Second quantization

In the course "Theorie E" second quantization for photons was introduced. Now we do the same for arbitrary particles, e.g., electrons or atoms.

I. BOSONS

We consider a system of many indistinguishable paricles which obey the Bose-Einstein statistics.

Let $|i\rangle = \phi_i(x)$ be the full ortho-normal system of one-particle states. By x we mean all the coordinates plus spin, i.e., $x = (\vec{r}, \sigma)$, where σ is the projection of the spin on the quantization axis. For $s = 1$, e.g., we have $\sigma = -1, 0, 1$. So a free particle in a box of volume $V = L^3$ having momentum $\hbar\vec{k}$, where $\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$, and $\sigma = 1$ would be described by

$$\phi_{\vec{k},1}(\vec{r}, \sigma) = \frac{1}{\sqrt{V}} e^{i\vec{k}\vec{r}} \delta_{\sigma,1} \tag{1}$$

For $s = 0$, the coordinate σ is unnecessary.

We characterize states of the system by occupation numbers, N_i, i.e, by number of particles which are in state i. Since the particles are indistinguishable this is the maximum information about the state of the system. We use the Dirac notation $|N_1, N_2, ...\rangle$ which describes a state with N_1 particles in state ϕ_1 etc. In usual Schrödinger representation this state reads

$$|N_1, N_2, ...\rangle = \left(\frac{N_1!N_2!\ldots}{N!}\right)^{1/2} \sum_P \phi_{P_1}(x_1)\phi_{P_2}(x_2)\ldots\phi_{P_N}(x_N) \ , \tag{2}$$

where $N = N_1 + N_2 + \ldots$ is the total number of particles. The permutation P counts all different arrangements of N_1 numbers 1, N_2 numbers 2 etc.

A. One-particle operators

Consider a one-particle operator. For example the z-coordinate operator $\hat{f}^{(1)} = z$ or the momentum in z direction $\hat{f}^{(1)} = -i\hbar\partial/\partial z$. For indistinguishable particles only the following operators are allowed

$$\hat{F}^{(1)} = \sum_a \hat{f}^{(1)}_{x_a} \ , \tag{3}$$

where the subscript x_a determines on which coordinate in (2) the operator $\hat{f}^{(1)}$ acts.

The operator $\hat{F}^{(1)}$ can change at most the state of one particle. Thus it can have only the following matrix elements

$$\langle N_1, N_2, \ldots | \hat{F}^{(1)} | N_1, N_2, \ldots \rangle \tag{4}$$

and

$$\langle \ldots, N_i, \ldots, N_j - 1, \ldots | \hat{F}^{(1)} | \ldots, N_i - 1, \ldots, N_j, \ldots \rangle \tag{5}$$

Combinatorics gives (exercise)

$$\langle N_1, N_2, \ldots | \hat{F}^{(1)} | N_1, N_2, \ldots \rangle = \sum_i N_i \langle i | \hat{f}^{(1)} | i \rangle \tag{6}$$

and

$$\langle \ldots, N_i, \ldots, N_j - 1, \ldots | \hat{F}^{(1)} | \ldots, N_i - 1, \ldots, N_j, \ldots \rangle = \sqrt{N_i N_j} \langle i | \hat{f}^{(1)} | j \rangle \tag{7}$$

B. Creation and annihilation operators

It is convenient to introduce the annihilation operator $\hat{a}_i$ defined by

$$\hat{a}_i | \ldots, N_i, \ldots \rangle = \sqrt{N_i} | \ldots, N_i - 1, \ldots \rangle \tag{8}$$

The same can be written as $\langle N_i - 1 | \hat{a}_i | N_i \rangle = \sqrt{N_i}$. The conjugated (creation) operator $\hat{a}_i^\dagger$ is given by

$$\langle N_i | \hat{a}_i^\dagger | N_i - 1 \rangle = \langle N_i - 1 | \hat{a}_i | N_i \rangle^* = \sqrt{N_i} \tag{9}$$

