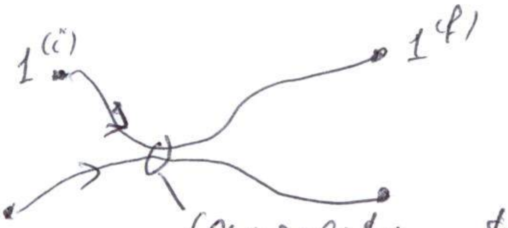
2^{nd} quantization

Books LL - III, Sect. IX (Identical particles)
Alt-Sim, CM-FT, Sect. 2 (2^{nd} quantization)

Goal: find the formal apparatus which is very convenient to built MB-QM or Q-St Phys.

Trivial input

all particles are distinguishable in cl/ph.



causality, trajectories cannot intersect in phase-space, we can follow trajectories and tell which particle occupies a given f-state

Toward QM: we can formaly find Hilbert space for dist.-particles with the basis

$$\underbrace{|\lambda_1, \lambda_2 \dots \lambda_N\rangle}_{\text{for } N\text{-particles}} = \underset{\uparrow \; 1^{st} \text{ particle}}{|\lambda_1\rangle} \otimes |\lambda_2\rangle \dots \underset{\uparrow \; N^{th} \text{ particle}}{|\lambda_N\rangle}$$

QM - particles became indistinguishable because of the uncertainty principle

or 2 ? trajectories are not
1 . defined, we cannot follow them

Consider two particles described by 2-p.w.f in 3d

$\Psi(\xi_1, \xi_2)$ and apply $\hat{P}_{1\leftrightarrow 2}$

(ξ_1 – 1st, ξ_2 – 2nd)

Postulate of our QM in 3d

$$\hat{P}\left(\hat{P}\,\Psi(\xi_1, \xi_2)\right) = \Psi(\xi_1, \xi_2) -$$

because Ψ must be single-valued

(Note: low-dim. system can be very different!)

+ particles 1 & 2 are indistinguishable ⇒

$\hat{P}$ can yield only a phase-factor (inessential)

$$\Psi(\xi_1, \xi_2) = e^{i\alpha}\,\Psi(\xi_2, \xi_1)$$

and $(e^{i\alpha})^2 \Rightarrow 1 \Rightarrow \alpha = 0, \pi$; $\boxed{e^{i\alpha} = \pm 1}$

$$\Psi(\xi_1, \xi_2) = \zeta\,\Psi(\xi_2, \xi_1)$$

where $\zeta = \begin{cases} +1 & \text{- for bosons (integer spin)} \\ -1 & \text{- for fermions (half-integer spin)} \end{cases}$

Conclusion: we must (anti) symmetrize states:

$$|\lambda_1, \lambda_2\rangle_{F/B} = \frac{1}{\sqrt{2}}\Big(\underbrace{|\lambda_1\rangle \otimes |\lambda_2\rangle + \zeta\,|\lambda_2\rangle \otimes |\lambda_1\rangle}\Big)$$

for correct norm.

linear combination of states, corresponding to distinguishable particles.

$|\lambda_1, \lambda_2\rangle$ is either symmetric or antisymmetric.

For N- particles

__Boson__ $|\lambda_1 \ldots \lambda_N\rangle = \left(\frac{\prod N_j!}{N!}\right) \sum_{\mathcal{P}} |\lambda_{p_1}\rangle \otimes \ldots \otimes |\lambda_{p_N}\rangle$

$\mathcal{P}$ - permutations of different indices p_i,

N_i - how many of these indices have a given value i

Note: $\sum_i N_i = N$

__Fermions:__ $|\lambda_1 \ldots \lambda_N\rangle = \frac{1}{\sqrt{N!}} \sum_{\mathcal{P}} \underbrace{\operatorname{sgn} \mathcal{P}}_{\text{sign of the permutation}} |\lambda_{p_1}\rangle \otimes \ldots \otimes |\lambda_{p_N}\rangle$ -

governed by a parity of transpositions which bring the permutation back to its original ordered form,

* add (3-1)

__Problem__ - the above repr. is very inconvenient for practical purposes because it contains redundant info. __Example__

$|1, 1, 1, 1, 2, 2, 4, 4, 4, \ldots\rangle$ can be

conveniently rewritten as

$|4, 2, 0, 3, \ldots\rangle$

number of particles in a given state

which are called __occupation numbers__

More detailed info is not needed in QM.

