sum_n \mathrm{e}^{-\mathrm{i}n\tau\omega}\mathrm{e}^{-|n|\tau\gamma}}_{\equiv S^{[\gamma,\omega_r]}(\omega)} \underbrace{\int_{-\infty}^{\infty} \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}\omega t'} f(t')}_{=\tilde{f}(\omega)}\,. \tag{3}$$

Where the sum

$$S^{[\gamma,\omega_r]}(\omega) \equiv \sum_{n\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}n\tau\omega}\mathrm{e}^{-|n|\tau\gamma} \overset{\tau=2\pi/\omega_r}{=} \sum_{n\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}2\pi n\omega/\omega_r}\mathrm{e}^{-2\pi|n|\gamma/\omega_r} \tag{4}$$

has the same form as a damped sum over Fourier modes,

$$S^{[\epsilon,L]}(x) \equiv \sum_{k\in\frac{2\pi}{L}\mathbb{Z}} \mathrm{e}^{-\mathrm{i}kx-\epsilon|k|} = \sum_{n\in\mathbb{Z}} \mathrm{e}^{-\mathrm{i}2\pi nx/L}\mathrm{e}^{-2\pi|n|\epsilon/L}\,, \tag{5}$$

which may be summed using a geometric series in the variables $\mathrm{e}^{-2\pi(\epsilon\pm\mathrm{i}x)/L}$ [siehe]:

$$S^{[\epsilon,L]}(x) = \frac{1-\mathrm{e}^{-4\pi\epsilon/L}}{1+\mathrm{e}^{-4\pi\epsilon/L}-2\mathrm{e}^{-2\pi\epsilon/L}\cos(2\pi x/L)} \simeq L\sum_{m\in\mathbb{Z}} \delta^{[\epsilon]}_{\mathrm{LP}}(x-mL)\,. \tag{6}$$

The result is a periodic sequence of peaks (shaded grey in sketch) at the positions $x \simeq mL$, each with the form of a Lorentzian function (LF), $\delta^{[\epsilon]}_{\mathrm{LP}}(x) = \frac{\epsilon/\pi}{x^2+\epsilon^2}$ for $x, \epsilon \ll L$. Using the association $x \mapsto \omega$, $\epsilon \mapsto \gamma$ and $L \mapsto \omega_r$ we obtain:

$$S^{[\gamma,\omega_r]}(\omega) \overset{(4,6)}{=} \omega_r \sum_{m\in\mathbb{Z}} \delta^{[\gamma]}_{\mathrm{LP}}(\omega-m\omega_r) \tag{7}$$

und
$$\tilde{p}_\gamma(\omega) \overset{(3,7)}{=} \omega_r \sum_{m\in\mathbb{Z}} \delta^{[\gamma]}_{\mathrm{LP}}(\omega-\omega_m)\tilde{f}(\omega)\,.$$

Thus the spectrum of a series of periodic pulses truncated by $|n| \lesssim 1/(\tau\gamma)$, corresponds to a frequency comb with broadened Lorentz functions as teeth, each with width $\simeq \gamma$.
Summary: This problem illuminates the following general relationships: (a) Because a periodic function $p(t)$ is defined by a discrete Fourier series representation, its Fourier integral representation $\tilde{p}(\omega)$ must then consist of a series of δ functions at the discrete Fourier frequencies ω_m. (b) For a periodic function, which is represented by $p(t) = \sum_n f(t-n\tau)$ for some source

function $f(t)$, the envelope of the frequency comb corresponds to the Fourier transform of the seed function $\tilde{p}_m = \tilde{f}(\omega_m)$. (c) Fourier reciprocity also applies in this case: the narrower the function $f(t)$, the the wider the form of the $\tilde{f}(\omega_m)$. (d) When $p(t)$ is multiplied with a carrier signal, whose frequency is is not commensurable with that of the comb, then the comb is shifted by an offset frequency. (e) If the $p(t)$ is only periodic within some bounded time interval, then the teeth of the frequency comb are broadened.

S.C7 Differential equations

S.C7.3 Linear first-order equations

ᴇC7.3.1 Separation of variables

a) The autonomous differential equation $\dot{x} = x^2$ can be solved by separation of variables and subsequent integration.

$$\frac{\mathrm{d}x}{\mathrm{d}t} = x^2 \quad \Rightarrow \quad \int_{x(t_0)}^{x(t)} \frac{\mathrm{d}\tilde{x}}{\tilde{x}^2} = \int_{t_0}^{t} \mathrm{d}\tilde{t} \quad \Rightarrow \quad -\frac{1}{x(t)} + \frac{1}{x(t_0)} = t - t_0\,.$$

Initial condition (i) is $x(0) = 1$: $\quad \Rightarrow \quad -\dfrac{1}{x(t)} + 1 = t \quad \Rightarrow \quad x(t) = \dfrac{1}{1-t}\,,$

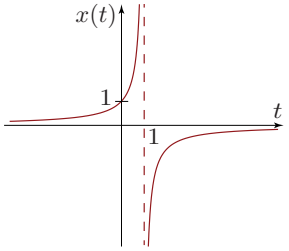
where the solution is defined on the interval $(-\infty, 1)$.

Initial condition (ii) is $x(2) = -1$: $\quad \Rightarrow \quad -\dfrac{1}{x(t)} - 1 = t - 2 \quad \Rightarrow \quad x(t) = \dfrac{1}{1-t}\,,$

where the solution is defined on the interval $(\infty, 1)$.

b) Graphical analysis of the equation $\dot{x} = x^2$:

(i) For all $x \neq 0$, $x^2 > 0$ and also $\dot{x} > 0$, i.e the curve has a monotonic increase. (ii) For $x = 1$, we have $\dot{x} = 1$, which fixes the slope at $x = 1$. For $x \to \pm\infty$, we have $\dot{x} \to \infty$. This suggests that there is a value for t where the curve diverges. According to the solution to the differential equation, this happens at $t = 1$.



ᴇC7.3.3 Separation of variables: barometric formula

With a linear temperature gradient, $T(x) = T_0 - b(x - x_0)$, separation of variables yields:

$$\frac{\mathrm{d}p(x)}{\mathrm{d}x} = -\alpha\frac{p(x)}{T(x)} = -\alpha\frac{p(x)}{T_0 + bx_0 - bx} \quad \Rightarrow \quad \int_{p_0}^{p}\frac{\mathrm{d}\tilde{p}}{\tilde{p}} = -\alpha\int_{x_0}^{x}\mathrm{d}\tilde{x}\frac{1}{T_0 + bx_0 - b\tilde{x}}$$

$$\Rightarrow \quad \ln\frac{p(x)}{p_0} = \frac{\alpha}{b}\ln\frac{T_0 + bx_0 - bx}{T_0} = \frac{\alpha}{b}\ln\left(\frac{T(x)}{T_0}\right) \quad \Rightarrow \quad \frac{p(x)}{p_0} = \left(\frac{T(x)}{T_0}\right)^{\frac{\alpha}{b}}\,.$$

This result is the so-called barometric height formula.

EC7.3.5 Substitution and separation of variables

(a) By inserting the substitution $y = ux$ and $y' = u'x + u$ into the differential equation $y' = f(y/x)$ we obtain a separable equation,

$$u'x + u = f(u) \quad \Rightarrow \quad \frac{\mathrm{d}u}{\mathrm{d}x} = \frac{f(u) - u}{x}\,,$$

since on the right-hand side of the boxed equation the u and x dependencies factorize.

(b) The equation $xy' = 2y + x$ is not directly separable, but it can be made separable by rearranging and substituting $y = ux$:

$$y' = 2y/x + 1 = f(y/x) \overset{y=ux}{=} f(u), \quad \text{with} \quad f(u) = 2u + 1\,.$$
$$\frac{\mathrm{d}u}{\mathrm{d}x} = \frac{f(u) - u}{x} = \frac{2u + 1 - u}{x} = \frac{u + 1}{x} \quad \Rightarrow \quad \int_{u_0}^{u} \mathrm{d}\tilde{u} \frac{1}{\tilde{u} + 1} = \int_{x_0}^{x} \mathrm{d}\tilde{x} \frac{1}{\tilde{x}}$$
$$\Rightarrow \quad \ln \frac{u + 1}{u_0 + 1} = \ln \frac{x}{x_0} \quad \Rightarrow \quad \frac{u + 1}{u_0 + 1} = \frac{x}{x_0}.$$

Initial condition: $y(x_0 = 1) = 0 \quad \Rightarrow \quad u_0 = u(x_0 = 1) = 0 \quad \Rightarrow \quad u + 1 = x.$
Solution: $u(x) = x - 1 \quad \Rightarrow \quad y(x) = ux = (x - 1)x\,.$ Initial condition: $y(1) = 0$. ✓

EC7.3.7 Inhomogeneous linear differential equation: variation of constant

(a) The general solution to the differential equation $\dot{x}_h(t) + 2x_h(t) = 0$ is: $x_h(t) = x_h(0)\mathrm{e}^{-2t}$.
(We find this by recognizing the integral, or by separating variables.)

(b) Variation of constants: ansatz: $x_p(t) = \tilde{c}(t)x_h(t) = c(t)\mathrm{e}^{-2t}$.
Insert this in the DE with $t_0 = 0,\ c(0) = 0$:

$$t = \dot{x}_p(t) + 2x_p(t) = \left[\dot{c}(t) - 2c(t) + 2c(t)\right]\mathrm{e}^{-2t} = \dot{c}(t)\mathrm{e}^{-2t} \quad \Rightarrow \quad \dot{c}(t) = t\mathrm{e}^{2t}\,.$$
$$\Rightarrow \quad c(t) = \int_0^t \mathrm{d}\tilde{t}\ \tilde{t}\mathrm{e}^{2\tilde{t}} \overset{\text{P.I.}}{=} \tfrac{1}{2}\tilde{t}\mathrm{e}^{2\tilde{t}}\Big|_0^t - \int_0^t \mathrm{d}\tilde{t}\ \tfrac{1}{2}\mathrm{e}^{2\tilde{t}} = \tfrac{1}{2}t\mathrm{e}^{2t} - \tfrac{1}{4}\mathrm{e}^{2\tilde{t}}\Big|_0^t = \tfrac{1}{2}t\mathrm{e}^{2t} - \tfrac{1}{4}\mathrm{e}^{2t} + \tfrac{1}{4}\,.$$
$$\Rightarrow \quad x_p(t) = c(t)\mathrm{e}^{-2t} = \tfrac{1}{2}t - \tfrac{1}{4} + \tfrac{1}{4}\mathrm{e}^{-2t}\,.$$

Initial condition is $x(0) = 0 \quad \Rightarrow \quad x_h(0) = 0$:

$$x(t) = x_h(t) + x_p(t) = x_h(0)\mathrm{e}^{-2t} + \tfrac{1}{2}t - \tfrac{1}{4} + \tfrac{1}{4}\mathrm{e}^{-2t}, \quad \Rightarrow \quad x(t) = \tfrac{1}{2}t - \tfrac{1}{4} + \tfrac{1}{4}\mathrm{e}^{-2t}\,.$$

S.C7.4 Systems of first order linear differential equations

ᴇC7.4.1 System of linear differential equations with non-diagonizable matrix

(a) Characteristic polynomial:

$$0 \stackrel{!}{=} \det(A-\lambda I) = (\tfrac{1}{3})^3 \begin{vmatrix} 7-3\lambda & 2 & 0 \\ 0 & 4-3\lambda & -1 \\ 2 & 0 & 4-3\lambda \end{vmatrix} = (\tfrac{1}{3})^3 \left[(7-3\lambda)(4-3\lambda)^2 - 4\right]$$
$$= -\lambda^3 + 5\lambda^2 - 8\lambda + 4 = -(\lambda-1)(\lambda-2)^2 \,.$$

Therefore there is a simple zero, $\lambda_1 = 1$, and a double zero, $\lambda_2 = \lambda_3 = 2$.

(b) We begin by finding the eigenvector $\mathbf{v}_1$ for λ_1:

$$\lambda_1 = 1: \qquad \mathbf{0} \stackrel{!}{=} (A-\lambda_1 \mathbb{1})\mathbf{v}_1 = \frac{1}{3}\begin{pmatrix} 4 & 2 & 0 \\ 0 & 1 & -1 \\ 2 & 0 & 1 \end{pmatrix} \mathbf{v}_1, \qquad \Rightarrow \qquad \mathbf{v}_1 = \frac{1}{3}\begin{pmatrix} -1 \\ 2 \\ 2 \end{pmatrix} .$$

The eigenvector $\mathbf{v}_1$ can be written down by inspection. It is nevertheless instructive to also determine it using Gaussian elimination:

$$\begin{array}{lcccc|c|l} [1]: & 4 & 2 & 0 & | & 0 & \\ [2]: & 0 & 1 & -1 & | & 0 & \\ [3]: & 2 & 0 & 1 & | & 0 & \end{array} \quad \longrightarrow \quad \begin{array}{l} [1]: \\ [2]: \\ [1]-2([2]+[3]): \end{array} \begin{array}{cccc|l} 4 & 2 & 0 & | & 0 \\ 0 & 1 & -1 & | & 0 \\ 0 & 0 & 0 & | & 0 \end{array}$$

$$\begin{array}{lcccc|c|l} [1]: & 4 & 2 & 0 & | & 0 & \\ [2]: & 0 & 1 & -1 & | & 0 & \\ [3]: & 0 & 0 & 0 & 1| & \alpha & \end{array} \quad \begin{array}{c} \swarrow \\ \longrightarrow \end{array} \quad \begin{array}{l} \frac{1}{4}[1]-\frac{1}{2}([2]+[3]): \\ [2]+[3]: \\ [3]: \end{array} \begin{array}{cccc|l} 1 & 0 & 0 & | & -\frac{1}{2}\alpha \\ 0 & 1 & 0 & | & \alpha \\ 0 & 0 & 1 & | & \alpha \end{array}$$

Since $(A-\lambda_1\mathbb{1}) = 0$, the rows of the extended matrix are not linearly independent, hence the second system yields a row that contains only zeros. Thus $\mathbf{v}_1$ involves one free parameter, which we chose as $v^3{}_1 = \alpha$ in the third system. By now taking, for example, $\alpha = \frac{2}{3}$, we obtain $\mathbf{v}_1 = \frac{1}{3}(-1,2,2)^T$.

Next we consider the eigenspace of λ_2:

$$\lambda_2 = 2: \qquad \mathbf{0} \stackrel{!}{=} (A-\lambda_2 \mathbb{1})\mathbf{v}_2 = \frac{1}{3}\begin{pmatrix} 1 & 2 & 0 \\ 0 & -2 & -1 \\ 2 & 0 & -2 \end{pmatrix} \mathbf{v}_2, \qquad \Rightarrow \qquad \mathbf{v}_2 = \frac{1}{3}\begin{pmatrix} 2 \\ -1 \\ 2 \end{pmatrix} .$$

$\mathbf{v}_2$, too, can be written down by inspection. But since λ_2 is a two-fold zero, the question immediately arises whether there exists another eigenvector associated with λ_2, linearly

independent from $\mathbf{v}_2$. To clarify this, we solve the above system by Gaussian elimination:

$$\begin{array}{lrrrcl}
[1]: & 1 & 2 & 0 & | & 0 \\
[2]: & 0 & -2 & -1 & | & 0 \\
[3]: & 2 & 0 & -2 & | & 0
\end{array}
\quad\longrightarrow\quad
\begin{array}{lrrrcl}
[1]: & 1 & 2 & 0 & | & 0 \\
-[2]: & 0 & 2 & 1 & | & 0 \\
2([1]+[2])-[3]: & 0 & 0 & 0 & | & 0
\end{array}$$

$$\begin{array}{lrrrcl}
[1]: & 1 & 2 & 0 & | & 0 \\
[2]: & 0 & 2 & 1 & | & 0 \\
[3]: & 0 & 0 & 1 & | & \alpha
\end{array}
\quad\begin{array}{c}\swarrow\\ \\ \longrightarrow\end{array}\quad
\begin{array}{lrrrcl}
[1]-[2]+[3]: & 1 & 0 & 0 & | & \alpha \\
\frac{1}{2}([2]-[3]): & 0 & 1 & 0 & | & -\frac{1}{2}\alpha \\
[3]: & 0 & 0 & 1 & | & \alpha
\end{array}$$

Since $(A-\lambda_2\mathbb{1})=0$, the rows of the extended matrix are not linearly independent. But although λ_2 is a *two*-fold zero of the characteristic polynomial, Gaussian elimination here yields only *one* row containing purely zeros, hence $\mathbf{v}_2$ involves only one free parameter. (In the third system we chose it as $v^3{}_2=\alpha$, and in the end used $\alpha=\frac{2}{3}$ to obtain $\mathbf{v}_2=\frac{1}{3}(2,-1,2)^T$.) Therefore the degenerate eigenvalue λ_2 has only *one* eigenvector, i.e. the eigenspace of λ_2 is only *one*-dimensional, just as the eigenspace of λ_1. Hence the matrix A is not diagonalizable. (For a diagonalizable matrix a two-fold zero would yield an extended matrix containing *two* rows consisting purely of zeros. The solution would then involve *two* independent parameters, so that it would be possible to construct *two* linearly independent eigenvectors, $\mathbf{v}_2$ and $\mathbf{v}_3$, both with eigenvalue λ_2.)

(c) To determine $\mathbf{v}_3$, we use Gaussian elimination to solve the equation $(A-\lambda_2\mathbb{1})\mathbf{v}_3=\mathbf{v}_2$:

$$\begin{array}{lrrrcl}
[1]: & 1 & 2 & 0 & | & 2 \\
[2]: & 0 & -2 & -1 & | & -1 \\
[3]: & 2 & 0 & -2 & | & 2
\end{array}
\quad\longrightarrow\quad
\begin{array}{lrrrcl}
[1]: & 1 & 2 & 0 & | & 2 \\
-[2]: & 0 & 2 & 1 & | & 1 \\
2[1]+2[2]-[3]: & 0 & 0 & 0 & | & 0
\end{array}$$

$$\begin{array}{lrrrcl}
[1]: & 1 & 2 & 0 & | & 2 \\
[2]: & 0 & 2 & 1 & | & 1 \\
[3]: & 0 & 0 & 1 & | & \alpha
\end{array}
\quad\begin{array}{c}\swarrow\\ \\ \longrightarrow\end{array}\quad
\begin{array}{lrrrcl}
[1]-2[2]+[3]: & 1 & 0 & 0 & | & 1+\alpha \\
\frac{1}{2}([2]-[3]): & 0 & 1 & 0 & | & \frac{1}{2}(1-\alpha) \\
[3]: & 0 & 0 & 1 & | & \alpha
\end{array}$$

The second system contains a row consisting purely of zeros, thus the solution has a free parameter; in the third system we choose it as $v^3{}_3=\alpha$. Setting, for example, $\alpha=-\frac{1}{3}$, we obtain $\mathbf{v}_3=\frac{1}{3}(2,2,-1)^T$. This choice is particularly convenient, since then $\mathbf{v}_1$, $\mathbf{v}_2$ and $\mathbf{v}_3$ form an orthonormal system. It yields the following similarity transformation S:

$$S=(\mathbf{v}_1,\mathbf{v}_2,\mathbf{v}_3)=\frac{1}{3}\begin{pmatrix}-1&2&2\\2&-1&2\\2&2&-1\end{pmatrix}=S^T=S^{-1}\,.$$

(d) For the coefficient $\mathbf{c}(0)$ we obtain:

$$\mathbf{c}(0)=S^{-1}\mathbf{x}(0)=\frac{1}{3}\begin{pmatrix}-1&2&2\\2&-1&2\\2&2&-1\end{pmatrix}\begin{pmatrix}1\\1\\1\end{pmatrix}=\begin{pmatrix}1\\1\\1\end{pmatrix}.$$

Thus the solution of the differential equation is:

$$\begin{aligned}\mathbf{x}(t) &= c^1(0)e^t\mathbf{v}_1 + \big(c^2(0) + tc^3(0)\big)e^{2t}\mathbf{v}_2 + c^3(0)e^{2t}\mathbf{v}_3 \\ &= \tfrac{1}{3}e^t\begin{pmatrix}-1\\2\\2\end{pmatrix} + \tfrac{1}{3}(1+t)e^{2t}\begin{pmatrix}2\\-1\\2\end{pmatrix} + \tfrac{1}{3}e^{2t}\begin{pmatrix}2\\2\\-1\end{pmatrix}.\end{aligned}$$

(e) Explicit check:

$$\begin{aligned}\dot{\mathbf{x}}(t) &= \tfrac{1}{3}e^t\begin{pmatrix}-1\\2\\2\end{pmatrix} + \tfrac{2}{3}(1+t)e^{2t}\begin{pmatrix}2\\-1\\2\end{pmatrix} + \tfrac{1}{3}e^{2t}\begin{pmatrix}2\\-1\\2\end{pmatrix} + \tfrac{2}{3}e^{2t}\begin{pmatrix}2\\2\\-1\end{pmatrix} \\ &= \tfrac{1}{3}e^t\begin{pmatrix}-1\\2\\2\end{pmatrix} + \tfrac{2}{3}(1+t)e^{2t}\begin{pmatrix}2\\-1\\2\end{pmatrix} + e^{2t}\begin{pmatrix}2\\1\\0\end{pmatrix}.\end{aligned}$$

On the other hand:

$$\begin{aligned}A\mathbf{x}(t) &= \tfrac{1}{3}e^t\begin{pmatrix}-1\\2\\2\end{pmatrix} + \tfrac{2}{3}(1+t)e^{2t}\begin{pmatrix}2\\-1\\2\end{pmatrix} + \tfrac{1}{9}e^{2t}\begin{pmatrix}7&2&0\\0&4&-1\\2&0&4\end{pmatrix}\begin{pmatrix}2\\2\\-1\end{pmatrix} \\ &= \tfrac{1}{3}e^t\begin{pmatrix}-1\\2\\2\end{pmatrix} + \tfrac{2}{3}(1+t)e^{2t}\begin{pmatrix}2\\-1\\2\end{pmatrix} + e^{2t}\begin{pmatrix}2\\1\\0\end{pmatrix} \overset{\checkmark}{=} \dot{\mathbf{x}}(t).\end{aligned}$$

S.C7.5 General nth order linear differential equation

ᴇC7.5.1 Inhomogeneous linear differential equation of order 2: driven overdamped harmonic oscillator

(a) Simplification of matrix equation:

$$\ddot{x} + 2\gamma\dot{x} + \Omega^2 x = f_{\mathrm{A}}(t), \quad x(0) = 0, \quad \dot{x}(0) = 1\,, \tag{1}$$

can be written as a first order matrix DE, using $\mathbf{x} \equiv (x, \dot{x})^T = (x^1, x^2)^T$ and $\ddot{x} = \dot{x}^2$.

