2

Second quantization

The purpose of this chapter is to introduce and apply the method of second quantization, a technique that underpins the formulation of quantum many-particle theories. The first part of the chapter focusses on methodology and notation, while the remainder is devoted to the development of applications designed to engender familiarity with and fluency in the technique. Specifically, we will investigate the physics of the interacting electron gas, charge density wave propagation in one-dimensional quantum wires, and spin waves in a quantum Heisenberg (anti)ferromagnet. Indeed, many of these examples and their descendants will reappear as applications in our discussion of methods of quantum field theory in subsequent chapters.

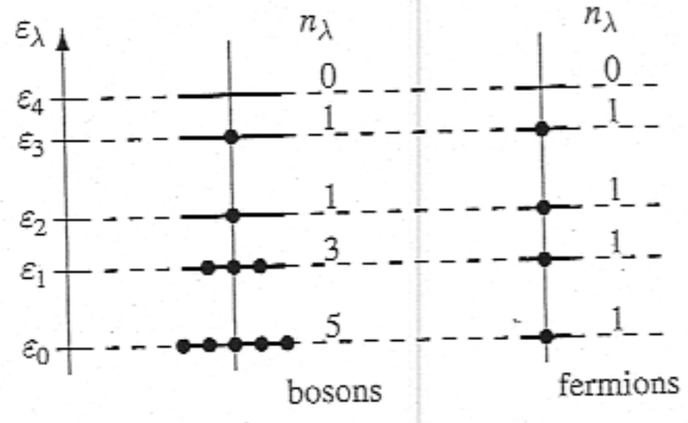
In the previous chapter we encountered two field theories that could conveniently be represented in the language of "second quantization," i.e. a formulation based on the algebra of certain ladder operators $\hat{a}_k$.[1] There were two remarkable facts about this formulation: firstly, second quantization provides a compact way of representing the *many-body* quasi-particle space of excitations; secondly, the properties of the ladder operators were encoded in a simple set of commutation relations (cf. Eq. (1.33)) rather than in some explicit Hilbert space representation.

Apart from a certain aesthetic appeal, these observations would not be of much relevance if it were not for the fact that the formulation can be generalized to a comprehensive and highly efficient formulation of many-body quantum mechanics in general. In fact, second quantization can be considered the first major cornerstone on which the theoretical framework of quantum field theory was built. This being so, extensive introductions to the concept can be found throughout the literature. We will therefore not develop the formalism in full mathematical rigor but rather proceed pragmatically by first motivating and introducing its basic elements, followed by a discussion of the "second quantized" version of standard operations of quantum mechanics (taking matrix elements, changing bases, representing operators, etc.). The second part of the chapter will be concerned with developing fluency in the method by addressing a number of applications. Readers familiar with the formalism may therefore proceed directly to these sections.

[1] The term "second quantization" is unfortunate. Historically, this terminology was motivated by the observation that the ladder operator algebra fosters an interpretation of quantum excitations as discrete "quantized" units. Fundamentally, however, there is nothing like "two" superimposed quantization steps in single- or many-particle quantum mechanics. Rather, one is dealing with a particular representation of the "first and only quantized" theory tailored to the particular problem at hand.

2.1 Introduction to second quantization

2.1.1 Motivation



We begin our discussion by recapitulating some fundamental notions of many-body quantum mechanics, as formulated in the traditional language of symmetrized/anti-symmetrized wavefunctions. Consider the (normalized) set of wavefunctions $|\lambda\rangle$ of some single-particle Hamiltonian $\hat{H}$: $\hat{H}|\lambda\rangle = \epsilon_\lambda|\lambda\rangle$, where ϵ_λ are the eigenvalues. With this definition, the normalized two-particle wavefunction $\psi_{\rm F}(\psi_{\rm B})$ of two fermions (bosons) populating levels λ_1 and λ_2 is given by the anti-symmetrized (symmetrized) product

$$\psi_{\rm F}(x_1, x_2) = \frac{1}{\sqrt{2}}\left(\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle - \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle\right),$$

$$\psi_{\rm B}(x_1, x_2) = \frac{1}{\sqrt{2}}\left(\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle + \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle\right).$$

In the Dirac bracket representation, the latter can be presented as

$$|\lambda_1, \lambda_2\rangle_{\rm F(B)} \equiv \frac{1}{\sqrt{2}}\left(|\lambda_1\rangle \otimes |\lambda_2\rangle + \zeta|\lambda_2\rangle \otimes |\lambda_1\rangle\right),$$

[2] **Enrico Fermi 1901–54**
Nobel Laureate in Physics in 1938 for his demonstrations of the existence of new radioactive elements produced by neutron irradiation, and for his related discovery of nuclear reactions brought about by slow neutrons. (Image © The Nobel Foundation.)

