Second quantization

Second quantization is a formalism to describe quantum systems, typically consisting of many identical particles. In this formalism the number of particles is not fixed and the wave functions are represented by operators. This gives rise to the name of the method – in the first quantization physical quantities such as momentum, position, energy, etc. get represented by operators. In the second quantization the wave functions get represented by operators.

In the beginning let us refresh our memory about the single-particle and many-particle Hilbert spaces

Consider a single-particle Hamiltonian with its eigenfunctions φ_λ:

$$\hat{h}\,\varphi_\lambda = \varepsilon_\lambda \varphi_\lambda \qquad (\lambda = \vec{k}, \sigma, \nu, \ldots \leftarrow \text{quantum numbers})$$

Hilbert space $\mathcal{H}_1$ is generated by a complete set φ_λ

Examples are:

a) A free particle: $\hat{h} = -\frac{\hbar^2}{2m}\nabla^2$

The eigenfunctions are labelled by the wavevectors $\vec{k}$:

$$\varphi_{\vec{k}} = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} \qquad V - \text{volume} \qquad \varepsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$$

b) A particle with spin 1/2 in a magnetic field

$\vec{B} = (0, 0, B)$ $\qquad \hat{h} = -\gamma B S_z = -\frac{q}{m} B S_z$

The Hilbert space has finite dimension (2), generated by the eigenstates $|\uparrow\rangle$ and $|\downarrow\rangle$

In the case of two identical particles the basis is given by the set of (anti) symmetrized functions

$$\psi_{\lambda,\nu}(1,2) = \frac{1}{\sqrt{2}}\left[\varphi_\lambda(1)\,\varphi_\nu(2) \pm \varphi_\lambda(2)\,\varphi_\nu(1)\right]$$

where φ_λ are single-particle states

The corresponding Hilbert space is denoted $\mathcal{F}_2$ and it is a subset of $\mathcal{H}_1 \otimes \mathcal{H}_1$. Because $\mathcal{F}_2$ is spanned only by (anti)symmetric functions it is only a subset of $\mathcal{H}_1 \otimes \mathcal{H}_2$

In the case of N identical fermions Hilbert space $\mathcal{F}_N$ is generated by

$$\psi_{\lambda_1 \dots \lambda_N}(1, \dots N) = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} (-1)^P \varphi_{\lambda_1}(P_1) \dots \varphi_{\lambda_N}(P_N) \qquad (*)$$

where the summation runs over all permutations $\{1, \dots N\}$.

It can be writtens as a familiar Slated determinant

$$\psi_{\lambda_1 \dots \lambda_N}(1, \dots N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_{\lambda_1}(1) & \varphi_{\lambda_1}(2) & \dots & \varphi_{\lambda_1}(N) \\ \varphi_{\lambda_2}(1) & \varphi_{\lambda_2}(2) & \dots & \varphi_{\lambda_2}(N) \\ \vdots & & \ddots & \vdots \\ \varphi_{\lambda_N}(1) & \varphi_{\lambda_N}(2) & \dots & \varphi_{\lambda_N}(N) \end{vmatrix}$$

For the case of N identical bosons the wavefunctions must be symmetric, so

$$\psi_{\lambda_1 \dots \lambda_N}(1, \dots N) = \sqrt{\frac{N_1! N_2! \dots}{N!}} \sum_{P \in S_N} \varphi_{\lambda_1}(P_1) \dots \varphi_{\lambda_N}(P_N)$$

where all terms in the sum come with the plus sign.

Examples of F_N are:

a) N non-interacting free particles

$$\hat{H} = \sum_{i=1}^{N} \hat{h}^{(i)} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m}$$

b) N distinguishable spins in a magnetic field

$$\hat{H} = -\gamma B \sum_{i=1}^{N} (S_i)_z$$

This corresponding Hilbert space has the dimension 2^N

Note that a different choice of a single-particle set φ_λ gives different many-particle basis. Nevertheless it spans the same Hilbert space $\mathcal{F}_N$

The formalism of second quantization introduces a different labelling of the basis states and also creation and annihilation operators that connect spaces with different number of particles

Because identical particles are indistinguishable we can never say (at least for a general state) that a particle is in a given single-particle state. Insted, we can change our description and characterize states (*) by the number of single-particle states occupied

$$|n_{\lambda_1}, n_{\lambda_2}, \dots\rangle = |\{n_\lambda\}\rangle = |0, \dots, 0, \underset{\uparrow \lambda_1}{5}, 0, \dots, 0, \underset{\uparrow \lambda_2}{1}, 0, \dots\rangle$$

Here on the right-hand side it is explicitly specified which states are occupied (and how many times if we deal with bosons) and which states are empty. For fermions the possible values are either 0 or 1. Such a representation is called the occupation number representation.