New variables: $\dot{x} = \dot{x}^1 = x^2, \qquad \ddot{x} = \dot{x}^2 = -\Omega^2 x^1 - 2\gamma x^2 + f_{\mathrm{A}}(t)\,.$

Matrix form: $$\underbrace{\begin{pmatrix}\dot{x}^1\\\dot{x}^2\end{pmatrix}}_{\dot{\mathbf{x}}} = \underbrace{\begin{pmatrix}0&1\\-\Omega^2&-2\gamma\end{pmatrix}}_{A}\underbrace{\begin{pmatrix}x^1\\x^2\end{pmatrix}}_{\mathbf{x}} + \underbrace{f_{\mathrm{A}}(t)\begin{pmatrix}0\\1\end{pmatrix}}_{\mathbf{b}(t)}.$$

Compact notation: $\dot{\mathbf{x}} = A\cdot\mathbf{x} + \mathbf{b}(t)\,.$ (2)

Initial values: $\mathbf{x}_0 = \mathbf{x}(0) = (x(0), \dot{x}(0))^T = (0,1)^T.$

(b) Homogeneous solution:
We first determine the eigenvalues λ_j and eigenvectors $\mathbf{v}_j$ ($j = +, -$) of A:

$$0 \stackrel{!}{=} \det(A - \lambda \mathbb{1}|) = \begin{vmatrix} -\lambda & 1 \\ -\Omega^2 & -2\gamma - \lambda \end{vmatrix} = \lambda(2\gamma + \lambda) + \Omega^2 = \lambda^2 + 2\gamma\lambda + \Omega^2 \,. \tag{3}$$

Eigenvalues (for $\gamma > \Omega$): $\boxed{\lambda_\pm = -\gamma \pm \gamma_\mathrm{r}, \text{ with } \gamma_\mathrm{r} \equiv \sqrt{\gamma^2 - \Omega^2} \text{ real}}$. (4)

Eigenvectors: $\mathbf{0} = (A - \lambda_j \mathbb{1})\mathbf{v}_j = \begin{pmatrix} -\lambda_j & 1 \\ -\Omega^2 & -2\gamma - \lambda_j \end{pmatrix} \mathbf{v}_j \quad \Rightarrow \quad \mathbf{v}_j = \begin{pmatrix} 1 \\ \lambda_j \end{pmatrix}$.

This works since $-\Omega^2 \cdot 1 + (-2\gamma - \lambda_j)\lambda_j \stackrel{(3)}{=} 0$ if λ_j is an eigenvalue.

Since $\mathbf{x}_j(t) = \mathbf{v}_j \mathrm{e}^{\lambda_j t}$ satisfies the homogeneous equation $\dot{\mathbf{x}}_j = A \cdot \mathbf{x}_j$, the first component of $\mathbf{x}_j(t)$, i.e. $x_j(t) = e^{\lambda_j t}$, fulfills the DE (1)$|_{f_\mathrm{A}(t)=0}$. Check that this is the case:

$$(\mathrm{d}_t^2 + 2\gamma \mathrm{d}_t + \Omega^2)\mathrm{e}^{\lambda_j t} = \left(\gamma_j^2 + 2\gamma\lambda_j + \Omega^2\right) \mathrm{e}^{\lambda_j t} \stackrel{(3)}{=} 0 \,. \quad \checkmark \tag{5}$$

The most general form of the homogeneous solution is $\mathbf{x}_\mathrm{h}(t) = \sum_j c_\mathrm{h}^j \mathbf{x}_j(t)$. For a given initial value $\mathbf{x}_0$, the coefficient vector $\mathbf{c}_\mathrm{h} = (c_\mathrm{h}^1, c_\mathrm{h}^2)^T$ is fixed by $\mathbf{x}_\mathrm{h}(0) = \sum_j \mathbf{v}_j c_\mathrm{h}^j = \mathbf{x}_0$, or in matrix notation, $S\mathbf{c}_\mathrm{h} = \mathbf{x}_0$, where the matrix $S = \{v^i{}_j\}$ has the eigenvectors $\mathbf{v}_j$ as columns, i.e. $S = (\mathbf{v}_1, \mathbf{v}_2)$:

$$S = \begin{pmatrix} 1 & 1 \\ \lambda_+ & \lambda_1 \end{pmatrix}, \quad S^{-1} = \frac{1}{\lambda_- - \lambda_+} \begin{pmatrix} \lambda_- & -1 \\ -\lambda_+ & 1 \end{pmatrix} \stackrel{(4)}{=} -\frac{1}{2\gamma_\mathrm{r}} \begin{pmatrix} \lambda_- & -1 \\ -\lambda_+ & 1 \end{pmatrix}, \tag{6}$$

$$\mathbf{c}_\mathrm{h} = S^{-1}\mathbf{x}_0 \Rightarrow \begin{pmatrix} c_\mathrm{h}^+ \\ c_\mathrm{h}^- \end{pmatrix} = -\frac{1}{2\gamma_\mathrm{r}} \begin{pmatrix} \lambda_- & -1 \\ -\lambda_+ & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{2\gamma_\mathrm{r}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \Rightarrow c_\mathrm{h}^\pm = \pm \frac{1}{2\gamma_\mathrm{r}} \,.$$

The homogeneous solution of the matrix DE (2)$|_{\mathbf{b}(t)=0}$ is thus

$$\mathbf{x}_\mathrm{h}(t) = \sum_j c_\mathrm{h}^j \mathbf{x}_j(t) = \frac{1}{2\gamma_\mathrm{r}} \left[\mathrm{e}^{\lambda_+ t} \begin{pmatrix} 1 \\ \lambda_+ \end{pmatrix} - \mathrm{e}^{\lambda_- t} \begin{pmatrix} 1 \\ \lambda_- \end{pmatrix} \right] \,,$$

and the homogeneous solution of the initial second order DE, (1)$|_{f_\mathrm{A}(t)=0}$, is

$$x_\mathrm{h}(t) = x_\mathrm{h}^1(t) = \boxed{\frac{1}{2\gamma_\mathrm{r}} \left[\mathrm{e}^{\lambda_+ t} - \mathrm{e}^{\lambda_- t}\right]} = \frac{\mathrm{e}^{-\gamma t}}{\gamma_\mathrm{r}} \sinh(\gamma_\mathrm{r} t) \,.$$

Check that $x_\mathrm{h}(t)$ has the required properties (not really necessary, since all relevant properties have already been checked above, but nevertheless instructive):

$$(\mathrm{d}_t^2 + 2\gamma \mathrm{d}_t + \Omega^2) x_\mathrm{h} = \frac{1}{2\gamma_\mathrm{r}} \left[\left(\gamma_+^2 + 2\gamma\gamma_+ + \Omega^2\right) \mathrm{e}^{\gamma_+ t} - \left(\gamma_-^2 + 2\gamma\gamma_- + \Omega^2\right) \mathrm{e}^{\gamma_- t} \right] \stackrel{(3)}{=} 0 \,. \checkmark$$

Initial value: $x_\mathrm{h}(0) = 0, \quad \dot{x}_\mathrm{h}(0) = 1 \,. \checkmark$ (7)

(c) Particular solution: The method of variation of constants looks for a particular solution of the matrix DE (2) of the form $\mathbf{x}_\mathrm{p}(t) = \sum_j c^j_\mathrm{p}(t)\mathbf{x}_j(t)$, with $c^j_\mathrm{p}(t)$ chosen such that

$$\sum_j \dot{c}^j_\mathrm{p}(t)\mathbf{x}_j(t) = \mathbf{b}(t)\,. \tag{8}$$

A solution to (8), with $c^j(0) = 0$ (and therefore $\mathbf{x}_\mathrm{p}(0) = \mathbf{0}$), is given by

$$c^j_\mathrm{p}(t) = \int_0^t \mathrm{d}\tilde{t}\,\tilde{b}^j(\tilde{t})\,\mathrm{e}^{-\lambda_j\tilde{t}}\,, \tag{9}$$

where the $\tilde{b}^j(t)$ originate from the decomposition of $\mathbf{b}(t) = \sum_j \mathbf{v}_j\tilde{b}^j(t)$ into eigenvectors. In components, $b^i(t) = v^i{}_j\tilde{b}^j(t)$, and in matrix notation, $\mathbf{b}(t) = S\tilde{\mathbf{b}}(t)$, $\tilde{\mathbf{b}}(t) = S^{-1}\mathbf{b}(t)$:

$$\begin{pmatrix}\tilde{b}^+(t)\\ \tilde{b}^-(t)\end{pmatrix} \overset{(6)}{=} -\frac{1}{2\gamma_\mathrm{r}}\begin{pmatrix}\lambda_- & -1\\ -\lambda_+ & 1\end{pmatrix} f_\mathrm{A}(t)\begin{pmatrix}0\\1\end{pmatrix} = \frac{f_\mathrm{A}(t)}{2\gamma_\mathrm{r}}\begin{pmatrix}1\\-1\end{pmatrix} \Rightarrow \boxed{\tilde{b}^\pm(t) = \pm\frac{f_\mathrm{A}(t)}{2\gamma_\mathrm{r}}}\,.$$

For the given driving function, we have $f_\mathrm{A}(t) = f_\mathrm{A}$ for $t \geq 0$, and therefore we obtain:

$$c^\pm_\mathrm{p}(t) \overset{(9)}{=} \pm\frac{f_\mathrm{A}}{2\gamma_\mathrm{r}}\int_0^t \mathrm{d}\tilde{t}\,\mathrm{e}^{-\lambda_\pm\tilde{t}} = \boxed{\pm\frac{f_\mathrm{A}}{2\gamma_\mathrm{r}\lambda_\pm}\left[1-\mathrm{e}^{-\lambda_\pm t}\right]}\,.$$

Check initial value: $c^j_\mathrm{p}(0) \overset{\checkmark}{=} 0$. Check that (8) holds:

$$\sum_j \dot{c}^j_\mathrm{p}(t)\mathbf{x}_j(t) \overset{(8)?}{=} \frac{f_\mathrm{A}}{2\gamma_\mathrm{r}}\left[\frac{\lambda_+\mathrm{e}^{-\lambda_+ t}}{\lambda_+}\begin{pmatrix}1\\\lambda_+\end{pmatrix}\mathrm{e}^{\lambda_+ t} - \frac{\lambda_-\mathrm{e}^{-\lambda_- t}}{\lambda_-}\begin{pmatrix}1\\\lambda_-\end{pmatrix}\mathrm{e}^{\lambda_- t}\right] = f_\mathrm{A}\begin{pmatrix}0\\1\end{pmatrix} \overset{\checkmark}{=} \mathbf{b}(t)\,.$$

The desired particular solution for $t > 0$ is therefore given by:

$$\begin{aligned}\mathbf{x}_\mathrm{p}(t) &= \sum_j c^j_\mathrm{p}(t)\mathbf{v}_j e^{\lambda_j t} = \frac{f_\mathrm{A}}{2\gamma_\mathrm{r}}\left[\frac{\mathrm{e}^{\lambda_+ t}-1}{\lambda_+}\begin{pmatrix}1\\\lambda_+\end{pmatrix} - \frac{\mathrm{e}^{\lambda_- t}-1}{\lambda_-}\begin{pmatrix}1\\\lambda_-\end{pmatrix}\right],\\ x_\mathrm{p}(t) &= x^1_\mathrm{p}(t) = \boxed{\frac{f_\mathrm{A}}{2\gamma_\mathrm{r}}\left[\frac{\mathrm{e}^{\lambda_+ t}-1}{\lambda_+} - \frac{\mathrm{e}^{\lambda_- t}-1}{\lambda_-}\right]}\,.\end{aligned}$$

Check that $x_\mathrm{p}(t)$ has the required properties (not really necessary, since all relevant properties have already been checked above, but nevertheless instructive):

$$\begin{aligned}(\mathrm{d}_t^2 + 2\gamma\mathrm{d}_t + \Omega^2)x_\mathrm{p}(t) &= \frac{f_\mathrm{A}}{2\gamma_\mathrm{r}}\left[\underbrace{(\lambda_+^2+2\gamma\lambda_+ +\Omega^2)}_{\overset{(4)}{=}0}\frac{\mathrm{e}^{\lambda_+ t}}{\lambda_+} - \underbrace{(\lambda_-^2+2\gamma\lambda_- +\Omega^2)}_{\overset{(4)}{=}0}\frac{\mathrm{e}^{\lambda_- t}}{\lambda_-} - \Omega^2\left(\frac{1}{\lambda_+}-\frac{1}{\lambda_-}\right)\right]\\ &= -\Omega^2\frac{f_\mathrm{A}}{2\gamma_\mathrm{r}}\left[\frac{\lambda_- - \lambda_+}{\lambda_-\lambda_+}\right] \overset{(4)}{=} \Omega^2\frac{f_\mathrm{A}}{2\gamma_\mathrm{r}}\frac{2\gamma_\mathrm{r}}{\Omega^2} = f_\mathrm{A}\,.\checkmark\end{aligned}$$

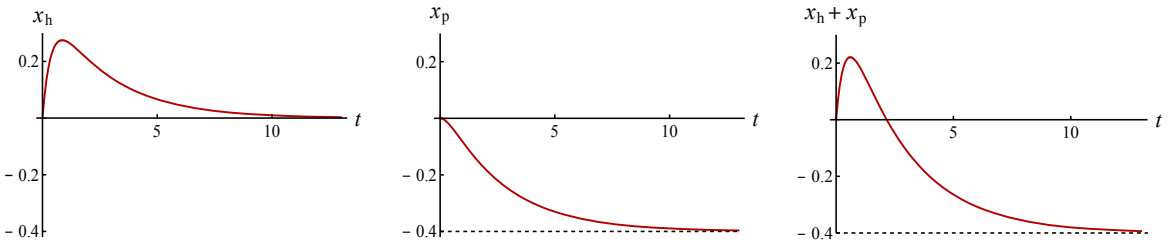
Initial value: $x_\mathrm{p}(0) = 0, \quad \dot{x}_\mathrm{p}(0) = 0\,.\quad\checkmark$ (10)

(d) Qualitative discussion: According to (7) and (10), the solution $x(t) = x_\mathrm{h}(t) + x_\mathrm{p}(t)$ of the inhomogeneous DEQ (1) has the required initial values $x(0) = 0$ and $\dot{x}(0) = 1$. Since $\lambda_\pm < 0$, the long time limit $t \to \infty$ is determined by the constant contribution of $x_\mathrm{p}(t)$ alone:

$$x_\mathrm{p}(t) \overset{t\to\infty}{\longrightarrow} x_\mathrm{p}(\infty) = -\frac{f_\mathrm{A}}{2\gamma_\mathrm{r}}\left[\frac{1}{\lambda_+} - \frac{1}{\lambda_-}\right] \overset{(4)}{=} \frac{f_\mathrm{A}}{\Omega^2}\,.$$

For $t > 0$, the driving force $F_\mathrm{A} = m f_\mathrm{A}$ is time-independent. Therefore, it leads to a constant shift in the equilibrium position from 0 to $x_\mathrm{p}(\infty) = f_\mathrm{A}/\Omega^2$. For this shift, the restoring force of the harmonic oscillator, $F_\mathrm{R} = -m\Omega^2 x_\mathrm{p}(\infty)$, cancels the driving force exactly, i.e. $F_\mathrm{A} + F_\mathrm{R} = 0$.

Concerning the sketch, for $f_\mathrm{A} < 0$: According to the given initial condition, $x(t)$ initially increases for small times (starting from 0), attains a maximum [at $\dot{x}_\mathrm{p}(t) = 0$, where $\mathrm{e}^{\lambda_+ t} = \mathrm{e}^{\lambda_- t}$ i.e. at $t = 1/(2\gamma_\mathrm{r})$], and thereafter tends to the long time limit from above, $x_\mathrm{p}(\infty) < 0$.



Parameters for the sketch: $\Omega = 1$, $\gamma = 1.5$, $f_\mathrm{A} = -0.4$.

ᴇC7.5.3 Coupled oscillations of two point masses

(a) Equations of motion:

in Matrix form:
$$\begin{pmatrix}\ddot{x}^1\\ \ddot{x}^2\end{pmatrix} = -\underbrace{\begin{pmatrix}\frac{K_1+K_{12}}{m_1} & -\frac{K_{12}}{m_1}\\ -\frac{K_{12}}{m_2} & \frac{K_2+K_{12}}{m_2}\end{pmatrix}}_{\equiv A}\begin{pmatrix}x^1\\ x^2\end{pmatrix}\,, \tag{1}$$

Compact notation:
$$\ddot{\mathbf{x}} = -A\mathbf{x}\,. \tag{2}$$

(b) Transformation into an eigenvalue problem:

Ansatz for solution:
$$\mathbf{x}(t) = \mathbf{v}\cos(\omega t)\,. \tag{3}$$

Differentiating the ansatz twice:
$$\ddot{\mathbf{x}}(t) = -\omega^2\mathbf{v}\cos(\omega t)\,. \tag{4}$$

Inserting (3), (4) in (2):
$$-\omega^2\mathbf{v}\cos(\omega t) = -A\mathbf{v}\cos(\omega t)\,,$$

Eigenvalue equation:
$$A\mathbf{v} = \omega^2\mathbf{v}\,. \tag{5}$$

(c) For $m_1 = m_2$, $K_2 = m_1\Omega^2$, $K_1 = 4K_2$ and $K_{12} = 2K_2$, we have: $A = \Omega^2 \begin{pmatrix} 6 & -2 \\ -2 & 3 \end{pmatrix}$

$\frac{1}{\Omega^2}$·[Eigenvalue equation (5)]: $\frac{1}{\Omega^2} A\mathbf{v} \overset{(5)}{=} \frac{\omega^2}{\Omega^2}\mathbf{v} = \lambda\mathbf{v}$, with $\lambda \equiv (\omega/\Omega)^2$. (6)

Determination of the eigenvalues λ_j of the matrix $\frac{1}{\Omega^2}A$:

Characteristic polynomial: $0 \overset{!}{=} \det \begin{pmatrix} 6-\lambda & -2 \\ -2 & 3-\lambda \end{pmatrix} = (6-\lambda)(3-\lambda) - 4$

$= \lambda^2 - 9\lambda + 14 = (\lambda - 7)(\lambda - 2)$.

Eigenvalues: $\lambda_1 = 2$, $\lambda_2 = 7$. (7)

Eigenvectors $\mathbf{v}_j$: $(A - \lambda_j \mathbb{1})\, \mathbf{v}_j = \mathbf{0}$.

$\lambda_1 = 2$: $\begin{pmatrix} 4 & -2 \\ -2 & 1 \end{pmatrix} \mathbf{v}_1 = \mathbf{0} \quad \Rightarrow \quad \mathbf{v}_1 = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix}$. (8)

$\lambda_2 = 7$: $\begin{pmatrix} -1 & -2 \\ -2 & -4 \end{pmatrix} \mathbf{v}_2 = \mathbf{0} \quad \Rightarrow \quad \mathbf{v}_2 = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ -1 \end{pmatrix}$. (9)

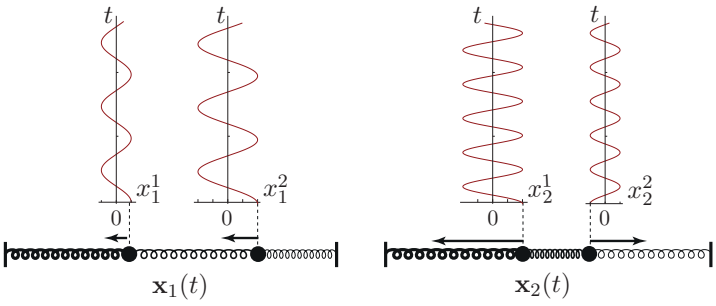
Eigenfrequency $\omega_j \overset{(6)}{=} \sqrt{\lambda_j}\Omega$: $\omega_1 \overset{(7)}{=} \sqrt{2}\Omega$, $\omega_2 \overset{(7)}{=} \sqrt{7}\Omega$.

Same-phase eigenmode: $\mathbf{x}_1(t) \overset{(3)}{=} \mathbf{v}_1 \cos(\omega_1 t) \overset{(8)}{=} \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ 2 \end{pmatrix} \cos(\sqrt{2}\Omega t)$.

Out-of-phase eigenmode: $\mathbf{x}_2(t) \overset{(3)}{=} \mathbf{v}_2 \cos(\omega_2 t) \overset{(9)}{=} \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ -1 \end{pmatrix} \cos(\sqrt{7}\Omega t)$.

(d) For the eigenmode $\mathbf{x}_1(t)$ (left sketch), both the masses swing in phase, and for $\mathbf{x}_2(t)$ (right sketch), both the masses swing out of phase. The latter requires stronger expansion and compression of the springs and therefore costs the out-of-phase mode more energy and thus has a higher frequency than the same-phase mode. The schematic sketch below illustrates the positions of the point masses at time $t = 0$ and the thick arrow illustrates their velocities a small time (e.g. half a period) later.

Remark: Both the masses at time $t = 0$ are displaced by ${x^1}_0$ and ${x^2}_0$ respectively, and the subsequent swinging is a superposition of both the eigenmodes, $\mathbf{x}(t) = \sum_j c^j \mathbf{x}_j(t)$, whose coefficients c^j are fixed by the initial displacement $\mathbf{x}_0 = ({x^1}_0, {x^2}_0)^T$, with $\mathbf{x}_0 = \sum_j c^j \mathbf{v}_j$.



