Lect 2: Field operators, Single-body operators two-body operators

§ Field operators — creation / annhilation operator in the Coordination representation.

As we explained in Lect. 1, we define creation / annhilation operators for an orthognal / complete single particle basis. What's the connetion between creation / annhilation operators for different choices of the single particle basis? We will answer this question below.

Suppose a set of creation / annhilation operators $a_i, a_i^\dagger$ $(i=1,2,\cdots)$ for the single particle basis $\{\psi_1(r), \psi_2(r), \cdots\}$. The system can be either bosonic or fermionic. We define

$$\hat{\psi}(r) = \sum_i \underset{\substack{\uparrow \\ \text{Single particle} \\ \text{wave function basis}}}{\psi_i(r)} \; a_i \;, \qquad \hat{\psi}^\dagger(r) = \sum_i \psi_i^*(r) \; a_i^\dagger$$

fermion or boson annhilation operator

$$\boxed{\text{ex: Check that } \quad \{\hat{\psi}(r), \hat{\psi}^\dagger(r')\} = \delta(r-r'), \quad \{\psi(r), \psi(r')\} = \{\psi^\dagger(r)\, \psi^\dagger(r')\} = 0}$$

Thus the physical meaning of $\hat{\psi}(r)$, $\hat{\psi}^\dagger(r)$ ~~is~~ are also a set of creation / annhilation operators. In fact, they are defined in the coordinate representation, where "r" is the index for the eigenstates in the coordinate representation.

For example, let us check the state by applying $\psi^\dagger(r)$ on the vaccum state $\psi^\dagger(r)|0\rangle$. Since it is a single particle state, let us write down explicitly its wavefunction $\langle r'|\psi^\dagger(r)|0\rangle = \sum_i \langle r'|a_i^\dagger|0\rangle \psi_i^*(r)$

$= \sum_i \langle r'|\psi_i\rangle \psi_i^*(r) = \sum_i \psi_i(r')\psi_i^*(r) = \delta(r'-r)$. This indeed means the creation of a particle at the position of r. We also see the result is independent of the choice of basis of ψ_i. If we chose $a_p, a_p^\dagger$ as operators in the momentum representation, for the plane wave states $\psi_p(r) = \frac{1}{\sqrt{V}} e^{ipr}$, we arrive at

$$\boxed{\begin{array}{ll} \psi(r) = \sum_p \frac{1}{\sqrt{V}} e^{ipr} a_p & \text{or} \quad \psi^\dagger(r) = \frac{1}{\sqrt{V}} \sum_p e^{-ipr} a_p^\dagger \\ a_p = \frac{1}{\sqrt{V}} \int dr\, e^{-ipr} \psi(r) & \quad a_p^\dagger = \frac{1}{\sqrt{V}} \int dr\, e^{ipr} \psi^\dagger(r) \end{array}}$$

Next we build up the connection between operators $a_i a_i^\dagger$ for the basis $\psi_i(r)$, $b_i b_i^\dagger$ for the basis $\phi_i(r)$

$$\Rightarrow \hat{\psi}(r) = \sum_i \psi_i(r) a_i = \sum \phi_i(r) b_i$$

$$\Rightarrow \boxed{a_i = \sum_j \langle \psi_i | \phi_j \rangle b_j \quad \text{and} \quad a_i^\dagger = \sum_j \langle \phi_j | \psi_i \rangle b_j^\dagger}$$

This is essentially Fourier transformation between two representations.

§ Single-body operators in the second quantization representation

$\hat{F} = \sum_{i=1}^{N} \hat{f}(i)$ in the first quantization, where $f(i)$ only depends on the variable of the i-th particle.

