Chap 1 Manybody wave function and Second quantization

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I. MANYBODY WAVE FUNCTION

A. One particle

Hamiltonian and Schrodinger equation for a single particle:

$$H^{(1)} = T + V; \tag{1}$$

$$H^{(1)}\phi_\alpha = \varepsilon_\alpha \phi_\alpha. \tag{2}$$

The index α can be a set of quantum numbers, e.g., $\alpha = (n, l, m)$. Whenever required, we will label, from low energy to high energy, $\alpha = \bar{1}, \bar{2}, \cdots$.

Orthogonality:

$$\langle \phi_\alpha | \phi_\beta \rangle = \delta_{\alpha\beta}. \tag{3}$$

Completeness:

$$\sum_\alpha |\phi_\alpha\rangle\langle\phi_\alpha| = \mathbf{1}. \tag{4}$$

The summation runs over all possible eigenstates, and $\mathbf{1}$ is the identity matrix in one-body Hilbert space $\mathcal{H}^{(1)}$.

B. N particles, non-interacting

Hamiltonian and Schrodinger equation for non-interacting N particles:

$$H = \sum_{i=1}^{N} H^{(1)}(r_i); \tag{5}$$

$$H\Psi(r_1, r_2, \cdots) = E\Psi(r_1, r_2, \cdots). \tag{6}$$

(Note: For simplicity, unless necessary, we often write $\mathbf{r}$ as r.) Since there is no interaction between particles, the Schrodinger equation is separable. Assume

$$\Psi(r_1, r_2, \cdots, r_N) = \phi(r_1)\phi(r_2)\cdots\phi(r_N), \tag{7}$$

then

$$H^{(1)}\phi_{\alpha_i}(r_i) = \varepsilon_{\alpha_i}\phi_{\alpha_i}(r_i), i = 1, 2, \cdots N. \tag{8}$$

Manybody eigenstate is a product of 1-particle states,

$$\begin{aligned} \Psi_{\alpha_1,\alpha_2,\cdots}(r_1, r_2, \cdots, r_N) &= \phi_{\alpha_1}(r_1)\phi_{\alpha_2}(r_2)\cdots\phi_{\alpha_N}(r_N) \\ &\equiv (r_1, r_2, \cdots, r_N | \Psi_{\alpha_1,\alpha_2,\cdots,\alpha_N}), \end{aligned} \tag{9}$$

with eigenvalues

$$E_{\alpha_1,\alpha_2,\cdots} = \varepsilon_{\alpha_1} + \varepsilon_{\alpha_2} + \cdots + \varepsilon_{\alpha_N}. \tag{10}$$

Notice that we have used a round bracket $|\cdots)$ to represent a product state. The angular bracket $|\cdots\rangle$ is reserved for later use. Orthogonality:

$$\big(\Psi_{\alpha'_1,\alpha'_2,\cdots,\alpha'_N}|\Psi_{\alpha_1,\alpha_2,\cdots,\alpha_N}\big) = \delta_{\alpha'_1\alpha_1}\delta_{\alpha'_2\alpha_2}\cdots\delta_{\alpha'_N\alpha_N} \tag{11}$$

Completeness:

$$\sum_{\alpha_1\alpha_2\cdots\alpha_N} |\Psi_{\alpha_1\alpha_2\cdots\alpha_N})(\Psi_{\alpha_1\alpha_2\cdots\alpha_N}| = \mathbf{1}. \tag{12}$$

The summation runs over all possible manybody eigenstates $\{\alpha_1\alpha_2\cdots\alpha_N\}$, and $\mathbf{1}$ is the identity matrix in manybody Hilbert space $\mathcal{H}^{(N)} = \underbrace{\mathcal{H}^{(1)}\otimes\mathcal{H}^{(1)}\otimes\cdots\otimes\mathcal{H}^{(1)}}_{N\ \textbf{times}}$.

C. Permutation symmetry for bosons and fermions

Definition of exchange operator:

$$P_{ij}\Psi(r_1\cdots r_i\cdots r_j\cdots) \equiv \Psi(r_1\cdots r_j\cdots r_i\cdots). \tag{13}$$

For any boson state and fermion state, we have

$$P_{ij}\Psi(r_1, r_2, \cdots) = \pm\Psi(r_1, r_2, \cdots). \tag{14}$$

In order for the eigenstates to satisfy this permutation symmetry, we need to symmetrize the state in Eq. (9).

For bosons,

$$\Psi^B_{\alpha_1,\alpha_2,\cdots}(r_1, r_2, \cdots) = \frac{1}{\sqrt{N!}}\sum_{\text{all}P} P\phi_{\alpha_1}(r_1)\phi_{\alpha_2}(r_2)\cdots, \tag{15}$$

where the summation runs over all possible permutations. Even though we have inserted a factor $1/\sqrt{N!}$, the state may still not be normalized (details later).

For fermions,

$$\Psi^F_{\alpha_1,\alpha_2,\cdots}(r_1, r_2, \cdots) = \frac{1}{\sqrt{N!}}\sum_{\text{all}P}(-1)^P P\phi_{\alpha_1}(r_1)\phi_{\alpha_2}(r_2)\cdots, \tag{16}$$

where $(-1)^P \equiv \pm 1$ for even/odd permutation.

Both summations in Eqs. (15) and (16) can be written in the following form,

$$\Psi^{B/F}_{\alpha_1,\alpha_2,\cdots}(r_1,r_2,\cdots)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_{\alpha_1}(r_1) & \phi_{\alpha_1}(r_2) & \cdots\\ \phi_{\alpha_2}(r_1) & \phi_{\alpha_2}(r_2) & \cdots\\ \vdots & & \ddots\end{vmatrix}_{\pm}. \tag{17}$$

For fermions, Eq. (16) is equal to the usual **determinant** $|\cdots|_-$, in which half of the terms have negative signs. For bosons, Eq. (15) is equal to the so-called **permanent** $|\cdots|_+$, in which all of the terms have positive signs. For fermions, Ψ^F is equal to zero if $\alpha_i=\alpha_j$ for any two states. This is the **Pauli exclusion principle**.

D. Normalization

In a bracket notation, Eqs. (15) and (16) (now free from the coordinate representation) are written as,

$$\begin{aligned}|\alpha_1,\alpha_2,\cdots\} &\equiv \frac{1}{\sqrt{N!}}\sum_{\text{all}P}(\pm1)^P P|\alpha_1\rangle|\alpha_2\rangle\cdots \\ &= \frac{1}{\sqrt{N!}}\sum_{\text{all}P}(\pm1)^P|\alpha_{P_1}\rangle|\alpha_{P_2}\rangle\cdots,\end{aligned} \tag{18}$$

where $(\alpha_{P_1},\alpha_{P_2},\cdots)$ is a permutation of $(\alpha_1,\alpha_2,\cdots)$.

