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2 Second Quantization

2.1 Harmonic Oscillator Algebra

There are two premises to construct the general normalized eigenstates of hermitian operator $a^\dagger a$.

1. The operator a satisfies $[a, a^\dagger] = 1$
2. $a^\dagger a|\alpha\rangle = \alpha|\alpha\rangle$, where $|\alpha\rangle$ is the **normalized** eigenstates of $a^\dagger a$.

Then,

$$\alpha = \langle\alpha|a^\dagger a|\alpha\rangle = \| a|\alpha\rangle \|^2 \geq 0 \tag{1}$$

The above implies that the eigenvalues are all real and nonnegative. By operator algebra, we observe that

$$[a^\dagger a, a] = [a^\dagger, a]\, a = -a \quad \Longrightarrow \quad (a^\dagger a)a = a(a^\dagger a - 1) \tag{2}$$
$$[a^\dagger a, a^\dagger] = a^\dagger\, [a^\dagger a, a^\dagger] = a^\dagger \quad \Longrightarrow \quad (a^\dagger a)a^\dagger = a^\dagger(a^\dagger a + 1) \tag{3}$$

From (2) we have, for an eigenstates $|\alpha\rangle$,

$$(a^\dagger a)a|\alpha\rangle = a(a^\dagger a - 1)\alpha\rangle = a(\alpha - 1)|\alpha\rangle = (\alpha - 1)a|\alpha\rangle \tag{4}$$

Therefore $a|\alpha\rangle$ is an eigenstates with eigenvalue $\alpha - 1$, unless $a|\alpha\rangle = 0$. Similarly, $a^\dagger|\alpha\rangle$ is an eigenstates with eigenvalue $\alpha + 1$, unless $a^\dagger|\alpha\rangle = 0$.
The norms of $a|\alpha\rangle$ $a^\dagger|\alpha\rangle$and is found from

$$\| a|\alpha\rangle \|^2 = \langle\alpha|a^\dagger a|\alpha\rangle = \alpha\langle\alpha|\alpha\rangle = \alpha \tag{5}$$
$$\| a^\dagger|\alpha\rangle \|^2 = \langle\alpha|aa^\dagger|\alpha\rangle = \langle\alpha|a^\dagger a + 1|\alpha\rangle = \alpha + 1 \tag{6}$$

and Now, suppose that $a^n|\alpha\rangle \neq 0$ for all n. Then by repeated application of Eq.(4), $a^n|\alpha\rangle$ is an eigenstate of $a^\dagger a$ with eigenvalue $\alpha - n$. This contradicts Eq.(1), because $\alpha - n < 0$ for sufficiently large n.

Therefore, we must have

$$a^n|\alpha\rangle \neq 0 \quad \text{but} \quad a^{n+1}|\alpha\rangle = 0 \tag{7}$$

for some nonnegative integer n. Let $|\alpha - n\rangle$ be a normalized eigenstates with eigenvalue $\alpha - n$. Then from Eqs.(5) and (7),

$$\sqrt{\alpha - n} = \| a|\alpha - n\rangle \| = 0, \tag{8}$$

and therefore $\alpha = n$. Remember that $a|\alpha - n\rangle \propto a^{n+1}|\alpha\rangle$.

This shows that the eigenvalues of $a^\dagger a$ must be nonnegative **integer**, and that there is a ground state $|0\rangle$ such that

$$a|0\rangle = 0 \tag{9}$$

If $|n\rangle$ is a normalized eigenstate with eigenvalue n, then, from Eq.(5),

$$|n-1\rangle = \frac{a|n\rangle}{\| a|n\rangle \|} = \frac{1}{\sqrt{n}}\; a|n\rangle \tag{10}$$

is a normalized eigenstate with eigenvalue $n-1$. Also

$$a^\dagger|n-1\rangle = \frac{1}{\sqrt{n}}\; a^\dagger a|n\rangle = \sqrt{n}|n\rangle \to |n\rangle = \frac{1}{\sqrt{n}}\, a^\dagger|n-1\rangle. \tag{11}$$

The last equation is a recurrence relation for the construction of eigenstates. We may then construct the eigenstates of $a^\dagger a$ as follows: First we find a state $|0\rangle$ such that $a|0\rangle = 0$. Then we define

$$|1\rangle = \; a^\dagger|0\rangle \;; \qquad |2\rangle = \; \frac{1}{\sqrt{2}} a^\dagger|1\rangle = \frac{1}{\sqrt{2}}(a^\dagger)^2|0\rangle \quad \cdots \tag{12}$$

and in general

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle \tag{13}$$

With this definition, the $|n\rangle$ are orthonormal and satisfy

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \tag{14}$$

$$a|n\rangle = \sqrt{n}|n-1\rangle \tag{15}$$

$$a^\dagger a|n\rangle = n|n\rangle \tag{16}$$

Orthonormality may be proved using following operator identity $[a,(a^\dagger)^n] = n(a^\dagger)^{n-1}$

$$\begin{aligned}
\langle n|m\rangle &= \frac{1}{\sqrt{n!m!}}\; \langle 0|a^n(a^\dagger)^m|0\rangle \\
&= \frac{1}{\sqrt{n!m!}}\; \big(\langle 0|a^{n-1}(a^\dagger)^m a|0\rangle + \langle 0|na^{n-1}(a^\dagger)^{m-1}|0\rangle\big) \\
&= \frac{1}{\sqrt{n!m!}}\; n\langle 0|a^{n-1}(a^\dagger)^{m-1}|0\rangle \\
&= \frac{1}{\sqrt{n!m!}}\; n(n-1)\langle 0|a^{n-2}(a^\dagger)^{m-2}|0\rangle \\
&\vdots \\
&= \frac{1}{\sqrt{n!m!}}\; n(n-1)\ldots(n-m-1)\langle 0|a^{n-m}|0\rangle \\
&= \frac{1}{\sqrt{n!m!}} n!\delta_{nm} \\
\therefore \langle n|m\rangle &= \delta_{nm}
\end{aligned} \tag{17}$$

Note that the first term of second equation vanishes due to the relation $a|0\rangle = 0$.

2.2 Field Quantization

Let us consider a real scalar field $\varphi(x)$ whose motion is described by the following Lagrangian

$$L(\dot\varphi,\varphi) = \frac{1}{2}\int d^3x \dot\varphi(x)\dot\varphi(x) - \frac{1}{2}\int d^3x \int d^3x' K(x-x')\varphi(x)\varphi(x') \tag{18}$$

The field $\varphi(x)$ can be thought as a phonon coordinates of one-dimensinal lattice. Namely,

$$\varphi(x_0) = x - x_0, \tag{19}$$

where x_0 is an equilibrium position of atomic ions. Define action S,

$$S = \int L\ dt = \frac{1}{2}\int dtd^3x\dot{\varphi}(x)\dot{\varphi}(x) - \frac{1}{2}\int dtd^3xd^3x'\varphi(x)\varphi(x')K(x-x') \quad (20)$$

Functional derivative of S is defined by

$$\delta S \equiv \int \frac{\delta S}{\delta\varphi(x)}\delta\varphi(x)dx \quad (21)$$

$$\delta S = S[\varphi+\delta\varphi] - S[\varphi] \quad (22)$$

$$= -\int dt\int d^3x\ \ddot{\varphi}\delta\varphi + \int dt\int d^3x\int d^3x'\delta\varphi(x)\varphi(x')K(x-x') \quad (23)$$

Then, the classical equation of motion

$$0 = \frac{\delta S}{\delta\varphi} = -\ddot{\varphi}(x) + \int d^3x' K(x-x')\varphi(x') \quad \text{(the system of harmonic oscillators)} \quad (24)$$