Thus

$$\hat{a}_i^\dagger | \ldots, N_i, \ldots \rangle = \sqrt{N_i + 1} | \ldots, N_i + 1, \ldots \rangle \tag{10}$$

Properties:

$$\hat{a}_i^\dagger \hat{a}_i | \ldots, N_i, \ldots \rangle = N_i | \ldots, N_i, \ldots \rangle \tag{11}$$

or in short $\hat{a}_i^\dagger \hat{a}_i = N_i$. Also $\hat{a}_i \hat{a}_i^\dagger = N_i + 1$. This gives the commutation relation

$$\hat{a}_i \hat{a}_i^\dagger - \hat{a}_i^\dagger \hat{a}_i = 1 \tag{12}$$

The state $|N_i\rangle$ is obtained by acting N_i times with the creation operator:

$$|N_i\rangle = \frac{(\hat{a}_i^\dagger)^{N_i}}{\sqrt{N_i!}} |0\rangle \ . \tag{13}$$

For different states i and j ($i \neq j$) we have $\hat{a}_i \hat{a}_j^\dagger - \hat{a}_j^\dagger \hat{a}_i = 0$ etc.

Now we can express the operator $\hat{F}^{(1)}$ in terms of the creation and annihilation operators:

$$\hat{F}^{(1)} = \sum_{ij} \langle i | f^{(1)} | j \rangle \hat{a}_i^\dagger \hat{a}_j \tag{14}$$

The equivalence is proven by comparing the matrix elements.

C. Two-particle operators

Consider now an operator $f^{(2)}$ acting on two-particle states. For example potential interaction between particles: $f^{(2)}\phi(x_1, x_2) = U(|\vec{r}_1 - \vec{r}_2|)\phi(x_1, x_2)$. Again, for indistinguishable particles only the following operators are allowed:

$$\hat{F}^{(2)} = \sum_{a<b} f^{(2)}_{ab} \ , \tag{15}$$

where the subscripts a and b determine on which pair of coordinates the operator $f^{(2)}$ acts. Analogously to the one-particle operators one obtains

$$\hat{F}^{(2)} = \frac{1}{2} \sum_{iklm} \langle ik| f^{(2)} |lm\rangle \, \hat{a}^\dagger_i \hat{a}^\dagger_k \hat{a}_l \hat{a}_m \ , \tag{16}$$

where

$$\langle ik| f^{(2)} |lm\rangle \equiv \int\int dx_1 dx_2 \, \phi^*_i(x_1)\phi^*_k(x_2)\hat{f}^{(2)}\phi_l(x_1)\phi_m(x_2) \ . \tag{17}$$

D. Example

Consider the Hamiltonian describing N pairwise interacting particles:

$$\hat{H} = \sum_a \hat{H}^{(1)}_a + \sum_{a<b} U^{(2)}(\vec{r}_a, \vec{r}_b) \ , \tag{18}$$

where the single-particle part it given by

$$\hat{H}^{(1)}_a = -\frac{\hbar^2}{2m}\Delta_a + U^{(1)}(\vec{r}_a) \tag{19}$$

Then in terms of creation and annihilation operators we obtain

$$\hat{H} = \sum_{ik} \langle i| \hat{H}^{(1)} |j\rangle \, \hat{a}^\dagger_i \hat{a}_j + \frac{1}{2} \sum_{iklm} \langle ik| U^{(2)} |lm\rangle \, \hat{a}^\dagger_i \hat{a}^\dagger_k \hat{a}_l \hat{a}_m \ . \tag{20}$$

If the states $|i\rangle$ are the eigenstates of $\hat{H}^{(1)}$, i.e., $\hat{H}^{(1)}|i\rangle = E_i |i\rangle$ we obtain

$$\hat{H} = \sum_i E_i \hat{a}^\dagger_i \hat{a}_i + \frac{1}{2} \sum_{iklm} \langle ik| U^{(2)} |lm\rangle \, \hat{a}^\dagger_i \hat{a}^\dagger_k \hat{a}_l \hat{a}_m \ . \tag{21}$$