The constraint on the number of particles N can be released by working in the extended space

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

called the Fock space. $\mathcal{F}_0$ contains a unique "vacuum" state (often denoted $|0\rangle$) that corresponds to no particles at all.

In the Fock space, creation operators are introduced that raise the number of particles in a given single-particle state by 1. For example, for fermions it reads

$$c^\dagger_{\lambda_1} |0, \dots 0, \underset{\uparrow \lambda_1}{0}, 0, \dots 1, 0, \dots\rangle = |0, \dots, 0, \underset{\uparrow \lambda_1}{1}, 0, \dots 1, 0\rangle$$

while particle creation in a single-particle state that

is already occupied gives zero:

$$c^+_{\lambda_2} |0,\dots,0,0,0,\dots,\underset{\uparrow}{1},0,\dots\rangle = 0$$

λ_2

The annihilation operator c_λ which lowers the occupation number for a single-particle state φ_λ by 1, does exactly opposite to what c^+_λ does.

The full basis of the Fock space $\mathcal{F}$ is generated by creation operators applied to the vacuum state $|0\rangle$:

$$c^+_{\lambda_1} \dots c^+_{\lambda_N} |0\rangle = |\dots, n_{\lambda_1}=1, \dots, n_{\lambda_N}=1, \dots\rangle$$

For bosons the number of particles in a given single-particle state is not restricted. We can introduce the annihilation and creation operators as follows:

$$b_{\lambda_i} |\dots, n_{\lambda_i}, \dots\rangle = \sqrt{n_{\lambda_i}}\, |\dots, n_{\lambda_i}-1, \dots\rangle$$

then

$$\langle n_{\lambda_i}-1 | b_{\lambda_i} | n_{\lambda_i}\rangle = \sqrt{n_{\lambda_i}}$$

Also, the action of $b^+_{\lambda_i}$ can be determined:

$$\langle n_{\lambda_i} | b^+_{\lambda_i} | n_{\lambda_i}-1\rangle = \langle n_{\lambda_i}-1 | b_{\lambda_i} | n_{\lambda_i}\rangle^* = \sqrt{n_{\lambda_i}}, \text{ so}$$

$$b^+_{\lambda_i} |n_{\lambda_i}\rangle = \sqrt{n_{\lambda_i}+1}\, |n_{\lambda_i}+1\rangle$$

The product of $b^+_{\lambda_i} b_{\lambda_i}$ when acting on a state can only multiply it by a constant

$$b^+_{\lambda_i} b_{\lambda_i} |n_{\lambda_i}\rangle = b^+_{\lambda_i} \sqrt{n_{\lambda_i}}\, |n_{\lambda_i}-1\rangle = \sqrt{(n_{\lambda_i}-1)+1}\,\sqrt{n_{\lambda_i}}\, |n_{\lambda_i}\rangle$$
$$= n_{\lambda_i} |n_{\lambda_i}\rangle$$

Similarly

$$b_{\lambda_i} b^+_{\lambda_i} |n_{\lambda_i}\rangle = b_{\lambda_i} \sqrt{n_{\lambda_i}+1}\, |n_{\lambda_i}+1\rangle = (n_{\lambda_i}+1) |n_{\lambda_i}\rangle$$

Combining the two expressions above we get

$$(b_{\lambda_i} b_{\lambda_i}^+ - b_{\lambda_i}^+ b_{\lambda_i})|n_{\lambda_i}\rangle = |n_{\lambda_i}\rangle$$

So $$[b_{\lambda_i}, b_{\lambda_i}^+] = 1$$

Since b_{λ_i} and b_{λ_j} (or $b_{\lambda_j}^+$) commute when $i \neq j$ (they change the occupation numbers of different single-particle states) we can write it more generally

$$[b_{\lambda_i}, b_{\lambda_j}^+] = \delta_{ij}$$ — fundamental commutation relations for bosonic creation and annihilation operators