If N is fixed then we can write any state of $\mathcal{F}^N$ as a linear combination

Note that anti-symmetrized fermionic state 3-1
has a form of Slatter determinant:

$$|\lambda_1 \dots \lambda_N\rangle = \frac{1}{\sqrt{N!}} \left| \begin{array}{ccc} \psi_{\lambda_1}(\xi_1) & \dots & \psi_{\lambda_1}(\xi_N) \\ \psi_{\lambda_2}(\xi_1) & \dots & \psi_{\lambda_2}(\xi_N) \\ - & - & - \\ \psi_{\lambda_N} & \dots & \psi_{\lambda_N} \end{array} \right| \text{ N-states}$$

$$\underbrace{\qquad\qquad\qquad\qquad}_{\text{N-particles.}}$$

Obviously, det = 0 if there are the same states
among λ_j - this is the Pauli principle:
2 (or more) fermions cannot occupy the same
states

$$|\psi\rangle = \sum_{n_i} c_{n_1, n_2 \ldots} \underbrace{|n_1, n_2, \ldots\rangle}_{\text{occupation numbers}}$$

where $\sum n_i = N$

States with undetermined number of particles belong to the so-called <u>Fock-space</u>

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{F}^N$$

Note $\mathcal{F}^0 \in \mathcal{F}$; $\mathcal{F}^0$ (vacuum space) contains only one state

$$|0\rangle \in \mathcal{F}^0$$

where there's no particle at all (recall GS for CM-systems, where excitations are absent)

<u>Next important step of the apparatus</u>

Let's define creation (raising) and annihilation (lowering) conjugated! operators as follows:

<u>bosons</u>

$$\hat{a}_j^{+} |\ldots n_j \ldots\rangle = \sqrt{n_j + 1}\, |\ldots n_j + 1 \ldots\rangle$$

$$\hat{a}_j |\ldots n_j \ldots\rangle = \sqrt{n_j}\, |\ldots n_j - 1 \ldots\rangle$$

increased / decreased by 1

Here n_j are integer (arbitrary!) occupation numbers fermions

$$\hat{a}_j^+ | \dots n_j \dots \rangle = (1-n_j)(-1)^{\epsilon_j} | \dots n_j + 1 \dots \rangle$$

$$\hat{a}_j | \dots n_j \dots \rangle = n_j (-1)^{\epsilon_j} | \dots n_j - 1 \dots \rangle$$

with $\epsilon_j = \sum_{k=1}^{j-1} n_k$, $\epsilon_1 = 0$ (implying a fixed order)

and $n_k = 0, 1$ ~~due~~ to the Pauli principle

Important (rigorous) statement: any state from the $\mathcal{F}$ can be constructed by action $\hat{a}^+$ on $|0\rangle$:

$$\boxed{|n_1, n_2, \dots \rangle = \prod_i \frac{1}{(n_i!)^{1/2}} (\hat{a}_i^+)^{n_i} |0\rangle}$$

which means that the rhp takes into account q-statistics automatically

$$\prod_i \frac{1}{(n_i!)^{1/2}} (\hat{a}_i^+)^{n_i} |0\rangle \text{ “}\equiv\text{” } \hat{S}_\xi [\varphi_1(\xi_1) \varphi_2(\xi_2) \dots]$$

$\hat{S}_\pm$ – symmetrization / antisymmetrization operators

Next step we need algebra of operators $\hat{a}^+, \hat{a}$

$$\cancel{\boxed{|n_1, n_2, \ldots\rangle = \prod_i \frac{1}{(n_i!)^{1/2}} (\hat{a}_i^{\dagger})^{n_i} |0\rangle}}$$

~~Conjugated operators are calle annihilation (lowering) operators. They are given by~~ see (4-1)

$$\cancel{\hat{a}_i |n_1, \ldots, n_i, \ldots\rangle = n_i^{1/2} \xi^{S_i} |n_1, \ldots, \underbrace{n_i - 1}_{\text{decreased by 1}}, \ldots\rangle}$$

Note that fermionic operators are nilpotents

$$(\hat{a}_i^{\dagger})^2 = (\hat{a}_j)^2 = 0$$

due to the Pauli principle - we can expect they anticommute. Indeed, startin from the definition one can directly show that (check!)

$$\boxed{[a_i, a_j^{\dagger}]_\xi = \delta_{i,j}; \quad [a_i, a_j]_\xi = [a_i^{\dagger}, a_j^{\dagger}]_\xi = 0}$$

they obbey the so-calle bosonic/fermionic algebra,

Here $[\ldots]_{\xi=1}$ - commutator $([\hat{a}, \hat{a}'] = \hat{a}\hat{a}' - \hat{a}'\hat{a})$