In analogy with the canonical conjugate momentum of classical mechanics one can define a conjugate momentum field to $\varphi(x)$:

$$\Pi(x) = \frac{\delta L}{\delta\dot{\varphi}(x)} = \dot{\varphi}(x) \quad (25)$$

■ **Hamiltonian** : Now by the standard procedure of constructing Hamiltonian from Lagrangian ($H(p,x) = p\dot{x} - L$)

$$H = \frac{1}{2}\int d^3x\Pi(x)\Pi(x) + \frac{1}{2}\int d^3x\int d^3x'K(x-x')\varphi(x)\varphi(x) \quad (26)$$

To **quantize** the above system let us **impose** the following commutation relations for $\hat{\varphi}(x)$ and $\hat{\Pi}(x)$. (Note that these fields are Hermitian.)

$$[\hat{\varphi}(x),\hat{\varphi}(x')] = [\hat{\Pi}(x),\hat{\Pi}(x')] = 0 \quad (27)$$

$$[\hat{\varphi}(x),\hat{\Pi}(x')] = i\hbar\delta^3(x-x') \quad (28)$$

This is an analogue of the commutation relation of quantum mechanics:

$$[\hat{x},\hat{x}] = [\hat{p},\hat{p}] = 0, \quad [\hat{x},\hat{p}] = i\hbar.$$

The quantum Hamiltonian is given by

$$\hat{H} = \frac{1}{2}\int d^3x\hat{\Pi}(x)\hat{\Pi}(x) + \frac{1}{2}\int d^3x\int d^3x'K(x-x')\hat{\varphi}(x)\hat{\varphi}(x) \quad (29)$$

Define

$$\tilde{\varphi}(k) = \int d^3x\hat{\varphi}(x)e^{-ik\cdot x} \quad , \quad \hat{\varphi}(x) = \int \frac{d^3k}{(2\pi)^3}\tilde{\varphi}(k)e^{ik\cdot x} \quad (30)$$

$$\tilde{\Pi}(k) = \int d^3x\hat{\Pi}(x)e^{-ik\cdot x} \quad , \quad \hat{\Pi}(x) = \int \frac{d^3k}{(2\pi)^3}\tilde{\Pi}(k)e^{ik\cdot x} \quad (31)$$

Since $\hat{\varphi}(x), \hat{\Pi}(x)$ are Hermitian

$$\tilde{\varphi}^\dagger(k) = \tilde{\varphi}(-k) \quad \tilde{\Pi}^\dagger(k) = \tilde{\Pi}(-k) \quad (32)$$

Commutation relations

$$[\tilde{\varphi}(k), \tilde{\varphi}(k')] = [\tilde{\Pi}(k), \tilde{\Pi}(k')] = 0 \tag{33}$$

$$[\tilde{\varphi}(k), \tilde{\Pi}(k')] = i\hbar(2\pi)^3\delta^3(k+k') \tag{34}$$

Let $w^2(k) = \int d^3x K(x) e^{-ik\cdot x}$, then

$$w^2(k) = w^{2*}(k) = w^2(-k) \quad (\text{from } K(x) = K(-x) = K^*(x)) \tag{35}$$

Hamiltonian

$$H = \frac{1}{2}\int \frac{d^3k}{(2\pi)^3}[\tilde{\Pi}(-k)\tilde{\Pi}(k) + w^2(k)\tilde{\varphi}(-k)\tilde{\varphi}(k)] \tag{36}$$

$$= \frac{1}{2}\int \frac{d^3k}{(2\pi)^3}[\tilde{\Pi}^\dagger(k)\tilde{\Pi}(k) + w^2(k)\tilde{\varphi}^\dagger(k)\tilde{\varphi}(k)] \tag{37}$$

Define annihilation and creation operators

$$a(k) = \frac{1}{\sqrt{2\hbar}}[\sqrt{w(k)}\tilde{\varphi}(k) + \frac{i}{\sqrt{w(k)}}\tilde{\Pi}(k)] \tag{38}$$

$$a^\dagger(k) = \frac{1}{\sqrt{2\hbar}}[\sqrt{w(k)}\tilde{\varphi}(-k) - \frac{i}{\sqrt{w(k)}}\tilde{\Pi}(-k)] \tag{39}$$

$$\tilde{\varphi}(k) = \sqrt{\frac{\hbar}{2w(k)}}[a(k) + a^\dagger(-k)] \tag{40}$$

$$\tilde{\Pi}(k) = -i\sqrt{\frac{\hbar w(k)}{2}}[a(k) - a^\dagger(-k)] \tag{41}$$

Commutation relation

$$[a(k), a(k')] = [a^\dagger(k), a^\dagger(k')] = 0 \quad , \quad [a(k), a^\dagger(k')] = (2\pi)^3\delta^3(k-k') \tag{42}$$

■ **Hamiltonian in terms of a and $a^\dagger$**

$$H = \frac{1}{2}\int \frac{d^3k}{(2\pi)^3}\hbar w(k)[a^\dagger(k)a(k) + a(k)a^\dagger(k)] \tag{43}$$

■ **Original field variables**

$$\hat{\varphi}(x) = \int \frac{d^3k}{(2\pi)^3}\sqrt{\frac{\hbar}{2w(k)}}[a(k)e^{ik\cdot x} + a^\dagger(k)e^{-ik\cdot x}] \tag{44}$$

$$\hat{\Pi}(x) = \int \frac{d^3k}{(2\pi)^3}\sqrt{\frac{\hbar w(k)}{2}}[-ia(k)e^{ik\cdot x} + ia^\dagger(k)e^{-ik\cdot x}] \tag{45}$$

2.3 Systems of Identical Particles

The Hilbert space $\mathcal{H}_N$ is the N^{th}tensor product of the single particle Hilbert space $\mathcal{H}$:

$$\mathcal{H}_N = \mathcal{H} \otimes \mathcal{H} \otimes \ldots \otimes \mathcal{H} \tag{46}$$

If $\{|\alpha\rangle\}$ is an orthogonal basis of $\mathcal{H}$, then the canonical orthogonal basis of $\mathcal{H}_N$is

$$|\alpha_1 \ldots \alpha_N) \equiv |\alpha_1\rangle \otimes |\alpha_2\rangle \ldots \otimes |\alpha_N\rangle \tag{47}$$

These basis states have the wave functions:

$$\begin{aligned}\psi_{\alpha_1\alpha_2\ldots\alpha_N}(\vec{r}_1\vec{r}_2\ldots\vec{r}_N) &= (\vec{r}_1\vec{r}_2\ldots\vec{r}_N|\alpha_1\cdots\alpha_N) \\ &= (\langle\vec{r}_1|\otimes\langle\vec{r}_2|\otimes\ldots\otimes\langle\vec{r}_N|)(|\alpha_1\rangle\otimes|\alpha_2\rangle\otimes\ldots\otimes|\alpha_N\rangle) \\ &= \phi_{\alpha_1}(\vec{r}_1)\phi_{\alpha_2}(\vec{r}_2)\ldots\phi_{\alpha_N}(\vec{r}_N) \qquad (48)\end{aligned}$$

The overlap of two vectors of the basis is given by:

$$(\alpha_1\alpha_2\ldots\alpha_N|\alpha'_1\alpha'_2\ldots\alpha_N) = \langle\alpha_1|\alpha'_1\rangle\langle\alpha_2|\alpha'_2\rangle\ldots\langle\alpha_N|\alpha'_N\rangle \qquad (49)$$

Since the basis $\{|\alpha\rangle\}$ is orthogonal, then the completeness of the basis $|\alpha_1\alpha_2\ldots\alpha_N)$ is

$$\sum_{\alpha_1\alpha_2\ldots\alpha_N}|\alpha_1\alpha_2\ldots\alpha_N)(\alpha_1\alpha_2\ldots\alpha_N| = 1 \qquad (50)$$