■ Bosons

$$\{\alpha_1,\alpha_2,\cdots|\alpha_1,\alpha_2,\cdots\}=\frac{1}{N!}\sum_{P,P'}\langle\alpha_{P'_1}|\alpha_{P_1}\rangle\langle\alpha_{P'_2}|\alpha_{P_2}\rangle\cdots, \tag{19}$$

in which $\langle\alpha_{P'_1}|\alpha_{P_1}\rangle=\delta_{P'_1P_1}...$ etc. If all of the particles live in different states, then after using

$$\begin{aligned}\alpha_{P'_1} &= \alpha_{P_1}\\ \alpha_{P'_2} &= \alpha_{P_2}\\ &\vdots\ ,\end{aligned} \tag{20}$$

we would have $N!$ terms (all of them being one) in the summation. Therefore,

$$\{\alpha_1,\alpha_2,\cdots|\alpha_1,\alpha_2,\cdots\}=1. \tag{21}$$

However, if there are n_1 particles live in state $\bar{1}$, n_2 particles live in state $\bar{2}$, ... etc (recall that $\bar{1},\bar{2}$ are the label of one-particle eigenstate from low energy to high energy), then there

are n_1 of the α_{P_i} states that are the same ($= \bar{1}$). Therefore, there are $n_1!$ different ways to match (using $\alpha_{P'_i} = \alpha_{P_i}$) members in that n_1-group, $n_2!$ different ways to match members in the n_2-group ... etc. As a result (pause and think),

$$\{\alpha_1, \alpha_2, \cdots | \alpha_1, \alpha_2, \cdots\} = n_1! n_2! \cdots . \tag{22}$$

That is, in general this ket state is not normalized. The normalized state should be defined as

$$\begin{aligned} &|\alpha_1, \alpha_2, \cdots\rangle = \frac{1}{\sqrt{n_1!}\sqrt{n_2!}\cdots} |\alpha_1, \alpha_2, \cdots\}, \\ &\langle \alpha_1, \alpha_2, \cdots | \alpha_1, \alpha_2, \cdots \rangle = 1. \end{aligned} \tag{23}$$

■ Fermions

Fermions do not have such a counting problem since no two particles can live in the same state. We can identify the normalized state $|\alpha_1, \alpha_2, \cdots\rangle$ as $|\alpha_1, \alpha_2, \cdots\}$ and

$$\begin{aligned} & \langle \alpha_1, \alpha_2, \cdots | \alpha_1, \alpha_2, \cdots \rangle \\ = & \frac{1}{N!} \sum_{P,P'} (-1)^{P'+P} \langle \alpha_{P'_1} | \alpha_{P_1} \rangle \langle \alpha_{P'_2} | \alpha_{P_2} \rangle \cdots , \\ = & \ 1. \end{aligned} \tag{24}$$

The factor $(-1)^{P'+P}$ must always be $+1$, since P' needs to be exactly the same as P, else some of the bracket $\langle \alpha_{P'_i} | \alpha_{P_i} \rangle$ would be zero.

II. CREATION AND ANNIHILATION OPERATORS

In the formulation of **second quantization**, operators are written in creation and annihilation operators.

A. Occupation number representation

After symmetrization (for bosons) or antisymmetrization (for fermions), a N-particle state becomes,

$$|\alpha_1\rangle |\alpha_2\rangle \cdots |\alpha_N\rangle \to |\alpha_1, \alpha_2, \cdots, \alpha_N\}. \tag{25}$$

Similarly, a $(N+1)$-particle state becomes,

$$|\alpha\rangle |\alpha_1\rangle |\alpha_2\rangle \cdots |\alpha_N\rangle \to |\alpha, \alpha_1, \alpha_2, \cdots, \alpha_N\}. \tag{26}$$

The **creation operator** maps a N-particle state to a $(N+1)$-particle state. It is defined as follows,

$$\begin{aligned} a_\alpha^\dagger|\alpha_1,\alpha_2,\cdots,\alpha_N\} &= |\alpha,\alpha_1,\alpha_2,\cdots,\alpha_N\} \\ &= (\pm 1)^{i-1}|\alpha_1,\alpha_2,\cdots,\underbrace{,\alpha,}_{i-\text{th}}\cdots,\alpha_N\}. \end{aligned} \tag{27}$$

For **annihilation operator** a_α, if α is the same as one of the α_i, but not the same as others, then

$$\begin{aligned} & a_{\alpha_i}|\alpha_1,\alpha_2,\cdots,\alpha_N\} \\ =\ & (\pm 1)^{i-1}|\alpha_1,\alpha_2,\cdots,(\text{no }\alpha_i),\cdots\alpha_N\}. \end{aligned} \tag{28}$$

For bosons, if there are multiple coincidence of α_i's with α, then

$$\begin{aligned} & a_\alpha|\alpha_1,\alpha_2,\cdots,\alpha_N\} \\ =\ & \sum_{i=1}^{N}\underbrace{\langle\alpha|\alpha_i\rangle}_{\delta_{\alpha\alpha_i}}|\alpha_1,\alpha_2,\cdots,(\text{no }\alpha_i),\cdots\alpha_N\}. \end{aligned} \tag{29}$$

For fermions, $|\alpha_1,\alpha_2,\cdots,\alpha_N\}$ with multiple coincidence is zero, of course.

■ Bosons

In addition to the $|\alpha_1,\alpha_2,\cdots\}$ notation, in which the slots are filled with quantum numbers for particles at position $r_1,r_2,\cdots$, we introduce the **occupation number representation**: $|n_1,n_2,\cdots\rangle$, in which the slots are filled with occupation numbers for states $\bar{1},\bar{2},\cdots$. If the state of the added particle $\alpha=\bar{\ell}$, then $n_\ell\to n_\ell+1$ (see Eq. (23)),

$$\begin{aligned} & |\underbrace{\alpha}_{r},\underbrace{\alpha_1}_{r_1},\underbrace{\alpha_2}_{r_2},\cdots,\underbrace{\alpha_N}_{r_N}\} \\ =\ & \sqrt{n_1!}\sqrt{n_2!}\cdots\sqrt{(n_\ell+1)!}\cdots \\ \times\ & |\underbrace{n_1}_{\bar{1}},\underbrace{n_2}_{\bar{2}},\cdots,\underbrace{n_\ell+1}_{\bar{\ell}},\cdots\rangle. \end{aligned} \tag{30}$$

Notice that the number of slots for $|\cdots\rangle$ could be infinite, if there are infinite numbers of single-particle eigen-states. Comparing Eqs. (27) and (30), we have

$$a_\ell^\dagger|n_1,n_2,\cdots,n_\ell,\cdots\rangle=\sqrt{n_\ell+1}|n_1,n_2,\cdots,n_\ell+1,\cdots\rangle. \tag{31}$$

The square-root is the important amplification factor for lasers to work.

Similarly, one can have the annihilation operator that maps a N-particle state to a $(N-1)$-particle state,

$$a_\ell|n_1, n_2, \cdots, n_\ell, \cdots\rangle \to |n_1, n_2, \cdots, n_\ell - 1, \cdots\rangle. \tag{32}$$

This follows naturally from Eq. (31):

$$\begin{aligned} & a_\ell|n_1, n_2, \cdots, n_\ell, \cdots\rangle \\ = & \sum_{\{n'\}} |\{n'\}\rangle\langle a_\ell^\dagger\{n'\}|n_1, n_2, \cdots\rangle \\ = & \sum_{\{n'\}} \sqrt{n'_\ell + 1}|\{n'\}\rangle\langle n'_1, \cdots, n'_\ell + 1, \cdots|n_1, \cdots, n_\ell \cdots\rangle \\ = & \sqrt{n_\ell}|n_1, n_2, \cdots, n_\ell - 1, \cdots\rangle. \end{aligned} \tag{33}$$

The ket $|\{n'\}\rangle$ is an abbreviation of $|n'_1, n'_2, \cdots\rangle$. We have inserted a completeness relation, and used a Hermitian conjugate operation to get the first equation.