Let us begin with a single particle basis in which f is diagonal,

$\hat{f}\,\psi_k = f_k \psi_k \quad (k = 1, 2, \cdots)$, then in the corresponding particle number occupation representation

$$\hat{F}\,|N_1 N_2 \cdots\rangle = (N_1 f_1 + N_2 f_2 + \cdots)\,|N_1 N_2 \cdots\rangle.$$

Check: let us go back to the first quantization

$$\hat{F} = \sum_{i=1}^{N} \hat{f}(i) \,,$$

For bosons: $|N_1 N_2 \cdots\rangle \rightarrow$

$$\psi^{B}_{N_1 N_2 \cdots}(x_1 \cdots x_N) = \sqrt{\frac{N_1!\,N_2!\cdots}{N!}} \sum_P \{\psi_1(x_1)\cdots\psi_1(x_{N_1})\}\{\psi_2(x_{N_1+1})\cdots\psi_2(x_{N_1+N_2})\}\cdots$$

$$\sum_{i=1}^{N} \hat{f}(x_i, P_i)\,\psi^{B}_{N_1 N_2}(x_1 \cdots x_N) = \sqrt{\frac{N_1!\cdots}{N!}} \sum_P \Big(\sum_{i=1}^{N} f(x_i, P_i)\Big)\{\psi_1(x_1)\cdots\psi_1(x_{N_1})\}\cdots$$

$$= \sqrt{\frac{N_1!\cdots}{N!}}\ \cancel{\sum_i}\ (N_1 f_1 + N_2 f_2 + \cdots) \sum_P \{\psi_1(x_1)\cdots\psi_1(x_{N_1})\}\{\psi_2(x_{N_1+1})\cdots\psi_2(x_{N_1+N_2})\}\cdots$$

$$= (N_1 f_1 + N_2 f_2 + \cdots)\,\psi^{B}_{N_1 N_2}(x_1 \cdots x_N)$$

Similarly results also apply for Fermions.

$$\Rightarrow \hat{F}|N_1 N_2 \cdots\rangle = \sum_k f_k \hat{n}_k |N_1 N_2 \cdots\rangle \Rightarrow$$

$$\hat{F} = \sum_k f_k a_k^\dagger a_k = \sum_k \underline{\langle \psi_k | \hat{f} | \psi_k \rangle} a_k^\dagger a_k \text{ in the diagonal basis.}$$

↑ matrix element in the single particle basis.

when written in the second quantization form, it applies for aribitary particle number N, thus now $\hat{F}$ is an operator defined in the Fock space.

Now let us change into a general basis $\phi_i(r)$ with associated Creation/annhillation operators $b, b^\dagger$, $\Rightarrow$

$$a_k = \sum_i \langle \psi_k | \phi_i \rangle b_i, \quad a_k^\dagger = \sum_j \langle \phi_j | \psi_k \rangle b_j^\dagger$$

$$\Rightarrow \hat{F} = \sum_{\substack{k \\ ij}} \langle \phi_j | \psi_k \rangle \langle \psi_k | f | \psi_k \rangle \langle \psi_k | \phi_i \rangle b_j^\dagger b_i$$

$$= \sum_{ij} \sum_{kk'} \langle \phi_j | \psi_k \rangle \underbrace{\langle \psi_k | f | \psi_{k'} \rangle}_{f_k \delta_{kk'}} \langle \psi_{k'} | \phi_i \rangle b_j^\dagger b_i$$

using $\sum_k |\psi_k\rangle\langle\psi_k| = I$.

$$= \sum_{ij} \langle \phi_j | f | \phi_i \rangle b_j^\dagger b_i$$

where $\underline{\langle \phi_j | f | \phi_i \rangle = \int dr\, \phi_j^*(r)\, f(r, p)\, \phi_i(r)}$.

Example: Kinetic energy. $H_0 = \sum_{i=1}^{N} \frac{\hbar^2 \hat{p}_i^2}{2m}$

in the momentum basis $\Rightarrow$ $H_0 = \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k$.