The wave functions of N Bosons or N Fermions are symmetric and anti-symmetric respectively.

$$\psi(\vec{r}_{P_1},\vec{r}_{P_2}\ldots\vec{r}_{P_N}) = \zeta^P\psi(\vec{r}_1,\vec{r}_2\ldots\vec{r}_N) \qquad (51)$$

where $\xi = 1$ for Boson,$\xi = -1$ for Fermion. In this context, these symmetry requirements are postulates. The symmetrization operator $\hat{\mathcal{P}}_{\mathcal{B}}$ and $\hat{\mathcal{P}}_{\mathcal{F}}$ are defined as

$$\hat{\mathcal{P}}_{\binom{\mathcal{B}}{\mathcal{F}}}\psi(\vec{r}_1\ldots\vec{r}_N) = \frac{1}{N!}\sum_P\zeta^P\psi(\vec{r}_{P_1},\vec{r}_{P_2}\ldots\vec{r}_{P_N}) \qquad (52)$$

The manifestly hermitian operator $\hat{\mathcal{P}}_{\binom{\mathcal{B}}{\mathcal{F}}}$ may be shown to be a projector as follows. For any wave function ψ of $\mathcal{H}_N$:

$$\hat{\mathcal{P}}^2_{\binom{\mathcal{B}}{\mathcal{F}}}\psi(\vec{r}_1\ldots\vec{r}_N) = \frac{1}{N!}\frac{1}{N!}\sum_P\sum_{P'}\zeta^P\zeta^{P'}\psi(\vec{r}_{P'P_1},\vec{r}_{P'P_2}\ldots\vec{r}_{P'P_N}) \qquad (53)$$

where $P'P$ denotes the group composition of P' and P. Since $\zeta^{P+P'} = \zeta^{P'P}$, the summation over P and P' can be replaced by a summation over $Q = P'P$ and P:

$$\begin{aligned}\hat{\mathcal{P}}^2_{\binom{\mathcal{B}}{\mathcal{F}}}\psi(\vec{r}_1\ldots\vec{r}_N) &= \frac{1}{N!}\sum_P\left(\frac{1}{N!}\sum_Q\zeta^Q\psi(\vec{r}_{Q_1},\ldots\vec{r}_{Q_N})\right) \\ &= \frac{1}{N!}\sum_P\hat{\mathcal{P}}_{\binom{\mathcal{B}}{\mathcal{F}}}\psi(\vec{r}_1\ldots\vec{r}_N) \\ &= \hat{\mathcal{P}}_{\binom{\mathcal{B}}{\mathcal{F}}}\psi(\vec{r}_1\ldots\vec{r}_N) \qquad (54)\end{aligned}$$

In the last step we used $\sum_P\frac{1}{N!} = 1$. The Eq. (54) implies that

$$\hat{\mathcal{P}}_F\psi_F = \psi_F, \quad \hat{\mathcal{P}}_B\psi_B = \psi_B,$$

which is just what we wanted. These operators project $\mathcal{H}_N$ onto the Hilbert space of Boson $\mathcal{B}_N$ and the Hilbert space of Fermions $\mathcal{F}_N$:

$$\mathcal{B}_N = \hat{\mathcal{P}}_{\mathcal{B}}\mathcal{H}_N \qquad (55)$$

$$\mathcal{F}_N = \hat{\mathcal{P}}_{\mathcal{F}}H_N \qquad (56)$$

Using these projector, a system of Bosons or Fermions with one particle in state α_1,one particle in state $\alpha_2 \cdots$, one particle in state α_N is represented as follow:

$$\begin{aligned}|\alpha_1 \dots \alpha_N\} &\equiv \sqrt{N!}\hat{\mathcal{P}}_{\binom{\mathcal{B}}{\mathcal{F}}}|\alpha_1 \cdots \alpha_N) \\ &= \frac{1}{\sqrt{N!}}\sum_P \zeta^P |\alpha_{P_1}\rangle \otimes |\alpha_{P_2}\rangle \dots \otimes |\alpha_{P_N}\rangle \end{aligned} \tag{57}$$

The closure relation in the $\mathcal{H}_N$ becomes a closure relation in $\mathcal{B}_N$ or $\mathcal{F}_N$:

$$\sum_{\alpha_1 \dots \alpha_N} \hat{\mathcal{P}}_{\binom{\mathcal{B}}{\mathcal{F}}}|\alpha_1 \dots \alpha_N)(\alpha_1 \cdots \alpha_N|\hat{\mathcal{P}}_{\binom{\mathcal{B}}{\mathcal{F}}} = \frac{1}{N!}\sum_{\alpha_1 \dots \alpha_N} |\alpha_1 \cdots \alpha_N\}\{\alpha_1 \dots \alpha_N| = 1 \tag{58}$$

Further, if the basis $|\alpha\rangle$ is orthogonal in $\mathcal{H}$, then the basis $|\alpha_1 \dots \alpha_N)$ is orthogonal in $\mathcal{H}_N$ and the basis $|\alpha_1 \dots \alpha_N\}$ orthogonal in $\mathcal{B}_N$ or $\mathcal{F}_N$.
The scalar product of two such vectors constructed from the same basis $|\alpha\rangle$ is:

$$\begin{aligned}\{\alpha'_1 \dots \alpha'_N|\alpha_1 \dots \alpha_N\} &= N!(\alpha'_1 \dots \alpha'_N|\hat{\mathcal{P}}^2_{\binom{\mathcal{B}}{\mathcal{F}}}|\alpha_1 \dots \alpha_N) \\ &= N!(\alpha'_1 \dots \alpha'_N|\hat{\mathcal{P}}_{\binom{\mathcal{B}}{\mathcal{F}}}|\alpha_1 \dots \alpha_N) \\ &= \sum_P \zeta^P \langle\alpha'_1|\alpha_{P_1}\rangle \dots \langle\alpha'_N|\alpha_{P_N}\rangle \\ &= \begin{cases}(-1)^P & \text{for Fermions} \\ n_1!n_2!\dots n_p! & \text{for Bosons}\end{cases} \\ &= \zeta^p \prod_\alpha n_\alpha! \end{aligned} \tag{59}$$

To normalize the states $|\alpha_1 \cdots \alpha_N\}$

$$\begin{aligned}|\alpha_1 \cdots \alpha_N\rangle &= \frac{1}{\sqrt{\prod_\alpha n_\alpha!}}|\alpha_1 \cdots \alpha_N\} \\ &= \frac{1}{\sqrt{N!\prod_\alpha n_\alpha!}}\sum_P \zeta^P |\alpha_{P_1}\rangle \otimes |\alpha_{P_2}\rangle \dots \otimes |\alpha_{P_N}\rangle \end{aligned} \tag{60}$$

the overlap between a tensor product $|\beta_1 \cdots \beta_N\rangle$ and the symmetrized or antisymmetrized state $|\alpha_1 \cdots \alpha_N\rangle$ is

$$\begin{aligned}(\beta_1 \dots \beta_N|\alpha_1 \dots \alpha_N\rangle &= \frac{1}{\sqrt{N!\prod_\alpha n_\alpha!}}\sum_P \zeta^P \langle\beta_1|\alpha_{P_1}\rangle\langle\beta_2|\alpha_{P_2}\rangle \dots \langle\beta_N|\alpha_{P_N}\rangle \\ &= \frac{1}{\sqrt{N!\prod_\alpha n_\alpha!}}\mathcal{S}(\langle\beta_i|\alpha_j\rangle) = \frac{1}{\sqrt{N!\prod_\alpha n_\alpha!}}\mathcal{S}(M_{ij}) \end{aligned} \tag{61}$$

$$\mathcal{S}(\langle\beta_i|\alpha_j\rangle) = \begin{cases}\text{For Bosons : } \mathrm{Per}(M_{ij}) \equiv \sum_P M_{1,P_1}M_{2,P_2}\dots M_{N,P_N} \\ \text{For Fermions : } \det(M_{ij}) \equiv \sum_P (-1)^P M_{1,P_1}M_{2,P_2}\dots M_{N,P_N}\end{cases} \tag{62}$$