By applying the creation operator repeatedly to the vacuum state $|0, 0, \cdots\rangle$ (abbreviated as $|\mathbf{0}\rangle$), one can reach any of the manybody state $|n_1, n_2, \cdots\rangle$ as follows,

$$|n_1, n_2, \cdots\rangle = \frac{1}{\sqrt{n_1!}}\frac{1}{\sqrt{n_2!}} \cdots \left(a_1^\dagger\right)^{n_1} \left(a_2^\dagger\right)^{n_2} \cdots |\mathbf{0}\rangle. \tag{34}$$

■ Fermions

The rules are simpler for fermions since the occupation number n_i ($\forall\ i$) can only be 0 or 1. If the state $\bar{\ell}$ is empty ($n_\ell = 0$), then

$$a_\ell^\dagger|n_1, n_2, \cdots, 0, \cdots\rangle = (-1)^\lambda|n_1, n_2, \cdots, 1, \cdots\rangle, \tag{35}$$

where $\lambda = \sum_{i=1}^{\ell-1} n_i$. If the state $\bar{\ell}$ is occupied ($n_\ell = 1$), then

$$a_\ell^\dagger|n_1, n_2, \cdots, 1, \cdots\rangle = 0. \tag{36}$$

One cannot add two fermions to the same state because of the exclusion principle.

On the other hand, for the annihilation operator, one has

$$\begin{aligned} a_\ell|n_1, n_2, \cdots, 1, \cdots\rangle &= (-1)^\lambda|n_1, n_2, \cdots, 0, \cdots\rangle, \\ a_\ell|n_1, n_2, \cdots, 0, \cdots\rangle &= 0, \end{aligned} \tag{37}$$

where $\lambda = \sum_{i=1}^{\ell-1} n_i$.

Also, a manybody state can be reached by applying the creation operator to the vacuum state (compare with Eq. (34)),

$$|n_1, n_2, \cdots\rangle = \left(a_1^\dagger\right)^{n_1} \left(a_2^\dagger\right)^{n_2} \cdots |\mathbf{0}\rangle. \tag{38}$$

Of course, the occupation numbers n_i ($\forall\ i$) can only be 0 or 1.

For example, the electrons in an electron gas are labelled by quantum numbers $(\mathbf{k}, s)$. The ground state of the electrons is a Fermi sphere in momentum space. The state of a filled Fermi sphere with radius k_F is

$$|FS\rangle = \prod_{k<k_F} a_{\mathbf{k}\uparrow}^\dagger a_{\mathbf{k}\downarrow}^\dagger |\mathbf{0}\rangle. \tag{39}$$

B. Commutation relations

Recall that

$$a_\alpha^\dagger |\alpha_1, \alpha_2, \cdots, \alpha_N\} = |\alpha, \alpha_1, \alpha_2, \cdots, \alpha_N\}.$$

Therefore,

$$\begin{aligned} a_\beta^\dagger a_\alpha^\dagger |\alpha_1, \alpha_2, \cdots, \alpha_N\} &= |\beta, \alpha, \alpha_1, \alpha_2, \cdots, \alpha_N\}, \\ a_\alpha^\dagger a_\beta^\dagger |\alpha_1, \alpha_2, \cdots, \alpha_N\} &= |\alpha, \beta, \alpha_1, \alpha_2, \cdots, \alpha_N\}. \end{aligned} \tag{41}$$

The two states on the RHS are identical for bosons, but differ by a sign for fermions. Since such a connection applies to any manybody state $|\alpha_1, \alpha_2, \cdots, \alpha_N\}$, we can remove the ket and simply write, **for bosons**,

$$a_\alpha^\dagger a_\beta^\dagger = a_\beta^\dagger a_\alpha^\dagger \quad \text{or} \quad [a_\alpha^\dagger, a_\beta^\dagger] = 0 \tag{42}$$

for any single-particle states α, β. Hermitian conjugate of this equation gives

$$[a_\alpha, a_\beta] = 0 \tag{43}$$

For fermions, one has

$$a_\alpha^\dagger a_\beta^\dagger = -a_\beta^\dagger a_\alpha^\dagger \quad \text{or} \quad \{a_\alpha^\dagger, a_\beta^\dagger\} = 0 \tag{44}$$

for any single-particle states α, β. Hermitian conjugate of this equation gives

$$\{a_\alpha, a_\beta\} = 0 \tag{45}$$

Notice that fermion creation operators *do not* commute, but anti-commute with each other. Also, if $\beta = \alpha$, then one has

$$\left(a_\alpha^\dagger\right)^2 = 0, \quad \forall\ \alpha. \tag{46}$$

This is again a reflection of the exclusion principle.

For combined operation of creation and annihilation operators, it is more convenient to use the occupation-number representation (Cf. Eq. (41)). One starts from fermions : From Eq. (35), we have,

$$a_\ell^\dagger|n_1, n_2, \cdots, 0, \cdots\rangle(-1)^\lambda|n_1, n_2, \cdots, 1, \cdots\rangle,$$

where $\lambda = \sum_{i=1}^{\ell-1} n_i$ Also, from Eq. (37),

$$a_\ell|n_1, n_2, \cdots, 1, \cdots\rangle = (-1)^\lambda|n_1, n_2, \cdots, 0, \cdots\rangle.$$

Combined operation gives ($\alpha = \bar{\ell}$)

$$\begin{aligned} a_\alpha a_\alpha^\dagger|n_1, n_2, \cdots, 0, \cdots\rangle &= |n_1, n_2, \cdots, 0, \cdots\rangle, \\ a_\alpha^\dagger a_\alpha|n_1, n_2, \cdots, 0, \cdots\rangle &= 0. \end{aligned} \tag{48}$$

One can also consider the possibility of $n_\ell = 1$ and write down another two equations. Both cases lead to $a_\alpha a_\alpha^\dagger + a_\alpha^\dagger a_\alpha = \mathbf{1}$, the identity operator. It's not difficult to show that, if the annihilation and creation operators act on different states, α and β, then $a_\alpha a_\beta^\dagger + a_\beta^\dagger a_\alpha = 0$. Therefore, in general, **for fermions**,

$$\{a_\alpha, a_\beta^\dagger\} = \delta_{\alpha\beta}. \tag{49}$$

It's left as an exercise to show that, **for bosons**, similar argument leads to

$$[a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta}. \tag{50}$$

Finally, for both bosons and fermions,

$$a_\alpha^\dagger a_\alpha|n_1, n_2, \cdots, n_\alpha, \cdots\rangle = n_\alpha|n_1, n_2, \cdots, n_\alpha, \cdots\rangle. \tag{51}$$

Therefore, $\hat{n}_\alpha \equiv a_\alpha^\dagger a_\alpha$ is also known as the **occupation number operator**.