where $\zeta = -1$ for fermions[2] while $\zeta = 1$ for bosons. Note that the explicit symmetrization of the wavefunctions is necessitated by quantum mechanical **indistinguishability**: For fermions (bosons) the wave function has to be anti-symmetric (symmetric) under particle exchange. More generally, an appropriately symmetrized N-particle wavefunction can be expressed in the form

$$|\lambda_1, \lambda_2, \ldots, \lambda_N\rangle \equiv \frac{1}{\sqrt{N!\prod_{\lambda=0}^{\infty}(n_\lambda!)}} \sum_{\mathcal{P}} \zeta^{(1-\operatorname{sgn}\mathcal{P})/2} |\lambda_{\mathcal{P}1}\rangle \otimes |\lambda_{\mathcal{P}2}\rangle \otimes \cdots \otimes |\lambda_{\mathcal{P}N}\rangle, \tag{2.1}$$

where n_λ represents the total number of particles in state λ (for fermions, Pauli exclusion enforces the constraint $n_\lambda \leq 1$) – see the schematic figure above. The summation runs over all $N!$ permutations of the set of quantum numbers $\{\lambda_1, \ldots, \lambda_N\}$, and $\operatorname{sgn}\mathcal{P}$ denotes the sign of the permutation $\mathcal{P}$. ($\operatorname{sgn}\mathcal{P} = 1\,[-1]$ if the number of transpositions of two elements which brings the permutation $(\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_N)$ back to its original form $(1, 2, \ldots, N)$ is even [odd].) The prefactor $1/\sqrt{N!\prod_\lambda(n_\lambda!)}$ normalizes the many-body wavefunction. In the fermionic case, this is known as a **Slater determinant**. Finally, notice that it will

be useful to assume that the quantum numbers $\{\lambda_i\}$ defining the state $|\lambda_1, \lambda_2, \ldots, \lambda_N\rangle$ are ordered according to some convention. (For example, for $\lambda_i = x_i$ a one-dimensional coordinate representation, we might order according to the rule $x_1 \leq x_2 \leq \cdots \leq x_N$.) Once an ordered sequence of states has been fixed we may – for notational convenience – label our quantum states by integers, $\lambda_i = 1, 2, \ldots$. Any initially non-ordered state (e.g. $|2, 1, 3\rangle$) can be brought into an ordered form ($|1, 2, 3\rangle$) at the cost of, at most, a change of sign.

INFO For the sake of completeness, let us spell out the connection between the **permutation group and many-body quantum mechanics** in a more mathematical language. The basic arena wherein N-body quantum mechanics takes place is the product space

$$\mathcal{H}^N \equiv \underbrace{\mathcal{H} \otimes \cdots \otimes \mathcal{H}}_{N \text{ copies}}$$

of N single-particle Hilbert[3] spaces. In this space, we have a linear representation of the permutation group, S^N,[4] assigning to each $\mathcal{P} \in S^N$ the permutation (no ordering of the λs implied at this stage)

$$\mathcal{P} : \mathcal{H}^N \to \mathcal{H}^N, \quad |\lambda_1\rangle \otimes \cdots \otimes |\lambda_N\rangle \mapsto |\lambda_{\mathcal{P}1}\rangle \otimes \cdots \otimes |\lambda_{\mathcal{P}N}\rangle.$$

The identification of all irreducible subspaces of this representation is a formidable task that, thanks to a fundamental axiom of quantum mechanics, we need not address in full. All we need to know is that S^N has two particularly simple one-dimensional irreducible representations: one wherein each $\mathcal{P} \in S^N$ acts as the identity transform $\mathcal{P}(\Psi) \equiv \Psi$ and, another, the alternating representation $\mathcal{P}(\Psi) = \operatorname{sgn} \mathcal{P} \cdot \Psi$. According to a basic postulate of quantum mechanics, the state vectors $\Psi \in \mathcal{H}^N$ describing bosons/fermions must transform according to the identity/alternating representation. The subset $\mathcal{F}^N \subset \mathcal{H}^N$ of all states showing this transformation behavior is the *physical* N-body quantum Hilbert space. To construct a basis of $\mathcal{F}^N$, one may apply the symmetrization operator $P^a \equiv \sum_{\mathcal{P}} \mathcal{P}$

[3] **David Hilbert 1862–1943**
His work in geometry had the greatest influence in that area after Euclid. A systematic study of the axioms of Euclidean geometry led Hilbert to propose 21 such axioms and he analyzed their significance. He contributed to many areas of mathematics.

[4] Recall that a **linear representation** of a group G is a mapping that assigns to each $g \in G$ a linear mapping $\rho_g : V \to V$ of some vector space V. For notational convenience one usually writes $g : V \to V$ instead of $\rho_g : V \to V$. Conceptually, however, it is often important to carefully discriminate between the abstract group elements g and the *matrices* (also g) assigned to them by a given representation. (Consider, for example the symmetry group $G = \mathrm{SU}(2)$ of quantum mechanical spin. SU(2) is the *two*-dimensional group of unitary matrices with determinant one. However, when acting in the Hilbert space of a quantum spin $S = 5/2$, say, elements of SU(2) are represented by $(2S + 1 = 11)$-dimensional matrices.) Two representations ρ and ρ' that differ only by a unitary transformation, $\forall g \in G : \rho_g = U\rho'_g U^{-1}$, are called unitary equivalent. If a transformation U can be found such that *all* representation matrices ρ_g assume a block structure, the representation is called reducible, and otherwise **irreducible**. Notice that the different sub-blocks of a reducible representation by themselves form irreducible representation spaces. The identification of all distinct irreducible representations of a given group is one of the most important objectives of group theory.

(anti-symmetrization operator $P^s \equiv \sum_{\mathcal{P}} \operatorname{sgn} \mathcal{P} \mathcal{P}$) to all basis vectors $|\lambda_1\rangle \otimes \cdots \otimes |\lambda_N\rangle$ of $\mathcal{H}^N$. Up to normalization, this operation obtains the states (2.1).