ᴇC7.5.5 Green's function of $(\mathrm{d}_t + a)$

(a) We first recall two properties of the δ-function: Firstly, it corresponds to the derivative of the θ-function $\mathrm{d}_t\theta(t) = \delta(t)$. Secondly, for an arbitrary function $b(t)$, it holds that $\delta(t)b(t) = \delta(t)b(0)$.
Now we verify the validity of the given ansatz for the Green's function:

Ansatz: $$G(t) = \theta(t)x_\mathrm{h}(t). \tag{1}$$

Let it satisfy the homogeneous solution: $$\tilde{D}(\mathrm{d}_t)x_\mathrm{h}(t) = 0\ , \tag{2}$$

with initial condition $$x_\mathrm{h}(0) = 1\ . \tag{3}$$

Then we have:
$$\begin{aligned}\mathrm{d}_t\big[\theta(t)x_\mathrm{h}(t)\big] &= \big[\mathrm{d}_t\theta(t)\big]x_\mathrm{h}(t) + \theta(t)\mathrm{d}_t x_\mathrm{h}(t)\\ &= \delta(t)x_\mathrm{h}(t) + \theta(t)\mathrm{d}_t x_\mathrm{h}(t)\ ,\\ &= \delta(t)\underbrace{x_\mathrm{h}(0)}_{\overset{(3)}{=}1} + \theta(t)\mathrm{d}_t x_\mathrm{h}(t)\ .\end{aligned} \tag{4}$$

$$\Rightarrow \qquad D(\mathrm{d}_t)G(t) \overset{(1)}{=} (\mathrm{d}_t + a)\big[\theta(t)x_\mathrm{h}(t)\big] \overset{(4)}{=} \delta(t) + \underbrace{\theta(t)\mathrm{d}_t x_\mathrm{h}(t) + a\theta(t)x_\mathrm{h}(t)}_{\theta(t)\,[D(\mathrm{d}_t)x_\mathrm{h}(t)] \overset{(2)}{=} 0} = \delta(t). \quad \checkmark$$

(b) The homogeneous equation $(\mathrm{d}_t + a)x_\mathrm{h}(t) = 0$, with initial condition $x_\mathrm{h}(0) = 1$, has the solution $x_\mathrm{h} = e^{-at}$. Consequently, the Green's function is:

$$\boxed{G(t) \overset{(1)}{=} \theta(t)\mathrm{e}^{-at}}\ . \tag{5}$$

(c) Fourier integral:
$$\tilde{\mathcal{G}}(\omega) = \int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}G(t) \overset{(5)}{=} \int_{-\infty}^{\infty}\mathrm{d}t\,\theta(t)\mathrm{e}^{(\mathrm{i}\omega - a)t} = \int_0^{\infty}\mathrm{d}t\,\mathrm{e}^{(\mathrm{i}\omega-a)t}$$
$$[e^{(\mathrm{i}\omega-a)\infty} = 0,\ \text{da } a > 0.] \qquad = \frac{1}{\mathrm{i}\omega - a}\left[e^{(\mathrm{i}\omega-a)t}\right]_0^{\infty} = \boxed{\frac{1}{a - \mathrm{i}\omega}}\ . \tag{6}$$

(d) Consistency check:

Defining Eqn for $G(t)$: $$D_t G(t) = \delta(t)\ , \qquad \text{with} \quad D(\mathrm{d}_t) = \mathrm{d}_t + a\ . \tag{7}$$

Fourier transform: $$\tilde{D}(-\mathrm{i}\omega)\tilde{\mathcal{G}}(\omega) = 1 \qquad \text{with} \quad \tilde{D}(-\mathrm{i}\omega) = -\mathrm{i}\omega + a\ . \tag{8}$$

(8) solve for $\tilde{\mathcal{G}}(\omega)$: $$\tilde{\mathcal{G}}(\omega) = \frac{1}{\tilde{D}(-\mathrm{i}\omega)} = \boxed{\frac{1}{-\mathrm{i}\omega + a}}\ . \qquad [= (6)\ \checkmark]\ . \tag{9}$$

Here, completeness is the main logic behind the steps (7) to (8):

Fourier representations of G, δ: $$G(t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\mathrm{e}^{-\mathrm{i}\omega t}\tilde{\mathcal{G}}(\omega)\ , \quad \delta(t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\mathrm{e}^{-\mathrm{i}\omega t}\ . \tag{10}$$

Inserting (10) in (7) :
$$\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\underbrace{[D(\mathrm{d}_t)]\,\mathrm{e}^{-\mathrm{i}\omega t}}_{=\tilde{D}(-\mathrm{i}\omega)\mathrm{e}^{-\mathrm{i}\omega t}}\tilde{\mathcal{G}}(\omega)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\mathrm{e}^{-\mathrm{i}\omega t}\,. \tag{11}$$

gives
$$\tilde{D}(-\mathrm{i}\omega)\tilde{\mathcal{G}}(\omega)=1. \qquad \text{[agrees with (8) ✓]} \tag{12}$$

(e) To solve the DE:
$$D(\mathrm{d}_t)x(t)=f(t), \qquad \text{with } f(t)=\mathrm{e}^{2at}\,. \tag{13}$$

Solution ansatz:
$$x(t)=\int_{-\infty}^{\infty}\mathrm{d}\tilde{t}\,G\left(t-\tilde{t}\right)f(\tilde{t})\overset{t'=t-\tilde{t}}{=}\int_{-\infty}^{\infty}\mathrm{d}t'\,G(t')f(t-t')\,. \tag{14}$$

This substitution simplifies the argument of G. In the current example, this is recommended since G here is a more complicated function that $f(t)$.

$$x(t)\overset{(5),(13)}{=}\int_{-\infty}^{\infty}\mathrm{d}t'\,\theta(t')\mathrm{e}^{-at'}\mathrm{e}^{2a(t-t')}=\mathrm{e}^{2at}\int_{0}^{\infty}\mathrm{d}t'\,\mathrm{e}^{-3at'}=\boxed{\frac{1}{3a}\mathrm{e}^{2at}}\,. \tag{15}$$

The solution may be verified via explicit insertion into the differential equation:
$$D(\mathrm{d}_t)x(t)\overset{(15)}{=}(\mathrm{d}_t+a)\frac{1}{3a}\mathrm{e}^{2at}=\frac{1}{3a}(2a+a)\mathrm{e}^{2at}=\mathrm{e}^{2at}\,. \quad ✓ \tag{16}$$

S.C7.6 General first-order differential equation

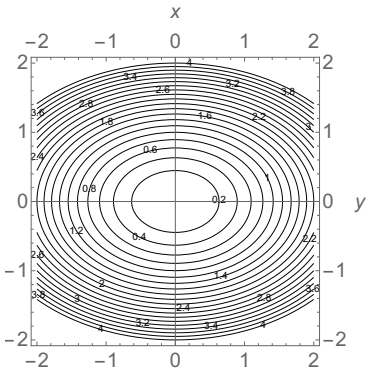
EC7.6.1 Field lines in two dimensions

Field lines are curves $\mathbf{r}(t)$ such that $\dot{\mathbf{r}}\parallel\mathbf{F}=(-ay,\,x)^T$, i.e. $\dot{x}(t)\sim -ay,\ \dot{y}(t)\sim x$.

This yeilds a DE for the field lines:

$$\frac{\mathrm{d}y}{\mathrm{d}x}=\frac{\dot{y}}{\dot{x}}=\frac{x}{-ay} \qquad \Rightarrow \qquad \int_{y_0}^{y}\mathrm{d}\tilde{y}(-a\tilde{y})=\int_{x_0}^{x}\mathrm{d}\tilde{x}\tilde{x}$$
$$\frac{-a}{2}\left(y^2-y_0^2\right)=\frac{1}{2}\left(x^2-x_0^2\right) \quad \Rightarrow \quad x^2+ay^2=\text{const.}$$

For $a>0$, this equation forms an ellipse.



S.C7.7 nth-order differential equation

S.C7.8 Linearizing differential equations

EC7.8.1 Fixed points of a differential equation in one dimension

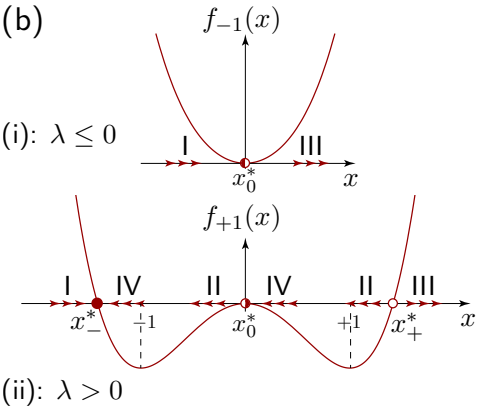
Differential equation: $\dot{x} = f_\lambda(x) = (x^2 - \lambda)^2 - \lambda^2$.

(a) Fixed points: $f_\lambda(x^*) = 0 \Rightarrow (x^*)^2 = \pm\lambda + \lambda$.

(i) For $\lambda \leq 0$ there is a single fixed point: $x_0^* = 0$.

(ii) For $\lambda > 0$ there are three fixed points: $x_-^* = -\sqrt{2\lambda}$, $x_0^* = 0$, $x_+^* = \sqrt{2\lambda}$.

(b)



(c) The stability of a fixed point is determined by the sign of $\dot{x} = f_\lambda(x)$ directly to the left and right of the fixed point, i.e. at $x = x^* \mp \epsilon$ (with $\epsilon \to 0^+$):

Left of x^*: for $\dot{x} = f_\lambda(x^* - \epsilon)$
- > 0, $x(t)$ increases $\Rightarrow$ flows towards x^*. (I)
- < 0, $x(t)$ decreases $\Rightarrow$ flows away from x^*. (II)

Right of x^*: for $\dot{x} = f_\lambda(x^* + \epsilon)$
- > 0 $x(t)$, increases $\Rightarrow$ flows away from x^*. (III)
- < 0 $x(t)$, decreases $\Rightarrow$ flows towards x^*. (IV)

Via a graphical analysis (see sketch) we find that:

(i) $\lambda \leq 0$: x_0^* is semistable (see I,III).

(ii) $\lambda > 0$: x_-^* is stable (see I,IV); x_0^* semistable (see II,IV); x_+^* unstable (see II,III).

EC7.8.3 Stability analysis in two dimensions

(a) Expressed in vector notation, the differential equation reads:

$$\begin{pmatrix}\dot{x}\\ \dot{y}\end{pmatrix} = \begin{pmatrix}2x^2 - xy\\ c(1-x)\end{pmatrix} \quad \Rightarrow \quad \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}), \quad \text{with} \quad \mathbf{x} = \begin{pmatrix}x\\ y\end{pmatrix}, \quad \mathbf{f}(x) = \begin{pmatrix}2x^2 - xy\\ c(1-x)\end{pmatrix}$$

Fixed point: $\mathbf{f}(\mathbf{x}^*) = \mathbf{0} \Rightarrow x^* = 1,\ y^* = 2x^* = 2,\ \mathbf{x}^* = \begin{pmatrix}1\\ 2\end{pmatrix}$

(b) Explicit insertion of $\mathbf{x} = \mathbf{x}^* + \boldsymbol{\eta} = \begin{pmatrix}1+\eta^1\\ 2+\eta^2\end{pmatrix}$ into the DE:

DE:
$$\dot{\mathbf{x}} = \dot{\boldsymbol{\eta}} = \begin{pmatrix}2(1+\eta^1)^2 - (1+\eta^1)(2+\eta^2)\\ c(1-(1+\eta^1))\end{pmatrix}$$

linear order:
$$= \begin{pmatrix}2\eta^1 - \eta^2\\ -c\eta^1\end{pmatrix} = \begin{pmatrix}2 & -1\\ -c & 0\end{pmatrix}\begin{pmatrix}\eta^1\\ \eta^2\end{pmatrix} = A\boldsymbol{\eta}.$$

(c) $\left(\frac{\partial f^i}{\partial x^j}\right) = \begin{pmatrix} \frac{\partial f^1}{\partial x} & \frac{\partial f^1}{\partial y} \\ \frac{\partial f^2}{\partial x} & \frac{\partial f^2}{\partial y} \end{pmatrix} = \begin{pmatrix} 4x-y & -x \\ -c & 0 \end{pmatrix} \quad \Rightarrow \quad \left(\frac{\partial f^i}{\partial x^j}\right)\Big|_{\mathbf{x}=\mathbf{x}^*} = \begin{pmatrix} 2 & -1 \\ -c & 0 \end{pmatrix} = A.\checkmark$

(d) Determination of the eigenvalues and eigenvectors of A:

Eigenvalues: $0 \stackrel{!}{=} \det(A-\lambda\mathbb{1}) = \begin{vmatrix} 2-\lambda & -1 \\ -c & -\lambda \end{vmatrix} = (2-\lambda)(-\lambda) - c = \lambda^2 - 2\lambda - c$

$\lambda_\pm = 1 \pm \frac{1}{2}\sqrt{4+4c} = 1 \pm \sqrt{1+c}\,.$

Eigenvectors: $\mathbf{0} \stackrel{!}{=} (A-\lambda_\pm\mathbb{1})\mathbf{v}_\pm = \begin{pmatrix} 2-\lambda_\pm & -1 \\ -c & -\lambda_\pm \end{pmatrix}\mathbf{v}_\pm \quad \Rightarrow \quad \mathbf{v}_\pm = \begin{pmatrix} \lambda_\pm \\ -c \end{pmatrix}.$

(e) For short times, the time-dependence of a displacement in the $\mathbf{v}_\pm$-direction is given by $\boldsymbol{\eta}_\pm(t) = \boldsymbol{\eta}_\pm(0)\mathrm{e}^{\lambda_\pm t}$. The fixed point is unstable in the $\mathbf{v}_+$-direction, since the eigenvalue λ_+ is strictly positive (we set $c > 0$). The fixed point is stable in the $\mathbf{v}_-$-direction (since $\lambda_- < 0$). The characteristic timescale, for which the displacement $\eta_\pm(t)$ grows or shrinks respectively, is given by $\tau_\pm = |\lambda_\pm|^{-1}$.

Check your results: For $c = 3$, we have $\lambda_\pm = 1 \pm 2 = \left\{ \begin{smallmatrix} 3 \\ -1 \end{smallmatrix} \right\}$, $\mathbf{v}_+ = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, $\mathbf{v}_- = \begin{pmatrix} -1 \\ -3 \end{pmatrix}$.

S.C7.9 Partial differential equations

S.C8 Functional calculus

S.C8.1 Definitions

S.C8.2 Functional derivative

S.C8.3 Euler-Lagrange equations

S.C9 Calculus of complex functions

S.C9.1 Holomorphic functions

EC9.1.1 Cauchy-Riemann equations

(a) $\mathrm{e}^z = \mathrm{e}^{x+\mathrm{i}y} = \mathrm{e}^x\mathrm{e}^{\mathrm{i}y} = \mathrm{e}^x\cos y + \mathrm{i}\mathrm{e}^x \sin y\,, \quad \Rightarrow \quad u(x,y) = \mathrm{e}^x\cos y,\ v(x,y) = \mathrm{e}^x\sin y\,.$

$$\begin{aligned} \partial_x u &= \mathrm{e}^x\cos y\,, & \partial_y v &= \mathrm{e}^x\cos y\,, & &\Rightarrow & \partial_x u &= \partial_y v\,.\checkmark \\ \partial_y u &= -\mathrm{e}^x\sin y\,, & \partial_x v &= \mathrm{e}^x\sin y\,, & &\Rightarrow & \partial_y u &= -\partial_x v\,.\checkmark \end{aligned}$$

The Cauchy-Riemann equations are satisfied. This was to be expected, because e^z depends on x and y only as a combined variable $z = x + \mathrm{i}y$.

(b) $\bar{z}^2 = (x - \mathrm{i}y)^2 = (x^2 - y^2) - \mathrm{i}2xy\,, \quad \Rightarrow \quad u(x,y) = x^2 - y^2\,,\ v(x,y) = -2xy\,.$

$$\begin{aligned} \partial_x u &= 2x\,, & \partial_y v &= -2x\,, & \Rightarrow \quad & \partial_x u \neq \partial_y v\,. \checkmark \\ \partial_y u &= -2y\,, & \partial_x v &= -2y\,, & \Rightarrow \quad & \partial_y u \neq -\partial_x v\,. \checkmark \end{aligned}$$

The Cauchy-Riemann equations are not satisfied. This was to be expected, because $\bar{z}^2$ does not depend on x and y as a combined variable $z = x + \mathrm{i}y$, but rather depends on $\bar{z} = x - \mathrm{i}y$.

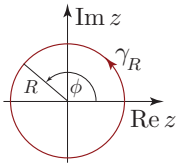
S.C9.2 Complex integration

ɛC9.2.1 Cauchy's theorem

Given: the analytic function $f(z) = \mathrm{e}^z$, with antiderivative $F(z) = \mathrm{e}^z$. A path integral of this function along a path $\gamma(t)$, with $t \in [0,1]$, has the form:

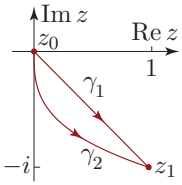
$$I_\gamma = \int_\gamma \mathrm{d}z\, f(z) = \int_0^1 \mathrm{d}t\, \frac{\gamma(t)}{\mathrm{d}t} f(\gamma(t)) = \int_{\gamma(0)}^{\gamma(1)} \mathrm{d}\gamma\, F'(\gamma) = F(\gamma(1)) - F(\gamma(0))\,.$$

(a) Parametrization of the circle: $\gamma_R(t) = R\,\mathrm{e}^{\mathrm{i}2\pi t}$, with $t \in [0,1]$.



$$\begin{aligned} I_{\gamma_R} &= \oint_{\gamma_R} \mathrm{d}z\, f(z) = \int_0^1 \mathrm{d}t \frac{\mathrm{d}\gamma_R}{\mathrm{d}t} f(\gamma(t)) = \int_0^1 \mathrm{d}t\, (\mathrm{i}2\pi R\,\mathrm{e}^{\mathrm{i}2\pi t})\, \mathrm{e}^{R\,\mathrm{e}^{\mathrm{i}2\pi t}} \\ &= \left[\mathrm{e}^{R\,\mathrm{e}^{\mathrm{i}2\pi t}}\right]_0^1 = \mathrm{e}^{R\,\mathrm{e}^{2\pi\mathrm{i}}} - \mathrm{e}^{R\,\mathrm{e}^0} = \mathrm{e}^{R\cdot 1} - \mathrm{e}^{R\cdot 1} = 0\,. \quad [\text{as expected} \checkmark] \end{aligned}$$

(b) (i) Parametrization of the line: $\gamma_1(t) = (1 - \mathrm{i})t$, with $t \in [0,1]$.



$$I_{\gamma_1} = \int_0^1 \mathrm{d}t \frac{\mathrm{d}\gamma_1}{\mathrm{d}t} f(\gamma(t)) = \int_0^1 \mathrm{d}t\, (1 - \mathrm{i})\mathrm{e}^{(1-\mathrm{i})t} = \left[\mathrm{e}^{(1-\mathrm{i})t}\right]_0^1 = \mathrm{e}^{1-\mathrm{i}} - 1\,.$$

(ii) Parametrization of the curve: $\gamma_2(t) = t^3 - \mathrm{i}t$, with $t \in [0,1]$.

$$I_{\gamma_2} = \int_0^1 \mathrm{d}t \frac{\mathrm{d}\gamma_2}{\mathrm{d}t} f(\gamma(t)) = \int_0^1 \mathrm{d}t\, (3t^2 - \mathrm{i})\mathrm{e}^{t^3 - \mathrm{i}t} = \left[\mathrm{e}^{t^3 - \mathrm{i}t}\right]_0^1 = \mathrm{e}^{1-\mathrm{i}} - 1\,.$$

As expected, we obtain $I_1 = I_2 = \mathrm{e}^{1-\mathrm{i}} - 1 = F(z_1) - F(z_0)$. ✓

S.C9.3 Singularities

EC9.3.1 Laurent series, residues

(a) The Taylor series of $p(z)$ about z_0 reads: $p(z) = \sum_{\bar{n}=0}^{k} \frac{p^{(\bar{n})}(z_0)}{\bar{n}!}(z-z_0)^{\bar{n}}$. Consequently, the Laurent series of $f_m(z)$ about z_0 has the following form:

$$f_m(z) = \frac{p(z)}{(z-z_0)^m} = \sum_{\bar{n}=0}^{k} \frac{p^{(\bar{n})}(z_0)}{\bar{n}!}(z-z_0)^{\bar{n}-m} \overset{n=\bar{n}-m}{=} \sum_{n=-m}^{k-m} \frac{p^{(n+m)}(z_0)}{(n+m)!}(z-z_0)^n .$$

(b) The Laurent series of $f_m(z) = \frac{z^3}{(z-2)^m}$ about $z_0 = 2$ follows from the Taylor series of $p(z) = z^3$ about z_0. With $p^{(1)}(z) = 3z^2$, $p^{(2)}(z) = 6z$ and $p^{(3)}(z) = 6$ we obtain:

$$p(z) = \sum_{\bar{n}=0}^{3} \frac{p^{(\bar{n})}(2)}{\bar{n}!}(z-2)^{\bar{n}} = 2^3 + 3\cdot 2^2(z-2) + \tfrac{1}{2!}6\cdot 2(z-2)^2 + \tfrac{1}{3!}6(z-2)^3 .$$

$$f_m(z) = \frac{p(z)}{(z-2)^m} = 8(z-2)^{-m} + 12(z-2)^{1-m} + 6(z-2)^{2-m} + (z-2)^{3-m} .$$

(c) The residues of $f_m(z)$ at $z_0 = 2$ (pole of order m) read:

$$\mathrm{Res}(f_m, 2) = \lim_{z\to 2} \frac{1}{(m-1)!}\frac{\mathrm{d}^{m-1}}{\mathrm{d}z^{m-1}}\left[(z-2)^m f_m(z)\right] = \lim_{z\to z_0} \frac{1}{(m-1)!}\frac{\mathrm{d}^{m-1}}{\mathrm{d}z^{m-1}}\left[z^3\right] .$$

$$\mathrm{Res}(f_1, 2) = \lim_{z\to 2} z^3 = 8 . \qquad \mathrm{Res}(f_2, 2) = \lim_{z\to 2} \frac{\mathrm{d}}{\mathrm{d}z} z^3 = \lim_{z\to 2} 3z^2 = 12 .$$

$$\mathrm{Res}(f_3, 2) = \lim_{z\to 2} \frac{1}{2!}\frac{\mathrm{d}^2}{\mathrm{d}z^2} z^3 = \lim_{z\to 2} \frac{3!}{2!} z = 6 . \qquad \mathrm{Res}(f_4, 2) = \lim_{z\to 2} \frac{1}{3!}\frac{\mathrm{d}^3}{\mathrm{d}z^3} z^3 = \lim_{z\to 2} \frac{3!}{3!} = 1 .$$

$$\mathrm{Res}(f_m, 2) = \lim_{z\to 2} \frac{1}{(m-1)!}\frac{\mathrm{d}^{m-1}}{\mathrm{d}z^{m-1}} z^3 = 0 \quad \text{for} \quad m \geq 5 .$$

As expected, the residue $\mathrm{Res}(f_m, 2)$ corresponds to the coefficient of $(z-2)^{-1}$ in the Laurent series of $f_m(z)$ presented in (b). ✓

S.C9.4 Residue theorem

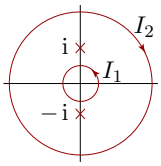
EC9.4.1 Circular contours, residue theorem

(a) With the parametrization $z(\phi) = R\mathrm{e}^{\mathrm{i}\phi}$ and $\phi \in [0, \pm k2\pi]$ for $I_\pm^{(k)}$ we obtain:

$$\left.\begin{aligned} I_+^{(k)} &= \oint_{|z|=R} \frac{\mathrm{d}z}{z} \\ I_-^{(k)} &= \oint_{|z|=R} \frac{\mathrm{d}z}{z} \end{aligned}\right\} = \int_0^{\pm k2\pi} \mathrm{d}\phi \, \frac{\mathrm{d}z(\phi)}{\mathrm{d}\phi}\frac{1}{z(\phi)} = \int_0^{\pm k2\pi} \mathrm{d}\phi \, \frac{\mathrm{i}R\mathrm{e}^{\mathrm{i}\phi}}{R\mathrm{e}^{\mathrm{i}\phi}} = \pm k2\pi\mathrm{i} .$$

Note: This result holds in general: when $g(z)$ has an isolated pole at z_0, and the contour γ_k circles this pole k times in the mathematically positive (resp. negative) direction, then $\oint_{\gamma_k} \mathrm{d}z\, g(z) = \pm k 2\pi\mathrm{i}\,\mathrm{Res}(g, z_0)$.