C. Change of basis

Under a unitary transformation, the one-particle state $|\alpha\rangle$ changes to $|\tilde{\alpha}\rangle$. They are related by the following unitary transformation,

$$|\tilde{\alpha}\rangle = \sum_{\alpha} |\alpha\rangle\langle\alpha|\tilde{\alpha}\rangle. \tag{52}$$

On such a new basis,

$$\begin{aligned} a^{\dagger}_{\tilde{\alpha}}|\tilde{\alpha}_1, \tilde{\alpha}_2, \cdots, \tilde{\alpha}_N\} &= |\tilde{\alpha}, \tilde{\alpha}_1, \tilde{\alpha}_2, \cdots, \tilde{\alpha}_N\} \\ &= \sum_{\alpha} \langle\alpha|\tilde{\alpha}\rangle|\alpha, \tilde{\alpha}_1, \tilde{\alpha}_2, \cdots, \tilde{\alpha}_N\} \\ &= \sum_{\alpha} \langle\alpha|\tilde{\alpha}\rangle a^{\dagger}_{\alpha}|\tilde{\alpha}_1, \tilde{\alpha}_2, \cdots, \tilde{\alpha}_N\}. \end{aligned} \tag{53}$$

Therefore, after striping off the ket state, we have

$$a^{\dagger}_{\tilde{\alpha}} = \sum_{\alpha} \langle\alpha|\tilde{\alpha}\rangle a^{\dagger}_{\alpha}. \tag{54}$$

That is, the creation operator transforms like $|\alpha\rangle$. Also,

$$a_{\tilde{\alpha}} = \sum_{\alpha} \langle\tilde{\alpha}|\alpha\rangle a_{\alpha}. \tag{55}$$

It can be shown that, if the new set $\{|\tilde{\alpha}\rangle\}$ is also an orthonormal set, then,

$$\begin{aligned} [a_{\tilde{\alpha}}, a^{\dagger}_{\tilde{\beta}}] &= \delta_{\tilde{\alpha}\tilde{\beta}} \quad \text{for bosons} \\ \{a_{\tilde{\alpha}}, a^{\dagger}_{\tilde{\beta}}\} &= \delta_{\tilde{\alpha}\tilde{\beta}} \quad \text{for fermions} \end{aligned} \tag{56}$$

That is, the canonical commutation relations remain invariant under a unitary transformation.

III. COORDINATE AND MOMENTUM REPRESENTATIONS

The ket states in previous Section are representation free. We will project such ket states to specific basis, such as coordinate basis, or momentum basis. Recall that the single-particle wave function is

$$\phi_{\alpha}(\mathbf{r}) = \langle\mathbf{r}|\alpha\rangle. \tag{57}$$

We can change the α-basis to r-basis using the unitary transformation (Eq. (54)), then

$$\psi^\dagger(\mathbf{r}) = \sum_\alpha \langle \alpha|\mathbf{r}\rangle a_\alpha^\dagger = \sum_\alpha \phi_\alpha^*(\mathbf{r}) a_\alpha^\dagger.$$

We have rewritten $a_r^\dagger$ as $\psi^\dagger(\mathbf{r})$. Such an operator that creates (or annihilates) a particle at a particular point in space is called a **field operator**. The inverse transformation is

$$a_\alpha^\dagger = \int d^3r \langle \mathbf{r}|\alpha\rangle \psi^\dagger(\mathbf{r}) = \int d^3r \phi_\alpha(\mathbf{r}) \psi^\dagger(\mathbf{r}). \tag{59}$$

For example, the quantum state $|\alpha\rangle$ of a particle in an empty box with volume V_0 can be labelled by momentum $\mathbf{k}$, and $\langle \mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V_0}$. Therefore,

$$\psi^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V_0}} \sum_k e^{-i\mathbf{k}\cdot\mathbf{r}} a_k^\dagger. \tag{60}$$

This is nothing but the Fourier expansion. Its inverse transformation is,

$$\begin{aligned} \psi^\dagger(\mathbf{k}) &= \int d^3r \langle \mathbf{r}|\mathbf{k}\rangle \psi^\dagger(\mathbf{r}) \\ &= \frac{1}{\sqrt{V_0}} \int d^3r e^{i\mathbf{k}\cdot\mathbf{r}} \psi^\dagger(\mathbf{r}). \end{aligned} \tag{61}$$

Solid state theorists prefer to move the $1/\sqrt{V_0}$ factor in Eq. (61) to Eq. (60). That is,

$$\begin{aligned} \psi^\dagger(\mathbf{r}) &= \frac{1}{V_0} \sum_k e^{-i\mathbf{k}\cdot\mathbf{r}} a_k^\dagger, \\ \psi^\dagger(\mathbf{k}) &= \int d^3r e^{i\mathbf{k}\cdot\mathbf{r}} \psi^\dagger(\mathbf{r}). \end{aligned} \tag{62}$$

We have assumed the system is inside a box with a finite volume, so the momentum $\mathbf{k}$ is quantized. If V_0 approaches infinity, then one can replace the summation with an integral,

$$\frac{1}{V_0} \sum_k \quad \to \quad \int \frac{d^3k}{(2\pi)^3}. \tag{63}$$

Consider another example: the hydrogen atom. The quantum numbers for a spinless electron are $\alpha = (n, l, m)$, and the field operator is

$$\psi^\dagger(\mathbf{r}) = \sum_{nlm} \phi_{nlm}^*(\mathbf{r}) a_{nlm}^\dagger. \tag{64}$$

According to Eq. (56), one has

$$\{\psi(\mathbf{r}), \psi^\dagger(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}'). \tag{65}$$

With the help of Eq. (59), the particle-number operator in the coordinate representation becomes

$$\begin{aligned} N &= \sum_\alpha a_\alpha^\dagger a_\alpha \\ &= \int d^3r d^3r' \sum_\alpha \langle \mathbf{r}|\alpha\rangle\langle\alpha|\mathbf{r}'\rangle \psi^\dagger(\mathbf{r})\psi(\mathbf{r}') \\ &= \int d^3r \psi^\dagger(\mathbf{r})\psi(\mathbf{r}). \end{aligned} \tag{66}$$

We have used a completeness relation to remove the α-summation, and used the orthogonality relation $\langle \mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}')$. Naturally, one can define the **particle-density operator** as

$$\rho(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r}). \tag{67}$$

This looks like the usual particle density in quantum mechanics. But beware that this is an operator relation, not a numerical relation.

IV. SECOND QUANTIZATION

A. One-body operator

To deal with manybody systems, we need an operator A that acts on N-body states $|\alpha_1\rangle|\alpha_2\rangle\cdots|\alpha_N\rangle$. For example, if $A_i^{(1)}$ is the operator for a particle at position $\mathbf{r}_i$, then A is the operator for all of the particles. The latter operates in a much larger, N-particle Hilbert space $\mathcal{H}^{(N)} = \mathcal{H}^{(1)} \otimes \mathcal{H}^{(1)} \otimes \cdots \otimes \mathcal{H}^{(1)}$.

The operator $A_i^{(1)}$ can be expanded using an explicit basis,

$$\begin{aligned} A_i^{(1)} &= \sum_{\alpha\beta} |\alpha\rangle\langle\alpha|A^{(1)}(\mathbf{r}_i)|\beta\rangle\langle\beta| \\ &= \sum_{\alpha\beta} A^{(1)}_{\alpha\beta}|\alpha\rangle\langle\beta|, \end{aligned} \tag{68}$$

where $A^{(1)}_{\alpha\beta} \equiv \langle\alpha|A^{(1)}|\beta\rangle$.