Example: using field operators $\psi(r)$, we can also express

$$\hat{F} = \int dr'' dr' \langle r''| f(r, \nabla_r) | r'\rangle \psi^\dagger(r'') \psi(r')$$

$$\langle r''| f(r, \nabla_r) | r'\rangle = \int dx\, \delta(x - r'') f(x, \nabla_x) \delta(r - r') = f(r'', \nabla_{r''}) \delta(r'' - r')$$

$$\hat{F} = \int dr'' dr' \{ f(r'', \nabla_{r''}) \delta(r'' - r') \} \psi^\dagger(r'') \psi(r')$$

$$= \int dr'' \psi^\dagger(r'') f(r'', \nabla_{r''}) \psi(r'')$$

$\Rightarrow$ The kinetic energy $\hat{H}_0 = \int dr\, \psi^\dagger(r) \frac{-\hbar^2 \nabla_r^2}{2m} \psi(r)$

In solid state physics, we often study lattice system. The coordinate representation is discretized: $|i\rangle \leftarrow \phi(r - R_i)$

$i = 1, 2, \cdots N$, R_i is the lattice site position

$$\Rightarrow H = \sum_{ij} a_i^\dagger a_j \langle i | h | j \rangle$$

$$= \sum_{ij} a_i^\dagger a_j \left\{ \int dr\, \phi^*(r - R_i) h(r, \nabla_r) \phi(r - R_j) \right\}$$

$$\approx -t \sum_i a_i^\dagger a_{i+1}$$

$\left[\begin{array}{l} \text{only keep the nearest neighbour hopping} \\ -t = \int dr\, \phi^*(r - R_i) h(r\, \nabla_r) \phi(r - R_{i+1}) \end{array} \right]$

§ Two-body operators

$$\hat{G} = \frac{1}{2} \sum_{i \neq j}^{N} \hat{g}(i,j), \quad \text{where } g(i,j) = g(j,i), \quad i,j \text{ are indices of two particles.}$$

Let us consider the special case in which $g(i,j)$ can be factorized into $\hat{g}(i,j) = \hat{u}(i)\hat{v}(j) + \hat{u}(j)\hat{v}(i)$, where u and v are single-body operators.

$$G = \frac{1}{2}\sum_{i\neq j}^{N} g(i,j) = \frac{1}{2}\sum_{i\neq j}^{N} \left(\hat{u}(i)\hat{v}(j) + \hat{u}(j)\hat{v}(i)\right) = \left(\sum_{i=1}^{N} u(i)\right)\left(\sum_{j=1}^{N} v(j)\right) - \left(\sum_{i=1}^{N} u(i)v(i)\right)$$

$$\sum_{i=1}^{N} u(i) = \sum_{lk} \langle l|\hat{u}|k\rangle a_l^{\dagger} a_k$$

$$\sum_{j=1}^{N} v(i) = \sum_{mn} \langle m|\hat{v}|n\rangle a_m^{\dagger} a_n$$

$$\sum_{i=1}^{N} u(i)v(i) = \sum_{lk} \langle l|\hat{u}\hat{v}|k\rangle a_l^{\dagger} a_k$$

$$\Rightarrow G = \sum_{lk}\sum_{mn} \langle l|\hat{u}|k\rangle\langle m|\hat{v}|n\rangle a_l^{\dagger} a_k a_m^{\dagger} a_n - \sum_{lk} \langle l|\hat{u}\hat{v}|k\rangle a_l^{\dagger} a_k$$

using $a_l^{\dagger} a_k a_m^{\dagger} a_n = a_l^{\dagger} a_m^{\dagger} a_n a_k + \delta_{mk} a_l^{\dagger} a_n$ (for both fermions and bosons).

$$\Rightarrow G = \sum_{lkmn} \langle l|u|k\rangle\langle m|v|n\rangle a_l^{\dagger} a_m^{\dagger} a_n a_k + \sum_{ln}\left[\sum_{m} \langle l|u|m\rangle\langle m|v|n\rangle a_l^{\dagger} a_n - \sum \langle l|uv|n\rangle a_l^{\dagger} a_n\right]$$

$$= \sum_{lkmn} \langle l|u|k\rangle\langle m|v|n\rangle a_l^{\dagger} a_m^{\dagger} a_n a_k$$