(b) The function $g(z)$ has two poles of order 1 at $z_\pm = \pm\mathrm{i}$:



$$g(z) = \frac{\mathrm{e}^{\mathrm{i}az}}{z^2+1} = \frac{\mathrm{e}^{\mathrm{i}z}}{(z-\mathrm{i})(z+\mathrm{i})} = \frac{\mathrm{e}^{\mathrm{i}z}}{(z-z_+)(z-z_-)}.$$

The corresponding residues are:

$$\mathrm{Res}(g, z_\pm) = \lim_{z\to z_\pm}\left[(z-z_\pm)\,\frac{\mathrm{e}^{\mathrm{i}az}}{(z-z_+)(z-z_-)}\right] = \frac{\mathrm{e}^{\mathrm{i}z_\pm}}{(z_\pm - z_\mp)} = \frac{\mathrm{e}^{\mp a}}{\pm 2\mathrm{i}}\,.$$

For $I_1 = \oint_{|z|=\frac{1}{2}} \mathrm{d}z\, g(z)$ both poles lie outside the integration contour, $\Rightarrow\ I_1 = 0$.

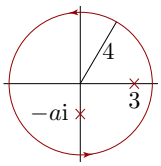
For $I_2 = \oint_{2\,\text{times: }|z|=2} \mathrm{d}z\, g(z)$ both poles lie inside the integration contour, hence we get

$$I_2(a) = -2\cdot 2\pi\mathrm{i}\Big[\mathrm{Res}(g, z_+) + \mathrm{Res}(g, z_-)\Big] = -4\pi\mathrm{i}\frac{\mathrm{e}^{-a}-\mathrm{e}^{a}}{2\mathrm{i}} = 4\pi\sinh a\,.$$

(c) The poles of $f(z)$ are located at the zeroes of the denominator. The hint then implies that the denominator contains a factor of $(z + a\mathrm{i})$. Using polynomial division, we can factorize as follows:

$$z^3 + (a\mathrm{i}-6)z^2 + (9 - a6\mathrm{i})z + 9a\mathrm{i} = (z+a\mathrm{i})(z^2-6z+9) = (z+a\mathrm{i})(z-3)^2\,.$$

Consequently $f(z)$ has one pole of order 1 at $z_a = -a\mathrm{i}$ and a pole of order 2 at $z_3 = 3$:



$$f(z) = \frac{z}{z^3 + (a\mathrm{i}-6)z^2 + (9-a6\mathrm{i})z + 9a\mathrm{i}} = \frac{z}{(z-z_a)(z-z_3)^2}\,.$$

The residues are thus:

$$\mathrm{Res}(f, z_a) = \lim_{z\to z_a}\big[(z-z_a)\,f(z)\big] = \frac{z_a}{(z_a-z_3)^2} = \frac{-a\mathrm{i}}{(-a\mathrm{i}-3)^2}\,.$$

$$\mathrm{Res}(f, z_3) = \lim_{z\to z_3}\frac{\mathrm{d}}{\mathrm{d}z}\big[(z-z_3)^2 g(z)\big] = \lim_{z\to z_3}\frac{\mathrm{d}}{\mathrm{d}z}\frac{z}{z-z_a} = \frac{(z_3-z_a)-z_3}{(z_3-z_a)^2} = \frac{a\mathrm{i}}{(3+a\mathrm{i})^2}\,.$$

The integration contour $|z| = 4$ encloses both poles for $a < 4$, however only encloses the pole at $z_2 = 3$ for $a > 4$. Hence:

$$I_3(a) = \oint_{|z|=4} \mathrm{d}z\, f(z) = \begin{cases} 2\pi\mathrm{i}\Big[\mathrm{Res}(f, -a\mathrm{i}) + \mathrm{Res}(f, 3)\Big] = 0\,, & \text{for } a < 4\,, \\ 2\pi\mathrm{i}\Big[\mathrm{Res}(f, 3)\Big] = -\frac{2\pi a}{(3+a\mathrm{i})^2}\,, & \text{for } a > 4\,. \end{cases}$$

To see that I_3 vanishes in the first case, we notice that: for $a < 4$, both poles lie inside the integration contour, and hence the circular contour with radius $|z| = 4$ may be extended to a circle with radius $R \to \infty$ without crossing any poles. Because the integrand vanishes as $f(z) \sim z^{-2} \sim R^{-2}$ for large arguments, while the integration measure only grows proportionally to R, the integral vanishes:

$$I_3(a<4) = \lim_{R\to\infty} \oint_{|z|=R} \mathrm{d}z\, f(z) = \lim_{R\to\infty} \oint_{|z|=R} \frac{\mathrm{d}z}{z} = \lim_{R\to\infty} \int_0^{2\pi} \mathrm{d}\phi \frac{\mathrm{i}R\mathrm{e}^{\mathrm{i}\phi}}{(\mathrm{i}R\mathrm{e}^{\mathrm{i}\phi})^2} = 0\,. \checkmark$$

Note: This is an example of the following general fact: If a complex path integral $I_\gamma = \oint_\gamma \mathrm{d}z f(z)$ encloses all poles of $f(z)$, then it may be extended to a circular path with radius $R \to \infty$, without crossing any poles. The integral $I_\gamma = \lim_{R\to\infty} \oint \mathrm{d}z f(z)$ will vanish as long as the integrand has the property $\lim_{|z|\to\infty}\big[z f(z)\big] = 0$.

Hence it follows that, for such functions, the sum of all the residues is always equal to zero – a useful consistency check! (Although this does not apply to part (b), because along the imaginary axis, where $z = \mathrm{i}y$ and $f(\mathrm{i}y) \propto e^{-ay}$, the limit $\lim_{y\to-\infty}\big[(\mathrm{i}y)f(\mathrm{i}y)\big] = \infty$.)

ᴇC9.4.3 Integrating by closing contour and using residue theorem

We regard the integral (with $a, b \in \mathbb{r}$) as a contour integral in the complex plane,

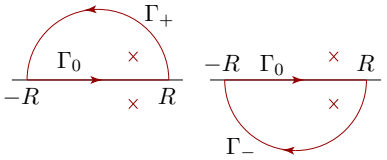
$$I(a,b) = \int_{-\infty}^{\infty} \mathrm{d}x\, f(x) = \lim_{R\to\infty} \int_{\Gamma_0} \mathrm{d}z\, f(z)\,, \quad \text{with} \quad f(z) = \frac{1}{z^2 - 2za + a^2 + b^2}\,,$$

where $\Gamma_0 : \{z(x) = x \,|\, x \in [-R, R]\}$ is a section of the real axis. The integrand has two poles of first order, at $z_\pm = a \pm \mathrm{i}|b|$ in the upper/lower half plane respectively:

$$f(z) = \frac{1}{(z - a - \mathrm{i}|b|)(z - a + \mathrm{i}|b|)} = \frac{1}{(z - z_+)(z - z_-)}\,.$$

Residues: $$\mathrm{Res}(f, z_\pm) = \lim_{z\to z_\pm}\big[(z - z_\pm) f(z)\big] = \lim_{z\to z_\pm} \frac{1}{(z - z_\mp)} = \frac{1}{z_\pm - z_\mp} = \frac{1}{\pm 2\mathrm{i}|b|}\,. \quad (1)$$

In order to use the residue theorem, we require a closed contour. We therefore insert the path Γ_0, a half circle about the origin with radius R. We can insert this circle in either the upper or lower half-planes; which we label Γ_+ and Γ_- respectively. The choice is arbitrary since in both cases $\int_{\Gamma_\pm} \mathrm{d}z\, f(z)$ vanishes in the limit $R \to \infty$. This can be seen as follows: The parametrization $\Gamma_\pm : \{z(\phi) = R\mathrm{e}^{\mathrm{i}\phi} | \phi \in [0, \pm\pi]\}$ gives



$$\int_{\Gamma_\pm} \mathrm{d}z\, f(z) = \int_0^{\pm\pi} \mathrm{d}\phi \frac{\mathrm{d}z(\phi)}{\mathrm{d}\phi} f(z(\phi)) \overset{R\to\infty}{\longrightarrow} \int_0^{\pm\pi} \mathrm{d}\phi \,(\mathrm{i}R\mathrm{e}^{\mathrm{i}\phi}) \frac{1}{(R\mathrm{e}^{\mathrm{i}\phi})^2} = 0\,.$$

The two different integrations paths, $\Gamma_0 \cup \Gamma_+ =$  and $\Gamma_0 \cup \Gamma_- =$  , both encircle a single pole, z_+ and z_- respectively. The different paths are traversed in the mathematically

positive or negative directions respectively, which contribute a plus or minus sign in the residue theorem, cancelling the sign from the poles, and thus giving the same result:

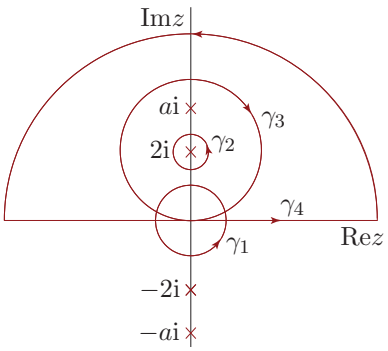
$$I(a,b) = \lim_{R\to\infty} \left\{ \begin{array}{l} \displaystyle\int_{\curvearrowleft} \mathrm{d}z\, f(z) \\ \displaystyle\int_{\curvearrowright} \mathrm{d}z\, f(z) \end{array} \right\} = \pm 2\pi\mathrm{i}\,\mathrm{Res}(f, z_\pm) \overset{(1)}{=} \pm 2\pi\mathrm{i}\,\frac{1}{\pm 2\mathrm{i}|b|} = \frac{\pi}{|b|}\,.$$

Note: The above strategy of enclosing a contour in the upper/lower half planes is always possible whenever $\lim_{|z|\to\infty}\big[zf(z)\big] = 0$. This applies, for example, to any rational function of the form $f(z) = p(z)/q(z)$, with polynomials $p(z)$ and $q(z)$ of degree n_p and n_q respectively, whenever $n_p \le n_q - 2$.

EC9.4.5 Various integration paths, residue theorem

(a) The function $f(z)$ has four poles of order 1, at $z_2^\pm = \pm 2\mathrm{i}$ and at $z_a^\pm = \pm a\mathrm{i}$:

$$f(z) = \frac{z^2}{(z^2+4)(z^2+a^2)} = \frac{z^2}{(z-z_2^+)(z-z_2^-)(z-z_a^+)(z-z_a^-)}\,.$$



The associated residues read:

$$\mathrm{Res}(f, z_2^\pm) = \lim_{z\to z_2^\pm}\big[(z-z_2^\pm)f(z)\big] = \frac{(z_2^\pm)^2}{(z_2^\pm - z_2^\mp)((z_2^\pm)^2+a^2)} = \frac{-4}{2(\pm 2\mathrm{i})(a^2-4)} = \frac{\pm\mathrm{i}}{a^2-4}\,.$$

$$\mathrm{Res}(f, z_a^\pm) = \lim_{z\to z_a^\pm}\big[(z-z_a^\pm)f(z)\big] = \frac{(z_a^\pm)^2}{((z_a^\pm)^2+4)(z_a^\pm - z_a^\mp)} = \frac{-a^2}{(a^2-4)2(\pm a\mathrm{i})} = \frac{\mp\mathrm{i}a}{2(a^2-4)}\,.$$

(b) The circular path γ_1 does not encircle any poles, and therefore $I_{\gamma_1} = \int_{\gamma_1} \mathrm{d}z\, f(z) = 0$.

γ_2 encloses the pole at z_2^+, and γ_3 encloses both the poles z_2^+ and z_a^+. Consequently, we have:

(c) $$I_{\gamma_1} = \int_{\gamma_1} \mathrm{d}z\, f(z) = 2\pi\mathrm{i}\,\mathrm{Res}(f, z_2^+) = -\frac{2\pi}{a^2-4}\,.$$

(d) $$I_{\gamma_3} = \int_{\gamma_3} \mathrm{d}z\, f(z) = -2\pi\mathrm{i}\big[\mathrm{Res}(f, z_2^+) + \mathrm{Res}(f, z_2^+)\big] = \frac{2\pi(1-\frac{1}{2}a)}{a^2-4}\,.$$

(e) The path γ_4 along the real axis can be calculated by closing it with a half-circle of radius $\to\infty$ in the upper or lower half planes, since $\lim_{|z|\to\infty}\big[zf(z)\big] = 0$. We choose the upper half-plane, because it allows us to use the fact that $\curvearrowleft$ encloses that same poles as γ_3. Because the direction of travel is reversed, we have $I_{\gamma_4} = I_{\curvearrowleft} = -I_{\gamma_3}$.

EC9.4.7 Inverse Fourier transform via contour closure

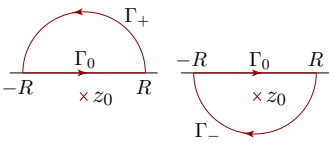
(a) We consider the Fourier integral (with $t \neq 0$) as a path integral in the complex plane:

$$G(t) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}\omega t}}{a - \mathrm{i}\omega} = \lim_{R\to\infty} \int_{\Gamma_0} \mathrm{d}z\, f(z)\,, \quad \text{with} \quad f(z) = \frac{1}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}zt}}{a - \mathrm{i}z} \quad (0 < a \in \mathbb{R})\,,$$

where $\Gamma_0 : \{z(x) = x \,|\, x \in [-R, R]\}$ is a section of the real axis. The integrand has a single pole of first order at $z_0 = -\mathrm{i}a$, with residue

$$\mathrm{Res}(f, z_0) = \lim_{z\to z_0} \big[(z - z_0) f(z)\big] = \lim_{z\to -\mathrm{i}a} \left[\frac{(z + \mathrm{i}a)}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}zt}}{-\mathrm{i}(z + \mathrm{i}a)}\right] = \frac{\mathrm{e}^{-at}}{-2\pi\mathrm{i}}\,. \tag{1}$$

In order to use the residue theorem, we require a closed contour. To this end, we close the path Γ_0 by a semicircle about the origin of radius R. We choose this semicircle to be in either the upper or lower half-plane depending on the sign of t, and we denote the resulting contours as Γ_+ and Γ_- respectively. This is in order to ensure that the semicircular integral $\int_{\Gamma_\pm} \mathrm{d}z\, f(z)$ vanishes as $R \to \infty$.



Using the parametrization $\Gamma_\pm$: $\{z(\phi) = R\mathrm{e}^{\mathrm{i}\phi} | \phi \in [0, \pm\pi]\}$ gives

$$\int_{\Gamma_\pm} \mathrm{d}z\, f(z) = \int_0^{\pm\pi} \mathrm{d}\phi\, \frac{\mathrm{d}z(\phi)}{\mathrm{d}\phi} f(z(\phi)) = \int_0^{\pm\pi} \mathrm{d}\phi \left(\mathrm{i}R\mathrm{e}^{\mathrm{i}\phi}\right) \frac{1}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}tR(\cos\phi + \mathrm{i}\sin\phi)}}{a - \mathrm{i}z}\,.$$

The vanishing of the integrand in the limit $R \to \infty$ is determined by the following factor:

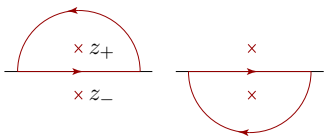
$$\mathrm{e}^{tR\sin\phi} \overset{R\to\infty}{\longrightarrow} \begin{cases} 0 & \text{for} \quad t\sin\phi < 0\,, \\ \infty & \text{for} \quad t\sin\phi > 0\,. \end{cases}$$

To ensure that the semicircular integral vanishes, we require the first case. Thus, for $t < 0$ or $t > 0$ we choose the contour such that $\sin\phi > 0$ or < 0 respectively, i.e. Γ_+ or Γ_-. The pole of $f(z)$ lies in the lower half plane, and so is not enclosed by the contour $\circlearrowleft = \Gamma_0 \cup \Gamma_+$. It is, however, enclosed by the contour $\circlearrowright = \Gamma_0 \cup \Gamma_-$ (which is traversed in the mathematically negative direction, and so picks up a negative sign in the residue theorem). Thus we conclude that:

$$\left.\begin{aligned} G(t < 0) &= I_{\circlearrowleft} \mathrm{d}z\, f(z) = 0\,. \\ G(t > 0) &= I_{\circlearrowright} \mathrm{d}z\, f(z) = -2\pi\mathrm{i}\,\mathrm{Res}(f, z_0) \overset{(1)}{=} \mathrm{e}^{-a|t|}\,. \end{aligned}\right\} \quad \Rightarrow \quad G(t) = \theta(t)\,\mathrm{e}^{-at}\,. \checkmark$$

(b) The procedure here is analogous to (a). The integral has the form $L(t) = \int_{-\infty}^{\infty} \mathrm{d}z\, f(z)$, with

$$f(z) = \frac{\mathrm{e}^{-\mathrm{i}zt}}{2\pi} \tilde{L}(z) = \frac{a\,\mathrm{e}^{-\mathrm{i}zt}}{\pi(z^2 + a^2)} = \frac{a\,\mathrm{e}^{-\mathrm{i}zt}}{\pi(z - z_+)(z - z_-)}\,.$$



Hence $f(z)$ has two poles of order 1, at $z_\pm = \pm \mathrm{i}a$, with residue

$$\mathrm{Res}(f, z_\pm) = \lim_{z \to z_\pm} \big[(z - z_\pm) f(z)\big] = \frac{a\,\mathrm{e}^{-\mathrm{i}z_\pm t}}{\pi(z_\pm - z_\mp)} = \frac{a\,\mathrm{e}^{\pm at}}{\pi(\pm 2\mathrm{i}a)} = \frac{\mathrm{e}^{\pm at}}{\pm 2\pi\mathrm{i}}\,. \tag{2}$$

For $t < 0$ or $t > 0$ we close the contour in the upper or lower half-planes respectively:

$$\left.\begin{aligned} L(t<0) &= I_{\curvearrowright} \mathrm{d}z\, f(z) = 2\pi\mathrm{i}\,\mathrm{Res}(f, z_+) \overset{(1)}{=} \mathrm{e}^{+at} \\ L(t>0) &= I_{\curvearrowleft} \mathrm{d}z\, f(z) = -2\pi\mathrm{i}\,\mathrm{Res}(f, z_-) \overset{(1)}{=} \mathrm{e}^{-at} \end{aligned}\right\} \quad \Rightarrow \quad L(t) = \mathrm{e}^{-a|t|}\,. \checkmark$$

As expected, the inverse Fourier transform of the Lorentz function has given us back the exponential function $\mathrm{e}^{-a|t|}$, which was the starting point for our calculations.

S.C9.5 Essential Singularities

S.C9.6 Riemann surfaces

SV Solutions: Vector Calculus

S.V1 Curves

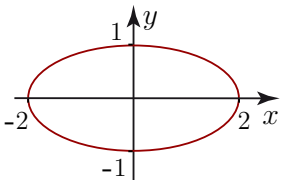
S.V1.2 Curve velocity

EV1.2.1 Velocity and acceleration

(a) Compact notation: $C(t) = \cos\left[\pi\left(1-\cos\omega t\right)\right]$, $S(t) = \sin\left[\pi((1-\cos\omega t)\right]$, with $C^2 + S^2 = 1$.
Derivatives: $\dot{C} = -\omega\pi\sin(\omega t)S$, $\dot{S} = \omega\pi\sin(\omega t)C$.

$$\begin{aligned}\mathbf{r}(t) &= \big(aC, S\big)^T, \qquad \dot{\mathbf{r}}(t) = \omega\pi\sin(\omega t)\big(-aS, C\big)^T \\ \ddot{\mathbf{r}}(t) &= \omega^2\pi\cos(\omega t)\big(-aS, C\big)^T - [\omega\pi\sin(\omega t)]^2\big(aC, S\big)^T \\ &= \omega\cot(\omega t)\dot{\mathbf{r}} - [\omega\pi\sin(\omega t)]^2\mathbf{r}\end{aligned}$$

(b) Parameter-free representation: $(x/a)^2 + y^2 = 1$. This traces out an ellipse. The illustration shows the case for $a = 2$.

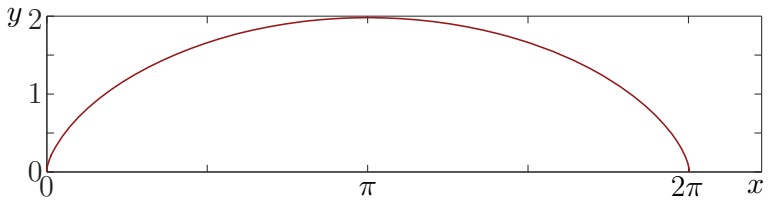


(c) $\mathbf{r}(t)\cdot\dot{\mathbf{r}}(t) = \pi\omega\sin(\omega t)\,CS(a^2-1)$; vanishes when $a = 1$, which is the special case of a circle. For a circular trajectory, the velocity vector is perpendicular to the position vector at every point.

S.V1.3 Curve length

EV1.3.1 Natural parametrization of a curve

(a)



(b) $\mathbf{r}(t) = \big(t-\sin t, 1-\cos t\big)^T$, $\dot{\mathbf{r}}(t) = \big(1-\cos t, \sin t\big)^T$

$\|\dot{\mathbf{r}}(t)\| = \sqrt{(1-\cos t)^2 + (\sin t)^2} = \sqrt{1-2\cos t+1} = 2|\sin(t/2)|$ $\quad\left[\cos 2A = 1-2\sin^2 A\right]$

For $t < 2\pi$, $\sin(t/2) > 0$, so the modulus signs may be omitted.

$$s(t) = \int_0^t \mathrm{d}u\, \|\dot{\mathbf{r}}(u)\| = \int_0^t \mathrm{d}u\, 2\sin(u/2) = -4\cos(u/2)\Big|_0^t = 4 - 4\cos(t/2)$$

(c) $t(s) = 2\arccos(1 - s/4) = 2\arccos\tilde{s}$, with $\tilde{s} = 1 - s/4$ [Inverse function of (b)]

$$\mathbf{r}_L(s) = \big(2\arccos\tilde{s} - \sin[2\arccos\tilde{s}]\,, 1 - \cos[2\arccos\tilde{s}]\,\big)^T$$
$$= \begin{pmatrix} 2\arccos\tilde{s} - 2\sin(\arccos\tilde{s})\cos(\arccos\tilde{s}) \\ 1 - \cos^2(\arccos\tilde{s}) + \sin^2(\arccos\tilde{s}) \end{pmatrix} = \begin{pmatrix} 2\arccos\tilde{s} - 2\sqrt{1-\tilde{s}^2}\tilde{s} \\ 1 - \tilde{s}^2 + 1 - \tilde{s}^2 \end{pmatrix}$$

S.V1.4 Line integral

ɛV1.4.1 Line integral: mountain hike

Strategy for the line integral $\int_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{F} = \int_I \mathrm{d}t\, \dot{\mathbf{r}}(t)\cdot\mathbf{F}(\mathbf{r}(t))$: find a parametrization $\mathbf{r}(t)$ of the curve, then determine $\dot{\mathbf{r}}(t)$, $\cdot\mathbf{F}(\mathbf{r}(t))$ and $\dot{\mathbf{r}}(t)\cdot\mathbf{F}(\mathbf{r}(t))$, then integrate.