Before defining the operator A, it is convenient to rewrite, following Feynman's notation (the $\times$ below is not the usual direct product $\otimes$),

$$|\alpha_1, \alpha_2, \cdots, \alpha_N\} \equiv |\alpha_1\rangle \times |\alpha_2\rangle \cdots |\alpha_N\rangle. \tag{69}$$

Operator A for a manybody system is connected with $A_i^{(1)}$ in the following way,

$$A = \sum_{i=1}^{N} A_i^{(1)}. \tag{70}$$

More precisely, it is

$$\begin{aligned} A|\alpha_1\rangle \times |\alpha_2\rangle \cdots |\alpha_N\rangle \;=\; & \left(A^{(1)}|\alpha_1\rangle\right) \times |\alpha_2\rangle \cdots |\alpha_N\rangle \\ & + \; |\alpha_1\rangle \times \left(A^{(1)}|\alpha_2\rangle\right) \cdots |\alpha_N\rangle \\ & + \; \cdots \\ & + \; |\alpha_1\rangle| \times |\alpha_2\rangle \cdots \left(A^{(1)}|\alpha_N\rangle\right). \end{aligned} \tag{71}$$

Let's first assume $A_i^{(1)} = |\alpha\rangle\langle\beta|$, then (see Eq. (29))

$$\begin{aligned} & A|\alpha_1\rangle \times |\alpha_2\rangle \cdots |\alpha_N\rangle \\ = \; & \sum_{i=1}^{N} \underbrace{\langle\beta|\alpha_i\rangle}_{\delta_{\beta\alpha_i}} |\alpha_1\rangle \times \cdots \times |\alpha\rangle \times \cdots |\alpha_N\rangle \\ = \; & a_\alpha^\dagger \sum_{i=1}^{N} (\pm 1)^{i-1} \delta_{\beta\alpha_i} |\alpha_1\rangle \times \cdots \times (\text{no } |\alpha_i\rangle) \times \cdots |\alpha_N\rangle \\ = \; & a_\alpha^\dagger a_\beta |\alpha_1\rangle \times |\alpha_2\rangle \cdots |\alpha_N\rangle. \end{aligned} \tag{72}$$

Notice that the summation here should be interpreted like the series in Eq. (72). The sign (± 1) is for bosons/fermions. In general, when $A = \sum_{\alpha\beta} A_{\alpha\beta}^{(1)} |\alpha\rangle\langle\beta|$, each term in the summation can be identified as $a_\alpha^\dagger a_\beta$ using the procedure above. As a result,

$$A = \sum_{\alpha\beta} A_{\alpha\beta}^{(1)} a_\alpha^\dagger a_\beta. \tag{73}$$

It looks as simple as the operator for a single particle (Eq. 68).

1. Example: Density operator

Firstly, we need to know the first quantized form of density. For a single particle, it is

$$\rho^{(1)}(\mathbf{r}) = \delta(\hat{\mathbf{r}} - \mathbf{r}). \tag{74}$$

Notice that $\hat{\mathbf{r}}$ is an operator, while $\mathbf{r}$ is just an ordinary vector. One can easily verify that $\langle\phi|\rho^{(1)}(\mathbf{r})|\phi\rangle = \phi^*(\mathbf{r})\phi(\mathbf{r})$. The Fourier transform of the density operator is

$$\begin{aligned} \rho^{(1)}(\mathbf{q}) \;&=\; \int dv e^{-i\mathbf{q}\cdot\mathbf{r}} \rho^{(1)}(\mathbf{r}) \\ &=\; e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}}. \end{aligned} \tag{75}$$

We have used a simpler notation dv for d^3r. For many particles (but still in first quantized form),

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} \delta(\hat{\mathbf{r}}_i - \mathbf{r}). \tag{76}$$

Its Fourier transform is

$$\rho(\mathbf{q}) = \sum_i e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}_i}. \tag{77}$$

To get the second quantized form, we need (see Eq. (73)),

$$\rho = \sum_{\alpha\beta} \rho^{(1)}_{\alpha\beta} a^\dagger_\alpha a_\beta. \tag{78}$$

a. Coordinate representation

In the coordinate representation, the matrix element in Eq. (78) is

$$\begin{aligned} \rho^{(1)}_{r'r''} &= \langle \mathbf{r}'|\rho^{(1)}(\mathbf{r})|\mathbf{r}''\rangle \\ &= \delta(\mathbf{r}' - \mathbf{r})\delta(\mathbf{r}' - \mathbf{r}''). \end{aligned} \tag{79}$$

Replace the α-summation in Eq. (78) by a r-integral, and rewrite $a^\dagger_r$ as $\psi^\dagger(\mathbf{r})$, then (following Eq. (78))

$$\begin{aligned} \rho(\mathbf{r}) &= \int dv' \int dv'' \delta(\mathbf{r}' - \mathbf{r})\delta(\mathbf{r}' - \mathbf{r}'')\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}'') \\ &= \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) \end{aligned} \tag{80}$$

This is the same as Eq. (67), and is similar to the usual expression $\rho(\mathbf{r}) = \phi^*(\mathbf{r})\phi(\mathbf{r})$. The difference is that $\phi(\mathbf{r})$ is a one-particle wave function, while $\psi(\mathbf{r})$ is a field operator.

b. Momentum representation

In momentum representation, the matrix element is

$$\begin{aligned} \rho^{(1)}_{k'k''} &= \langle \mathbf{k}'|\rho^{(1)}(\mathbf{q})|\mathbf{k}''\rangle \\ &= \int dv' \int dv'' \langle \mathbf{k}'|\mathbf{r}'\rangle\langle \mathbf{r}'|e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}}|\mathbf{r}''\rangle\langle \mathbf{r}''|\mathbf{k}''\rangle. \end{aligned} \tag{81}$$

The matrix element $\langle \mathbf{r}'|e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}}|\mathbf{r}''\rangle = e^{-i\mathbf{q}\cdot\mathbf{r}''}\delta(\mathbf{r}' - \mathbf{r}'')$. Also, $\langle \mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V_0}$, so we get

$$\rho^{(1)}_{k'k''} = \delta(\mathbf{k}'' - \mathbf{k}' - \mathbf{q}). \tag{82}$$

Therefore,

$$\begin{aligned}\rho(\mathbf{q}) &= \sum_{k'k''} \rho^{(1)}_{k'k''} a^\dagger_{k'} a_{k''} \\ &= \sum_{k'} a^\dagger_{k'} a_{k'+q}.\end{aligned} \tag{83}$$

2. Example: Hamiltonian for non-interacting particles

Consider the following Hamiltonian for a single particle,

$$H^{(1)} = \frac{p^2}{2m} + V^{(1)}(\mathbf{r}). \tag{84}$$

For a non-interacting manybody system, it becomes

$$H = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + V^{(1)}(\mathbf{r}_i) \right]. \tag{85}$$

Inter-particle interaction $V(\mathbf{r}_i - \mathbf{r}_j)$ will be discussed in the next Section.