Some readers may wonder why we mention these representation-theoretic aspects. Being pragmatic, all we really need to know is the symmetrization/anti-symmetrization postulate, and its implementation through (2.1). Notice, however, that one may justly question what we actually mean when we talk about the permutation exchange of quantum numbers. For example, when we compare wavefunctions that differ by an exchange of coordinates, we should, at least in principle, be able to tell by what physical operation we effect this exchange (for, otherwise, we cannot really compare them other than in a formal and, in fact, in an ambiguous sense).

Oddly enough, decades passed before this crucial issue in quantum mechanics was critically addressed. In a now seminal work by Leinaas and Myrheim[5] it was shown that the standard paradigm of permutation exchange is far from innocent. In particular, it turned out that its applicability is in an essential way tied to the dimensionality of space! Specifically, in two-dimensional spaces (in a sense, also in $d = 1$) a more elaborate scheme is needed. (Still one may use representation-theoretic concepts to describe particle exchange. However, the relevant group – the **braid group** – now differs from the permutation group.) Physically, these phenomena manifest themselves in the emergence of quantum particles different from both bosons and fermions. For a further discussion of these "**anyons**" we refer to Chapter 9.

While representations like (2.1) *can* be used to represent the full Hilbert space of many-body quantum mechanics, a moment's thought shows that this formulation is not at all convenient.

- It takes little imagination to anticipate that practical computation in the language of Eq. (2.1) will be cumbersome. For example, to compute the overlap of two wavefunctions one needs to form no less than $(N!)^2$ different products.
- The representation is tailor-made for problems with fixed particle number N. However, we know from statistical mechanics that for $N = \mathcal{O}(10^{23})$ it is much more convenient to work in a grand canonical formulation where N is allowed to fluctuate.
- Closely related to the above, in applications one will often ask questions such as, "What is the amplitude for injection of a particle into the system at a certain space-time coordinate (x_1, t_1) followed by annihilation at some later time (x_2, t_2)?" Ideally, one would work with a representation that supports the intuition afforded by thinking in terms of such processes: i.e. a representation where the quantum numbers of *individual* quasi-particles rather than the entangled set of quantum numbers of *all* constituents are fundamental.

The "second quantized" formulation of many-body quantum mechanics, as introduced in the next subsection, will remove all these difficulties in an elegant and efficient manner.

[5] J. M. Leinaas and J. Myrheim, On the theory of identical particles, Il *Nuovo Cimento* B **37** (1977), 1–23.

2.1.2 The apparatus of second quantization

Occupation number representation and Fock space

Some of the disadvantages of the representation (2.1) can be cured with relatively little effort. In our present notation, quantum states are represented by "N-letter words" of the form $|1, 1, 1, 1, 2, 2, 3, 3, 3, 4, 6, 6, \ldots\rangle$. Obviously, this notation contains a lot of redundancy. A more efficient encoding of the state above might read $|4, 2, 3, 1, 0, 2, \ldots\rangle$, where the ith number signals how many particles occupy state number i; no more information is needed to characterize a symmetrized state. (For fermions, these occupation numbers take a value of either zero or one.) This defines the "**occupation number representation.**" In the new representation, the basis states of $\mathcal{F}^N$ are specified by $|n_1, n_2, \ldots\rangle$, where $\sum_i n_i = N$. Any state $|\Psi\rangle$ in $\mathcal{F}^N$ can be obtained by a linear superposition

$$|\Psi\rangle = \sum_{\substack{n_1, n_2, \ldots \\ \sum n_i = N}} c_{n_1, n_2, \ldots} |n_1, n_2, \ldots\rangle.$$

As pointed out above, eventually we will want to emancipate ourselves from the condition of a fixed particle number N. A Hilbert space large enough to accommodate a state with an undetermined number of particles is given by

$$\mathcal{F} \equiv \bigoplus_{N=0}^{\infty} \mathcal{F}^N. \tag{2.2}$$

Notice that the direct sum contains a curious contribution $\mathcal{F}^0$, the "vacuum space." This is a one-dimensional Hilbert space which describes the sector of the theory with no particles present. Its single normalized basis state, the **vacuum state**, is denoted by $|0\rangle$. We will soon see why it is convenient to add this strange animal to our family of basis states. The space $\mathcal{F}$ is called **Fock space**[6] and it defines the principal arena of quantum many-body theory.

[6] **Vladimir Aleksandrovich Fock 1898–1974**
One of the main participants in the history of the general theory of relativity in Russia. His groundbreaking contributions to many-body theory include the introduction of Fock space and the development of perhaps *the* most important many-particle approximation scheme, the Hartree–Fock approximation (see Chapter 5).

To obtain a basis of $\mathcal{F}$, we need only take the totality of our previous basis states $\{|n_1, n_2, \ldots\rangle\}$, and drop the condition $\sum_i n_i = N$ on the occupation numbers. A general many-body state $|\Psi\rangle$ can then be represented by a linear superposition $|\Psi\rangle = \sum_{n_1, n_2, \ldots} c_{n_1, n_2, \ldots} |n_1, n_2, \ldots\rangle$. Notice that states of *different* particle numbers may contribute to the linear superposition forming $|\Psi\rangle$. We shall see that such mixtures play an important role, for example in the theory of superconductivity.