For example, consider free ($U^{(1)} = 0$) but interacting ($U^{(2)} = U(|\vec{r}_a - \vec{r}_b|)$) particles. Then, the convenient basis is

$$|\vec{p}\rangle = \frac{1}{\sqrt{V}} e^{\frac{i\vec{p}\vec{r}}{\hbar}} \tag{22}$$

and we obtain

$$\hat{H} = \sum_{\vec{p}} \frac{(\vec{p})^2}{2m} \hat{a}^{\dagger}_{\vec{p}} \hat{a}_{\vec{p}} + \frac{1}{2V} \sum_{\vec{p},\vec{q}_1,\vec{q}_2} U(|\vec{q}_1 - \vec{q}_2|) \hat{a}^{\dagger}_{\vec{p}+\frac{\vec{q}_1}{2}} \hat{a}^{\dagger}_{\vec{p}-\frac{\vec{q}_1}{2}} \hat{a}_{\vec{p}+\frac{\vec{q}_2}{2}} \hat{a}_{\vec{p}-\frac{\vec{q}_2}{2}} \ . \tag{23}$$

Another way to parametrize the momenta of interacting particles would be, for example,

$$\hat{H} = \sum_{\vec{p}} \frac{(\vec{p})^2}{2m} \hat{a}^{\dagger}_{\vec{p}} \hat{a}_{\vec{p}} + \frac{1}{2V} \sum_{\vec{p}_1,\vec{p}_1,\vec{q}} U(\vec{q}) \hat{a}^{\dagger}_{\vec{p}_1+\vec{q}} \hat{a}^{\dagger}_{\vec{p}_2-\vec{q}} \hat{a}_{\vec{p}_2} \hat{a}_{\vec{p}_1} \ . \tag{24}$$

E. Field operators

More compact and intuitive form one obtains by defining the field operators:

$$\hat{\Psi}(x) = \sum_i \phi_i(x) \hat{a}_i \quad \text{and} \quad \hat{\Psi}^{\dagger}(x) = \sum_i \phi^*_i(x) \hat{a}^{\dagger}_i \tag{25}$$

The wave functions have the property ($\sum_i |i\rangle \langle i| = \hat{1}$)

$$\sum_i \phi^*_i(x) \phi_i(x') = \delta(x - x') = \delta(\vec{r} - \vec{r}') \delta_{\sigma,\sigma'} \tag{26}$$

From this we derive

$$\hat{\Psi}(x) \hat{\Psi}^{\dagger}(x') - \hat{\Psi}^{\dagger}(x') \hat{\Psi}(x) = \delta(x - x') \tag{27}$$

and all other commutators vanish ($[\hat{\Psi}, \hat{\Psi}] = 0$ and $[\hat{\Psi}^{\dagger}, \hat{\Psi}^{\dagger}] = 0$).

Physical meaning: $\hat{\Psi}^{\dagger}(x_0)$ creates a particle at x_0 (that is at $\vec{r}_0$ with spin projection σ_0). Indeed, since $\hat{a}^{\dagger}_i |0\rangle$ corresponds to the state with wave function $\phi_i(x)$, we obtain that $\hat{\Psi}^{\dagger}(x_0) |0\rangle$ corresponds to the wave function $\sum_i \phi^*_i(x_0) \phi_i(x) = \delta(x - x_0)$.

F. One- and two-particle operators in terms of field operators

$$\hat{F}^{(1)} = \sum_{ij} \langle i| f^{(1)} |j\rangle \hat{a}^{\dagger}_i \hat{a}_j = \sum_{ij} \int dx \phi^*_i(x) f^{(1)} \phi_j(x) \hat{a}^{\dagger}_i \hat{a}_j = \int dx \hat{\Psi}^{\dagger}(x) f^{(1)} \hat{\Psi}(x) \tag{28}$$

For example density of a single particle at x_0 is given by $f^{(1)}_{\rho}(x_0) = \delta(x - x_0)$. This gives for the total density of many particles

$$F^{(1)}_{\rho}(x_0) = \hat{\rho}(x_0) = \hat{\Psi}^{\dagger}(x_0) \hat{\Psi}(x_0) \tag{29}$$