a. *Energy-eigenstate representation*

Recall Eq. (1),

$$H^{(1)}\phi_\alpha = \varepsilon_\alpha \phi_\alpha.$$

The Hamiltonian matrix is diagonalized in the eigenstate basis,

$$H^{(1)}_{\alpha\beta} = \varepsilon_\alpha \delta_{\alpha\beta}. \tag{87}$$

Therefore, the second quantized form is quite simple,

$$H = \sum_{\alpha\beta} H^{(1)}_{\alpha\beta} a^\dagger_\alpha a_\beta = \sum_\alpha \varepsilon_\alpha a^\dagger_\alpha a_\alpha. \tag{88}$$

b. *Coordinate representation*

The Hamiltonian matrix in the coordinate basis is

$$\langle \mathbf{r}|H^{(1)}|\mathbf{r}'\rangle = -\frac{\hbar^2}{2m}\nabla^2 \delta(\mathbf{r}-\mathbf{r}') + V^{(1)}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}'). \tag{89}$$

Therefore, the second quantized Hamiltonian is

$$\begin{aligned} H &= \int dv dv' \langle \mathbf{r}|H^{(1)}|\mathbf{r}'\rangle \psi^\dagger(\mathbf{r})\psi(\mathbf{r}') \\ &= \int dv \psi^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V^{(1)}(\mathbf{r})\right] \psi(\mathbf{r}). \end{aligned} \tag{90}$$

Recall that the first quantized version is written as Eq. (85).

The Heisenberg equation for field operator is

$$[\psi, H] = i\hbar \frac{\partial \psi}{\partial t}, \tag{91}$$

which leads to

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V^{(1)}(\mathbf{r})\right] \psi(\mathbf{r}, t) = i\hbar \frac{\partial \psi}{\partial t}. \tag{92}$$

Even though this looks exactly the same as the Schrodinger for a single particle, it is actually an equation for the field operator. It is as if we have promoted the single-particle wave function to a field operator. That is why the present formulation is called the **second quantization**.

c. Momentum representation

The Hamiltonian matrix in the momentum basis is (recall that $\langle \mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V_0}$)

$$\begin{aligned} \langle \mathbf{k}|H^{(1)}|\mathbf{k}'\rangle &= \frac{\hbar^2 k^2}{2m}\langle \mathbf{k}|\mathbf{k}'\rangle + \int dv \langle \mathbf{k}|\mathbf{r}\rangle V^{(1)}(\mathbf{r}) \langle \mathbf{r}|\mathbf{k}'\rangle \\ &= \frac{\hbar^2 k^2}{2m}\delta_{kk'} + \frac{1}{V_0}\int dv V^{(1)}(\mathbf{r}) e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}. \end{aligned} \tag{93}$$

The second integral is actually the Fourier transform of $V^{(1)}(\mathbf{r})$: $V^{(1)}(\mathbf{k}-\mathbf{k}')$. The second quantized Hamiltonian is

$$\begin{aligned} H &= \sum_k \sum_{k'} \langle \mathbf{k}|H^{(1)}|\mathbf{k}'\rangle a_k^\dagger a_{k'} \\ &= \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k + \frac{1}{V_0}\sum_k \sum_{k'} V^{(1)}(\mathbf{k}-\mathbf{k}') a_k^\dagger a_{k'}. \end{aligned} \tag{94}$$

The potential term can also be written as (see Eq. (83))

$$\frac{1}{V_0}\sum_k \sum_q V^{(1)}(\mathbf{q}) a_k^\dagger a_{k-q} = \frac{1}{V_0}\sum_q V^{(1)}(\mathbf{q})\rho(-\mathbf{q}). \tag{95}$$

Some useful operators in first and second quantized form are summarized in Table 1.

TABLE I One-body operator

	1st quantization	2nd quantization
particle density $\rho(\mathbf{r})$	$\sum_i \delta(\hat{\mathbf{r}}_i - \mathbf{r})$	$\psi^\dagger(\mathbf{r})\psi(\mathbf{r})$
$\rho(\mathbf{q})$	$\sum_i e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}_i}$	$\sum_k a_k^\dagger a_{k+q}$
current density $\mathbf{j}(\mathbf{r})$	$\frac{1}{2m}\sum_i [\hat{\mathbf{p}}_i\delta(\hat{\mathbf{r}}_i - \mathbf{r}) + \delta(\hat{\mathbf{r}}_i - \mathbf{r})\hat{\mathbf{p}}_i]$	$\frac{\hbar}{2mi}\left[\psi^\dagger(\mathbf{r})\nabla\psi(\mathbf{r}) - \left(\nabla\psi^\dagger(\mathbf{r})\right)\psi(\mathbf{r})\right]$
$\mathbf{j}(\mathbf{q})$	$\frac{1}{2m}\sum_i \left(\hat{\mathbf{p}}_i e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}_i} + e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}_i}\hat{\mathbf{p}}_i\right)$	$\frac{\hbar}{2m}\sum_k (2\mathbf{k}+\mathbf{q})\, a_k^\dagger a_{k+q}$
one-body potential $V(\mathbf{r})$	$\sum_i V^{(1)}(\hat{\mathbf{r}}_i - \mathbf{r})$	$\int dv\ \psi^\dagger(\mathbf{r})V^{(1)}(\mathbf{r})\psi(\mathbf{r})$.
$V(\mathbf{q})$	$V^{(1)}(\mathbf{q})\sum_i e^{i\mathbf{q}\cdot\hat{\mathbf{r}}_i}$	$\sum_k V^{(1)}(\mathbf{q}) a_{k+q}^\dagger a_k$
magnetic moment density $\mathbf{m}(\mathbf{r})$	$\sum_i \boldsymbol{\sigma}_i\delta(\hat{\mathbf{r}}_i - \mathbf{r})$	$\boldsymbol{\psi}^\dagger(\mathbf{r})\boldsymbol{\sigma}\boldsymbol{\psi}(\mathbf{r})$ $[\boldsymbol{\psi}$ is a spinor]
$\mathbf{m}(\mathbf{q})$	$\sum_i \boldsymbol{\sigma}_i e^{-i\mathbf{q}\cdot\hat{\mathbf{r}}_i}$	$\sum_k \boldsymbol{\psi}_k^\dagger\boldsymbol{\sigma}\boldsymbol{\psi}_{k+q}$

B. Two-body operator

Two-body operators act on two particles at a time. A typical example is the interaction potential $V(\mathbf{r}_i - \mathbf{r}_j)$. In general, the operator for the whole system can be written as

$$A = \frac{1}{2}\sum_{i\neq j} A_{ij}^{(2)}. \tag{96}$$

One term in the summation,

$$\begin{aligned} A_{ij}^{(2)} &= \sum_{\alpha\alpha'\beta\beta'} |\alpha\rangle|\alpha'\rangle\langle\alpha|\langle\alpha'|A_{ij}^{(2)}|\beta\rangle|\beta'\rangle\langle\beta|\langle\beta'| \\ &= \sum_{\alpha\alpha'\beta\beta'} A^{(2)}_{\alpha\alpha'\beta'\beta}|\alpha\rangle|\alpha'\rangle\langle\beta|\langle\beta'|, \end{aligned} \tag{97}$$

in which α and β label quantum states of particle i; α' and β' label quantum states of particle j. Notice that we have switched the subscripts β, β' of $A^{(2)}$. Some textbooks prefer not to switch them.