In coordinate representation,

$$\text{For Bosons : } \psi_{\beta_1 \dots \beta_N}(x_1 \cdots x_N) = (x_1 \dots x_N|\beta_1 \dots \beta_N\rangle = \frac{1}{\sqrt{N!\prod_\alpha n_\alpha!}}\mathrm{Per}(\phi_{\beta_i}(x_j)) \tag{63}$$

$$\text{For Fermions : } \psi_{\beta_1 \dots \beta_N}(x_1 \cdots x_N) = (x_1 \dots x_N|\beta_1 \dots \beta_N\rangle = \frac{1}{\sqrt{N!}}\det(\phi_{\beta_i}(x_j)) \tag{64}$$

The completeness relation in $\mathcal{B}_N$ or $\mathcal{F}_N$ is

$$\sum_{\alpha_1 \dots \alpha_N} \frac{\prod_\alpha n_\alpha!}{N!}|\alpha_1 \dots \alpha_N\rangle\langle\alpha_1 \dots \alpha_N| = 1 \tag{65}$$

2.4 Many-Body Operators

Let $\hat{O}$ be an arbitrary operator in $\mathcal{B}_N$ or $\mathcal{F}_N$. For any states, and any permutation P:

$$(\beta_{P_1}\dots\beta_{P_N}|\hat{O}|\beta'_{P_1}\dots\beta'_{P_N}) = (\beta_1\dots\beta_N|\hat{O}|\beta'_1\dots\beta'_N) \tag{66}$$

We begin by considering the case of one-body operators. An Operator $\hat{U}$ is a one-body operator if the action of $\hat{U}$ on a state $|\alpha_1\dots\alpha_N)$ of N particles is the sum of the action of $\hat{U}$ on each particle:

$$\hat{U}|\alpha_1\dots\alpha_N) = \sum_{i=1}^{N}\hat{U}_i|\alpha_1\dots\alpha_N) \tag{67}$$

The matrix element of a one-body operator $\hat{U}$ between two states $|\alpha_1\dots\alpha_N)$ and $|\beta_1\dots\beta_N)$ is given by

$$(\alpha_1\dots\alpha_N|\hat{U}|\beta_1\dots\beta_N) = \sum_{i=1}^{N}(\alpha_1\dots\alpha_N|\hat{U}_i|\beta_1\dots\beta_N) \tag{68}$$

$$= \sum_{i=1}^{N}\prod_{k\neq i}\langle\alpha_k|\beta_k\rangle\langle\alpha_i|\hat{U}_i|\beta_i\rangle \tag{69}$$

and thus for two non-orthogonal states:

$$\frac{(\alpha_1\dots\alpha_N|\hat{U}|\beta_1\dots\beta_N)}{(\alpha_1\dots\alpha_N|\beta_1\dots\beta_N)} = \sum_{i=1}^{N}\frac{\langle\alpha_i|\hat{U}_i|\beta_i\rangle}{\langle\alpha_i|\beta_i\rangle} \tag{70}$$

Similarly, for two-body operator $\hat{V}$ $\quad(\hat{V}_{ij} = \hat{V}_{ji} \quad \rightarrow$ symmetry requirement)

$$\hat{V}|\alpha_1\dots\alpha_N) = \sum_{1\leq i<j\leq N}\hat{V}_{ij}|\alpha_1\dots\alpha_N) \tag{71}$$

$$= \frac{1}{2}\sum_{1\leq i\neq j\leq N}\hat{V}_{ij}|\alpha_1\dots\alpha_N) \tag{72}$$

The matrix elements of $\hat{V}$ are given by :

$$(\alpha_1\dots\alpha_N|\hat{V}|\beta_1\dots\beta_N) = \frac{1}{2}\sum_{i\neq j}(\alpha_1\dots\alpha_N|\hat{V}_{ij}|\beta_1\dots\beta_N) \tag{73}$$

$$= \frac{1}{2}\sum_{ij}\prod_{\substack{k\neq i\\k\neq j}}\langle\alpha_k|\beta_k\rangle(\alpha_i\alpha_j|\hat{V}|\beta_i\beta_j) \tag{74}$$

and for non-orthogonal states,

$$\frac{(\alpha_1\dots\alpha_N|\hat{V}|\beta_1\dots\beta_N)}{(\alpha_1\dots\alpha_N|\beta_1\dots\beta_N)} = \frac{1}{2}\sum_{i\neq j}\frac{(\alpha_i\alpha_j|\hat{V}|\beta_i\beta_j)}{\langle\alpha_i|\beta_i\rangle\langle\alpha_j|\beta_j\rangle} \tag{75}$$

2.5 Creation and Annihilation Operators

Creation and annihilation operators generate the entire Hilbert space by their action on a single reference state and provide a basis for the algebra of operators on Hilbert space.

Creation operator and Fock space For each single-particle state $|\lambda\rangle$ (such as momentum state $|\mathbf{k}\rangle$)of the single-particle space $\mathcal{H}$, we define a Boson or Fermion creation operator $a^\dagger_\lambda$ by its action on any symmetrized or antisymmetrized state of $\mathcal{B}_N$ of $\mathcal{F}_N$ as follows:

$$a^\dagger_\lambda|\lambda_1 \dots \lambda_N\} \equiv |\lambda\lambda_1 \dots \lambda_N\} \tag{76}$$
$$a^\dagger_\lambda|\lambda_1 \dots \lambda_N\rangle = \sqrt{n_\lambda + 1}|\lambda\lambda_1 \dots \lambda_N\rangle \tag{77}$$

The second equation of the above follows directly from the definition of $|\lambda_1 \dots \lambda_N\rangle$. In the case of Fermions,

$$a^\dagger_\lambda|\lambda_1 \dots \lambda_N\rangle = \begin{cases} |\lambda\lambda_1 \dots \lambda_N\rangle & \text{if the state } |\lambda\rangle \text{ is not present in } |\lambda_1 \dots \lambda_N\rangle \\ 0 & \text{if the state } |\lambda\rangle \text{ is present in } |\lambda_1 \dots \lambda_N\rangle \end{cases} \tag{78}$$

It is useful to define the vacuum state, denoted by $|0\rangle$, which represents an empty state.

$$a^\dagger_\lambda|0\rangle = |\lambda\rangle \tag{79}$$

The creation operators $a^\dagger_\lambda$ do not operate within one space $\mathcal{B}_n$ or $\mathcal{F}_n$, but rather operate from any space $\mathcal{B}_n$ or $\mathcal{F}_n$ to $\mathcal{B}_{n+1}$ or $\mathcal{F}_{n+1}$. Hence it is useful to define **Fock** space as the direct sum of the Boson or Fermion spaces with arbitrary number of particles.

$$\begin{aligned} \mathcal{B} &= \mathcal{B}_0 \oplus \mathcal{B}_1 \oplus \mathcal{B}_2 \oplus \dots = \oplus_{n=0}^{\infty}\mathcal{B}_n \\ \mathcal{F} &= \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \dots = \oplus_{n=0}^{\infty}\mathcal{F}_n \\ \mathcal{B}_0 &= \mathcal{F}_0 = |0\rangle \\ \mathcal{B}_1 &= \mathcal{F}_1 = \mathcal{H} \end{aligned}$$