Foundations of second quantization

The occupation number representation introduced above provides a step in the right direction, but it does not yet solve our main problem. Lingering behind the compact

representation $|n_1, n_2, \ldots\rangle$ are the formidable sums over the permutation group appearing in Eq. (2.1). Surely, we need a representation of the theory wherein we are spared the need to explicitly symmetrize an $\mathcal{O}(10^{23})$ number of particles every time a matrix element is computed! The formalism of "second quantization" introduced below elegantly removes this obstacle.

Let us begin by recalling an elementary fact of linear algebra: a linear map $A : V \to V$ of a vector space into itself is fully determined by defining the images $w_i \equiv Av_i$ of the action of A on a basis $\{v_i\}$. Now let us use this scheme to introduce a set of linear operators acting in Fock space. For every $i = 1, 2, \ldots$, we define operators $a_i^\dagger : \mathcal{F} \to \mathcal{F}$ through

$$a_i^\dagger |n_1, \ldots, n_i, \ldots\rangle \equiv (n_i + 1)^{1/2} \zeta^{s_i} |n_1, \ldots, n_i + 1, \ldots\rangle, \tag{2.3}$$

where $s_i = \sum_{j=1}^{i-1} n_j$. In the fermionic case, the occupation numbers n_i have to be understood mod 2. Specifically, $(1+1) = 0 \bmod 2$, i.e. the application of $a_i^\dagger$ to a state with $n_i = 1$ annihilates this state.

Notice that by virtue of this definition we are able to generate every basis state of $\mathcal{F}$ by repeated application of $a_i^\dagger$s to the vacuum state. (From a formal point of view, this fact alone is motivation enough to add the vacuum space to the definition of Fock space.) Indeed, repeated application of Eq. (2.3) leads to the important relation

$$\boxed{|n_1, n_2, \ldots\rangle = \prod_i \frac{1}{(n_i!)^{1/2}} \left(a_i^\dagger\right)^{n_i} |0\rangle.} \tag{2.4}$$

Notice that Eq. (2.4) presents a strong statement: the complicated permutation "entanglement" implied in the definition (2.1) of the Fock states can be generated by straightforward application of a set of linear operators to a single reference state. Physically, N-fold application of operators $a^\dagger$ to the empty vacuum state generates an N-particle state, which is why the $a^\dagger$s are commonly called **creation operators**. Of course, the introduction of creation operators might still turn out to be useless, i.e. consistency with the properties of the Fock states (such as the fact that, in the fermionic case, the numbers $n_i = 0, 1$ are defined only mod 2), imply complicated correlations between the different $a_i^\dagger$. However, as we shall demonstrate below, this is not the case.

Consider two operators $a_i^\dagger$ and $a_j^\dagger$ for $i \neq j$. From the definition (2.3), one may readily verify that $\left(a_i^\dagger a_j^\dagger - \zeta a_j^\dagger a_i^\dagger\right) |n_1, n_2, \ldots\rangle = 0$. Holding for every basis vector, this relation implies that $\left[a_i^\dagger, a_j^\dagger\right]_\zeta = 0$, where

$$[\hat{A}, \hat{B}]_\zeta \equiv \hat{A}\hat{B} - \zeta \hat{B}\hat{A},$$

i.e. $[\,,\,]_{\zeta=1} \equiv [\,,\,]$ is the commutator and $[\,,\,]_{\zeta=-1} \equiv \{\,,\,\}$ the anti-commutator. Turning to the case $i = j$, we note that, for fermions, the two-fold application of $a_i^{\dagger 2}$ to *any* state leads to its annihilation. Thus, $a_i^{\dagger 2} = 0$ is nilpotent, a fact that can be formulated as $\left[a_i^\dagger, a_i^\dagger\right]_+ = 0$. For bosons we have, of course, $\left[a_i^\dagger, a_i^\dagger\right] = 0$ (identical operators commute!). Summarizing, we have found that the creation operators obey the commutation relation

$$\forall i, j: \quad \left[a_i^\dagger, a_j^\dagger\right]_\zeta = 0. \tag{2.5}$$

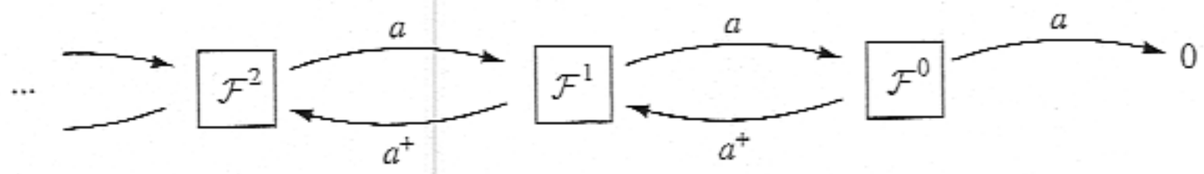


Figure 2.1 Visualization of the generation of the Fock subspaces $\mathcal{F}^N$ by repeated action of creation operators on the vacuum space $\mathcal{F}^0$.