Let's first assume $A^{(2)}_{ij} = |\alpha\rangle|\alpha'\rangle\langle\beta|\langle\beta'|$, then (for $i < j$)

$$\begin{aligned} & A^{(2)}_{ij}|\alpha_1\rangle \times \cdots |\alpha_N\rangle \\ = & \sum_{i<j}\langle\beta|\alpha_i\rangle\langle\beta'|\alpha_j\rangle|\alpha_1\rangle \times \cdots |\alpha\rangle \cdots |\alpha'\rangle \cdots |\alpha_N\rangle \\ = & \; a^\dagger_\alpha a^\dagger_{\alpha'} \sum_{i\neq j}(\pm 1)^{i-1}(\pm 1)^{j-2}\delta_{\beta\alpha_i}\delta_{\beta'\alpha_j} \\ & |\alpha_1\rangle \times \cdots (\text{no } |\alpha_i\rangle) \cdots (\text{no } |\alpha_j\rangle) \cdots |\alpha_N\rangle \\ = & \; a^\dagger_\alpha a^\dagger_{\alpha'} a_{\beta'} a_\beta |\alpha_1\rangle \times |\alpha_2\rangle \cdots |\alpha_N\rangle. \end{aligned} \tag{98}$$

That is, $|\alpha\rangle|\alpha'\rangle\langle\beta|\langle\beta'|$ can be identified with $a^\dagger_\alpha a^\dagger_{\alpha'} a_{\beta'} a_\beta$. The same is true if $i > j$. In general, when $A^{(2)}_{ij}$ is a superposition of many terms, one has

$$A = \frac{1}{2}\sum_{\alpha\alpha'\beta\beta'} A^{(2)}_{\alpha\alpha'\beta'\beta} a^\dagger_\alpha a^\dagger_{\alpha'} a_{\beta'} a_\beta. \tag{99}$$

1. Example: Inter-particle interaction

a. Coordinate representation

The matrix elements of $V^{(2)}(\mathbf{r}_i - \mathbf{r}_j)$ is

$$\begin{aligned} V^{(2)}_{rr'r''r'''} &= \langle \mathbf{r}\mathbf{r}'|V^{(2)}(\mathbf{r}_i - \mathbf{r}_j)|\mathbf{r}'''\mathbf{r}''\rangle \\ &= V^{(2)}(\mathbf{r} - \mathbf{r}')\delta(\mathbf{r} - \mathbf{r}''')\delta(\mathbf{r}' - \mathbf{r}''). \end{aligned} \tag{100}$$

Replace the summations in Eq. (100) by integrals over coordinates and write a_r as $\psi(\mathbf{r})$, we will get

$$V = \frac{1}{2}\int dv dv' \psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')V^{(2)}(\mathbf{r} - \mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}). \tag{101}$$

The quartic operator can be written in terms of the density operator,

$$\begin{aligned} & \psi^\dagger(\mathbf{r})\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}) \\ = & \; \psi^\dagger(\mathbf{r})\psi(\mathbf{r})\psi^\dagger(\mathbf{r}')\psi(\mathbf{r}') - \psi^\dagger(\mathbf{r})\psi(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') \\ = & \; \rho(\mathbf{r})\rho(\mathbf{r}') - \rho(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}'). \end{aligned} \tag{102}$$

The second term contributes to a self-interaction energy in Eq. (101). Therefore, the substraction helps removing the self-interaction in the first term.

b. Momentum representation

Expanding the field operator using plane waves,

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{V_0}} \sum_k a_k e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{103}$$

then the inter-particle interaction becomes

$$\begin{aligned} V &= \frac{1}{2V_0^2} \sum_{k_1,k_2,k_3,k_4} a^\dagger_{k_4} a^\dagger_{k_3} a_{k_2} a_{k_1} \\ &\times \int dv dv' V^{(2)}(\mathbf{r}-\mathbf{r}') e^{i(\mathbf{k}_1-\mathbf{k}_4)\cdot\mathbf{r}} e^{i(\mathbf{k}_2-\mathbf{k}_3)\cdot\mathbf{r}'}. \end{aligned} \tag{104}$$

Write the interaction potential as

$$V^{(2)}(\mathbf{r}-\mathbf{r}') = \frac{1}{V_0} \sum_q V^{(2)}(\mathbf{q}) e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}, \tag{105}$$

then the space integral gives $V_0 \delta_{\mathbf{k}_4,\mathbf{k}_1+\mathbf{q}} \delta_{\mathbf{k}_3,\mathbf{k}_2-\mathbf{q}}$. Finally,

$$V = \frac{1}{2V_0} \sum_{k_1,k_2,q} V^{(2)}(\mathbf{q}) a^\dagger_{k_1+q} a^\dagger_{k_2-q} a_{k_2} a_{k_1}. \tag{106}$$

One can visualize the item in the summation as follows: two incoming particles with momenta $\mathbf{k}_1$ and $\mathbf{k}_2$ are scattered by the potential and become outgoing particles with momenta $\mathbf{k}_1 + \mathbf{q}$ and $\mathbf{k}_2 - \mathbf{q}$. The total momentum is conserved (elastic scattering), but there is a transfer of momentum $\mathbf{q}$ from particle 2 to particle 1.

V. GENERAL DISCUSSION

A. Spin degree of freedom

From now on, we will focus only on systems of electrons (or fermions). Non-interacting (or weakly interacting) electrons are referred to as electron gas. When interaction plays an important role, we will call them as electron liquid. For spinful electrons in an empty box, the Hamiltonian in coordinate representation is

$$\begin{aligned} H &= \sum_s \int dv\ \psi^\dagger_s(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V^{(1)}_s(\mathbf{r}) \right] \psi_s(\mathbf{r}) \\ &+ \frac{1}{2} \sum_{s,s'} \int dv dv' \psi^\dagger_s(\mathbf{r}) \psi^\dagger_{s'}(\mathbf{r}') V^{(2)}_{ss'}(\mathbf{r}-\mathbf{r}') \psi_{s'}(\mathbf{r}') \psi_s(\mathbf{r}), \end{aligned} \tag{107}$$

in which we have allowed for spin-dependent external potential $V_s^{(1)}(\mathbf{r})$ and electron interaction $V_{ss'}^{(2)}(\mathbf{r}-\mathbf{r}')$. The Hamiltonian in momentum representation is

$$\begin{aligned} H &= \sum_{ks} \frac{\hbar^2 k^2}{2m} a_{ks}^\dagger a_{ks} + \frac{1}{V_0} \sum_{kqs} V_s^{(1)}(\mathbf{q}) a_{k+q,s}^\dagger a_{ks} \\ &+ \frac{1}{2V_0} \sum_{ks,k's',q} V_{ss'}^{(2)}(\mathbf{q}) a_{k+q,s}^\dagger a_{k'-q,s'}^\dagger a_{k's'} a_{ks}. \end{aligned} \tag{108}$$

The subscripts $(\mathbf{k}, s)$ are good quantum numbers for (non-interacting) electrons in an empty box, which has free-particle energy $\varepsilon_k^0 = \hbar^2 k^2/2m$. For electrons in a lattice without spin-orbit coupling, the proper label for quantum states is $(n, \mathbf{k}, s)$, where n is the band index, and $\mathbf{k}$ is the quasi-momentum for Bloch electron. Also, the free-particle energy ε_k^0 has to be replaced by Bloch energy ε_{nk}.