$[\ldots]_{\xi=-1}$ - anticommutator $(\{\hat{a}, \hat{a}'\} = \hat{a}\hat{a}' + \hat{a}'\hat{a})$

Note that $\hat{a}_i^{\dagger} \hat{a}_i |\{n\}\rangle \overset{def}{\equiv} \hat{n}_i |\{n\}\rangle \overset{check}{=} n_i |\{n\}\rangle$

counts a number of particles in the state

Final step changing the basis to the basis of the occupation numbers. Example: interacting systems

$$\hat{H} = \overbrace{\sum_a \hat{H}_a^{(1)}}^{\hat{H}^{(1)}} + \overbrace{\sum_{a>b} \hat{H}_{a,b}^{(2)}}^{\hat{H}^{(2)}}$$

over all particles

Here $\hat{H}^{(1)}_a$ - single particle operators which act on variables of the particle "a" (kinetic energy, external fields / potentials, etc.)

$\hat{H}^{(2)}_{a,b}$ (or $\hat{H}^{(2)}(\xi_a, \xi_b)$) - two particle operators (like pair-interactions)

Goal: change from summations over particles to summations over states. Equivalence of both approaches can be shown by comparing matrix elements of operators in different representations.

Let's demonstrate how it work for a diagonal (in a given basis) operator by using $\hat{n}$-operators

Consider

$$\langle \{n'\} | \sum_a \hat{H}^{(1)}_a | \{n\} \rangle \quad (1)$$

all occupation numbers are here

introduce $h^{(1)}_j = \langle \lambda_j | \hat{H}^{(1)}_a | \lambda_j \rangle$ to transform

$$(1) \to \langle \{n'\} | \sum_j h^{(1)}_j n_j | \{n\} \rangle \quad (2)$$

Matrix element of $\hat{H}^{(1)}_a$

multiplicity of each state

Using properties of $\hat{n}_j$:

$$(2) \to \langle \{n'\} | \sum_j h^{(1)}_j \hat{n}_j | \{n\} \rangle$$

which allows us to conclude that

$$\hat{H}^{(1)} = \sum_i h_i^{(1)} \hat{a}_i^+ \hat{a}_i$$

In a general case (non-diagonal operator):

$$\hat{H}^{(1)} = \sum_{ik} \langle \lambda_i | \hat{H}_a^{(1)} | \lambda_k \rangle \hat{a}_{\lambda_i}^+ \hat{a}_{\lambda_k}$$

And similar for 2-particle operators

$$\hat{H}^{(2)} = \underbrace{\frac{1}{2}}_{\text{to avoid double-counting}} \sum_{\text{all}} \langle \lambda_i \lambda_k | \hat{H}_{ab}^{(2)} | \lambda_l \lambda_m \rangle \hat{a}_{\lambda_i}^+ \hat{a}_{\lambda_k}^+ \hat{a}_{\lambda_l} \hat{a}_{\lambda_m}$$

<u>Examples</u> the density operator

$$\hat{\rho}(r_0) = |r_0\rangle\langle r_0|$$

with the matrix element

$$\langle \psi | \hat{\rho}(r_0) | \psi \rangle = |\psi(r_0)|^2$$

Let's choose the position basis $|r\rangle$ and let coordinates be discrete (the lattice) $\Rightarrow$

$$\hat{\rho}(r_0) = \sum_{r,r'} \underbrace{\langle r | r_0 \rangle}_{\delta_{r,r_0}} \underbrace{\langle r_0 | r' \rangle}_{\delta_{r_0,r'}} \hat{a}_r^+ \hat{a}_{r'} = \hat{a}_{r_0}^+ \hat{a}_{r_0}$$

(use the above eq.)

Here $\hat{a}_{r_0}^+ / \hat{a}_{r_0}$ creates / annihilates a particle on the site r_0

The kinetic energy

$$\hat{H}_{kin} = \underbrace{\varepsilon}_{\text{dispersion relation } (\hbar=1)}(\underbrace{\hat{k}}_{\text{momentum operator (diagonal)}})$$

Using the basis $|k\rangle$ we find

$$\hat{H}_{kin} = \sum_{k_1,k_2} \underbrace{\langle k_1 | \varepsilon(\hat{k}) | k_2 \rangle}_{\delta_{k_1,k_2}\, \varepsilon(k_1)} \hat{a}^+_{k_1} \hat{a}_{k_2} =$$

$$= \sum_k \varepsilon(k)\, \hat{a}^+_k \hat{a}_k$$ – properly weighted sum of partial kinetic energies.