② by switching $lk \leftrightarrow mn$

$$\Rightarrow G = \sum_{mn,lk} \langle m|\hat{u}|n\rangle\langle l|\hat{v}|k\rangle\, a_m^+ a_l^+ a_k a_n$$

$$= \sum_{mn,lk} \langle m|\hat{u}|n\rangle\langle l|\hat{v}|k\rangle\, a_l^+ a_m^+ a_n a_k$$

$$\Rightarrow G = \frac{1}{2}\sum_{mnlk} \{\langle l|\hat{u}|k\rangle\langle m|\hat{v}|n\rangle + \langle m|\hat{u}|n\rangle\langle l|\hat{v}|k\rangle\}\, a_l^+ a_m^+ a_n a_k$$

define $\boxed{\langle l m | g | k n\rangle = \int dr_1 dr_2\, \phi_l^*(r_1)\phi_m^*(r_2)\, g(r_1, r_2)\, \phi_n(r_2)\phi_k(r_1)}$

$$= \frac{1}{2}\left[\int dr_1 dr_2\, \phi_l^*(r_1)\phi_m^*(r_2)\,[\hat{u}(r_1)\hat{v}(r_2) + \hat{u}(r_2)\hat{v}(r_1)]\,\phi_n(r_2)\phi_k(r_1)\right]$$

$$= \frac{1}{2}\{\langle l|\hat{u}|k\rangle\langle m|\hat{v}|n\rangle + \langle m|\hat{u}|n\rangle\langle l|\hat{v}|k\rangle\}$$

$$\Rightarrow \boxed{G = \frac{1}{2}\sum_{mnlk} \langle l m| g(1,2)|k n\rangle\, a_l^+ a_m^+ a_n a_k.}$$

Generally speaking, $g(i,j)$ can be expanded into a sum of a set of us and vs, thus the above expression should still be valid!

Example: for Coulomb interaction between electrons

$$V = \frac{1}{2}\sum_{i\neq j} \frac{e^2}{|r_i - r_j|} \quad \Rightarrow g = \frac{e^2}{|r_1 - r_2|}$$

$$G = \frac{1}{2}\int dr_1 dr_2 dr_3 dr_4 \; \langle r_1 r_2 | g | r_4 r_3 \rangle \; \psi^\dagger(r_1)\psi^\dagger(r_2)\psi(r_3)\psi(r_4)$$

$$\langle r_1 r_2 | g | r_4 r_3 \rangle = \int dx dy \; \delta(x-r_1)\delta(y-r_2)\, g(x,y)\, \delta(x-r_4)\delta(y-r_3)$$

$$= \delta(r_1-r_4)\delta(r_2-r_3)\frac{e^2}{|r_1-r_2|}$$

$$\Rightarrow G = \frac{1}{2}\int dr_1 dr_2 \; \psi^\dagger(r_1)\psi^\dagger(r_2)\frac{e^2}{|r_1-r_2|}\psi(r_2)\psi(r_1)$$

Ex: transfer into momentum space, plug in

$$\psi(r) = \frac{1}{\sqrt{V}}\sum_k e^{ikr}\, a_k$$

$$G = \left(\frac{1}{\sqrt{V}}\right)^4 \cdot \frac{1}{2} \sum_{\substack{k_1 k_2 \\ k_3 k_4}} \int_{dr_2}^{dr_1} e^{-ik_1 r_1} e^{-ik_2 r_2} \frac{e^2}{|r_1-r_2|} e^{ik_3 r_2} e^{ik_4 r_1}$$

$$a^\dagger_{k_1} a^\dagger_{k_2} a_{k_3} a_{k_4}$$

$$\int dr_1 dr_2 \to \int dR\, dr \quad \text{where} \quad R = \frac{r_1+r_2}{2} \qquad r = r_1 - r_2$$

$$\Rightarrow \int dR\, dr \quad e^{-ik_1(R+\frac{r}{2}) - ik_2(R-\frac{r}{2})}\, e^{ik_3(R-\frac{r}{2}) + ik_4(R+\frac{r}{2})}\, \frac{e^2}{r}$$