Analogously

$$\hat{F}^{(2)} = \frac{1}{2} \sum_{iklm} \langle ik| f^{(2)} |lm\rangle \hat{a}^{\dagger}_i \hat{a}^{\dagger}_k \hat{a}_l \hat{a}_m$$

$$
\begin{aligned}
&= \frac{1}{2}\sum_{iklm}\int\int dx_1 dx_2\, \phi_i^*(x_1)\phi_k^*(x_2)\hat{f}^{(2)}\phi_l(x_1)\phi_m(x_2)\hat{a}_i^\dagger\hat{a}_k^\dagger\hat{a}_l\hat{a}_m \\
&= \frac{1}{2}\int\int dx_1 dx_2\, \hat{\Psi}^\dagger(x_1)\hat{\Psi}^\dagger(x_2)\hat{f}^{(2)}\hat{\Psi}\ (x_1)\hat{\Psi}\ (x_2) \\
&= \frac{1}{2}\int\int dx_1 dx_2\, \hat{\Psi}^\dagger(x_1)\hat{\Psi}^\dagger(x_2)\hat{f}^{(2)}\hat{\Psi}\ (x_2)\hat{\Psi}\ (x_1)\ , \qquad (30)
\end{aligned}
$$

The order is not important for bosons. However, for fermions discussed below, only the last form is correct.

Consider again the Hamiltonian describing N pairwise interacting particles:

$$
\hat{H} = \sum_a \hat{H}_a^{(1)} + \sum_{a<b} U^{(2)}(\vec{r}_a, \vec{r}_b)\ , \qquad (31)
$$

where the single-particle part it given by

$$
\hat{H}_a^{(1)} = -\frac{\hbar^2}{2m}\Delta_a + U^{(1)}(\vec{r}_a) \qquad (32)
$$

In terms of the field operators we obtain

$$
\begin{aligned}
\hat{H} \ &= \int dx \left\{ -\frac{\hbar^2}{2m}\hat{\Psi}^\dagger(x)\Delta\hat{\Psi}(x) + \hat{\Psi}^\dagger(x)U^{(1)}(x)\hat{\Psi}(x) \right\} \\
&+ \frac{1}{2}\int\int dx_1 dx_2\, \hat{\Psi}^\dagger(x_1)\hat{\Psi}^\dagger(x_2)U^{(2)}(x_1, x_2)\hat{\Psi}\ (x_2)\hat{\Psi}\ (x_1) \qquad (33)
\end{aligned}
$$

II. FERMIONS

The wave functions must be antisymmetric. This means that the occupation numbers are either 0 or 1, $N_i = 0, 1$. This is called Pauli principle. The wave function for N particles occupying states $i = 1, ..., N$ is given by

$$
|1_1, 1_2, ..., 1_N\rangle = \left(\frac{1}{N!}\right)^{1/2} \sum_P (-1)^P \phi_{P_1}(x_1)\phi_{P_2}(x_2)\ldots\phi_{P_N}(x_N)\ , \qquad (34)
$$

To fix the signs one chooses a certain order of states. For example, the permutation with $P_1 < P_2 < \ldots < P_N$ will be assigned the positive sign.

A. One-particle operators

Consider a one-particle operator. For example the z-coordinate operator $\hat{f}^{(1)} = z$ or the momentum in z direction $\hat{f}^{(1)} = -i\hbar\partial/\partial z$. For indistinguishable particles only the following operators are allowed

$$
\hat{F}^{(1)} = \sum_a \hat{f}_{x_a}^{(1)}\ , \qquad (35)
$$

where the subscript x_a determines on which coordinate in (34) the operator $\hat{f}^{(1)}$ acts.