If we now turn to the case of fermions we can find that

$$c_{\lambda_i}^+ c_{\lambda_i} |n_{\lambda_i}\rangle = \begin{cases} 0 & , n_{\lambda_i} = 0 \\ 1|n_{\lambda_i}\rangle & , n_{\lambda_i} = 1 \end{cases}$$

$$c_{\lambda_i} c_{\lambda_i}^+ |n_{\lambda_i}\rangle = \begin{cases} 1|n_{\lambda_i}\rangle & , n_{\lambda_i} = 0 \\ 0 & , n_{\lambda_i} = 1 \end{cases}$$

which gives

$$(c_{\lambda_i} c_{\lambda_i}^+ + c_{\lambda_i}^+ c_{\lambda_i})|n_{\lambda_i}\rangle = 1|n_{\lambda_i}\rangle \qquad n_{\lambda_i} = 0, 1$$

and the fundamental commutation relation is

$$\{c_{\lambda_i}, c_{\lambda_j}^+\} = \delta_{ij}$$

↑ anticommutator

Let us now consider how creation and annihilation operators transform upon changing the single-particle basis. Suppose c_λ^+ correspond to the basis $\{|\lambda\rangle\}$. If we change to a new basis $\{|\nu\rangle\}$ what are c_ν^+ in terms of c_λ^+ ?

$$|\nu\rangle = \sum_\lambda \underbrace{\langle\lambda|\nu\rangle}_{\text{elements of the transformation matrix } A_{\lambda\nu}} |\lambda\rangle$$

$$\| \qquad\qquad \|$$

$$a_\nu^+ |0\rangle = \sum_\lambda \langle\lambda|\nu\rangle\, a_\lambda^+ |0\rangle$$

It follows then that

$$a_\nu^+ = \sum_\lambda \langle\lambda|\nu\rangle\, a_\lambda^+$$

Taking the conjugate of the above equation gives

$$a_\nu = \sum_\lambda \langle\nu|\lambda\rangle\, a_\lambda$$

Hence the change of basis only requires the calculation of matrix elements $\langle\nu|\lambda\rangle$

By convention, the field operator $\Psi(\vec{r})$ is associated with the basis of position states $|\vec{r}\rangle$:

$$\Psi(\vec{r}) = \sum_\lambda \langle\vec{r}|\lambda\rangle\, c_\lambda \qquad \Psi^+(\vec{r}) = \sum_\lambda \langle\lambda|\vec{r}\rangle\, c_\lambda^+$$

Using the (anti)commutation relations we can find that

$$\{\Psi(\vec{r}), \Psi(\vec{r}')\} = 0 \qquad \{\Psi(\vec{r}), \Psi^+(\vec{r}')\} = \delta(\vec{r}-\vec{r}')$$

Indeed

$$\{\Psi(\vec{r}), \Psi^+(\vec{r}')\} = \sum_{\lambda\nu} \langle\vec{r}|\lambda\rangle c_\lambda \langle\nu|\vec{r}'\rangle c_\nu^+ + \sum_{\lambda\nu} \langle\nu|\vec{r}'\rangle c_\nu^+ \langle\vec{r}|\lambda\rangle c_\lambda =$$

$$= \sum_{\lambda\nu} \langle\vec{r}|\lambda\rangle\langle\nu|\vec{r}'\rangle \delta_{\lambda\nu} = \langle\vec{r}|\vec{r}'\rangle = \delta(\vec{r}-\vec{r}')$$

The total number of particles is then given by

$$\hat{N} = \sum_\lambda c_\lambda^+ c_\lambda = \int \hat{\rho}(\vec{r})\, d\vec{r}$$

where $\hat{\rho}(\vec{r}) = \Psi^+(\vec{r})\Psi(\vec{r})$ is the local density operator

Example: In the momentum basis

$$\Psi(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} c_{\vec{k}}$$

where $c_{\vec{k}}$ destroys a particle with momentum $\vec{k}$

$\Psi^+(\vec{r})$ is the sum of all possible ways to add a particle to the system at position $\vec{r}$ through any of the basis states $\Psi_\lambda(\vec{r})$

$\Psi(\vec{r})$ and $\Psi^+(\vec{r})$ are second quantized operators defined in every point in space. They are called quantum field operators.