$$= \int dR\; e^{-i(k_1+k_2-k_3-k_4)\cdot R} \int dr\; e^{-i(k_1-k_2+k_3-k_4)\cdot\frac{r}{2}}\, \frac{e^2}{r}$$

$$\swarrow$$

$$\Rightarrow \delta(k_1+k_2=k_3+k_4)\cdot V$$

set $k_3 = k_2 - q$

$k_4 = k_1 + q$

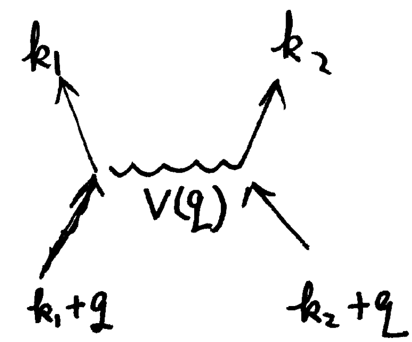
$$\Rightarrow \quad k_1 - k_2 + 2q = k_4 - k_3$$

$$\Rightarrow k_1 - k_2 + (k_3 - k_4) = -2q$$

$$\Rightarrow \int dR\, dr \;\cdots\; = \mathrm{Vol}\cdot\int dr\, e^{i\vec{q}\cdot\vec{r}}\,\frac{e^2}{r} = \mathrm{Vol}.\; V(q)$$

$\uparrow$ Fourier transform of $\frac{e^2}{r}$

$$\Rightarrow\; G = \frac{1}{2V}\sum_{\substack{k_1 k_2 \\ q}} V(q)\, a^{+}_{k_1} a^{+}_{k_2} a_{k_2-q}\, a_{k_1+q}$$



if add electron spin, we have

$$G = \frac{1}{2V}\sum_{k_1,k_2,q} v(q)\, a^{+}_{k_1\sigma}\, a^{+}_{k_2\sigma'}\, a_{k_2-q\,\sigma'}\, a_{k_1+q,\sigma}$$

This expression can also be obtained directly through the momentum representation. we define $a^{+}_{k\sigma}$, $a_{k\sigma}$ for the creation/annilation operators for the momentum ~~sb~~ spin basis $|k\sigma\rangle = e^{ikr}|\chi_\sigma\rangle$

$$\Rightarrow\; G = \frac{1}{2}\sum_{\substack{k_1 k_2\\ k_3 k_4}} \left\langle \begin{matrix} k_1 & k_2 \\ \sigma_1 & \sigma_2 \end{matrix} \right| \frac{e^2}{|r_1-r_2|} \left| \begin{matrix} k_4 & k_3 \\ \sigma_4 & \sigma_3 \end{matrix} \right\rangle a^{+}_{k_1\sigma_1} a^{+}_{k_2\sigma_2} a_{k_3\sigma_3} a_{k_4\sigma_4}$$

where
$$\left\langle \begin{matrix} k_1 & k_2 \\ \sigma_1 & \sigma_2 \end{matrix} \right| \frac{e^2}{|r_1-r_2|} \left| \begin{matrix} k_4 & k_3 \\ \sigma_4 & \sigma_3 \end{matrix} \right\rangle = \frac{\langle \chi_{\sigma_1}|\chi_{\sigma_3}\rangle\langle\chi_{\sigma_2}|\chi_{\sigma_4}\rangle}{V^2}\int dr_1 dr_2\, e^{-ik_1r_1-ik_2r_2}\,\frac{e^2}{|r_1-r_2|}\, e^{ik_4r_1}\, e^{ik_3r_2}$$

$$= \delta_{\sigma_1\sigma_3}\,\delta_{\sigma_2\sigma_4}\;\frac{1}{V}\;V(q)\cdot\delta(k_1+k_2=k_3+k_4)\quad \text{where } q = k_3-k_1$$

$$\Rightarrow \boxed{G = \frac{1}{2V}\sum_{k_1k_2q,\sigma\sigma'} v(q)\; a^{\dagger}_{k_1\sigma}\, a^{\dagger}_{k_2\sigma'}\, a_{k_2-q\sigma'}\, a_{k_1+q\sigma}}$$