Now, quantum mechanics is a unitary theory so, whenever one meets a new operator $\hat{A}$, one should determine its Hermitian adjoint $\hat{A}^\dagger$. To understand the action of the Hermitian adjoints $\left(a_i^\dagger\right)^\dagger = a_i$ of the creation operators we may take the complex conjugates of all basis matrix elements of (2.3):

$$\left\langle n_1, \ldots, n_i, \ldots \left| a_i^\dagger \right| n_1', \ldots, n_i', \ldots \right\rangle = \left(n_i'+1\right)^{1/2} \zeta^{s_i'} \delta_{n_1,n_1'} \ldots \delta_{n_i,n_i'+1} \cdots$$

$$\Rightarrow \quad \langle n_1', \ldots, n_i', \ldots | a_i | n_1, \ldots, n_i, \ldots \rangle^* = n_i^{1/2} \zeta^{s_i} \delta_{n_1',n_1} \ldots \delta_{n_i',n_i-1} \cdots$$

Holding for every bra $\langle n_1', \ldots, n_i', \ldots |$, the last line tells us that

$$a_i | n_1, \ldots, n_i, \ldots \rangle = n_i^{1/2} \zeta^{s_i} | n_1, \ldots, n_i - 1, \ldots \rangle, \tag{2.6}$$

a relation that identifies a_i as an operator that *annihilates* particles. The action of creation and **annihilation operators** in Fock space is illustrated in Fig. 2.1. Creation operators $a^\dagger : \mathcal{F}^N \to \mathcal{F}^{N+1}$ increase the particle number by one, while annihilation operators $a : \mathcal{F}^N \to \mathcal{F}^{N-1}$ lower it by one; the application of an annihilation operator to the vacuum state, $a_i|0\rangle = 0$, annihilates it. (Do not confuse the vector $|0\rangle$ with the number zero.)

Taking the Hermitian adjoint of Eq. (2.5) we obtain $[a_i, a_j]_\zeta = 0$. Further, a straightforward calculation based on the definitions (2.3) and (2.6) shows that $\left[a_i, a_j^\dagger\right]_\zeta = \delta_{ij}$. Altogether, we have shown that the creation and annihilation operators satisfy the algebraic closure relation

$$\boxed{\left[a_i, a_j^\dagger\right]_\zeta = \delta_{ij}, \quad [a_i, a_j]_\zeta = 0, \quad \left[a_i^\dagger, a_j^\dagger\right]_\zeta = 0.} \tag{2.7}$$

Given that the full complexity of Fock space is generated by application of $a_i^\dagger$s to a single reference state, the simplicity of the relations obeyed by these operators seems remarkable and surprising.

INFO Perhaps less surprising is that, behind this phenomenon, there lingers some mathematical structure. Suppose we are given an abstract algebra $\mathcal{A}$ of objects a_i, $a_i^\dagger$ satisfying the relation (2.7). (Recall that an algebra is a vector space whose elements can be multiplied by each other.) Further suppose that $\mathcal{A}$ is irreducibly represented in some vector space V, i.e. that there is a mapping assigning to each $a_i \in \mathcal{A}$ a linear mapping $a_i : V \to V$, such that every vector $|v\rangle \in V$ can be reached from any other

$|w\rangle \in V$ by (possibly iterated) application of operators a_i and $a_i^\dagger$ (irreducibility).[7] According to the **Stone–von Neumann theorem** (a) such a representation is unique (up to unitary equivalence), and (b) there is a unique state $|0\rangle \in V$ that is annihilated by every a_i. All other states can then be reached by repeated application of $a_i^\dagger$s. The precise formulation of this theorem, and its proof – a good practical exercise in working with creation/annihilation operators – are left as Problem 2.4.1. From the Stone–von Neumann theorem, we can infer that the Fock space basis could have been constructed in reverse. Not knowing the basis $\{|n_1, n_2, \ldots\rangle\}$, we could have started from a set of operators obeying the commutation relations (2.7) acting in some *a priori* unknown space $\mathcal{F}$. Outgoing from the unique state $|0\rangle$, the prescription (2.4) would then have yielded an equally unique basis of the entire space $\mathcal{F}$ (up to unitary transformations). In other words, the algebra (2.7) fully characterizes the operator action and provides information equivalent to the definitions (2.3) and (2.6).

Practical aspects

Our next task will be to promote the characterization of Fock space bases introduced above to a full reformulation of many-body quantum mechanics. To this end, we need to find out how changes from one single-particle basis $\{|\lambda\rangle\}$ to another $\{|\tilde{\lambda}\rangle\}$ affect the operator algebra $\{a_\lambda\}$. (In this section we shall no longer use integers to identify different elements of a given single-particle basis. Rather, we use Greek labels λ, i.e. $a_\lambda^\dagger$ creates a particle in state λ.) Equally important, we need to understand in what way generic operators acting in many-particle Hilbert spaces can be represented in terms of creation and annihilation operators.

- **Change of basis:** Using the resolution of identity $\mathrm{id} = \sum_{\lambda=0}^{\infty} |\lambda\rangle\langle\lambda|$, the relations $|\tilde{\lambda}\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\tilde{\lambda}\rangle$, $|\lambda\rangle \equiv a_\lambda^\dagger|\Omega\rangle$, and $|\tilde{\lambda}\rangle \equiv a_{\tilde{\lambda}}^\dagger|\Omega\rangle$ immediately give rise to the transformation law

$$\boxed{a_{\tilde{\lambda}}^\dagger = \sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a_\lambda^\dagger, \qquad a_{\tilde{\lambda}} = \sum_\lambda \langle\tilde{\lambda}|\lambda\rangle a_\lambda.} \tag{2.8}$$

In many applications, we will be dealing with *continuous* sets of quantum numbers (such as continuous position coordinates). In these cases, the quantum numbers are commonly denoted by a bracket notation $a_\lambda \rightsquigarrow a(x) = \sum_\lambda \langle x|\lambda\rangle a_\lambda$ and the summations appearing in the transformation formula above translate to integrals: $a_\lambda = \int dx \langle\lambda|x\rangle a(x)$.