Suitable bases for the Fock space utilize unnormalized or normalized states of the proper symmetry.
The closure relation in the Fock space may be written

$$\begin{aligned} 1 =& |0\rangle\langle 0| + \sum_{N=1}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \dots \lambda_N} |\lambda_1 \dots \lambda_N\}\{\lambda_1 \dots \lambda_N| \\ =& |0\rangle\langle 0| + \sum_{N=1}^{\infty} \frac{1}{N!} \sum_{\lambda_1 \dots \lambda_N} \left(\prod_\lambda n_\lambda!\right) |\lambda_1 \dots \lambda_N\rangle\langle\lambda_1 \dots \lambda_N| \end{aligned} \tag{80}$$

Any basis vector $|\lambda_1 \dots \lambda_N\}$ or $|\lambda_1 \dots \lambda_N\rangle$ may be generated by repeated action of the creation operators on the vacuum $|0\rangle$

$$\begin{aligned} |\lambda_1 \dots \lambda_N\} &= a^\dagger_{\lambda_1} a^\dagger_{\lambda_2} \dots a^\dagger_{\lambda_N}|0\rangle \\ |\lambda_1 \dots \lambda_N\rangle &= \frac{1}{\sqrt{\prod_\lambda n_\lambda!}}\ a^\dagger_{\lambda_1} a^\dagger_{\lambda_2} \dots a^\dagger_{\lambda_N}|0\rangle \end{aligned} \tag{81}$$

Commutation relations between creation operators The symmetry or antisymmetry properties of the many particle states, referring Eq.(51), impose commutation or anticommutation relations between the creation operators. For any state $|\lambda_1 \dots \lambda_N\rangle$ and any single particle states $|\lambda\rangle$ and $|\mu\rangle$, we obtain: ζ is +1 for Bosons and -1 for Fermions (recall even/odd permutation).

$$\begin{aligned} a^\dagger_\lambda a^\dagger_\mu|\lambda_1 \dots \lambda_N\} &= |\lambda\mu\lambda_1 \dots \lambda_N\} \\ &= \zeta|\mu\lambda\lambda_1 \dots \lambda_N\} \\ &= \zeta a^\dagger_\mu a^\dagger_\lambda|\lambda_1 \dots \lambda_N\} \end{aligned} \tag{82}$$
$$\implies \quad a^\dagger_\lambda a^\dagger_\mu - \zeta a^\dagger_\mu a^\dagger_\lambda = 0 \tag{83}$$

$$\therefore [a_\lambda^\dagger, a_\mu^\dagger]_- = a_\lambda^\dagger a_\mu^\dagger - a_\mu^\dagger a_\lambda^\dagger = [a_\lambda^\dagger, a_\mu^\dagger] = 0 \quad \text{for Bosons}$$
$$[a_\lambda^\dagger, a_\mu^\dagger]_+ = a_\lambda^\dagger a_\mu^\dagger + a_\mu^\dagger a_\lambda^\dagger = \{a_\lambda^\dagger, a_\mu^\dagger\} = 0 \quad \text{for Fermions} \tag{84}$$

Eq.82 is the Hilbert space represented in the 2nd quantized fashion.

Annihilation operator The operators $a_\lambda^\dagger$ are not hermitian, and therefore we define the annihilation operators a_λ as the adjoints of the creation operators $a_\lambda^\dagger$. The commutation relations of annihilation operators follow immediately from the adjoint of Eq.(84)

$$\therefore [a_\lambda, a_\mu]_- = 0 \quad \text{for Bosons}$$
$$[a_\lambda, a_\mu]_+ = 0 \quad \text{for Fermions} \tag{85}$$

Let us recall the definition of adjoint:

$$\langle A|\hat{O}^\dagger|B\rangle = \Big(\langle B|\hat{O}|A\rangle\Big)^* = (\hat{O}|A\rangle)^\dagger|B\rangle. \tag{86}$$

Then it is easy to understand Eq. (87). The action of a_λ to the right is obtained by evaluating its matrix element.

$$\{\alpha_1 \dots \alpha_m|a_\lambda|\beta_1 \dots \beta_n\} = \{\lambda\alpha_1 \dots \alpha_m|\beta_1 \dots \beta_n\} \tag{87}$$

The r.h.s is non-zero only if m+1=n, so one effect of a_λ acting to the right is to decrease the number of particles in the state on which it acts by one. When acting on the vacuum it yields 0 for any state $|\lambda\rangle$:

$$a_\lambda|0\rangle = 0 \quad \overset{D.C.}{\Longleftrightarrow} \quad \langle 0|a_\lambda^\dagger = 0 \tag{88}$$

Next, let's calculate the action of a_λ on a many-particle state. Using closure relation,

$$a_\lambda|\beta_1 \dots \beta_n\} = \sum_{P=0}^{\infty} \frac{1}{P!} \sum_{\alpha_1 \dots \alpha_P} |\alpha_1 \dots \alpha_P\}\{\alpha_1 \dots \alpha_P|a_\lambda|\beta_1 \dots \beta_n\}$$
$$= \sum_{P=0}^{\infty} \frac{1}{P!} \sum_{\alpha_1 \dots \alpha_P} \{\lambda\alpha_1 \dots \alpha_P|\beta_1 \dots \beta_n\}|\alpha_1 \dots \alpha_P\} \tag{89}$$

Only the terms with $P = (n-1)$ and the set $\{\lambda, \alpha_1, \dots, \alpha_P\}$ equal to a permutation of $\{\beta_1, \dots, \beta_n\}$ are non-vanishing. So,

$$a_\lambda|\beta_1 \dots \beta_n\} = \sum_{i=1}^{n} \zeta^{i-1}\delta_{\lambda\beta_i}|\beta_1 \dots \beta_{i-1}\beta_{i+1} \dots \beta_n\} \quad (\beta_i \text{ has been removed.})$$
$$a_\lambda|\beta_1 \dots \beta_n\rangle = \frac{1}{\sqrt{n_\lambda}} \sum_{i=1}^{n} \zeta^{i-1}\delta_{\lambda\beta_i}|\beta_1 \dots \beta_{i-1}\beta_{i+1} \dots \beta_n\rangle \tag{90}$$

In the occupation number representation

$$a_\lambda|n_{\beta_1}n_{\beta_2} \dots n_\lambda \dots\rangle = \sqrt{n_\lambda}|n_{\beta_1}n_{\beta_2} \dots (n_\lambda - 1) \dots\rangle \quad \text{(for Bosons)} \tag{91}$$

$$a_\lambda|\beta_1 \dots \beta_n\rangle = \begin{cases} (-1)^{\lambda-1}|\beta_1 \dots \beta_{\lambda-1}\beta_{\lambda+1} \dots \beta_n\rangle & \text{if the state } |\lambda\rangle \text{ is occupied.} \\ 0 & \text{if the state } |\lambda\rangle \text{ is unoccupied.} \end{cases} \quad \text{(for Fermions)} \tag{92}$$

For concreteness, let us consider a case with $n = 3$ for fermions.

$$\frac{1}{2!}\{\lambda a_1 a_2|\beta_1\beta_2\beta_3\}.$$

For this to be non-vanishing we have to require

$$\begin{aligned}
\lambda a_1 a_2 &= \beta_1\beta_2\beta_3(+1), \quad \lambda a_1 a_2 = \beta_2\beta_3\beta_1(+1), \quad \lambda a_1 a_2 = \beta_3\beta_1\beta_2(+1), \\
\lambda a_1 a_2 &= \beta_2\beta_1\beta_3(-1), \quad \lambda a_1 a_2 = \beta_3\beta_2\beta_1(-1), \quad \lambda a_1 a_2 = \beta_1\beta_3\beta_2(-1).
\end{aligned} \tag{93}$$