Given: $\mathbf{r}_0 \equiv (0,0)^T$, $\mathbf{r}_1 \equiv (3,3a)^T$, $\mathbf{r}_2 \equiv (2,4a)^T$, $\mathbf{F}(\mathbf{r}) = \mathbf{F}_g + \mathbf{F}_w = (-y^2, -10)^T$.

Hiker 1: Path γ_1 is a straight line from $\mathbf{r}_0$ to $\mathbf{r}_1$ and hence has the form $y(x) = ax$. A possible parametrization, with $t = x \in (0,3)$ as curve parameter, is:

γ_1 :
$$\mathbf{r}(t) = (x(t), y(x))^T = (t, at)^T$$
$$\dot{\mathbf{r}}(t) = (1, a)^T,$$
$$\mathbf{F}(\mathbf{r}(t)) = \big(-y^2(t), -10\big)^T = (-a^2, -10)^T$$
$$\big[\dot{\mathbf{r}}(t)\cdot\mathbf{F}(\mathbf{r}(t))\big]_{\gamma_1} = -(a^2 + 10a)$$
$$W[\gamma_1] = -\int_{\gamma_1} \mathrm{d}\mathbf{r}\cdot\mathbf{F} = \int_0^3 \mathrm{d}t\, [a^2t^2 + 10a] = \big[\tfrac{1}{3}a^2t^3 + 10at\big]_0^3 = 9a^2 + 30a\,.$$

Hiker 2: Path γ_2 is a parabola with apex $\mathbf{r}_2 = (2,4a)^T$ and has the form $y(x) = -k(x-2)^2 + 4a$. Inserting $\mathbf{r}_0 = (0,0)^T$ or $\mathbf{r}_1 = (3,3a)^T$ yields the curvature, $k = a$. A possible parametrization, with $t = x \in (0,3)$ as curve parameter, is:

γ_2 :
$$\mathbf{r}(t) = (x(t), y(x))^T = (t, -a(t-2)^2 + 4a)^T$$
$$\dot{\mathbf{r}}(t) = (1, -2a(t-2))^T,$$
$$\mathbf{F}(\mathbf{r}(t)) = \big(-y^2(t), -10\big)^T = (-[-a(t-2)^2 + 4a]^2, -10)^T$$
$$\big[\dot{\mathbf{r}}(t)\cdot\mathbf{F}(\mathbf{r}(t))\big]_{\gamma_1} = -[-a(t-2)^2 + 4a]^2 + 20a(t-2)$$
$$W[\gamma_2] = -\int_{\gamma_2} \mathrm{d}\mathbf{r}\cdot\mathbf{F} = \int_0^3 \mathrm{d}t\, \Big[[-a(t-2)^2 + 4a]^2 - 20a(t-2)\Big]$$

$$= \int_0^3 \mathrm{d}t \left[a^2(t-2)^4 - 8a^2(t-2)^2 + 16a^2 - 20at + 40a\right]$$
$$= \left[\tfrac{1}{5}a^2(t-2)^5 - \tfrac{8}{3}a^2(t-2)^3 - 10at^2 + (16a^2+40a)t\right]_0^3$$
$$= \left(\tfrac{1}{5} - \tfrac{8}{3} + 48 + \tfrac{32}{5} - \tfrac{64}{3}\right)a^2 + (-90+120)\,a = \tfrac{153}{5}a^2 + 30a\,.$$

S.V2 Curvilinear Coordinates

S.V2.1 Polar coordinates

ᴇV2.1.1 Coordinate calculations

Cylindrical coordinates: $\rho = \sqrt{x^2+y^2}$, $\phi = \arctan(y/x) + n_\phi\pi$, $z = z$,
Spherical coordinates: $r = \sqrt{x^2+y^2+z^2}$, $\theta = \arccos(z/r)$, $\phi = \arctan(y/x) + n_\phi\pi$,

with $\theta \in (0,\pi)$, and $n_\phi \in \mathbb{Z}$ chosen such that $\phi \in (0,2\pi)$ lies in the correct quadrant.

P_1: $(x,y,z) = (3,-2,4)$, $(\rho,\phi,z) = (\sqrt{13}, 5.69, 4)$, $(r,\theta,\phi) = (\sqrt{29}, 0.73, 5.69)$
$x>0, y<0 \quad\Rightarrow\quad \phi$ lies in the 4th quadrant $\quad\Rightarrow\quad \phi \in (3\pi/2, 2\pi)$
$\phi = \arctan(-2/3) + 2\pi \approx -0.59 + 6.28 = 5.69$ (equals $326°$)
$\theta = \arccos(4/\sqrt{29}) \approx 0.73$ (equals $42°$)

P_2: $(x,y,z) = (1,1,1)$, $(\rho,\phi,z) = (\sqrt{2}, \pi/4, 1)$, $(r,\theta,\phi) = (\sqrt{3}, 0.96, \pi/4)$
$x>0, y>0 \quad\Rightarrow\quad \phi$ lies in the 1st quadrant $\quad\Rightarrow\quad \phi \in (0,\pi/2)$
$\phi = \arctan(1/1) = \pi/4$ (equals $45°$)
$\theta = \arccos(1/\sqrt{3}) \approx 0.96$ (equals $55°$)

P_3: $(x,y,z) = (-3,0,-2)$, $(\rho,\phi,z) = (3, \pi, -2)$, $(r,\theta,\phi) = (\sqrt{13}, 2.16, \pi)$
$x<0, y=0 \quad\Rightarrow\quad \phi$ lies on the negative x-axis $\quad\Rightarrow \phi = \pi$ (equals $180°$)
$\theta = \arccos(-2/\sqrt{13}) \approx 2.16$ (equals $124°$)

S.V2.2 Coordinate transformations

S.V2.3 Coordinate basis and local basis

S.V2.4 Cylindrical and spherical coordinates

ɛV2.4.1 Cylindrical coordinates: velocity, kinetic energy, angular momentum

In terms of the cylindrical coordinates $y_1 = \rho$, $y_2 = \phi$, $y_3 = z$, the Cartesian coordinates $x_i = x_i(y_i)$ are given by $x_1 = x = \rho\cos\phi$, $x_2 = y = \rho\sin\phi$, $x_3 = z$. We also have $\mathbf{e}_{x_i} \cdot \mathbf{e}_{x_j} = \delta_{ij}$.

Position vector: $\mathbf{r} = x\,\mathbf{e}_x + y\,\mathbf{e}_y + z\,\mathbf{e}_z = \rho\cos\phi\,\mathbf{e}_x + \rho\sin\phi\,\mathbf{e}_y + z\mathbf{e}_z = \rho\,\mathbf{e}_\rho + z\mathbf{e}_z$.

(a) Construction of the basis vectors: $\mathbf{v}_{y_i} = \partial\mathbf{r}/\partial y_i$, $v_{y_i} = \|\partial\mathbf{r}/\partial y_i\|$, $\mathbf{e}_{y_i} = \mathbf{v}_{y_i}/v_{y_i}$.

$$\begin{aligned}
&\mathbf{v}_\rho = \cos\phi\,\mathbf{e}_x + \sin\phi\,\mathbf{e}_y, && v_\rho = (\sin^2\phi + \cos^2\phi)^{\frac{1}{2}} = 1, && \mathbf{e}_\rho = \cos\phi\,\mathbf{e}_x + \sin\phi\,\mathbf{e}_y\,.\\
&\mathbf{v}_\phi = -\rho\sin\phi\,\mathbf{e}_x + \rho\cos\phi\,\mathbf{e}_y, && v_\phi = (\rho^2\sin^2\phi + \rho^2\cos^2\phi)^{\frac{1}{2}} = \rho, && \mathbf{e}_\phi = -\sin\phi\,\mathbf{e}_x + \cos\phi\,\mathbf{e}_y\,.\\
&\mathbf{v}_z = \mathbf{e}_z, && v_z = 1, && \mathbf{e}_z = \mathbf{e}_z\,.
\end{aligned}$$

Normalization is guaranteed by construction: $\mathbf{e}_\rho \cdot \mathbf{e}_\rho = \mathbf{e}_\phi \cdot \mathbf{e}_\phi = \mathbf{e}_z \cdot \mathbf{e}_z = 1$.
Orthogonality:

$$\begin{aligned}
&\mathbf{e}_\rho \cdot \mathbf{e}_\phi = (\cos\phi\,\mathbf{e}_x + \sin\phi\,\mathbf{e}_y)\cdot(-\sin\phi\,\mathbf{e}_x + \cos\phi\,\mathbf{e}_y) = -\cos\phi\sin\phi + \sin\phi\cos\phi = 0\,,\\
&\mathbf{e}_\rho \cdot \mathbf{e}_z = (\cos\phi\,\mathbf{e}_x + \sin\phi\,\mathbf{e}_y)\cdot\mathbf{e}_z = 0\,, \quad \mathbf{e}_\phi \cdot \mathbf{e}_z = (-\sin\phi\,\mathbf{e}_x + \cos\phi\,\mathbf{e}_y)\cdot\mathbf{e}_z = 0\,.
\end{aligned}$$

Hence: $\mathbf{e}_{y_i} \cdot \mathbf{e}_{y_j} = \delta_{ij}$. ✓

(b) Cross product: $\mathbf{e}_\rho \times \mathbf{e}_\rho = \mathbf{e}_\phi \times \mathbf{e}_\phi = \mathbf{e}_z \times \mathbf{e}_z = \mathbf{0}$.

$$\begin{aligned}
&\mathbf{e}_\rho \times \mathbf{e}_\phi = (\cos\phi\,\mathbf{e}_x + \sin\phi\,\mathbf{e}_y)\times(-\sin\phi\,\mathbf{e}_x + \cos\phi\,\mathbf{e}_y) = \cos^2\phi\,\mathbf{e}_z - \sin^2\phi(-\mathbf{e}_z) = \mathbf{e}_z\,,\\
&\mathbf{e}_\phi \times \mathbf{e}_z = (-\sin\phi\,\mathbf{e}_x + \cos\phi\,\mathbf{e}_y)\times\mathbf{e}_z = -\sin\phi(-\mathbf{e}_y) + \cos\phi\,\mathbf{e}_x = \mathbf{e}_\rho\,,\\
&\mathbf{e}_z \times \mathbf{e}_\rho = \mathbf{e}_z \times (\cos\phi\,\mathbf{e}_x + \sin\phi\,\mathbf{e}_y) = \cos\phi\,\mathbf{e}_y + \sin\phi(-\mathbf{e}_x) = \mathbf{e}_\phi\,.
\end{aligned}$$

Hence: $\mathbf{e}_{y_i} \times \mathbf{e}_{y_j} = \varepsilon_{ijk}\mathbf{e}_{y_k}$. ✓

Remark: In 3 dimensions a set of *orthonormal* basis vectors "automatically" satisfy the cross product formula. Above, the explicit calculations show that the cross product is cyclic in it's arguments. Alternatively, you can convince yourself of this using a sketch.

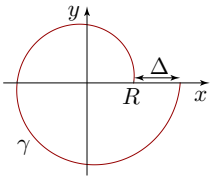
(c) $$\mathbf{v} = \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{r}(\rho,\phi,z) = \dot\rho\partial_\rho\mathbf{r} + \dot\phi\partial_\phi\mathbf{r} + \dot z\partial_z\mathbf{r} \overset{(a)}{=} \dot\rho\,\mathbf{e}_\rho + \rho\dot\phi\,\mathbf{e}_\phi + \dot z\,\mathbf{e}_z\,.$$

(d) $$T = \tfrac{1}{2}m\mathbf{v}^2 = \tfrac{1}{2}m\big(\dot\rho\,\mathbf{e}_\rho + \rho\dot\phi\,\mathbf{e}_\phi + \dot z\,\mathbf{e}_z\big)^2 = \tfrac{1}{2}m\big[\dot\rho^2 + \rho^2\dot\phi^2 + \dot z^2\big]\,.$$

(e) $$\begin{aligned}
\mathbf{L} &= m(\mathbf{r}\times\mathbf{v}) = m(\rho\,\mathbf{e}_\rho + z\mathbf{e}_z)\times(\dot\rho\,\mathbf{e}_\rho + \rho\dot\phi\,\mathbf{e}_\phi + \dot z\,\mathbf{e}_z)\\
&= m\big[\rho^2\dot\phi\;(\mathbf{e}_\rho\times\mathbf{e}_\phi) + z\dot\rho(\mathbf{e}_z\times\mathbf{e}_\rho) + \rho\dot z(\mathbf{e}_\rho\times\mathbf{e}_z) + z\rho\dot\phi(\mathbf{e}_z\times\mathbf{e}_\phi)\big]\\
&= m\big[-z\rho\dot\phi\,\mathbf{e}_\rho + (z\dot\rho - \rho\dot z)\mathbf{e}_\phi + \rho^2\dot\phi\,\mathbf{e}_z\big]\,.
\end{aligned}$$

E V2.4.3 Line integral in polar coordinates: spiral

(a) $\mathbf{r} = \rho\,\mathbf{e}_\rho\,, \quad \partial_\phi \mathbf{r} = \partial_\phi \rho\,\mathbf{e}_\rho + \rho\,\mathbf{e}_\phi\,, \quad \mathbf{F}_1(\mathbf{r}) = \mathbf{e}_\phi\,.$



$$W_1[\gamma_S] = \int_0^{2\pi} \mathrm{d}\phi\,(\partial_\phi \mathbf{r})\cdot\mathbf{F}_1 = \int_0^{2\pi} \mathrm{d}\phi(\partial_\phi\rho\,\mathbf{e}_\rho + \rho\,\mathbf{e}_\phi)\cdot\mathbf{e}_\phi = \int_0^{2\pi}\mathrm{d}\phi\,\rho$$
$$= \int_0^{2\pi}\mathrm{d}\phi\,(R + \tfrac{1}{2\pi}\Delta\phi) = \Big[R\phi + \tfrac{1}{4\pi}\Delta\phi^2\Big]_0^{2\pi} = 2\pi R + \pi\Delta\,.$$

(b) Along the straight path γ_G we use Cartesian coordinates:

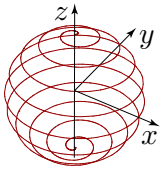
$$\mathbf{r} = x\mathbf{e}_x\,, \quad \partial_x\mathbf{r} = \mathbf{e}_x\,, \quad \mathbf{F}_1(\mathbf{r}) = \mathbf{e}_x\,.$$
$$W_2[\gamma_G] = \int_R^{R+\Delta}\mathrm{d}x\,(\partial_x\mathbf{r})\cdot\mathbf{F}_2 = \int_R^{R+\Delta}\mathrm{d}x\,\mathbf{e}_x\cdot\mathbf{e}_x = \int_R^{R+\Delta}\mathrm{d}x = \Delta\,.$$

Along the spiral path γ_S we use polar coordinates, with $\mathbf{F}_2 = \mathbf{e}_x = \cos\phi\,\mathbf{e}_\rho - \sin\phi\,\mathbf{e}_\phi$.

$$W_2[\gamma_S] = \int_0^{2\pi}\mathrm{d}\phi\,(\partial_\phi\mathbf{r})\cdot\mathbf{F}_2 = \int_0^{2\pi}\mathrm{d}\phi(\partial_\phi\rho\,\mathbf{e}_\rho + \rho\,\mathbf{e}_\phi)\cdot(\cos\phi\,\mathbf{e}_\rho - \sin\phi\,\mathbf{e}_\phi)$$
$$= \int_0^{2\pi}\mathrm{d}\phi\,\big[\tfrac{1}{2\pi}\Delta\cos\phi + (R + \tfrac{1}{2\pi}\phi\Delta)(-\sin\phi)\big]$$
$$= 0 + 0 - \tfrac{1}{2\pi}\Delta\int_0^{2\pi}\mathrm{d}\phi\,\phi\sin\phi \overset{\text{part. int.}}{=} -\tfrac{1}{2\pi}\Delta(-2\pi) = \Delta\,.$$

Discussion: Since $\mathbf{F}_2$ is a gradient field (with $\mathbf{F}_2 = \boldsymbol{\nabla}x$), the value of a line integral depends only on the starting point and endpoint of its path. These are the same for γ_G and γ_S, hence $W[\gamma_G] = W[\gamma_S]$.

E V2.4.5 Line integral in spherical coordinates: satellite in orbit



(a) During the flight, $t_D = \pi/\omega_1$, θ varies linearly from 0 to $\omega_1 t_D = \pi$, and ϕ varies from 0 to $\omega_2 t_D = 10(2\pi)$. Therefore the spiral winds itself around the north-south axis 10 times.

(b) $\mathbf{r}(t) = r(t)\,\mathbf{e}_r(t)\,, \quad$ with $\quad r = r_0\,, \quad \theta(t) = \omega_1 t\,, \quad \phi(t) = \omega_2 t\,.$

$$\dot{\mathbf{r}} = \dot{r}\,\mathbf{e}_r + r\dot{\theta}\,\mathbf{e}_\theta + r\dot{\phi}\sin\theta\,\mathbf{e}_\phi = r_0\omega_1\,\mathbf{e}_\theta + r_0\omega_2\sin(\omega_1 t)\,\mathbf{e}_\phi\,.$$

(c) $$L[\gamma] = \int_0^{\pi/\omega_1}\mathrm{d}t\;\|\mathbf{v}(t)\| = \int_0^{\pi/\omega_1}\mathrm{d}t\,r_0\sqrt{\omega_1^2 + \omega_2^2\sin^2(\omega_1 t)}\,.$$

(d) $\mathbf{F} = -F_0\sin\theta\,\mathbf{e}_\phi\,, \quad \dot{\mathbf{r}}(t)\cdot\mathbf{F}(\mathbf{r}(t)) = -F_0 r_0\omega_2\sin^2(\omega_1 t)\,,$ since $\mathbf{e}_\theta\cdot\mathbf{e}_\phi = 0\,,\ \mathbf{e}_\phi\cdot\mathbf{e}_\phi = 1\,.$

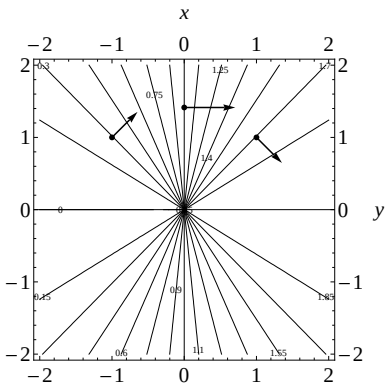
$$W[\gamma] = \int_\gamma \mathrm{d}\mathbf{r}\cdot\mathbf{F} = \int_0^{\pi/\omega_1}\mathrm{d}t\,\dot{\mathbf{r}}(t)\cdot\mathbf{F}(\mathbf{r}(t)) = -F_0 r_0\omega_2\int_0^{\pi/\omega_1}\mathrm{d}t\;\sin^2(\omega_1 t)$$
$$= -F_0 r_0\omega_2\frac{1}{2}\Big[t - \frac{1}{\omega_1}\sin(\omega_1 t)\cos(\omega_1 t)\Big]_0^{\pi/\omega_1} = -F_0\pi r_0\frac{\omega_2}{2\omega_1}\,.$$

S.V2.5 Local coordinate bases and linear algebra

S.V3 Fields

S.V3.1 Scalar fields

ᴇV3.1.1 Gradient of a mountain slope



(a) The gradient and total differential are given by:

$$\boldsymbol{\nabla} h_{\mathbf{r}} = \begin{pmatrix} \partial_x h \\ \partial_y h \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{x^2+y^2} - x\cdot\frac{2x}{2\sqrt{x^2+y^2}}}{x^2+y^2} \\ \frac{-x\cdot\frac{2y}{2\sqrt{x^2+y^2}}}{x^2+y^2} \end{pmatrix} = \frac{y}{r^3}\begin{pmatrix} y \\ -x \end{pmatrix} .$$

$$\mathrm{d}h_{\mathbf{r}}(\mathbf{n}) = (\partial_x h)n_x + (\partial_y h)n_y = \frac{y}{r^3}(yn_x - xn_y) .$$

(b) The direction of the steepest increase of the slope is given by the gradient vector $\boldsymbol{\nabla} h_{\mathbf{r}} = (y/r^3)(y,-x)^T$. It is parallel to the unit vector $\hat{\mathbf{n}}_{\parallel} = \boldsymbol{\nabla} h_{\mathbf{r}}/\|\boldsymbol{\nabla} h_{\mathbf{r}}\| = \mathrm{sign}(y)(y,-x)^T/r$.

(c) The contour lines at the point $\mathbf{r}$ are perpendicular to the gradient vector $\boldsymbol{\nabla} h_{\mathbf{r}}$ and therefore run along the unit vector $\hat{\mathbf{n}}_{\perp} = \mathrm{sign}(y)(x,y)^T/r$. (Verify that $\mathrm{d}h_{\mathbf{r}}(\hat{\mathbf{n}}_{\perp}) = 0$, which confirms that h does not change along the direction of $\hat{\mathbf{n}}_{\perp}$.)

(d) The arrows with starting points $\mathbf{r}_1 = (-1,1)^T$, $\mathbf{r}_2 = (0,\sqrt{2})^T$ and $\mathbf{r}_3 = (1,1)^T$ depict the vectors $\boldsymbol{\nabla} h_{\mathbf{r}_1} = 2^{-3/2}(1,1)^T$, $\boldsymbol{\nabla} h_{\mathbf{r}_2} = 2^{-1/2}(1,0)^T$ and $\boldsymbol{\nabla} h_{\mathbf{r}_3} = 2^{-3/2}(1,-1)^T$, respectively.

(e) Yes: For $x = y \geq 0$, $h(x,x) = 1 + 1/\sqrt{2}$ is constant. Therefore, this defines a contour line which is at a height of $1 + 1/\sqrt{2}$.

(f) The contour line at a height of $h(\mathbf{r}) \equiv H$ is defined by the equation

$$H \equiv \frac{x}{\sqrt{x^2+y^2}} + 1.$$

For a given value of x, we rearrange the equation, then square both sides and solve for y:

$$\begin{aligned} (H-1)^2[x^2+y^2] &= x^2 \\ (H-1)^2 y^2 &= x^2[1-(H-1)^2] \qquad \Rightarrow \qquad y = x\left[\frac{1}{(H-1)^2} - 1\right]^{1/2} . \end{aligned}$$

Check: The contour at $y = x$ implies that $H = 1 + 1/\sqrt{2}$, and is therefore consistent with (iv).

(g) Regions where the slope is completely flat locally are given by the equation $\boldsymbol{\nabla} h_{\mathbf{r}} = \mathbf{0}$. This is satisfied when $y = 0$ with $x \neq 0$. The line $\{(x,0)|x<0\}$ defines the 'valley', and is at a height of $h = 0$. The line $\{(x,0)|x>0\}$ defines the 'ridge' of the slope and is at a height of $h = 2$.