Example The transformation from the coordinate to the Fourier momentum representation in a finite one-dimensional system of length L would read

$$a_k = \int_0^L dx\, \langle k|x\rangle a(x), \qquad a(x) = \sum_k \langle x|k\rangle a_k, \tag{2.9}$$

where $\langle k|x\rangle \equiv \langle x|k\rangle^* = e^{-ikx}/\sqrt{L}$.

[7] To appropriately characterize the representation, we need to be a bit more precise. Within $\mathcal{A}$, a_i and $a_i^\dagger$ are independent objects, i.e. in general there exists no notion of Hermitian adjointness in $\mathcal{A}$. We require, though, that the representation assigns to $a_i^\dagger$ the Hermitian adjoint (in V) of the image of a_i. Also, we have to require that $[a_i, a_j^\dagger] \in \mathcal{A}$ be mapped onto $[a_i, a_j^\dagger] : V \to V$ where, in the latter expression, the commutator involves the ordinary product of matrices $a_i, a_j^\dagger : V \to V$.

- **Representation of operators (one-body):** Single-particle or one-body operators $\hat{\mathcal{O}}_1$ acting in the N-particle Hilbert space $\mathcal{F}^N$ generally take the form $\hat{\mathcal{O}}_1 = \sum_{n=1}^{N} \hat{o}_n$, where $\hat{o}_n$ is an ordinary single-particle operator acting on the nth particle. A typical example is the kinetic energy operator $\hat{T} = \sum_n \hat{p}_n^2/2m$, where $\hat{p}_n$ is the momentum operator acting on the nth particle. Other examples include the one-particle potential operator $\hat{V} = \sum_n V(\hat{x}_n)$, where $V(x)$ is a scalar potential, the total spin operator $\sum_n \hat{\mathbf{S}}_n$, etc. Since we have seen that, by applying field operators to the vacuum space, we can generate the Fock space in general and any N-particle Hilbert space in particular, it must be possible to represent any operator $\hat{\mathcal{O}}_1$ in an a-representation.

  Now, although the representation of n-body operators is, after all, quite straightforward, the construction can, at first sight, seem daunting. A convenient way of finding such a representation is to express the operator in terms of a basis in which it is diagonal, and only later transform to an arbitrary basis. For this purpose it is useful to define the **occupation number operator**

$$\boxed{\hat{n}_\lambda = a_\lambda^\dagger a_\lambda} \tag{2.10}$$

with the property that, for bosons or fermions (exercise), $\hat{n}_\lambda \left(a_\lambda^\dagger\right)^n |0\rangle = n \left(a_\lambda^\dagger\right)^n |0\rangle$. Since $\hat{n}_\lambda$ commutes with all $a_{\lambda' \neq \lambda}^\dagger$, Eq. (2.4) readily implies that $\hat{n}_{\lambda_j} |n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle = n_{\lambda_j} |n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle$, i.e., $\hat{n}_\lambda$ simply counts the number of particles in state λ (hence the name "occupation number operator"). Let us now consider a one-body operator, $\hat{\mathcal{O}}_1$, which is diagonal in the basis $|\lambda\rangle$, with $\hat{o} = \sum_i o_{\lambda_i} |\lambda_i\rangle\langle\lambda_i|$, $o_{\lambda_i} = \langle\lambda_i|\hat{o}|\lambda_i\rangle$. With this definition, one finds that

$$\begin{aligned}\left\langle n'_{\lambda_1}, n'_{\lambda_2}, \ldots \middle| \hat{\mathcal{O}}_1 \middle| n_{\lambda_1}, n_{\lambda_2}, \ldots \right\rangle &= \sum_i o_{\lambda_i} n_{\lambda_i} \left\langle n'_{\lambda_1}, n'_{\lambda_2}, \ldots \middle| n_{\lambda_1}, n_{\lambda_2}, \ldots \right\rangle \\ &= \left\langle n'_{\lambda_1}, n'_{\lambda_2}, \ldots \middle| \sum_i o_{\lambda_i} \hat{n}_{\lambda_i} \middle| n_{\lambda_1}, n_{\lambda_2}, \ldots \right\rangle.\end{aligned}$$

Since this equality holds for any set of states, one can infer the second quantized representation of the operator $\hat{\mathcal{O}}_1$,

$$\hat{\mathcal{O}}_1 = \sum_{\lambda=0}^{\infty} o_\lambda \hat{n}_\lambda = \sum_{\lambda=0}^{\infty} \langle\lambda|\hat{o}|\lambda\rangle a_\lambda^\dagger a_\lambda.$$

The result is straightforward: a one-body operator engages a single particle at a time – the others are just spectators. In the diagonal representation, one simply counts the number of particles in a state λ and multiplies by the corresponding eigenvalue of the one-body operator. Finally, by transforming from the diagonal representation to a general basis, one obtains the general result,

$$\boxed{\hat{\mathcal{O}}_1 = \sum_{\mu\nu} \langle\mu|\hat{o}|\nu\rangle a_\mu^\dagger a_\nu.} \tag{2.11}$$

[8] **Wolfgang Pauli 1900–58**
Nobel Laureate in Physics in 1945 "for the discovery of the Exclusion Principle, also called the Pauli Principle." (Image © The Nobel Foundation.)