Thus we obtain

$$\begin{aligned}
a_\lambda|\beta_1\beta_2\beta_3\} &= \frac{1}{2!}\Big(|\beta_2\beta_3\} + |\beta_3\beta_1\} + |\beta_1\beta_2\} \\
&- |\beta_1\beta_3\} - |\beta_2\beta_1\} - |\beta_3\beta_2\}\Big) \\
&= |\beta_2\beta_3\} - |\beta_1\beta_3\} + |\beta_1\beta_2\}.
\end{aligned} \tag{94}$$

Commutation relation between creation and annihilation operators We consider the case in which $|\lambda\rangle$ and $|\mu\rangle$ are two states belonging to the orthonormal basis. Then,

$$a_\lambda a_\mu^\dagger|\alpha_1\ldots\alpha_n\} = a_\lambda|\mu\alpha_1\ldots\alpha_n\}$$

$$= \delta_{\lambda\mu}|\alpha_1\ldots\alpha_n\} + \sum_{i=1}^{n}\zeta^i\delta_{\lambda\alpha_i}|\mu\alpha_1\ldots\alpha_{i-1}\alpha_{i+1}\ldots\alpha_n\} \tag{95}$$

$$a_\mu^\dagger a_\lambda\,|\alpha_1\ldots\alpha_n\} = \sum_{i=1}^{n}\zeta^{i-1}\delta_{\lambda\alpha_i}|\mu\alpha_1\ldots\alpha_{i-1}\alpha_{i+1}\ldots\alpha_n\} \tag{96}$$

$$\Longrightarrow \quad a_\lambda a_\mu^\dagger - \zeta a_\mu^\dagger a_\lambda = \delta_{\lambda\mu} \tag{97}$$

$$\begin{aligned}
\therefore [a_\lambda, a_\mu^\dagger]_- &= \delta_{\lambda\mu} \quad \text{for Bosons} \\
[a_\lambda, a_\mu^\dagger]_+ &= \delta_{\lambda\mu} \quad \text{for Fermions}
\end{aligned} \tag{98}$$

It is remarkable that symmetry requirement (51) imposes all of our commutation and anticommutation relation of creation and annihilation operators, (84), (85) and (98).

Creation and annihilation operators in another basis Creation and annihilation operators in another basis may be obtained straight forwardly from the operators $\{a_\alpha^\dagger, a_\alpha\}$. Consider a transformation which transforms the orthonormal basis $\{|\alpha\rangle\}$ into another basis $\{|\tilde{\alpha}\rangle\}$ as follows. Insert a closure relation! The quick way.....

$$|\tilde{\alpha}\rangle = \sum_\alpha |\alpha\rangle\langle\alpha|\tilde{\alpha}\rangle = \sum_\alpha\langle\alpha|\tilde{\alpha}\rangle|\alpha\rangle \tag{99}$$

By this equation and the definition of creation operators $a_{\tilde{\alpha}}^\dagger$ and $a_\alpha^\dagger$.

$$\begin{aligned}
a_{\tilde{\alpha}}^\dagger|\tilde{\alpha}_1\cdots\tilde{\alpha}_n\} &= |\tilde{\alpha}\tilde{\alpha}_1\cdots\tilde{\alpha}_n\} \\
&= \sum_\alpha\langle\alpha|\tilde{\alpha}\rangle|\alpha\tilde{\alpha}_1\cdots\tilde{\alpha}_n\} \\
&= \sum_\alpha\langle\alpha|\tilde{\alpha}\rangle a_\alpha^\dagger|\tilde{\alpha}_1\cdots\tilde{\alpha}_n\}
\end{aligned} \tag{100}$$

Since this result holds for a set of basis states $|\tilde{\alpha}_1 \cdots \tilde{\alpha}_n\}$, the creation operators satisfy the operator equation

$$a^\dagger_{\tilde{\alpha}} = \sum_\alpha \langle \alpha|\tilde{\alpha}\rangle a^\dagger_\alpha \tag{101}$$

and annihilation operators satisfy the adjoint equation

$$a_{\tilde{\alpha}} = \sum_\alpha \langle \tilde{\alpha}|\alpha\rangle a_\alpha \tag{102}$$

An easy way to remember these relations is to use the following association:

$$a^\dagger_\lambda \leftrightarrow |\lambda\rangle, \quad a_\lambda \leftrightarrow \langle\lambda|. \tag{103}$$

Commutation and anticommutation relations for $a^\dagger_{\tilde{\alpha}}$ and $a_{\tilde{\beta}}$ are computed straight forwardly from Eqs.(101) and (102).

$$\begin{aligned}[a_{\tilde{\beta}}, a^\dagger_{\tilde{\alpha}}]_{-\zeta} &= \sum_{\alpha\beta} \langle\tilde{\beta}|\beta\rangle\langle\alpha|\tilde{\alpha}\rangle [a_\beta, a^\dagger_\alpha]_{-\zeta} \\ &= \sum_\alpha \langle\tilde{\beta}|\alpha\rangle\langle\alpha|\tilde{\alpha}\rangle \\ &= \langle\tilde{\beta}|\tilde{\alpha}\rangle\end{aligned} \tag{104}$$

and similarly,

$$[a^\dagger_{\tilde{\alpha}}, a^\dagger_{\tilde{\beta}}]_{-\zeta} = [a_{\tilde{\alpha}}, a_{\tilde{\beta}}]_{-\zeta} = 0 \tag{105}$$

Of particular importance is the $\{|x\rangle\}$ basis, where $|x\rangle$ represents $|\overrightarrow{r}\sigma\tau\rangle$. In this case, the creation and annihilation operators are traditionally denoted by $\hat{\psi}^\dagger(x)$ and $\hat{\psi}(x)$ called *field operators*. Their commutation relations follow from Eq.(104).

$$[\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(y)]_{-\zeta} = [\hat{\psi}(x), \hat{\psi}(y)]_{-\zeta} = 0 \tag{106}$$

$$[\hat{\psi}(x), \hat{\psi}^\dagger(y)]_{-\zeta} = \delta(x-y) \tag{107}$$

The expansion of these operators on a basis $\{|\alpha\rangle\}$ follows from Eqs.(101) and (102).

$$\hat{\psi}^\dagger(x) = \sum_\alpha \langle\alpha|x\rangle a^\dagger_\alpha = \sum_\alpha \phi^*_\alpha(x) a^\dagger_\alpha \tag{108}$$

$$\hat{\psi}(x) = \sum_\alpha \langle x|\alpha\rangle a_\alpha = \sum_\alpha \phi_\alpha(x) a_\alpha \tag{109}$$

where $\phi_\alpha(x)$ is the coordinate representation wave function of the state $|\alpha\rangle$.

Representing an operator in terms of $a^\dagger$ & a In addition to generating all the many-particle states in the Fock space by repeated action on the vacuum, a fundamental property of creation and annihilation operators is that they provide a basis for all in the Fock space.