(h) At the point $\mathbf{r} = \mathbf{0} = (0,0)^T$, we find an infinitely steep i.e. vertical 'wall'. This is evident from the fact that the gradient vector $\boldsymbol{\nabla} h_{\mathbf{r}}$ is not well defined at that point and it depends on the direction from which $\mathbf{r}$ approaches the point $\mathbf{0}$. For example, on the one hand $\lim_{x\to 0}\left[\boldsymbol{\nabla} h_{(x,0)}\right] = (0,0)^T$ (the valley and the ridges remain flat even for arbitrarily small $|x|$), while on the other hand, $\lim_{y\to 0}\left[\boldsymbol{\nabla} h^T_{(0,y)}\right] = \lim_{y\to 0}(1/|y|, 0) = (\infty, 0)^T$ (the gradient in the x-direction along the line $x = 0$ is greater for smaller values of $|y|$). Actually, the 'vertical' part of the 'wall' is infinitesimally narrow because for all $\mathbf{r} \neq \mathbf{0}$, $\boldsymbol{\nabla} h_{\mathbf{r}}$ is well defined and finite.

ᴇV3.1.3 Gradient of $\ln(1/r)$

$$\phi(\mathbf{r}) = \ln\frac{1}{r}, \quad r = \sqrt{x^2+y^2+z^2}$$

$$\boldsymbol{\nabla}\phi = \begin{pmatrix}\partial_x\\ \partial_y\\ \partial_z\end{pmatrix}\phi = \phi'(r)\begin{pmatrix}\partial_x\\ \partial_y\\ \partial_z\end{pmatrix} r = \frac{1}{r}\cdot\left(-\frac{1}{2}\right)\frac{1}{(x^2+y^2+z^2)^{1/2}}\begin{pmatrix}2x\\ 2y\\ 2z\end{pmatrix}$$

$$= -\frac{1}{r^2}\begin{pmatrix}x\\ y\\ z\end{pmatrix} = -\frac{\hat{\mathbf{r}}}{r}$$

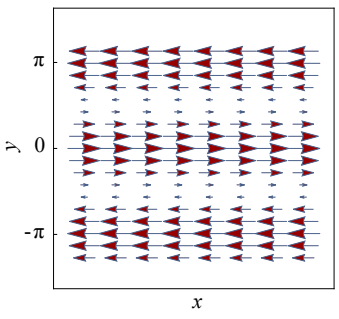
$$|\boldsymbol{\nabla}\phi|^2 = \frac{1}{r^4}(x^2+y^2+z^2) = \frac{1}{r^2} \qquad \Rightarrow \qquad |\boldsymbol{\nabla}\phi| = 1 \quad \text{at} \quad r = 1$$

This describes a spherical surface around the origin with radius 1.

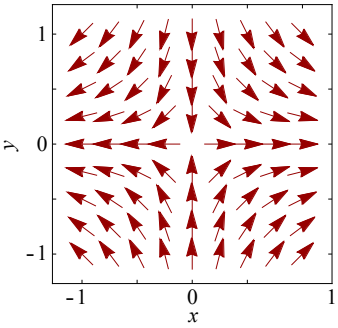
S.V3.2 Gradient fields

ᴇV3.2.1 Scetching a vector field

(a) The direction of the vector field $\mathbf{A}(\mathbf{r})$ is always parallel to $\mathbf{e}_x$, independent of $\mathbf{r}$. For a fixed value of y the field has a fixed value, independent of x, depicted by arrows that all have the same length and direction. For a fixed value of x, the length and direction of the arrows change periodically with y, as $\cos(y)$. In particular, $\mathbf{A} = \mathbf{e}_x$ for $y = n2\pi$, $\mathbf{A} = -\mathbf{e}_x$ for $y = (n+\frac{1}{2})2\pi$, and $\mathbf{A} = \mathbf{0}$ for $y = (n+\frac{1}{2})\pi$, with $n \in \mathbb{Z}$.



(b) The norm of the vector field $\mathbf{B}(\mathbf{r})$ is independent of $\mathbf{r}$, $\|\mathbf{B}(\mathbf{r})\| = 1$, thus all arrows have the same length. On the x axis we have $\mathbf{B}(\mathbf{r}) = \frac{x}{|x|}\mathbf{e}_x = \mathrm{sign}(x)\mathbf{e}_x$, thus the arrows point outward (away from the origin). On the y axis we have $\mathbf{B}(\mathbf{r}) = -\mathrm{sign}(y)\mathbf{e}_y$, thus the arrows point inward (toward the origin). On the diagonal $x = y$ we have $\mathbf{B}(\mathbf{r}) = \mathrm{sign}(x)\frac{1}{\sqrt{2}}(1,-1)^T$, thus for $x > 0$ (or $x < 0$) all arrows point with slope -1 towards the bottom right (bzw. or the top left). Analogously for the other diagonal. Arrow directions between axes and diagonals follow by interpolation.



In both figures the axes labels refer to the units used for $\mathbf{r}$-arrows from the domain of the map. The unit of length for arrows from the codomain has not been specified, hence only their direction and relative length carries any significance, not their absolute length. Moreover, the size of the arrow heads has been chosen proportional to the arrow length; this makes it visually clearer how the field strength varies.

EV3.2.3 Potential of a vector field

(a) Along the integration path $\gamma_1 = \{\mathbf{r}(t) = (t,t,t)^T \mid 0 < t < 1\}$, we have $\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = (1,1,1)^T$ for the velocity vector, and $\mathbf{A}(\mathbf{r}(\mathbf{t})) = (2t^2 + t^3, t^2, 3t^3)^T$ for the vector field. Hence:

$$\int_{\gamma_1} \mathrm{d}\mathbf{r} \cdot \mathbf{A}(\mathbf{r}) = \int_0^1 \mathrm{d}t\, \tfrac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} \cdot \mathbf{A}(\mathbf{r}(t)) = \int_0^1 \mathrm{d}t\, (3t^2 + 4t^3) = 2$$

(b)

$$\mathbf{A}(\mathbf{r}) = \begin{pmatrix} A_x(\mathbf{r}) \\ A_y(\mathbf{r}) \\ A_z(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} 2xy + z^3 \\ x^2 \\ 3xz^2 \end{pmatrix} \quad \Rightarrow \quad \begin{aligned} \partial_x A_y - \partial_y A_x &= -2x + 2x = 0 \\ \partial_y A_z - \partial_z A_y &= 0 - 0 = 0 \\ \partial_z A_x - \partial_x A_z &= -3z^2 + 3z^2 = 0 \end{aligned}$$

Therefore, $\partial_i A_j - \partial_j A_i = 0$ holds. Furthermore, since the domain of $\mathbf{A}(\mathbf{r})$, which is $\mathbb{R}^3$, is simply connected, I_1 is independent of the path γ_1 between $\mathbf{0}$ and $\mathbf{b}$.

(c) Choose a suitable parametrization, e.g. $\gamma_{\mathbf{r}} = \{\mathbf{r}'(t) = t\mathbf{r} = (tx, ty, tz) \mid , 0 < t < 1\}$.

$$\begin{aligned} \mathbf{r}'(t) &= \big(x'(t), y'(t), z'(t)\big)^T = t\mathbf{r} = (tx, ty, tz)^T, \qquad \dot{\mathbf{r}}'(t) = \mathbf{r} = (x,y,z)^T, \\ \mathbf{A}(\mathbf{r}'(t)) &= \Big(2x'(t)y'(t) + z'^3(t), x'^2(t), 3x'(t)z'^2(t)\Big)^T \\ &= \big(2(tx)(ty) + (tz)^3, (tx)^2, 3(tx)(tz)^2\big)^T \\ \dot{\mathbf{r}}(t) \cdot \mathbf{A}(\mathbf{r}(t)) &= 2x^2yt^2 + xz^3t^3 + yx^2t^2 + 3xz^3t^3 = 3x^2yt^2 + 4xz^3t^3 \\ \phi(\mathbf{r}) = \int_{\gamma_{\mathbf{r}}} \mathrm{d}\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}') &= \int_0^1 \mathrm{d}t\, \dot{\mathbf{r}}(t) \cdot \mathbf{A}(\mathbf{r}(t)) = \int_0^1 \mathrm{d}t \left(3x^2yt^2 + 4xz^3t^3\right) = x^2y + xz^3 \end{aligned}$$

(d) Consistency check:

$$\nabla\phi(\mathbf{r}) = \begin{pmatrix}\partial_x\\ \partial_y\\ \partial_z\end{pmatrix}(x^2y + xz^3) = \begin{pmatrix}2xy + z^3\\ x^2\\ 3xz^2\end{pmatrix}. \qquad \text{Evidently} \quad \nabla\phi(\mathbf{r}) \overset{\checkmark}{=} \mathbf{A}(\mathbf{r})\,.$$

(e)

$$I_1 = \int_{\gamma_1} \mathrm{d}\mathbf{r}\cdot\mathbf{A}(\mathbf{r}) = \int_{\gamma_1} \mathrm{d}\mathbf{r}\cdot\nabla\phi(\mathbf{r}) = \phi(\mathbf{b}) - \phi(\mathbf{0}) = 1^2\cdot 1 + 1\cdot 1^3 - 0 = 2$$

This is in agreement with part (a) of the exercise! ✓

ᴇV3.2.5 Line integral of magnetic field of a current-carrying conductor

(a) All components of the curl of the given field, $\mathbf{B} = \frac{c}{x^2+y^2}(-y, x, 0)^T$, vanish away from the z axis ($\sqrt{x^2+y^2} \neq 0$):

$$\partial_z B_x - \partial_x B_z = 0\,, \quad \partial_z B_y - \partial_y B_z = 0\,.$$
$$\partial_x B_y - \partial_y B_x = c\left[\frac{(x^2+y^2)-2x^2}{(x^2+y^2)^2} - (-)\frac{(x^2+y^2)-2y^2}{(x^2+y^2)^2}\right] = 0\,.$$

(b) Along the circular path γ_K with radius R around the origin, with $t \in [0, 2\pi]$, one finds:

$$\mathbf{r}(t) = \big(x(t), y(t), z(t)\big)^T = R(\cos(t), \sin(t), 0)^T, \qquad \dot{\mathbf{r}}(t) = R(-\sin(t), \cos(t), 0)^T$$
$$\mathbf{B}(\mathbf{r}(t)) = \frac{c}{x(t)^2+y(t)^2}(-y(t), x(t), 0)^T = \frac{cR}{R^2}(-\sin(t), \cos(t), 0)^T$$
$$\dot{\mathbf{r}}(t)\cdot\mathbf{B}(\mathbf{r}(t)) = c\big[\sin^2(t) + \cos^2(t)\big] = c$$
$$W[\gamma_K] = \int_{\gamma_K}\mathrm{d}\mathbf{r}\cdot\mathbf{F} = \int_0^{2\pi}\mathrm{d}t\,\dot{\mathbf{r}}(t)\cdot\mathbf{F}(\mathbf{r}(t)) = \int_0^{2\pi}\mathrm{d}t\,c = 2\pi c\,.$$

(c) The line integral has four contributions, corresponding to the four edges of the rectangle:

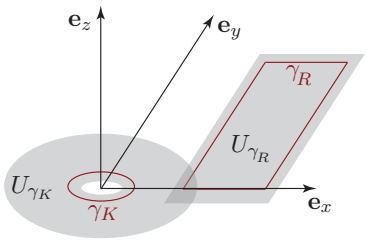
$$\frac{1}{c}W[\gamma_R] = \int_1^2 \mathrm{d}x\frac{0}{x^2+0^2} + \int_0^3 \mathrm{d}y\frac{2}{2^2+y^2} + \int_2^1 \mathrm{d}x\frac{-3}{x^2+3^2} + \int_3^0 \mathrm{d}y\frac{1}{1^2+y^2}$$
$$\overset{\tilde{y}=\frac{y}{2},\,\tilde{x}=\frac{x}{3}}{=} 0 + \int_0^{\frac{3}{2}}\mathrm{d}\tilde{y}\frac{1}{1+\tilde{y}^2} + \int_{\frac{1}{3}}^{\frac{2}{3}}\mathrm{d}\tilde{x}\frac{1}{\tilde{x}^2+1^2} - \int_0^3 \mathrm{d}y\frac{1}{1^2+y^2}$$
$$= [\arctan(\tfrac{3}{2}) - \arctan(0)] + [\arctan(\tfrac{2}{3}) - \arctan(\tfrac{1}{3})] - [\arctan(3) - \arctan(0)]$$
$$= \tfrac{\pi}{2} - \tfrac{\pi}{2} = 0\,,$$

since $\arctan(\frac{A}{B}) + \arctan(\frac{B}{A}) = \frac{\pi}{2}$ holds for arbitrary positive numbers A and B.

(d) The line integral $W[\gamma] = \oint_\gamma \mathrm{d}\mathbf{r} \cdot \mathbf{B}$ along a closed curve $\gamma \in \mathbb{R}^3$ vanishes if, and only if, there exists a domain U_γ with the following properties: (i) the domain U_γ encloses the entire curve ($\gamma \subset U_\gamma$); the curl of the field $\mathbf{B}$ vanishes throughout the domain U_γ ($\boldsymbol{\nabla} \times \mathbf{B} = \mathbf{0}$ for all $\mathbf{r} \in U_\gamma$); (iii) the domain U_γ is *simply connected*. In other words: the line integral vanishes if, and only if, it is possible to shrink the integration path down to a point, *without* leaving the domain on which the curl vanishes.

The curl of the present vector field $\mathbf{B}$ vanishes, according to (a), in a domain that is not simply connected: $\mathbb{R}^3$ without the z axis, $\mathbb{R}^3/\{(0,0,z)^T | z \in \mathbb{R}\}$ [or, for fixed $z = 0$, the xy plane without the origin, $\mathbb{R}^2/(0,0)^T$]. Therefore the line integral $W[\gamma]$ along a closed curve γ vanishes if, and only if, the curve does *not* encircle the z axis. This is the case for the rectangular path γ_R of part (c), but not for the circular path γ_K of part (b).

The figure shows examples of two domains (shaded), a rectangle U_{γ_R} and a ring U_{γ_K}, that satisfy properties (i) and (ii): (i) both domains enclose the corresponding integration paths, γ_R or γ_K, respectively, and (ii) the curl of $\mathbf{B}$ vanishes throughout both domains. However, property (iii) holds only for the first domain: the rectangle U_{γ_R} is simply connected, the ring U_{γ_K} is not.

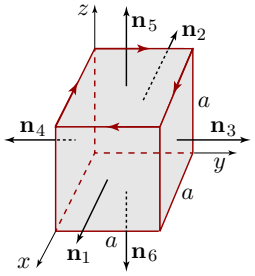


Conclusion: $\boldsymbol{\nabla} \times \mathbf{B} = \mathbf{0}$ is a necessary, but not a sufficient condiction for $\oint \mathrm{d}\mathbf{r} \cdot \mathbf{B} = 0$. The latter requires $\boldsymbol{\nabla} \times \mathbf{B} = \mathbf{0}$ to hold on a *simply connected* domain.

S.V3.3 Sources of vector fields

EV3.3.1 Gauss' theorem – cube (Cartesian coordinates)

C is a cube with edge length a (see sketch). Let S_1 to S_6 be its 6 faces with normal vectors $\mathbf{n}_{1,2} = \pm\mathbf{e}_x$, $\mathbf{n}_{3,4} = \pm\mathbf{e}_y$, $\mathbf{n}_{5,6} = \pm\mathbf{e}_z$. We seek the flux $\Phi = \int_{\partial C} \mathrm{d}\mathbf{S} \cdot \mathbf{v}$ of the vector field $\mathbf{v}(\mathbf{r}) = (x^2, y^2, z^2)^T$.



(a) Direct calculation of $\Phi = \sum_{i=1}^6 \Phi_i$, with $\Phi_i = \int_{S_i} \mathrm{d}\mathbf{S} \cdot \mathbf{v}$:

$$\Phi_1 + \Phi_2 = \int_0^a \mathrm{d}y \int_0^a \mathrm{d}z \left[\underbrace{(\mathbf{n}_1 \cdot \mathbf{v})_{x=a}}_{a^2} + \underbrace{(\mathbf{n}_2 \cdot \mathbf{v})_{x=0}}_{0} \right] = a^4 \,.$$

Analogously: $\Phi_3 + \Phi_4 = \Phi_5 + \Phi_6 = a^4$. We thus obtain $\Phi = 3a^4$.

(b) Alternatively, using Gauss's theorem: $\Phi = \int_{\partial C} \mathrm{d}\mathbf{S} \cdot \mathbf{v} \overset{\text{Gauss}}{=} \int_C \mathrm{d}V \, \boldsymbol{\nabla} \cdot \mathbf{v}$.

$$\Phi = \int_0^a \int_0^a \int_0^a \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \, \boldsymbol{\nabla} \cdot \mathbf{v} = \int_0^a \int_0^a \int_0^a \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \, (2x + 2y + 2z)$$
$$= \left[x^2\right]_0^a \cdot \left[y\right]_0^a \cdot \left[z\right]_0^a + \left[x\right]_0^a \cdot \left[y^2\right]_0^a \cdot \left[z\right]_0^a + \left[x\right]_0^a \cdot \left[y\right]_0^a \cdot \left[z^2\right]_0^a = 3a^4 \,. \quad [= \text{(a)} \checkmark]$$

EV3.3.3 Calculating volume of cylinder using Gauss' theorem

The surface of the cylinder Z consists of a bottom, middle, and top, $\partial Z = B \cup M \cup T$. Let $\mathbf{v}$ be a vector field with the property that $\boldsymbol{\nabla} \cdot \mathbf{v} = 1$, then the volume V_Z of the cylinder is determined as follows, by integrating the flux through the surface:

Volume of Z: $$V_Z = \int_Z \mathrm{d}V = \int_Z \mathrm{d}V(\boldsymbol{\nabla} \cdot \mathbf{v}) = \int_{\partial Z} \mathrm{d}\mathbf{S} \cdot \mathbf{v} \ = \Phi_B + \Phi_M + \Phi_T \ .$$

In cylindrical coordinates, $\mathbf{r} = \rho \mathbf{e}_\rho + z\mathbf{e}_z$, the surface elements of the three sides of the cylinder are as follows:

Middle: $\mathrm{d}\mathbf{S} = R\,\mathrm{d}\phi\,\mathrm{d}z\,\mathbf{e}_\rho$, $\rho = R$,
Top: $\mathrm{d}\mathbf{S} = \rho\,\mathrm{d}\rho\,\mathrm{d}\phi\,\mathbf{e}_z$, $z = h$,
Bottom: $\mathrm{d}\mathbf{S} = -\rho\,\mathrm{d}\rho\,\mathrm{d}\phi\,\mathbf{e}_z$, $z = 0$.

If we choose $\mathbf{v} = z\mathbf{e}_z$, then $\boldsymbol{\nabla} \cdot \mathbf{v} = 1$, and so $\mathrm{d}\mathbf{S} \cdot \mathbf{v} = 0$ for the bottom and middle, thus only the top face contributes:

$$V_Z = \Phi_D = \int_D \mathrm{d}\mathbf{S} \cdot \mathbf{v} \ = \int_0^{2\pi} \mathrm{d}\phi \int_0^R \mathrm{d}\rho\, \rho h = \pi R^2 h \,. \checkmark$$

Alternatively, albeit less elegantly, one could also choose for example $\mathbf{v} = \frac{1}{3}\mathbf{r}$, which also fulfils the condition $\boldsymbol{\nabla} \cdot \mathbf{v} = 1$. Since $\mathbf{r} = \rho\,\mathbf{e}_\rho + z\,\mathbf{e}_z$, we get:

Middle: $$\Phi_M = \frac{1}{3}\int_M \mathrm{d}\mathbf{S} \cdot \mathbf{v} = \frac{1}{3}\int_0^{2\pi} d\phi \int_0^h dz\, R^2 = \frac{2}{3}\pi h R^2 \ .$$

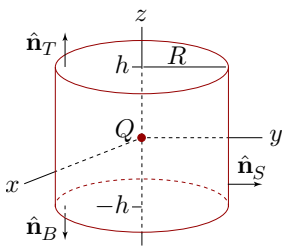
Top: $$\Phi_T = \frac{1}{3}\int_T \mathrm{d}\mathbf{S} \cdot \mathbf{v} = \frac{1}{3}\int_0^R \rho\, d\rho \int_0^{2\pi} d\phi\, h = \frac{1}{3}\frac{1}{2}R^2 2\pi h = \frac{1}{3}\pi h R^2 \ .$$

Bottom: $$\Phi_B = \frac{1}{3}\int_B \mathrm{d}\mathbf{S} \cdot \mathbf{v} = \frac{-1}{3}\int_0^R \rho\, d\rho \int_0^{2\pi} d\phi \cdot 0 = 0 \ .$$

Combined: $$V_Z = \Phi_M + \Phi_D + \Phi_B = \frac{2}{3}\pi h R^2 + \frac{1}{3}\pi h R^2 = \pi R^2 h \,. \checkmark$$

EV3.3.5 Flux integral: flux of electric field through cylinder

We choose the symmetry axis of the cylinder to be the z-axis, and use cylindrical coordinates:



Position vector: $$\mathbf{r} = \rho\,\mathbf{e}_\rho + z\,\mathbf{e}_z \,, \quad r^2 = \rho^2 + z^2 \,.$$

Electric field: $$\mathbf{E}(\mathbf{r}) = E_0 \frac{\mathbf{r}}{r^3} = E_0 \frac{\rho\,\mathbf{e}_\rho + z\mathbf{e}_z}{(\rho^2 + z^2)^{\frac{3}{2}}} \,.$$

(a) The calculations of the flux through both the top (T) and the bottom (B) both proceed in exactly the same way; as such we will show only one calculation (The plus/minus sign is for the top/bottom faces). The geometry of the problem is especially easy, so we may simply present the surface integral without any prior calculation:

$$\Phi_{T/B} = \int_0^{2\pi} \mathrm{d}\phi \int_0^R \mathrm{d}\rho\, \rho\, (\hat{\mathbf{n}}_{T/B} \cdot \mathbf{E})_{z=\pm h} = 2\pi \int_0^R \mathrm{d}\rho\, \rho\, \frac{E_0 h}{(\rho^2+h^2)^{\frac{3}{2}}} = -\left[\frac{2\pi E_0 h}{(\rho^2+h^2)^{\frac{1}{2}}}\right]_0^R$$

$$= 2\pi E_o h \left[\frac{1}{h} - \frac{1}{(R^2+h^2)^{\frac{1}{2}}}\right].$$

Explanation: The above form of the surface integral results from the following considerations:

For the top/bottom, we have: $z = \pm h\,, \quad \mathbf{r}(\rho,\phi) = \rho\,\mathbf{e}_\rho \mp h\mathbf{e}_z\,.$

Tangent vectors: $\partial_\rho \mathbf{r} = \mathbf{e}_\rho, \quad \partial_\phi \mathbf{r} = \rho \mathbf{e}_\phi \quad \Rightarrow \quad \partial_\rho \mathbf{r} \times \partial_\phi \mathbf{r} = \rho\,\mathbf{e}_z\,.$

The vector $\partial_\rho \mathbf{r} \times \partial_\phi \mathbf{r}$ is therefore parallel to $\mathbf{e}_z$, and hence normal to the top/bottom surfaces, as expected. We choose the sign of the corresponding normal vector, $\hat{\mathbf{n}}_T$ or $\hat{\mathbf{n}}_B$ respectively, so that it points *outwards*, hence:

Normal vector: $\hat{\mathbf{n}}_{T/B} = \pm \dfrac{\partial_\rho \mathbf{r} \times \partial_\phi \mathbf{r}}{\|\partial_\rho \mathbf{r} \times \partial_\phi \mathbf{r}\|} = \pm \mathbf{e}_z\,, \quad \hat{\mathbf{n}}_{T/B} \cdot \mathbf{E}\Big|_{z=\pm h} = E_0 \dfrac{(\pm 1)(\pm h)}{(\rho^2 + (\pm h)^2)^{\frac{3}{2}}}\,.$

Surface element: $\mathrm{d}\mathbf{S}_{T/B} = \mathrm{d}S\, \hat{\mathbf{n}}_{T/B}, \quad \mathrm{d}S = \mathrm{d}\rho\, \mathrm{d}\phi\, \|\partial_\rho \mathbf{r} \times \partial_\phi \mathbf{r}\| = \mathrm{d}\rho\, \mathrm{d}\phi\, \rho.$

As expected, $\mathrm{d}S = \|\mathrm{d}\mathbf{S}\| = \mathrm{d}\rho\, \mathrm{d}\phi\, \rho$ corresponds to the surface element for polar coordinates.