The operator $\hat{F}^{(1)}$ can change at most the state of one particle. Thus it can have only the following matrix elements

$$\langle N_1, N_2, \ldots | \hat{F}^{(1)} | N_1, N_2, \ldots \rangle \ , \tag{36}$$

where $N_i = 0, 1$ and

$$\langle \ldots, 1_i, \ldots, 0_j, \ldots | \hat{F}^{(1)} | \ldots, 0_i, \ldots, 1_j, \ldots \rangle \tag{37}$$

or

$$\langle \ldots, 0_i, \ldots, 1_j, \ldots | \hat{F}^{(1)} | \ldots, 1_i, \ldots, 0_j, \ldots \rangle \tag{38}$$

Order is now important, so the way we write assumes $i < j$.

Combinatorics gives (exercise)

$$\langle N_1, N_2, \ldots | \hat{F}^{(1)} | N_1, N_2, \ldots \rangle = \sum_i N_i \langle i | \hat{f}^{(1)} | i \rangle \tag{39}$$

and

$$\langle \ldots, 1_i, \ldots, 0_j, \ldots | \hat{F}^{(1)} | \ldots, 0_i, \ldots, 1_j, \ldots \rangle = \langle i | \hat{f}^{(1)} | j \rangle \ (-1)^{\theta_{ij}} \tag{40}$$

where $\theta_{ij} \equiv \sum_{k=i+1}^{k=j-1} N_k$. That is the sign is determined by the number of occupied states between i and j.

B. Creation and annihilation operators

We define

$$\hat{a}_i | \ldots, 1_i, \ldots \rangle = (-1)^{\theta_{i\infty}} | \ldots, 0_i, \ldots \rangle \tag{41}$$

and

$$\hat{a}_i^\dagger | \ldots, 0_i, \ldots \rangle = (-1)^{\theta_{i\infty}} | \ldots, 1_i, \ldots \rangle \tag{42}$$

That is the sign is determined by the number of occupied states with $k > i$.

Than, by comparing the matrix elements we obtain

$$\hat{F}^{(1)} = \sum_{ij} \langle i | f^{(1)} | j \rangle \, \hat{a}_i^\dagger \hat{a}_j \tag{43}$$

This definition shows that in order to get signs right we have to act with creation operators in a certain order. Namely

$$|1_1, 1_2, ..., 1_N\rangle = \hat{a}_N^\dagger \ldots \hat{a}_2^\dagger \hat{a}_1^\dagger |0\rangle \tag{44}$$

That is every time $\hat{a}_i^\dagger$ acts there are no yet states occupied to the right of i. We should annihilate the states in the opposite order, i.e.,

$$|0\rangle = \hat{a}_1 \hat{a}_2 \dots \hat{a}_N |1_1, 1_2, ..., 1_N\rangle \tag{45}$$

From here we obtain the anti-commutation relations for $i \neq j$:
$\hat{a}_i \hat{a}_j + \hat{a}_j \hat{a}_i = 0$, $\hat{a}_i^\dagger \hat{a}_j^\dagger + \hat{a}_j^\dagger \hat{a}_i^\dagger = 0$, $\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j \hat{a}_i^\dagger = 0$ etc.
For $i = j$ we obtain $\hat{a}_i^\dagger \hat{a}_i = N_i$, while $\hat{a}_i \hat{a}_i^\dagger = 1 - N_i$. Thus $\hat{a}_i \hat{a}_i^\dagger + \hat{a}_i^\dagger \hat{a}_i = 1$.

C. Two-particle operators

Consider now an operator $f^{(2)}$ acting on two-particle states. For example potential interaction between particles: $f^{(2)}\phi(x_1, x_2) = U(|\vec{r}_1 - \vec{r}_2|)\phi(x_1, x_2)$. Again, for indistinguishable particles only the following operators are allowed:

$$\hat{F}^{(2)} = \sum_{a<b} f_{ab}^{(2)} \ , \tag{46}$$

where the subscripts a and b determine on which pair of coordinates the operator $f^{(2)}$ acts.