A convenient technique for representing an operator in terms of creation and annihilation operators is to first use a basis in which it is diagonal and then transform to general basis. To represent the operator in the diagonal basis, we define the number operator $\hat{n}_\alpha$:

$$\hat{n}_\alpha = a^\dagger_\alpha a_\alpha \tag{110}$$

The action of $\hat{n}_\alpha$ on a state $|\phi\rangle$ is to count the number of particles in state $|\alpha\rangle$ in the state $|\phi\rangle$:

$$\begin{aligned}\hat{n}_\alpha|\alpha_1\cdots\alpha_N\} &= a^\dagger_\alpha a_\alpha|\alpha_1\cdots\alpha_N\} \\ &= \sum_{i=1}^N \zeta^{i-1}\delta_{\alpha\alpha_i} a^\dagger_\alpha|\alpha_1\cdots\hat{\alpha}_i\cdots\alpha_N\} \\ &= \sum_{i=1}^N \zeta^{i-1}\delta_{\alpha\alpha_i}|\alpha_i\alpha_1\cdots\alpha_N\} \\ &= \sum_{i=1}^N (\zeta^{i-1})^2\delta_{\alpha\alpha_i}|\alpha_1\cdots\alpha_i\cdots\alpha_N\} \\ &= \left(\sum_{i=1}^N \delta_{\alpha\alpha_i}\right)|\alpha_1\cdots\alpha_N\} \end{aligned} \tag{111}$$

where $\sum_{i=1}^N \delta_{\alpha\alpha_i}$ yields the number of particles in the state $|\alpha\rangle$ in $|\alpha_1\cdots\alpha_N\}$. The operator $\hat{N}$ which counts the total number of particles in a state is given by:

$$\hat{N} = \sum_\alpha \hat{n}_\alpha = \sum_\alpha a^\dagger_\alpha a_\alpha \tag{112}$$

Now consider an one-body operator $\hat{U}$, which is diagonal in the orthonormal basis $|\alpha\rangle$.

$$\hat{U}|\alpha\rangle = U_\alpha|\alpha\rangle \tag{113}$$

$$U_\alpha = \langle\alpha|U|\alpha\rangle \tag{114}$$

Using Eq. (59), we obtain

$$\begin{aligned}\{\alpha'_1\cdots\alpha'_N|\hat{U}|\alpha_1\cdots\alpha_N\} &= \sum_P \zeta^P \sum_{i=1}^N \prod_{k\neq i}\langle\alpha'_{Pk}|\alpha_k\rangle\langle\alpha'_{P_i}|U_i|\alpha_i\rangle \\ &= \left(\sum_{i=1}^N U_{\alpha_i}\right)\{\alpha'_1\cdots\alpha'_N|\alpha_1\cdots\alpha_N\} \\ &= \{\alpha'_1\cdots\alpha'_N|\sum_\alpha U_\alpha\hat{n}_\alpha|\alpha_1\cdots\alpha_N\} \end{aligned} \tag{115}$$

Obtain the operator equation

$$\hat{U} = \sum_\alpha U_\alpha\hat{n}_\alpha = \sum_\alpha \langle\alpha|U|\alpha\rangle a^\dagger_\alpha a_\alpha \tag{116}$$

In order to obtain the action of $\hat{U}$, we must sum over all states $|\alpha\rangle$ multiplying U_α by the number of particles in state $|\alpha\rangle$.

Now transform from the diagonal representation to a general basis using Eqs.(101) and (102) then

$$\begin{aligned}\hat{U} &= \sum_{\alpha\lambda\mu} U_\alpha\langle\lambda|\alpha\rangle\langle\alpha|\mu\rangle a^\dagger_\lambda a_\mu \\ &= \sum_{\lambda\mu}\langle\lambda|U|\mu\rangle a^\dagger_\lambda a_\mu \end{aligned} \tag{117}$$

where

$$\begin{aligned}\langle\lambda|U|\mu\rangle &= \sum_\alpha\sum_{\alpha'}\langle\lambda|\alpha\rangle\langle\alpha|U|\alpha'\rangle\langle\alpha'|\mu\rangle \\ &= \sum_\alpha \langle\lambda|\alpha\rangle U_\alpha \langle\alpha|\mu\rangle \\ &= \int dxdy\ \phi_\lambda^*(x)\langle x|U|y\rangle\phi_\mu(y) \end{aligned} \tag{118}$$

For example, using field operators in the $\{\overrightarrow{x}\}$ representation, the kinetic operator $\hat{T}$ and a local one-body operator $\hat{U}$ may be written

$$\begin{aligned}\hat{T} &= \sum_{\lambda\mu}\langle\lambda|U|\mu\rangle a_\lambda^\dagger a_\mu^\dagger \\ &= \int dxdy\ \langle x|\frac{-\hbar^2}{2m}\nabla^2|y\rangle\psi^\dagger(x)\psi(y) \\ &= \int dxdy\ \frac{-\hbar^2}{2m}\nabla_y^2\ \langle x|y\rangle\psi^\dagger(x)\psi(y) \\ &= \int dxdy\ \frac{-\hbar^2}{2m}\nabla_y^2\ \delta(x-y)\psi^\dagger(x)\psi(y) \\ &= -\frac{\hbar^2}{2m}\int d^3x\ \hat{\psi}^\dagger(\overrightarrow{x})\nabla^2\hat{\psi}(\overrightarrow{x}) \end{aligned} \tag{119}$$

$$\hat{U} = \int d^3x\ U(\overrightarrow{x})\psi^\dagger(\overrightarrow{x})\hat{\psi}(\overrightarrow{x}) \tag{120}$$

in the $\{\overrightarrow{p}\}$ representation, the kinetic energy is:

$$\hat{T} = \int d^3p\ \frac{\hat{\overrightarrow{p}}^2}{2m}\hat{\psi}^\dagger(\overrightarrow{p})\hat{\psi}(\overrightarrow{p}) \tag{121}$$

A two-body operator $\hat{U}$ may be expressed in terms of creation and annihilation operators.

$$\hat{V}|\alpha\beta) = V_{\alpha\beta}|\alpha\beta) \tag{122}$$

$$V_{\alpha\beta} = (\alpha\beta|V|\alpha\beta) \tag{123}$$

Calculate a general matrix element as before.

$$\begin{aligned}\{\alpha_1'\cdots\alpha_N'|V|\alpha_1\cdots\alpha_N\} &= \sum_P \zeta^P\frac{1}{2}\sum_{i\neq j}\prod_{\substack{k\neq i\\k\neq j}}\langle\alpha_{P_k}'|\alpha_k\rangle(\alpha_{P_i}'\alpha_{P_j}'|\hat{V}|\alpha_i\alpha_j) \\ &= \left(\frac{1}{2}\sum_{i\neq j}^N V_{\alpha_i\alpha_j}\right)\{\alpha_1'\cdots\alpha_N'|\alpha_1\cdots\alpha_N\} \end{aligned} \tag{124}$$

The factor $\frac{1}{2}\sum_{i\neq j}^N V_{\alpha_i\alpha_j}$ is a sum all over distinct pairs of particles present in the state $|\alpha_1\cdots\alpha_N\rangle$. Needs to construct an operator $\hat{P}_{\alpha\beta}$ which counts the number of pairs of particles in the state $|\alpha\rangle$ and $|\beta\rangle$. If $|\alpha\rangle$ and $|\beta\rangle$ are different, the number of pair is $n_\alpha n_\beta$ whereas if $|\alpha\rangle = |\beta\rangle$ the number of pairs is $n_\alpha(n_\alpha - 1)$. Hence the operator which counts pairs may be written

$$\begin{aligned}\hat{P}_{\alpha\beta} &= \hat{n}_\alpha\hat{n}_\beta - \delta_{\alpha\beta}\hat{n}_\alpha \\ &= a_\alpha^\dagger a_\alpha a_\beta^\dagger a_\beta - \delta_{\alpha\beta}a_\alpha^\dagger a_\alpha \\ &= a_\alpha^\dagger \xi a_\beta^\dagger a_\alpha a_\beta \\ &= a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha \end{aligned} \tag{125}$$

So Eq.(124) may be written

$$\{\alpha'_1 \cdots \alpha'_N|\hat{V}|\alpha_1 \cdots \alpha_N\} = \{\alpha'_1 \cdots \alpha'_N|\frac{1}{2}\sum_{\alpha\beta} V_{\alpha\beta}\hat{P}_{\alpha\beta}|\alpha_1 \cdots \alpha_N\} \tag{126}$$

Hence $\hat{V}$ satisfies the operator equation

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta} V_{\alpha\beta}\hat{P}_{\alpha\beta} = \frac{1}{2}\sum_{\alpha\beta}(\alpha\beta|V|\alpha\beta)a^\dagger_\alpha a^\dagger_\beta a_\beta a_\alpha \tag{127}$$