To cement these ideas, let us consider some specific examples: representing the matrix elements of the single-particle spin operator as $(S_i)_{\alpha\alpha'} = \frac{1}{2}(\sigma_i)_{\alpha\alpha'}$, where α, α' is a two-component spin index and σ_i are the Pauli[8] spin matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2.12}$$

the **spin operator** of a many-body system assumes the form

$$\hat{\mathbf{S}} = \sum_{\lambda} a^{\dagger}_{\lambda\alpha'} \mathbf{S}_{\alpha'\alpha} a_{\lambda\alpha}. \tag{2.13}$$

(Here, λ denotes the set of additional quantum numbers, e.g. a lattice site index.)
When second quantized in the position representation, one can show that the **one-body Hamiltonian** for a free particle is given as a sum of kinetic and potential energy as

$$\hat{H} = \int d^d r \; a^{\dagger}(\mathbf{r}) \left[\frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}) \right] a(\mathbf{r}), \tag{2.14}$$

where $\hat{\mathbf{p}} = -i\hbar\partial$.

EXERCISE Starting with momentum representation (in which the kinetic energy is diagonal), transform to the position representation and thereby establish Eq. (2.14).

The **local density operator** $\hat{\rho}(\mathbf{r})$, measuring the particle density at a certain coordinate $\mathbf{r}$, is simply given by

$$\hat{\rho}(\mathbf{r}) = a^{\dagger}(\mathbf{r}) a(\mathbf{r}). \tag{2.15}$$

Finally, the **total occupation number operator**, obtained by integrating over the particle density, is defined by $\hat{N} = \int d^d r \; a^{\dagger}(\mathbf{r}) a(\mathbf{r})$. In a theory with discrete quantum numbers, this operator assumes the form $\hat{N} = \sum_{\lambda} a^{\dagger}_{\lambda} a_{\lambda}$.

- **Representation of operators (two-body):** Two-body operators $\hat{\mathcal{O}}_2$ are needed to describe pairwise interactions between particles. Although pair-interaction potentials are straightforwardly included in classical many-body theories, their embedding into conventional many-body quantum mechanics is made cumbersome by particle indistinguishability. As compared with the conventional description, the formulation of interaction processes within the language of second quantization is considerably more straightforward.

  Initially, let us consider particles subject to the symmetric two-body potential $V(\mathbf{r}_m, \mathbf{r}_n) \equiv V(\mathbf{r}_n, \mathbf{r}_m)$ between two particles at position $\mathbf{r}_m$ and $\mathbf{r}_n$. Our aim is to find an operator $\hat{V}$ in second quantized form whose action on a many-body state gives

(presently, it is more convenient to use the original representation (2.1) rather than the occupation number representation)

$$\hat{V}|\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N\rangle = \sum_{n<m}^{N} V(\mathbf{r}_n, \mathbf{r}_m)|\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N\rangle = \frac{1}{2}\sum_{n\neq m}^{N} V(\mathbf{r}_n, \mathbf{r}_m)|\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N\rangle.$$

When this is compared with the one-point function, one might immediately guess that

$$\hat{V} = \frac{1}{2}\int d^d r \int d^d r' a^\dagger(\mathbf{r})a^\dagger(\mathbf{r}')V(\mathbf{r}, \mathbf{r}')a(\mathbf{r}')a(\mathbf{r}).$$

That this is the correct answer can be confirmed by applying the operator to a many-body state:

$$\begin{aligned} a^\dagger(\mathbf{r})a^\dagger(\mathbf{r}')a(\mathbf{r}')a(\mathbf{r})|\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\rangle &= a^\dagger(\mathbf{r})a^\dagger(\mathbf{r}')a(\mathbf{r}')a(\mathbf{r})a^\dagger(\mathbf{r}_1)\cdots a^\dagger(\mathbf{r}_N)|\Omega\rangle \\ &= \sum_{n=1}^{N}(-\zeta)^{n-1}\delta(\mathbf{r}-\mathbf{r}_n)a^\dagger(\mathbf{r}_n)\overbrace{a^\dagger(\mathbf{r}')a(\mathbf{r}')}^{\hat{\rho}(\mathbf{r}')}a^\dagger(\mathbf{r}_1)\cdots a^\dagger(\mathbf{r}_{n-1})a^\dagger(\mathbf{r}_{n+1})\cdots a^\dagger(\mathbf{r}_N)|\Omega\rangle \\ &= \sum_{n=1}^{N}(-\zeta)^{n-1}\delta(\mathbf{r}-\mathbf{r}_n)\sum_{m(\neq n)}^{N}\delta(\mathbf{r}'-\mathbf{r}_m)a^\dagger(\mathbf{r}_n)a^\dagger(\mathbf{r}_1)\cdots a^\dagger(\mathbf{r}_{n-1})a^\dagger(\mathbf{r}_{n+1})\cdots a^\dagger(\mathbf{r}_N)|\Omega\rangle \\ &= \sum_{n,m\neq n}^{N}\delta(\mathbf{r}-\mathbf{r}_n)\delta(\mathbf{r}'-\mathbf{r}_m)|\mathbf{r}_1, \mathbf{r}_2, \cdots \mathbf{r}_N\rangle. \end{aligned}$$