We obtain

$$\hat{F}^{(2)} = \frac{1}{2} \sum_{iklm} \langle ik| f^{(2)} |lm\rangle \, \hat{a}_i^\dagger \hat{a}_k^\dagger \hat{a}_m \hat{a}_l \ , \tag{47}$$

where

$$\langle ik| f^{(2)} |lm\rangle \equiv \int\int dx_1 dx_2 \, \phi_i^*(x_1)\phi_k^*(x_2)\hat{f}^{(2)}\phi_l(x_1)\phi_m(x_2) \ . \tag{48}$$

Pay attention to the order of operators in (47). In order to keep the signs right we have to create and annihilate in opposite order (here with respect to coordinates x_a and x_b).

Recall that $x = (\vec{r}, \sigma)$, i.e., it includes the spin variable (index). The integration $\int dx$ means then $\int dx \equiv \sum_\sigma \int d^3r$.

D. Field operators

More compact and intuitive form one obtains by defining the field operators:

$$\hat{\Psi}(x) = \sum_i \phi_i(x)\hat{a}_i \quad \text{and} \quad \hat{\Psi}^\dagger(x) = \sum_i \phi_i^*(x)\hat{a}_i^\dagger \tag{49}$$

The wave functions have the property ($\sum_i |i\rangle \langle i| = \hat{1}$)

$$\sum_i \phi_i^*(x)\phi_i(x') = \delta(x - x') = \delta(\vec{r} - \vec{r}')\delta_{\sigma,\sigma'} \tag{50}$$

From this we derive

$$\hat{\Psi}(x)\hat{\Psi}^{\dagger}(x') + \hat{\Psi}^{\dagger}(x')\hat{\Psi}(x) = \delta(x - x') \tag{51}$$

and all other anti-commutators vanish ($\left\{\hat{\Psi}, \hat{\Psi}\right\}_{+} = 0$ and $\left\{\hat{\Psi}^{\dagger}, \hat{\Psi}^{\dagger}\right\}_{+} = 0$).

Physical meaning: $\hat{\Psi}^{\dagger}(x_0)$ creates a particle at x_0 (that is at $\vec{r}_0$ with spin projection σ_0). Indeed, since $\hat{a}_i^{\dagger}|0\rangle$ corresponds to the state with wave function $\phi_i(x)$, we obtain that $\hat{\Psi}^{\dagger}(x_0)|0\rangle$ corresponds to the wave function $\sum_i \phi_i^*(x_0)\phi_i(x) = \delta(x - x_0)$.

E. One- and two-particle operators in terms of field operators

$$\hat{F}^{(1)} = \sum_{ij} \langle i| f^{(1)} |j\rangle \hat{a}_i^{\dagger}\hat{a}_j = \sum_{ij} \int dx \phi_i^*(x) f^{(1)} \phi_j(x) \hat{a}_i^{\dagger}\hat{a}_j = \int dx \hat{\Psi}^{\dagger}(x) f^{(1)} \hat{\Psi}(x) \tag{52}$$

For example density of a single particle at x_0 is given by $f_{\rho}^{(1)}(x_0) = \delta(x - x_0)$. This gives for the total density of many particles

$$F_{\rho}^{(1)}(x_0) = \hat{\rho}(x_0) = \hat{\Psi}^{\dagger}(x_0)\hat{\Psi}(x_0) \tag{53}$$

Analogously

$$\begin{aligned}
\hat{F}^{(2)} &= \frac{1}{2} \sum_{iklm} \langle ik| f^{(2)} |lm\rangle \hat{a}_i^{\dagger}\hat{a}_k^{\dagger}\hat{a}_m\hat{a}_l \\
&= \frac{1}{2} \sum_{iklm} \int\int dx_1 dx_2\, \phi_i^*(x_1)\phi_k^*(x_2) \hat{f}^{(2)} \phi_l(x_1)\phi_m(x_2) \hat{a}_i^{\dagger}\hat{a}_k^{\dagger}\hat{a}_m\hat{a}_l \\
&= \frac{1}{2} \int\int dx_1 dx_2\, \hat{\Psi}^{\dagger}(x_1)\hat{\Psi}^{\dagger}(x_2) \hat{f}^{(2)} \hat{\Psi}\ (x_2)\hat{\Psi}\ (x_1)\ ,
\end{aligned} \tag{54}$$

The order is important.