Now let us consider how we can represent an arbitrary single-particle operator $\hat{O}$ acting in N-particle Hilbert space, f_N. It generally takes the form

$$\hat{O} = \sum_{n=1}^{N} \hat{o}_n$$

where $\hat{o}_n$ is an ordinary single-particle operator

Example:

a) The kinetic energy operator $\hat{T} = \sum_{n=1}^{N} \frac{p_n^2}{2m}$

b) One-particle potential $\hat{V} = \sum_{n=1}^{N} V(\vec{r}_n)$

c) Total spin operator $\sum_{n=1}^{N} \vec{s}_n$

There exist some basis $|\lambda\rangle$ in which $\hat{O}$ is diagonal

We can use the spectral expansion for $\hat{o}$

$$\hat{o} = \sum_{\lambda}' |\lambda\rangle o_\lambda \langle\lambda|$$

where $o_\lambda = \langle\lambda|\hat{o}|\lambda\rangle$

$$\hat{n}_\lambda |\lambda_1 \dots \lambda_N\rangle = \frac{a_\lambda^+ a_{\lambda_1} \dots a_{\lambda_n}^+ a_{\lambda_n} |0\rangle}{\sqrt{\prod_i n_{\lambda_i}!}} = \sum_{i=1}^{N} \delta_{\lambda\lambda_i} |\lambda_1 \dots \lambda_N\rangle$$

Then using the fact that

$$\langle \lambda_1' \dots \lambda_N' | \hat{O} | \lambda_1 \dots \lambda_N \rangle = \left(\sum_{i=1}^{N} o_{\lambda_i} \right) \langle \lambda_1' \dots \lambda_N' | \lambda_1 \dots \lambda_N \rangle$$

$$= \langle \lambda_1' \dots \lambda_N' | \sum_{\lambda=0}^{\infty}{}' o_\lambda \hat{n}_\lambda | \lambda_1 \dots \lambda_N \rangle \qquad \hat{n}_\lambda = c_\lambda^+ c_\lambda$$

Since the equality holds for any set of states we can conclude that

$$\hat{O} = \sum_{\lambda=0}^{\infty} o_\lambda \hat{n}_\lambda = \sum_{\lambda=0}^{\infty} \langle \lambda | \hat{o} | \lambda \rangle c_\lambda^+ c_\lambda$$

Finally we can transform this to a general basis

$$\left(c_\lambda^+ = \sum_\mu \langle \mu | \lambda \rangle c_\mu^+ \qquad c_\lambda = \sum_\nu \langle \lambda | \nu \rangle c_\nu \right)$$

$$\hat{O} = \sum_{\lambda\mu\nu} \langle \mu | \lambda \rangle o_\lambda \langle \lambda | \nu \rangle c_\mu^+ c_\nu = \sum_{\mu\nu} \langle \mu | \hat{o} | \nu \rangle c_\mu^+ c_\nu$$

Example: The total spin operator is given by

$$\vec{S} = \sum_{\alpha\beta} c_\alpha^+ \vec{S}_{\alpha\beta} c_\beta \qquad \vec{S}_{\alpha\beta} = \frac{1}{2} \vec{\sigma}_{\alpha\beta}$$

where $\alpha, \beta = \uparrow, \downarrow$ is the spin quantum number

$$S^z = \frac{1}{2}\left(\hat{n}_\uparrow - \hat{n}_\downarrow\right)$$

It is also possible to generalize for the case of 2-body operators:

$$\hat{V} = \frac{1}{2} \sum_{i \neq j} \hat{v}(i,j)$$

$$\hat{V} = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle c_\alpha^+ c_\beta^+ c_\delta c_\gamma$$

Example:

$$\hat{V} = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \qquad \hat{V} = \frac{1}{2} \sum_{\{\vec{k}_i, \sigma_i\}} \left\langle \vec{k}_1\sigma_1, \vec{k}_2\sigma_2 \left| \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \right| \vec{k}_4\sigma_4, \vec{k}_3\sigma_3 \right\rangle \cdot c_{\vec{k}_1\sigma_1}^+ c_{\vec{k}_2\sigma_2}^+ c_{\vec{k}_3\sigma_3} c_{\vec{k}_4\sigma_4}$$

and

$$\left\langle \vec{k}_1\sigma_1, \vec{k}_2\sigma_2 \left| \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \right| \vec{k}_4\sigma_4, \vec{k}_3\sigma_3 \right\rangle = \frac{\delta_{\sigma_1\sigma_4}\, \delta_{\sigma_2\sigma_3}}{\text{Volume}}\, \delta\left(k_1 + k_2 - k_3 - k_4\right)$$