(b) The calculation of the flux through the side (S) proceeds as follows:

$$\Phi_S = \int_0^{2\pi} \mathrm{d}\phi\, R \int_{-h}^{h} \mathrm{d}z\, (\hat{\mathbf{n}}_S \cdot \mathbf{E})_{\rho=R} = 2\pi R \int_{-h}^{h} \mathrm{d}z\, \frac{E_0 R}{(R^2+z^2)^{\frac{3}{2}}} = \left[\frac{2\pi E_0 z}{(R^2+z^2)^{\frac{1}{2}}}\right]_{-h}^{h}$$

$$= \frac{4\pi E_o h}{(R^2+h^2)^{\frac{1}{2}}}\,.$$

Explanation: The above form of the surface integral results from the following considerations:

On the side, we have: $\rho = R\,, \quad \mathbf{r}(\phi, z) = R\,\mathbf{e}_\rho + z\mathbf{e}_z\,.$

Tangent vectors: $\partial_\phi \mathbf{r} = R\mathbf{e}_\phi\,, \quad \partial_z \mathbf{r} = \mathbf{e}_z \quad \Rightarrow \quad \partial_\phi \mathbf{r} \times \partial_z \mathbf{r} = R\,\mathbf{e}_\rho\,.$

The vector $\partial_\phi \mathbf{r} \times \partial_z \mathbf{r}$ is thus parallel to $\mathbf{e}_\rho$, and is therefore normal to the side and directed outwards, as expected. The corresponding normal vector reads:

Normal vector: $\hat{\mathbf{n}}_S = \dfrac{\partial_\rho \mathbf{r} \times \partial_\phi \mathbf{r}}{\|\partial_\phi \mathbf{r} \times \partial_z \mathbf{r}\|} = \mathbf{e}_\rho\,, \quad \hat{\mathbf{n}}_S \cdot \mathbf{E}\Big|_{\rho=R} = E_0 \dfrac{R}{(R^2+z^2)^{\frac{3}{2}}}\,.$

Surface element: $\mathrm{d}\mathbf{S}_S = \mathrm{d}S\, \hat{\mathbf{n}}_S, \quad \mathrm{d}S = \mathrm{d}\phi\, \mathrm{d}z\, \|\partial_\phi \mathbf{r} \times \partial_z \mathbf{r}\| = \mathrm{d}\phi\, R\, \mathrm{d}z.$

As expected, $\mathrm{d}S$ is the product of the line element for integration along a circle with radius R, $R\,\mathrm{d}\phi$, and the line element in the z-direction, $\mathrm{d}z$.

The integral for Φ_s may be calculated as follows (with $s = z/R$):

$$I = \int \mathrm{d}s \frac{1}{(1+s^2)^{\frac{3}{2}}} \quad \text{[Substitution: } s = \sinh y,\ \mathrm{d}s = \mathrm{d}y \cosh y,\ \sqrt{1+s^2} = \cosh y.\text{]}$$
$$= \int \mathrm{d}y \frac{\cosh y}{\cosh^3 y} = \int \mathrm{d}y \frac{1}{\cosh^2 y} = \tanh y = \frac{\sinh y}{\cosh y} = \frac{s}{(1+s^2)^{\frac{1}{2}}} .$$

Check: $\frac{\mathrm{d}}{\mathrm{d}s} \frac{s}{(1+s^2)^{\frac{1}{2}}} = \frac{1}{(1+s^2)^{\frac{1}{2}}} - \frac{s^2}{(1+s^2)^{\frac{3}{2}}} = \frac{1+s^2-s^2}{(1+s^2)^{\frac{3}{2}}} = \frac{1}{(1+s^2)^{\frac{3}{2}}} \cdot \checkmark$

For the total outward flux, Φ_S cancels the second term in $\Phi_T + \Phi_B$, with the result: $\Phi_Z = \Phi_T + \Phi_B + \Phi_S = 4\pi E_0 = 4\pi Q$.

This is an example of Gauss's law for electrostatics: the flux of an electric field through a closed surface, which encloses an electric charge Q_{tot}, is always equal to $\Phi = 4\pi Q_{\mathrm{tot}}$.

E V3.3.7 Gauss' theorem – cylinder (cylindrical coordinates)

(a)
$$\nabla \cdot \mathbf{v} = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(z\rho^2\right) = 2z$$

(b) The top and bottom faces don't contribute, since $\mathrm{d}\mathbf{S} \propto \mathbf{e}_z \perp \mathbf{v}$.
The flux through the side is given by

$$\int_S \mathrm{d}\mathbf{S} \cdot \mathbf{v} = \int_{\text{Mantel}} \mathrm{d}\mathbf{S} \cdot \mathbf{v} = \int_0^{2\pi} \mathrm{d}\phi \int_0^H \mathrm{d}z \, (R\mathbf{e}_\rho) \cdot (Rz\mathbf{e}_\rho) = \pi H^2 R^2$$

(c)
$$\int_{V_S} \mathrm{d}\mathbf{S} \cdot \mathbf{v} = \int_V \mathrm{d}V \nabla \cdot \mathbf{v}$$
$$= \int_0^{2\pi} \mathrm{d}\phi \int_0^H \mathrm{d}z \int_0^R \mathrm{d}\rho \rho \, (2z) = \pi H^2 R^2$$

S.V3.4 Circulation of vector fields

E V3.4.1 Gradient, divergence, curl

$$f = x^2 y + y^2 z\ , \quad \nabla f = (\partial_x f, \partial_y f, \partial_z f)^T = \left(2xy, x^2 + 2yz, y^2\right)^T$$
$$\mathbf{v} = (xyz, y^2, z^2)^T$$
$$\nabla \cdot \mathbf{v} = \partial_x v_x + \partial_y v_y + \partial_z v_z = yz + 2y + 2z$$
$$\nabla \times \mathbf{v} = (\partial_y v_z - \partial_z v_y, \partial_z v_x - \partial_x v_z, \partial_x v_y - \partial_y v_x)^T = (0, xy, -xz)^T$$

E V3.4.3 Source fields have no curl

$$\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\varphi)=\partial_i\partial_j\varphi\,\epsilon_{ijk}\mathbf{e}_k \overset{\text{(i)}}{=} \partial_j\partial_i\varphi\,\epsilon_{ijk}\mathbf{e}_k \overset{\text{(ii)}}{=} \partial_i\partial_j\varphi\,\epsilon_{jik}\mathbf{e}_k \overset{\text{(iii)}}{=} -\partial_i\partial_j\varphi\,\epsilon_{ijk}\mathbf{e}_k=-\boldsymbol{\nabla}\times(\boldsymbol{\nabla}\varphi)$$
$$\overset{\text{(iv)}}{\Rightarrow}\ \boldsymbol{\nabla}\times(\boldsymbol{\nabla}\varphi)=\mathbf{0}$$

Explanation of steps: (i) Follows from Schwarz's theorem. (ii) Change of summation indices: $i\leftrightarrow j$. (iii) Anti-symmetric property of the Levi-Civita tensor under exchange of indices. (iv) $A=-A\Rightarrow A=0$.

E V3.4.5 Nabla identities

(a)
$$\boldsymbol{\nabla}f=\mathrm{e}^{-x^2}\begin{pmatrix}-2xz\\0\\1\end{pmatrix},\quad \boldsymbol{\nabla}g=\begin{pmatrix}0\\z^{-1}\\-yz^{-2}\end{pmatrix},$$
$$\boldsymbol{\nabla}\cdot\mathbf{A}=2xy\,,\quad \boldsymbol{\nabla}\times\mathbf{A}=-x^2\mathbf{e}_z\,,\quad \boldsymbol{\nabla}\cdot\mathbf{B}=0,\quad \boldsymbol{\nabla}\times\mathbf{B}=\mathbf{0}\,.$$

(b) Equations (i) and (ii) are vector equations, which we will consider for a specific component, say i. In contrast, (iii) is scalar equation.

(i) $$\left[\boldsymbol{\nabla}(fg)\right]^i=\partial_i(fg)=f(\partial_i g)+g(\partial_i f)=f(\boldsymbol{\nabla}g)^i+g(\boldsymbol{\nabla}f)^i$$

(ii)
$$\begin{aligned}&\left[\mathbf{A}\times(\boldsymbol{\nabla}\times\mathbf{B})+\mathbf{B}\times(\boldsymbol{\nabla}\times\mathbf{A})+(\mathbf{A}\cdot\boldsymbol{\nabla})\mathbf{B}+(\mathbf{B}\cdot\boldsymbol{\nabla})\mathbf{A}\right]^i\\
&=\epsilon_{ijk}A^j(\boldsymbol{\nabla}\times\mathbf{B})^k+\epsilon_{ijk}B^j(\boldsymbol{\nabla}\times\mathbf{A})^k+A^j\partial_jB^i+B^j\partial_jA^i\\
&=\underbrace{\epsilon_{ijk}\epsilon_{klm}}_{=\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl}}\left(A^j\partial_lB^m+B^j\partial_lA^m\right)+A^j\partial_jB^i+B^j\partial_jA^i\\
&=A^j\partial_iB^j-A^j\partial_jB^i+B^j\partial_iA^j-B^j\partial_jA^i+A^j\partial_jB^i+B^j\partial_jA^i\\
&=A^j\partial_iB^j+B^j\partial_iA^j=\partial_i\left(A^jB^j\right)=\left[\boldsymbol{\nabla}(\mathbf{A}\cdot\mathbf{B})\right]^i\end{aligned}$$

(iii) $$\boldsymbol{\nabla}\cdot(f\mathbf{A})=\partial_i\left(fA^i\right)=f\partial_iA^i+A^i\partial_if=f(\boldsymbol{\nabla}\cdot\mathbf{A})+\mathbf{A}^i(\boldsymbol{\nabla}f)_i=f(\boldsymbol{\nabla}\cdot\mathbf{A})+\mathbf{A}\cdot(\boldsymbol{\nabla}f)$$

(c) Using the results from (a) we obtain:

(i)
$$\boldsymbol{\nabla}(fg)=\boldsymbol{\nabla}(y\mathrm{e}^{-x^2})=\mathrm{e}^{-x^2}\begin{pmatrix}-2xy\\1\\0\end{pmatrix}$$
$$f(\boldsymbol{\nabla}g)+g(\boldsymbol{\nabla}f)=z\mathrm{e}^{-x^2}\begin{pmatrix}0\\z^{-1}\\-yz^{-2}\end{pmatrix}+yz^{-1}\mathrm{e}^{-x^2}\begin{pmatrix}-2xz\\0\\1\end{pmatrix}=\mathrm{e}^{-x^2}\begin{pmatrix}0-2xy\\1+0\\-yz^{-1}+yz^{-1}\end{pmatrix}$$
$$=\mathrm{e}^{-x^2}\begin{pmatrix}-2xy\\1\\0\end{pmatrix}=\boldsymbol{\nabla}(fg)\quad\checkmark$$

(ii) $\boldsymbol{\nabla}(\mathbf{A}\cdot\mathbf{B}) = \boldsymbol{\nabla}\left(x^2y\right) = \begin{pmatrix} 2xy \\ x^2 \\ 0 \end{pmatrix}$

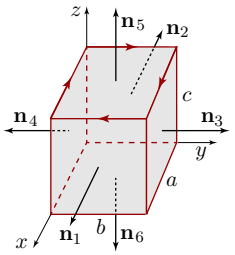
$$\begin{aligned}\mathbf{A}\times(\boldsymbol{\nabla}\times\mathbf{B}) + \mathbf{B}\times(\boldsymbol{\nabla}\times\mathbf{A}) + (\mathbf{A}\cdot\nabla)\,\mathbf{B} + (\mathbf{B}\cdot\boldsymbol{\nabla})\,\mathbf{A} \\ = 0 + \mathbf{e}_x\times\left(-x^2\mathbf{e}_z\right) + x^2y\partial_x\mathbf{B} + \partial_x\mathbf{A} = 0 + x^2\mathbf{e}_y + 0 + 2xy\mathbf{e}_x \\ = \begin{pmatrix} 2xy \\ x^2 \\ 0 \end{pmatrix} = \boldsymbol{\nabla}(\mathbf{A}\cdot\mathbf{B}) \quad \checkmark\end{aligned}$$

(iii) $\boldsymbol{\nabla}\cdot(f\mathbf{A}) = \boldsymbol{\nabla}\cdot\begin{pmatrix} z\mathrm{e}^{-x^2}x^2y \\ 0 \\ 0 \end{pmatrix} = yz\mathrm{e}^{-x^2}\left(-2x^3+2x\right)$

$$\begin{aligned}f(\boldsymbol{\nabla}\cdot\mathbf{A}) + \mathbf{A}\cdot(\boldsymbol{\nabla}f) = z\mathrm{e}^{-x^2}(2xy) + \begin{pmatrix} x^2y \\ 0 \\ 0 \end{pmatrix}\cdot\begin{pmatrix} -2xz\mathrm{e}^{-x^2} \\ 0 \\ 0 \end{pmatrix} = \mathrm{e}^{-x^2}\left(2xyz - 2x^3yz\right) \\ = yz\mathrm{e}^{-x^2}\left(-2x^3+2x\right) = \boldsymbol{\nabla}\cdot(f\mathbf{A}) \quad \checkmark\end{aligned}$$

E V3.4.7 Stokes' theorem – cube (Cartesian coordinates)

C is a cuboid with edge lengths a, b and c (see sketch). Let S_1 to S_6 be its 6 sides with normal vectors $\mathbf{n}_{1,2} = \pm\mathbf{e}_x$, $\mathbf{n}_{3,4} = \pm\mathbf{e}_y$, $\mathbf{n}_{5,6} = \pm\mathbf{e}_z$. We seek the flux $\Phi = \int_{\partial C}\mathrm{d}\mathbf{S}\cdot\mathbf{v}$ of the vector field $\mathbf{v}(\mathbf{r}) = (\frac{1}{2}x^2 + x^2y, \frac{1}{2}x^2y^2, 0)^T$.



(a) Direct calculation of $\Phi = \sum_{i=1}^{6}\Phi_i$, with $\Phi_i = \int_{S_i}\mathrm{d}\mathbf{S}\cdot\mathbf{v}$:

$$\Phi_1+\Phi_2 = \int_0^b\mathrm{d}y\int_0^c\mathrm{d}z\,\Big[\underbrace{(\mathbf{n}_1\cdot\mathbf{v})_{x=a}}_{a^2(\frac{1}{2}+y)} + \underbrace{(\mathbf{n}_2\cdot\mathbf{v})_{x=0}}_{0}\Big] = \tfrac{1}{2}a^2(b+b^2)c\,.$$

$$\Phi_3+\Phi_4 = \int_0^a\mathrm{d}x\int_0^c\mathrm{d}z\,\Big[\underbrace{(\mathbf{n}_3\cdot\mathbf{v})_{y=b}}_{\frac{1}{2}x^2b^2} + \underbrace{(\mathbf{n}_4\cdot\mathbf{v})_{y=0}}_{0}\Big] = \tfrac{1}{6}a^3b^2c\,.$$

Analogously: $\Phi_5+\Phi_6 = 0$, da $\mathbf{n}_5\cdot\mathbf{v} = \mathbf{n}_6\cdot\mathbf{v} = 0$. Therefore $\Phi = \frac{1}{2}a^2bc(1+b+\frac{1}{3}ab)$.

(b) Alternative method, using Gauss's theorem: $\Phi = \int_{\partial C}\mathrm{d}\mathbf{S}\cdot\mathbf{v} \overset{\text{Gauss}}{=} \int_C\mathrm{d}V\,\boldsymbol{\nabla}\cdot\mathbf{v}$.

$$\begin{aligned}\Phi &= \int_0^a\int_0^b\int_0^c\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,\boldsymbol{\nabla}\cdot\mathbf{v} = \int_0^a\int_0^a\int_0^a\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\,(x+2xy+x^2y) \\ &= \left[\tfrac{1}{2}x^2\right]_0^a\cdot\left[y\right]_0^b\cdot\left[z\right]_0^c + \left[x^2\right]_0^a\cdot\left[\tfrac{1}{2}y^2\right]_0^b\cdot\left[z\right]_0^c + \left[\tfrac{1}{3}x^3\right]_0^a\cdot\left[\tfrac{1}{2}y^2\right]_0^b\cdot\left[z\right]_0^c \\ &= \tfrac{1}{2}a^2bc(1+b+\tfrac{1}{3}ab)\,.\ [= \text{(a)}\ \checkmark]\end{aligned}$$

ɛV3.4.9 Gradient, divergence, curl, Laplace in cylindrical coordinates

(a) Position vector: $\mathbf{r} = (\rho\cos\phi, \rho\sin\phi, z)^T$.

$$\begin{aligned}
\partial_\rho \mathbf{r} &\equiv b_\rho \mathbf{e}_\rho, \quad \text{with} \quad b_\rho = 1\ , \ \mathbf{e}_\rho = (\cos\phi, \sin\phi, 0)^T\ .\\
\partial_\phi \mathbf{r} &\equiv b_\phi \mathbf{e}_\phi, \quad \text{with} \quad b_\phi = \rho\ , \ \mathbf{e}_\phi = (-\sin\phi, \cos\phi, 0)^T\ .\\
\partial_z \mathbf{r} &\equiv b_z \mathbf{e}_z, \quad \text{with} \quad b_z = 1\ , \ \mathbf{e}_z = (0, 0, 1)^T\ .
\end{aligned}$$

(b) Gradient: $$\boldsymbol{\nabla} f = \mathbf{e}_\rho \frac{1}{b_\rho}\partial_\rho f + \mathbf{e}_\phi \frac{1}{b_\phi}\partial_\phi f + \mathbf{e}_z \frac{1}{b_z}\partial_z f = \mathbf{e}_\rho \partial_\rho f + \mathbf{e}_\phi \frac{1}{\rho}\partial_\phi f + \mathbf{e}_z \partial_z f\ .$$

(c) Divergence:

$$\begin{aligned}
\boldsymbol{\nabla}\cdot\mathbf{B} &= \frac{1}{b_\rho b\phi b_z}\Big[\partial_\rho\left(b_\phi b_z B_\rho\right) + \partial_\phi\left(b_z b_\rho B_\phi\right) + \partial_z\left(b_\rho b_\phi B_z\right)\Big]\\
&= \frac{1}{\rho}\Big[\partial_\rho\left(\rho B_\rho\right) + \partial_\phi\left(B_\phi\right) + \partial_z\left(\rho B_z\right)\Big]\\
&= \frac{1}{\rho}\partial_\rho\left(\rho B_\rho\right) + \frac{1}{\rho}\partial_\phi B_\phi + \partial_z B_z\ .
\end{aligned}$$

(d) Curl:

$$\begin{aligned}
\boldsymbol{\nabla}\times\mathbf{B} &= \mathbf{e}_\rho \frac{1}{b_\phi b_z}\Big[\partial_\phi\left(b_z B_z\right) - \partial_z\left(b_\phi B_\phi\right)\Big] + \mathbf{e}_\phi \frac{1}{b_z b_\rho}\Big[\partial_z\left(b_\rho B_\rho\right) - \partial_\rho\left(b_z B_z\right)\Big]\\
&\quad + \mathbf{e}_z \frac{1}{b_\rho b_\phi}\Big[\partial_\rho\left(b_\phi B_\phi\right) - \partial_\phi\left(b_\rho B_\rho\right)\Big]\\
&= \mathbf{e}_\rho \frac{1}{\rho}\Big[\partial_\phi\left(B_z\right) - \partial_z\left(\rho B_\phi\right)\Big] + \mathbf{e}_\phi\Big[\partial_z\left(B_\rho\right) - \partial_\rho\left(B_z\right)\Big] + \mathbf{e}_z \frac{1}{\rho}\Big[\partial_\rho\left(\rho B_\phi\right) - \partial_\phi\left(B_\rho\right)\Big]\\
&= \mathbf{e}_\rho\Big[\frac{1}{\rho}\partial_\phi B_z - \partial_z B_\phi\Big] + \mathbf{e}_\phi\Big[\partial_z B_\rho - \partial_\rho B_z\Big] + \mathbf{e}_z \frac{1}{\rho}\Big[\partial_\rho\left(\rho B_\phi\right) - \partial_\phi B_\rho\Big]\ .
\end{aligned}$$

(e) Laplace: $\boldsymbol{\nabla}^2 f = \boldsymbol{\nabla}\cdot\boldsymbol{\nabla} f$

$$= \frac{1}{\rho}\partial_\rho\big(\rho\partial_\rho f\big) + \frac{1}{\rho}\partial_\phi\Big(\frac{1}{\rho}\partial_\phi f\Big) + \partial_z\big(\partial_z f\big) = \frac{1}{\rho}\partial_\rho\big(\rho\partial_\rho f\big) + \frac{1}{\rho^2}\partial_\phi^2 f + \partial_z^2 f\ .$$

(f) Curl-Gradient:

$$\mathbf{D} \equiv \boldsymbol{\nabla} f = \mathbf{e}_u \underbrace{\frac{1}{b_u}\partial_u f}_{\equiv D_u} + \mathbf{e}_v \underbrace{\frac{1}{b_v}\partial_v f}_{\equiv D_v} + \mathbf{e}_w \underbrace{\frac{1}{b_w}\partial_w f}_{\equiv D_w}\ .$$

$$\boldsymbol{\nabla}\times\mathbf{D} = \mathbf{e}_u \frac{1}{b_v b_w}\Big[\partial_v\left(b_w D_w\right) - \partial_w\left(b_v D_v\right)\Big] + \circlearrowright_{u\,v\,w} + \circlearrowright_{u\,v\,w}\ .$$

$$\begin{aligned}\boldsymbol{\nabla}\times(\boldsymbol{\nabla}f) &= \mathbf{e}_u\frac{1}{b_v b_w}\Big[\partial_v\Big(b_w\frac{1}{b_w}\partial_w f\Big)-\partial_w\Big(b_v\frac{1}{b_v}\partial_v f\Big)\Big] \;+\; \circlearrowright_{u,v,w} \;+\; \circlearrowright_{u,v,w}\\ &= \mathbf{e}_u\frac{1}{b_v b_w}\Big[\partial_v\partial_w-\partial_w\partial_v\Big]f \;+\; \circlearrowright_{u,v,w} \;+\; \circlearrowright_{u,v,w}\\ &= \mathbf{0} \quad \text{[using Schwarz's theorem]}\,. \quad \checkmark\end{aligned}$$