Multiplying by $V(\mathbf{r}, \mathbf{r}')/2$, and integrating over $\mathbf{r}$ and $\mathbf{r}'$, one confirms the validity of the expression. It is left as an exercise to confirm that the naive expression $\frac{1}{2}\int d^d r \int d^d r' V(\mathbf{r}, \mathbf{r}')\hat{\rho}(\mathbf{r})\hat{\rho}(\mathbf{r}')$ does not reproduce the two-body operator. More generally, turning to a non-diagonal basis, it is straightforward to confirm that a general two-body operator can be expressed in the form

$$\boxed{\hat{\mathcal{O}}_2 = \sum_{\lambda\lambda'\mu\mu'} \mathcal{O}_{\mu,\mu',\lambda,\lambda'}a^\dagger_\mu a^\dagger_{\mu'}a_\lambda a_{\lambda'}} \tag{2.16}$$

where $\mathcal{O}_{\mu,\mu',\lambda,\lambda'} \equiv \langle\mu, \mu'|\hat{\mathcal{O}}_2|\lambda, \lambda'\rangle$.

As well as the pairwise **Coulomb interaction** formulated above, another important interaction, frequently encountered in problems of quantum magnetism, is the **spin–spin interaction**. From our discussion of the second-quantized representation of spin $\hat{\mathbf{S}}$ above, we can infer that the general spin–spin interaction can be presented in second-quantized form as

$$\hat{V} = \frac{1}{2}\int d^d r \int d^d r' \sum_{\alpha\alpha'\beta\beta'} J(\mathbf{r}, \mathbf{r}')\mathbf{S}_{\alpha\beta}\cdot\mathbf{S}_{\alpha'\beta'}a^\dagger_\alpha(\mathbf{r})a^\dagger_{\alpha'}(\mathbf{r}')a_{\beta'}(\mathbf{r}')a_\beta(\mathbf{r}),$$

where $J(\mathbf{r}, \mathbf{r}')$ denotes the exchange interaction.

In principle, one may proceed in the same manner and represent general n-body interactions in terms of second-quantized operators. However, as $n > 2$ interactions appear infrequently, we refer to the literature for discussion.

This completes our formal introduction to the method of second quantization. To remove some of the abstraction, and to develop fluency in the operation of the method, we will close this chapter by addressing a number of problems chosen from the realm of condensed matter. In doing so, we will see that, although second quantization provides merely a representation and not a solution, its application often leads to considerable simplification of the analysis of many-particle systems. To further motivate our discussion, we will endeavor to classify some of the characteristic "phases" of the interacting electron gas in solid state media. The effective model Hamiltonians that appear below provide the input for subsequent applications of the methods of quantum field theory considered in this text.

It is, however, important to emphasize that the present text is necessarily limited in its scope. Although a detailed survey of modern aspects of condensed physics is a worthwhile and welcome enterprise, we do not wish to detract from our main focus, the development of modern *methods* of quantum field theory in the condensed matter setting. Readers primarily interested in methodological aspect may safely skip the next sections and turn directly to Chapter 3 below. For later reference, it is worthwhile keeping in mind that the physical *motivation* for the study of various prototypical model systems considered later in the text is given in Section 2.2.

2.2 Applications of second quantization

Starting from the prototype Hamiltonian (1.1) introduced in Chapter 1, we have already explored generic aspects of lattice dynamics in condensed matter systems. In much of the remaining text we will explore examples from the complementary sector focussing on the electronic degrees of freedom. Drawing on the first of the principles discussed in Chapter 1, we will begin our discussion by reducing the full many-body Hamiltonian to a form that contains the essential elements of the electron dynamics. As well as the pure electron sub-Hamiltonian H_e, the reduced Hamiltonian will involve the interaction between the electrons and the positively charged ionic background lattice. However, typically, lattice distortions due to both the motion of the ions and the ion–ion interaction couple only indirectly. (Exercise: Try to think of a prominent example where the electron sector is *crucially* influenced by the dynamics of the host lattice.) To a first approximation, we may, therefore, describe the electron system through the simplified Hamiltonian, $\hat{H} = \hat{H}_0 + \hat{V}_{ee}$, where

$$\left.\begin{aligned} \hat{H}_0 &= \int d^d r\, a_\sigma^\dagger(\mathbf{r}) \left[\frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}) \right] a_\sigma(\mathbf{r}) \\ \hat{V}_{ee} &= \frac{1}{2} \int d^d r \int d^d r'\, V_{ee}(\mathbf{r}-\mathbf{r}') a_\sigma^\dagger(\mathbf{r}) a_{\sigma'}^\dagger(\mathbf{r}') a_{\sigma'}(\mathbf{r}') a_\sigma(\mathbf{r}), \end{aligned}\right\} \tag{2.17}$$

$V(\mathbf{r}) = \sum_I V_{ei}(\mathbf{R}_I - \mathbf{r})$ denotes the lattice potential experienced by the electrons, and the coordinates of the lattice ions $\mathbf{R}_I$ are assumed fixed. For completeness, we have also endowed the electrons with a spin index, $\sigma = \uparrow / \downarrow$. The Hamiltonian defines the problem of the interacting electron gas embedded in a solid state system.

Despite its seemingly innocuous structure, the interacting electron Hamiltonian (2.17) accommodates a wide variety of electron phases from metals and magnets to insulators.