B. Tight-binding model

In the tight-binding model, the electrons hop from one atom to another. The operator a_{nks} for a Bloch state has to be replaced by a_l, where l contains information such as band index n, lattice site $\mathbf{R}$, and spin s. The **Wannier function** (sometimes atomic orbitals are used instead) is

$$\langle \mathbf{r}|l\rangle = \langle \mathbf{r}|n, \mathbf{R}, s\rangle = w_n(\mathbf{r}-\mathbf{R})\chi_s, \tag{109}$$

where χ_s is a spinor,

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{110}$$

They have the following orthogonality and completeness relations:

$$\chi_s^\dagger \chi_{s'} = \delta_{ss'}, \quad \sum_s \chi_s \chi_s^\dagger = \mathbf{1}_{2\times 2}. \tag{111}$$

The Hamiltonian for non-interacting electrons is

$$H_0 = \sum_{\tilde{l}\tilde{m}s} H_{\tilde{l}\tilde{m}}^{(1)} a_{\tilde{l}s}^\dagger a_{\tilde{m}s}, \tag{112}$$

where $\tilde{l} = (n, \mathbf{R})$, and $H_{\tilde{l}\tilde{m}}^{(1)} = \langle \tilde{l}|\frac{p^2}{2m} + V^{(1)}(\mathbf{r})|\tilde{m}\rangle$, assuming $V^{(1)}$ is a spin-independent potential. We have contracted the spin degree of freedom in the matrix elements.

If the interaction is also spin-independent, then

$$V_{ee} = \frac{1}{2} \sum_{lmm'l'} V^{(2)}_{\tilde{l}\tilde{m}\tilde{m}'\tilde{l}'} a^\dagger_l a^\dagger_m a_{m'} a_{l'}, \tag{113}$$

where

$$\begin{aligned} & V^{(2)}_{\tilde{l}\tilde{m}\tilde{m}'\tilde{l}'} \\ = & \int dv_1 dv_2 w^*_{n_l}(\mathbf{r}_1 - \mathbf{R}_l) w^*_{n_m}(\mathbf{r}_2 - \mathbf{R}_m) V^{(2)}(\mathbf{r}_1 - \mathbf{r}_2) \\ \times & \; w_{n_{m'}}(\mathbf{r}_2 - \mathbf{R}_{m'}) w_{n_{l'}}(\mathbf{r}_1 - \mathbf{R}_{l'}). \end{aligned} \tag{114}$$

In reality, one may keep only the nearest-neighbor and the next-nearest-neighbor couplings. Furthermore, one might be able to use the **one-band approximation**, assuming that the electrons only reside on one band n, then (n is omitted for simplicity), then

$$\begin{aligned} H &= H_0 + V_{ee} \\ &= \sum_{RR's} H^{(1)}_{RR'} a^\dagger_{Rs} a_{R's} \\ &+ \frac{1}{2} \sum_{\substack{R_1 R_2 R'_2 R'_1 \\ ss'}} V^{(2)}_{R_1 R_2 R'_2 R'_1} a^\dagger_{R_1 s} a^\dagger_{R_2 s'} a_{R'_2 s'} a_{R'_1 s}, \end{aligned} \tag{115}$$

in which we have assumed that the one-body and two-body potentials are spin-independent.

The simplest possible model (with interaction) is to keep only the nearest-neighbor hopping in the first term, and only the on-site energy in the second term. That is,

$$\begin{aligned} H &= t \sum_{<RR'>s} a^\dagger_{Rs} a_{R's} + U \sum_R a^\dagger_{R\uparrow} a^\dagger_{R\downarrow} a_{R\downarrow} a_{R\uparrow} \\ &= t \sum_{<RR'>s} a^\dagger_{Rs} a_{R's} + U \sum_R n_{R\uparrow} n_{R\downarrow}, \end{aligned} \tag{116}$$

where n_{Rs} is the occupation-number operator. Notice that there are only two parameters: the hopping amplitude t and the on-site energy U. This is the famous **Hubbard model** proposed by Hubbard more than 50 years ago to study narrow-band materials, such as transition metal oxides. It is also considered as the underlying model for high temperature superconductors. Despite enormous effort from numerous researchers, the phase diagrams for the Hubbard model in dimension two and higher remain inconclusive. (see the article by J. Quintanilla and C. Hooley in Phys. World, June, 2009)

C. What do we calculate

Most of the time we are interested in obtaining some of the following properties:

▷ Ground state energy

▷ Phase diagram (comparing lowest energies of different phases)

▷ Other ground state properties, such as charge order or spin order (correlation function), density of states ... etc.

▷ Low-lying excitations (quasi-particles, collective excitations)

▷ Linear response function (conductivity, susceptibility ... etc)

▷ Other quantities of experimental interest.

Of course, whether the result is satisfactory or not depends on whether, at the first place, the simplified model captures the essential ingredients of the phenomena we intend to study.

D. How do we calculate

The Hilbert space $\mathcal{H}^{(N)}$ of a manybody system is mind bogglingly big. In classical mechanics, if the solution space of a particle has dimension d, then the solution space of the whole system is Nd. However, in quantum mechanics, the latter is d^N. This causes major problem for analytical and numerical calculations, and many different methods have been proposed:

▷ Mean field approximation (MFA)

▷ Equation of motion (EOM) method

▷ Perturbation expansion using Green's function (diagram expansion)

▷ Variational method

▷ Density functional theory (DFT)

▷ Quantum Monte Carlo (QMC) method

▷ Density matrix renormalization group (DMRG)

▷ Tensor network renormalization group

▷ $\cdots$

The first 3 are perturbative calculations in essence. The last 4 are numerical methods. Variation method first requires guess work, and then numerical computation.

Homework:

1. Under an unitary transformation, an ortho-normalized set $\{|\alpha\rangle\}$ is transformed to another ortho-normalized set $\{|\tilde{\alpha}\rangle\}$. Show that the anti-commutation relation (for fermions) is invariant under the unitary transformation.

$$\{a_\alpha, a_\beta^\dagger\} = \delta_{\alpha\beta} \ \rightarrow \{a_{\tilde{\alpha}}, a_{\tilde{\beta}}^\dagger\} = \delta_{\tilde{\alpha}\tilde{\beta}}.$$

2. Show that, if

$$H = \int dv \psi^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V^{(1)}(\mathbf{r}) \right] \psi(\mathbf{r}),$$

then the field operator satisfies the following equation of motion,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V^{(1)}(\mathbf{r}) \right] \psi(\mathbf{r}, t) = i\hbar \frac{\partial \psi}{\partial t}.$$

3. Start from

$$\mathbf{j}^{(1)}(\mathbf{r}) = \frac{1}{2m} \left[\hat{\mathbf{p}}\delta(\hat{\mathbf{r}} - \mathbf{r}) + \delta(\hat{\mathbf{r}} - \mathbf{r})\hat{\mathbf{p}} \right],$$

first find out its Fourier transform $\mathbf{j}^{(1)}(\mathbf{q})$, then show that (see Table 1)

$$\mathbf{j}(\mathbf{q}) = \frac{\hbar}{2m} \sum_k (2\mathbf{k} + \mathbf{q}) \, a_k^\dagger a_{k+q}.$$

References

[1] Chap 6 of R.P. Feynman, *Statistical Mechanics, a set of lectures*, Addison-Wesley Publishing Company, 1990.

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