ᴇV3.4.11 Gradient, divergence, curl (spherical coordinates)

(a) Cartesian: $\mathbf{r}=(x,y,z)^T$, $\quad r=\sqrt{x^2+y^2+z^2}$.
Since both f and $\mathbf{v}$ depend on the radius r, it is recommended to calculate the partial derivatives beforehand: The scalar field f depends only on the radius $f(\mathbf{r})=1/r$. Consequently, calculate the partial derivative of $f(r(x,y,z))$ with respect to x_i according to the chain rule as follows:

$$\begin{aligned}\partial_i r &= \partial r/\partial x_i = x_i/r \qquad \text{with} \qquad x_i = x,y,z\,. && (1)\\ \partial_r f &= \partial_r(1/r) = -1/r^2\,. && (2)\\ \partial_i f &= (\partial_r f)(\partial_i r) = (\partial_r f)(x_i/r) \overset{(1,2)}{=} -x_i/r^3\,, && (3)\\ \boldsymbol{\nabla} f &= \begin{pmatrix}\partial_x f\\ \partial_y f\\ \partial_z f\end{pmatrix} \overset{(3)}{=} -\frac{1}{r^3}\begin{pmatrix}x\\ y\\ z\end{pmatrix} \overset{(2)}{=} -\frac{1}{r^3}\,\mathbf{r}\,. && (4)\end{aligned}$$

The vector field $\mathbf{v}=(\mathrm{e}^{-r/a}/r)\mathbf{r}$ has the form $\mathbf{v}=(v_x,v_y,v_z)^T$, with $v_i=R(r)x_i$, where

$$\begin{aligned}R &= \frac{\mathrm{e}^{-r/a}}{r}\,, \qquad \text{with} \qquad \partial_i R=(\partial_r R)(\partial_i r)=(\partial_r R)(x_i/r)\,, && (5)\\ \partial_r R &= \Big(-\frac{1}{r^2}-\frac{1}{ar}\Big)\,\mathrm{e}^{-r/a} = \Big(-\frac{1}{r}-\frac{1}{a}\Big)\,R\,. && (6)\end{aligned}$$

In the following, we use Einstein summation notation (e.g. $x_i x_i = r^2$).

$$\begin{aligned}\boldsymbol{\nabla}\cdot\mathbf{v} &= \partial_i v_i = \big(\partial_i R\big)x_i + R\big(\partial_i x_i\big)\\ &\overset{(5)}{=} \big(\partial_r R\big)\underbrace{(x_i/r)x_i}_{=\,r^2/r\,=\,r} + 3R \overset{(6)}{=} \Big[-1-\frac{r}{a}+3\Big]\,R = \Big[2-\frac{r}{a}\Big]\,\frac{\mathrm{e}^{-r/a}}{r}\,.\end{aligned}$$

$$\begin{aligned}\boldsymbol{\nabla}\times\mathbf{v} &= \partial_i v_j \varepsilon_{ijk}\mathbf{e}_k = \partial_i(Rx_j)\varepsilon_{ijk}\mathbf{e}_k = \big[(\partial_i R)x_j + R(\partial_i x_j)\big]\varepsilon_{ijk}\mathbf{e}_k\\ &= \big[(\partial_r R)(x_i/r)x_j + R\delta_{ij}\big]\varepsilon_{ijk}\mathbf{e}_k = \mathbf{0} \quad \text{[using anti-symmetry of } \varepsilon_{ijk}\text{]}\,.\end{aligned}$$

$$\begin{aligned}\boldsymbol{\nabla}^2 f &= \partial_i[\partial_i f] \overset{(3)}{=} \partial_i\Big[-x_i/r^3\Big] = -\Big[(\partial_i x_i)/r^3 + x_i\partial_i(1/r^3)\Big]\\ &= -\Big[3/r^3 + x_i\partial_r(1/r^3)(\partial_i r)\Big] = -\Big[3/r^3 + \underbrace{x_i(-3/r^4)(x_i/r)}_{-3r^2/r^5}\Big] = 0\,.\end{aligned}$$

(b) Spherical coordinates:

$$f(r,\theta,\phi) = 1/r\,, \qquad \mathbf{v}(r,\theta,\phi) = \mathrm{e}^{-r/a}\mathbf{e}_r, \quad \Rightarrow \quad v_r = \mathrm{e}^{-r/a}, \quad v_\theta = 0, \quad v_\phi = 0\,.$$

$$\boldsymbol{\nabla} f = \left(\mathbf{e}_r\partial_r + \mathbf{e}_\theta\frac{1}{r}\partial_\theta + \mathbf{e}_\phi\frac{1}{r\sin\theta}\partial_\phi\right)\frac{1}{r} = -\frac{1}{r^2}\mathbf{e}_r\,.$$

$$\begin{aligned}\boldsymbol{\nabla}\cdot\mathbf{v} &= \frac{1}{r^2}\partial_r\left(r^2 v_r\right) + \frac{1}{r\sin\theta}\partial_\theta\left(\sin\theta v_\theta\right) + \frac{1}{r\sin\theta}\partial_\phi v_\phi \\ &= \frac{1}{r^2}\partial_r\left(r^2\mathrm{e}^{-r/a}\right) = \frac{1}{r^2}\left(2r - \frac{r^2}{a}\right)\mathrm{e}^{-r/a} = \left(2 - \frac{r}{a}\right)\frac{\mathrm{e}^{-r/a}}{r}\,.\end{aligned}$$

$$\begin{aligned}\boldsymbol{\nabla}\times\mathbf{v} &= \mathbf{e}_r\frac{1}{r\sin\theta}\left(\partial_\theta\left(\sin\theta v_\phi\right) - \partial_\phi v_\theta\right) + \mathbf{e}_\theta\frac{1}{r}\left(\frac{1}{\sin\theta}\partial_\phi v_r - \partial_r\left(r v_\phi\right)\right) \\ &\quad + \mathbf{e}_\phi\frac{1}{r}\left(\partial_r\left(r v_\theta\right) - \partial_\theta v_r\right) = \mathbf{0}\,.\end{aligned}$$

$$\boldsymbol{\nabla}^2 f = \frac{1}{r^2}\partial_r\left(r^2\partial_r f\right) + \frac{1}{r^2\sin\theta}\partial_\theta\left(\sin\theta\partial_\theta f\right) + \frac{1}{r^2\sin^2\theta}\partial_\phi^2 f = \frac{1}{r^2}\partial_r\left(-r^2\frac{1}{r^2}\right) = 0\,.$$

The results calculated in Cartesian and spherical coordinates are in agreement with each other, but the latter calculate is a bit more elegant since it uses the fact that f and $\mathbf{v}$ depend only on r, and r and $\mathbf{e}_r$, respectively.

ɛV3.4.13 Stokes' theorem – magnetic dipole (spherical coordinates)

(a) Magnetic field:
$$\begin{aligned}\mathbf{B} &= \frac{1}{c}\frac{3r\mathbf{e}_r(m\mathbf{e}_z\cdot r\mathbf{e}_r) - m\mathbf{e}_z r^2}{r^5} \\ &= \frac{m}{c}\frac{1}{r^3}\left(3\mathbf{e}_r(\mathbf{e}_z\cdot\mathbf{e}_r) - \mathbf{e}_z\right) \overset{\mathbf{e}_r\cdot\mathbf{e}_z=\cos(\theta)}{=} \frac{m}{cr^3}\left(3\cos(\theta)\mathbf{e}_r - \mathbf{e}_z\right)\,.\end{aligned}$$

Surface element: $\mathrm{d}\mathbf{S} = \mathrm{d}S\mathbf{e}_r = \sin\theta R^2\,\mathrm{d}\phi\,\mathrm{d}\theta\,\mathbf{e}_r\,.$

Flux:
$$\begin{aligned}\Phi &= \int_H \mathrm{d}\mathbf{S}\cdot\mathbf{B} = \frac{m}{cR^3}\int_0^{2\pi}\mathrm{d}\phi\int_0^{\pi/2}\mathrm{d}\theta\, R^2\sin(\theta)(3\cos(\theta) - \mathbf{e}_z\cdot\mathbf{e}_r) \\ &= \frac{m}{cR^3}2\pi R^2\underbrace{\int_0^{\pi/2}\mathrm{d}\theta\, 2\sin(\theta)\cos(\theta)}_{\sin^2(\theta)|_0^{\pi/2}=1} = \frac{2\pi m}{cR}\,.\end{aligned}$$

(b) Stoke's theorem: $\int_H \mathrm{d}\mathbf{S}\cdot\mathbf{B} = \oint_\gamma \mathrm{d}\mathbf{r}\mathbf{A}$. Hence we must calculate the line integral over the circle with radius R, $\mathbf{r}(\phi) = R\mathbf{e}_r$ with $\theta = \pi/2$, $\phi\in[0,2\pi]$:

Vector field in Spherical coordinates : $\mathbf{A} = \frac{1}{c}\frac{m\mathbf{e}_z\times r\mathbf{e}_r}{r^3} = \frac{1}{c}\frac{m}{r^2}\mathbf{e}_\phi\,.$

Line element : $\mathrm{d}\mathbf{r}(\phi) = \mathrm{d}\phi\partial_\phi\mathbf{r} = R\mathrm{d}\phi\mathbf{e}_\phi\,.$

Consequently : $\mathrm{d}\mathbf{r}(\phi)\cdot\mathbf{A} = R\mathrm{d}\phi\mathbf{e}_\phi\cdot\frac{1}{c}\frac{m}{R^2}\mathbf{e}_\phi = \frac{m}{cR}\mathrm{d}\phi\,.$

Flux: $$\Phi = \oint_\gamma d\mathbf{r}\cdot\mathbf{A} = \frac{m}{cR}\int_0^{2\pi}\mathrm{d}\phi = \frac{2\pi m}{cR}\,. \quad \checkmark$$

E V3.4.15 Stokes' theorem – magnetic field of infinite current-carrying wire (cylindrical coordinates)

(a) Cartesian coordinates, with $\sqrt{x^2+y^2}\neq 0$:

$$\mathbf{B} = \frac{2I}{c}\frac{1}{x^2+y^2}\Big(-y,x,0\Big)^T.$$

$$\boldsymbol{\nabla}\cdot\mathbf{B}(\mathbf{r}) = \sum_i \partial_i B^i = \frac{2I}{c}\left(-\frac{2x(-y)}{(x^2+y^2)^2} - \frac{2yx}{(x^2+y^2)^2}\right) = 0\,.$$

$$\boldsymbol{\nabla}\times\mathbf{B} = \begin{pmatrix}\partial_y B^z - \partial_z B^y\\ \partial_z B^x - \partial_x B^z\\ \partial_x B^y - \partial_y B^x\end{pmatrix} = \frac{2I}{c}\begin{pmatrix}0\\0\\ \frac{1}{x^2+y^2} - \frac{2x^2}{(x^2+y^2)^2} + \frac{1}{x^2+y^2} - \frac{2y^2}{(x^2+y^2)^2}\end{pmatrix} = \mathbf{0}\,.$$

(b) Cylindrical coordinates, with $\rho>0$:

$$\mathbf{B} = \mathbf{e}_\phi\frac{2I}{c}\frac{1}{\rho}, \quad \Rightarrow \quad B^\rho = B^z = 0, \quad B^\phi = \frac{2I}{c}\frac{1}{\rho}\,. \tag{1}$$

$$\boldsymbol{\nabla}\cdot\mathbf{B} = \frac{1}{\rho}\partial_\rho\left(\rho B^\rho\right) + \frac{1}{\rho}\partial_\phi B^\phi + \partial_z B^z = 0\,. \tag{2}$$

$$\boldsymbol{\nabla}\times\mathbf{B} = \mathbf{e}_\rho\left(\frac{1}{\rho}\partial_\phi B^z - \partial_z B^\phi\right) + \mathbf{e}_\phi\left(\partial_z B^\rho - \partial_\rho B^z\right) + \mathbf{e}_z\frac{1}{\rho}\left(\partial_\rho\left(\rho B^\phi\right) - \partial_\phi B^\rho\right) \tag{3}$$

$$= \mathbf{e}_z\frac{2I}{c}\frac{1}{\rho}\underbrace{\partial_\rho\left(\frac{\rho}{\rho}\right)}_{=\partial_\rho 1=0} = \mathbf{0}\,. \tag{4}$$

The results of the calculations in Cartesian and cylindrical coordinates agree of course, however the last calculation is somewhat more elegant, since it exploits the fact that $\mathbf{B}$ depends only on ρ and $\mathbf{e}_\phi$.

(c) Parametrization of the path: $\mathbf{r}(\phi) = \mathbf{e}_\rho R$, with $\phi\in[0,2\pi]$, and $\frac{\mathbf{r}(\phi)}{\mathrm{d}\phi} = \mathbf{e}_\phi R$.

$$\oint_{\gamma_D}\mathrm{d}\mathbf{r}\cdot\mathbf{B} = \int_0^{2\pi}\mathrm{d}\phi\,\underbrace{\frac{\mathbf{r}(\phi)}{\mathrm{d}\phi}}_{=\mathbf{e}_\phi R}\cdot\mathbf{B}(\mathbf{r}) = \int_0^{2\pi}\mathrm{d}\phi\,RB^\phi \overset{(1)}{=} \int_0^{2\pi}\mathrm{d}\phi\,R\frac{2I}{cR} = 2\pi\frac{2I}{c} = \frac{4\pi I}{c}\,. \tag{5}$$

(d) Using Stokes's theorem, we see immediately that:

$$\int_D \mathrm{d}\mathbf{S}\cdot(\boldsymbol{\nabla}\times\mathbf{B}) \overset{\text{Stokes}}{=} \oint_{\gamma_D}\mathrm{d}\mathbf{r}\cdot\mathbf{B} \overset{(5)}{=} \frac{4\pi I}{c}\,. \tag{6}$$

(e) On the one hand, it follows from (a) that $\boldsymbol{\nabla}\times\mathbf{B}=0$ for all spatial points with $\rho>0$, i.e. for all points except those that lie directly on the z-axis. On the other hand, it follows from (d) that the flux integral of $\boldsymbol{\nabla}\times\mathbf{B}$ does not vanish over the disk D, but rather is equal to $4\pi I/c$. This appears paradoxical at first: How can the surface integral of a vector field yield a finite value if it apparently vanishes everywhere? It would appear that this is because the calculation in part (a) does not hold for the case $\rho=0$. The fact that the integrand is equal to zero everywhere except for a single value of the integration variable, and that the integral is finite in total, tells us that we must be dealing with a δ-function. Therefore, $\boldsymbol{\nabla}\times\mathbf{B}$ must be proportional to a two dimensional δ-function:

$$\boldsymbol{\nabla}\times\mathbf{B}=C\,\mathbf{e}_z\,\delta(x)\delta(y)\,. \tag{7}$$

The direction of $\boldsymbol{\nabla}\times\mathbf{B}$ is equal to $\mathbf{e}_z$ from symmetry arguments, since $\mathbf{B}$ is in the $\mathbf{e}_\phi$-direction, and $\mathbf{e}_z$ is the sole unit vector that stays parallel to $\mathbf{e}_\phi$ for all angles ϕ. The constant C can be determined as follows:

$$\frac{4\pi I}{c}\overset{(6)}{=}\int_D \mathrm{d}\mathbf{S}\cdot(\boldsymbol{\nabla}\times\mathbf{B})\overset{(7)}{=}\int_D \mathrm{d}S\,\mathbf{e}_z\cdot C\,\mathbf{e}_z\,\delta(x)\delta(y)=C\underbrace{\int_D \mathrm{d}S\,\delta(x)\delta(y)}_{=1},\Rightarrow\ C=\frac{4\pi I}{c}\,. \tag{8}$$

(f) From (7) and (8), it follows that $\boldsymbol{\nabla}\times\mathbf{B}=4\pi\,\mathbf{j}(\mathbf{r})/c$, with $\mathbf{j}(\mathbf{r})=\mathbf{e}_z\,I\delta(x)\delta(y)$. This corresponds to Ampere's law (one of the Maxwell's equations), where $\mathbf{j}(\mathbf{r})$ is the current density of an infinitesimally thin conductor with current I along z-axis.

E V3.4.17 Gauss' theorem – electrical dipole potential (spherical coordinates)

(a)

We have: $\partial_i x_i = x_i/r$ with $x_i = x, y, z$.

$$\mathbf{E}=-\nabla\Phi=-\begin{pmatrix}\partial_x\Phi\\ \partial_y\Phi\\ \partial_z\Phi\end{pmatrix}=-\frac{p}{4\pi\varepsilon_0}\begin{pmatrix}-\frac{3zx}{r^5}\\ -\frac{3zy}{r^5}\\ -\frac{3z^2}{r^5}+\frac{1}{r^3}\end{pmatrix}=\frac{p}{4\pi\varepsilon_0}\left(3\frac{z}{r^5}\mathbf{r}-\frac{1}{r^3}\mathbf{e}_z\right)\,.$$

(b) In spherical coordinates, the field takes on the form $\Phi(\mathbf{r})=\frac{p}{4\pi\varepsilon_0}\frac{\cos\theta}{r^2}$.

$$\mathbf{E}=-\nabla\Phi=-\left(\mathbf{e}_r\partial_r+\mathbf{e}_\theta\frac{1}{r}\partial_\theta+\mathbf{e}_\phi\frac{1}{r\sin\theta}\partial_\phi\right)\Phi=\frac{p}{4\pi\varepsilon_0}\left(\frac{2\cos\theta}{r^3}\mathbf{e}_r+\frac{\sin\theta}{r^3}\mathbf{e}_\theta\right)\,.$$

Since $\mathbf{e}_z=\cos\theta\mathbf{e}_r-\sin\theta\mathbf{e}_\theta$, this corresponds to the Cartesian result:

$$\mathbf{E}=\frac{p}{4\pi\varepsilon_0}\Big(3\underbrace{\frac{\cos\theta}{r^3}}_{z/r^4}\mathbf{e}_r-\frac{1}{r^3}\underbrace{(\cos\theta\mathbf{e}_r-\sin\theta\mathbf{e}_\theta)}_{\mathbf{e}_z}\Big)$$

(c)

$$\nabla \cdot \mathbf{E} = \sum_i \frac{\partial}{\partial x_i} E_i = \frac{p}{4\pi\varepsilon_0} \left(\frac{9z}{r^5} + \frac{3z}{r^5} - 15\frac{z}{r^6} \left(\frac{x^2}{r} + \frac{y^2}{r} + \frac{z^2}{r} \right) + \frac{3}{r^4}\frac{z}{r} \right) = 0$$

$$\nabla \times \mathbf{E} = \frac{p}{4\pi\varepsilon_0} \begin{pmatrix} -\frac{15z^2y}{r^7} + \frac{3y}{r^5} - \frac{3y}{r^5} + \frac{15z^2y}{r^7} \\ \frac{3x}{r^5} - \frac{15z^2x}{r^7} + \frac{15z^2x}{r^7} - \frac{3x}{r^5} \\ -\frac{15zyx}{r^7} + + \frac{15zxy}{r^7} \end{pmatrix} = \mathbf{0}$$

(d)

$$\begin{aligned} \nabla \cdot \mathbf{E} &= \frac{1}{r^2}\partial_r \left(r^2 E_r \right) + \frac{1}{r\sin\theta}\partial_\theta \left(\sin\theta E_\theta \right) + \frac{1}{r\sin\theta}\partial_\phi E_\phi \\ &= \frac{p}{4\pi\varepsilon_0} \left(\frac{1}{r^2}\partial_r \left(\frac{2\cos\theta}{r} \right) + \frac{1}{r\sin\theta}\partial_\theta \left(\frac{\sin^2\theta}{r^3} \right) = \frac{-2\cos\theta}{r^4} + \frac{2\cos\theta}{r^4} \right) = 0 \\ \nabla \times \mathbf{E} &= \mathbf{e}_r \frac{1}{r\sin\theta} \left(\partial_\theta \left(E_\phi \sin\theta \right) - \partial_\phi E_\theta \right) + \mathbf{e}_\theta \frac{1}{r} \left(\frac{1}{\sin\theta}\partial_\phi E_r - \partial_r \left(E_r \right) \right) + \mathbf{e}_\phi \frac{1}{r} \left(\partial_r \left(r E_\theta \right) - \partial_\theta E_r \right) \\ &= \frac{p}{4\pi\varepsilon_0} \mathbf{e}_\phi \frac{1}{r} \left(\underbrace{\partial_r \left(\frac{\sin\theta}{r^2} \right)}_{-2\frac{\sin\theta}{r^3}} - \underbrace{\partial_\theta \left(\frac{2\cos\theta}{r^3} \right)}_{-2\frac{\sin\theta}{r^3}} \right) = \mathbf{0} \end{aligned}$$

(e) The mathematical Gauss' theorem gives:

$$\int_S \mathrm{d}\mathbf{S} \cdot \mathbf{E} = \int_{V_S} \mathrm{d}V \underbrace{\nabla \cdot \mathbf{E}}_{=0} \stackrel{?}{=} 0 \,.$$

Since $\nabla \cdot \mathbf{E} = 0$ for all $\mathbf{r} \neq 0$, it is an obvious deduction that the integral $\int_{V_S} \mathrm{d}V \nabla \cdot \mathbf{E}$ also vanishes. [According to the exercise, it is enough to just deduce this exactly and therefore is not covered in detail. However, there is still a subtlety which is exactly the issue which needs to be addressed and we elaborate on that below:] The components of $\mathbf{E}$, however, diverge *at* the origin, which raises the question as to whether the volume integral $\int_{V_S} \mathrm{d}V \, \nabla \cdot \mathbf{E}$ can even have a finite value. . (The latter is for e.g. the case for the potential of a point charge.) For checking condition, we calculate the flux integral directly as an integral over the spherical surface S, with area element $\mathrm{d}\mathbf{S} = \mathrm{d}S\mathbf{e}_r$ and $\mathrm{d}S = \mathrm{d}\phi\mathrm{d}\theta \sin\theta R^2$:

$$\int_S \mathrm{d}\mathbf{S} \cdot \mathbf{E} = \int_S \mathrm{d}S \underbrace{\mathbf{e}_r \cdot \mathbf{E}}_{E_r}(r = R) = \frac{3pR^2}{4\pi\varepsilon_0 R^3} \int_0^{2\pi} \mathrm{d}\phi \underbrace{\int_0^\pi \mathrm{d}\theta \sin\theta\cos\theta}_{0} = 0 \,.$$

The flux integral indeed yields zero and thus gives the result for the physical Gauss' theorem as $Q/\varepsilon = \int_S \mathrm{d}\mathbf{S} \cdot \mathbf{E} = 0$. This again demonstrates the physical fact that the total charge of an electric dipole is equal to zero.

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