The action of a two-body operator is obtained by summing over pairs of single-particles states $|\alpha\rangle$ and $|\beta\rangle$ and multiplying the matrix element $(\alpha\beta|V|\alpha\beta)$ by the number of pairs of such particles present in the physical state. Transforming from the diagonal representation to an arbitrary basis, the general expression for a two-body potential is

$$\hat{V} = \frac{1}{2}\sum_{\lambda\mu\nu\rho}(\lambda\mu|V|\nu\rho)a^\dagger_\lambda a^\dagger_\mu a_\rho a_\nu \tag{128}$$

Perhpas the easies way to remember is to use the state-operator association.

$$\begin{aligned}\hat{V} &= \frac{1}{2}\sum_{\lambda\mu\nu\rho}|\lambda\mu)(\lambda\mu|\hat{V}|\nu\rho)\,(\nu\rho| \\ &\to \frac{1}{2}\sum_{\lambda\mu\nu\rho} a^\dagger_\lambda a^\dagger_\mu\, a_\rho a_\nu.\end{aligned} \tag{129}$$

The last step comes from the observation

$$(\nu\rho| \leftrightarrow |\nu\rho) = a^\dagger_\nu a^\dagger_\rho \leftrightarrow a_\rho a_\nu.$$

For example, Coulomb potential is (spin neglected)

$$\begin{aligned}\hat{V} &= \frac{1}{2}\sum_{\lambda\mu\nu\rho}(\lambda\mu|V|\nu\rho)a^\dagger_\lambda a^\dagger_\mu a_\rho a_\nu \\ &= \frac{1}{2}\sum_{x_1x_2}\sum_{y_1y_2}(x_2\ y_2|\frac{e^2}{|\hat{x}-\hat{y}|}|x_1\ y_1)\ \psi^\dagger(x_2)\ \psi^\dagger(y_2)\ \psi(y_1)\ \psi(x_1) \\ &= \frac{1}{2}\int dx_1dx_2dy_1dy_2\ \frac{e^2}{|x_1-y_1|}\ (x_2\ y_2|x_1\ y_1)\ \psi^\dagger(x_2)\ \psi^\dagger(y_2)\ \psi(y_1)\ \psi(x_1) \\ &= \frac{1}{2}\int dx_1dx_2dy_1dy_2\ \frac{e^2}{|x_1-y_1|}\ \delta(x_2-x_1)\delta(y_2-y_1)\ \psi^\dagger(x_2)\ \psi^\dagger(y_2)\ \psi(y_1)\ \psi(x_1) \\ &= \frac{1}{2}\int dxdy\ \frac{e^2}{|x-y|}\ \psi^\dagger(x)\ \psi^\dagger(y)\ \psi(y)\ \psi(x) \\ &= \frac{1}{2}\int d^3x\ d^3y\ \frac{e^2}{|\overrightarrow{x}-\overrightarrow{y}|}\ \psi^\dagger(\overrightarrow{x})\ \psi^\dagger(\overrightarrow{y})\ \psi(\overrightarrow{y})\ \psi(\overrightarrow{x})\end{aligned} \tag{130}$$

3 Examples

3.1 Electrons in solid

Let us express the electrons moving in periodic potential interacting each other through Coulomb interaction with spin degrees of freedom included. In the first quantized version the Hamiltonian is

$$\hat{H} = \sum_i \left(\frac{\mathbf{p}_i^2}{2m} + U(\mathbf{x}_i)\right) + \frac{1}{2}\sum_{i,j} V(\mathbf{x}_i - \mathbf{x}_j). \tag{131}$$

Now the quantum number includes the spin degrees of freeom, so that the matrix elements should be evaluated in the following fashion. $\lambda = x\alpha$, where x is a position while α is spin quantum number.

$$(\lambda\mu|\hat{U}|\nu\rho) = (x'\alpha', y'\beta'|\hat{U}|x\alpha, y\beta) = U(x-y)\delta(x-x')\delta(y-y')\delta_{\alpha\alpha'}\delta_{\beta\beta'}.$$

Then the complete Hamiltonian can be written in the second quantized form:

$$\begin{aligned} \hat{H} &= \int d^3x \sum_\alpha \psi^\dagger_\alpha(\vec{x})\Big[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\Big]\psi_\alpha(\vec{x}) \\ &+ \frac{1}{2}\int d^3x d^3y \sum_{\alpha\beta} \psi^\dagger_\alpha(\vec{x})\psi^\dagger_\beta(\vec{y})\psi_\beta(\vec{y})\psi_\alpha(\vec{x})U(\vec{x}-\vec{y}). \end{aligned} \tag{132}$$

In momentum space

$$\begin{aligned} |x\rangle &= \sum_p |p\rangle\langle p|x\rangle \\ \psi^\dagger(x) &= \sum_p \psi^\dagger(p)\langle p|x\rangle = \sum_p \psi^\dagger(p)e^{-ipx} \\ \psi(x) &= \sum_p \psi(p)e^{ipx}, \quad V(x-y) = \int \frac{d^nq}{(2\pi)^n} V(q)e^{-iq\cdot(x-y)}. \end{aligned} \tag{133}$$

The momentum space representation of interaction term is

$$\hat{V} = \sum_{\alpha\beta} \frac{1}{2} \int \frac{d^np_1 d^np_2 d^nq}{(2\pi)^{3n}} \psi^\dagger_{p_1\alpha}\psi^\dagger_{p_2\beta}\psi_{p_2-q\beta}\psi_{p_1+q\alpha}V(q). \tag{134}$$

3.2 Density Operators

The density operator in the first quantized version is

$$\rho(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i). \tag{135}$$

Each particle is labelled by i. Remember that the second quantized one-particle operator (namely bilinear) is determined by one-particle matrix elements. Note that in the above expression $\mathbf{r}_i$ are operators, while is mere dummy variable for integration. The second quantized quantized density operator can be obtained in the following way:

$$\begin{aligned} \rho(\mathbf{r}) &= \int dxdy\langle x|\delta(r-r_i)|y\rangle\psi^\dagger(x)\psi(y) \\ &= \int dxdy\langle x|\delta(r-y)|y\rangle\psi^\dagger(x)\psi(y) \\ &= \int dxdy\delta(x-y)\delta(r-y)\psi^\dagger(x)\psi(y) = \psi^\dagger(r)\psi(r). \end{aligned} \tag{136}$$

Thus we arrive at

$$\rho(\mathbf{r}) = \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) = \sum_{\lambda,\lambda'} a^\dagger_\lambda a_{\lambda'}\, \phi^*_\lambda(\mathbf{r})\phi_{\lambda'}(\mathbf{r}). \tag{137}$$

$$N = \int d\mathbf{r}\rho(\mathbf{r}) = \Big(\int d\mathbf{r}\phi^*_\lambda(\mathbf{r})\phi_{\lambda'}(\mathbf{r})\Big)\sum_{\lambda,\lambda'} a^\dagger_\lambda a_{\lambda'} = \sum_\lambda a^\dagger_\lambda a_\lambda.$$

Note that $\int d\mathbf{r}\phi^*_\lambda(\mathbf{r})\phi_{\lambda'}(\mathbf{r}) = \delta_{\lambda\lambda'}$. In momentum space

$$\rho(\mathbf{q}) = \int e^{-i\mathbf{q}\cdot\mathbf{x}}\rho(\mathbf{x}) = \sum_{\mathbf{k}} a^\dagger_{\mathbf{k}+\mathbf{q}}a_{\mathbf{k}}. \tag{138}$$

The current operators in the first quantized version is

$$\mathbf{J}(\mathbf{r}) = e\frac{1}{2}\sum_i \Big[\mathbf{v}_i\delta(\mathbf{r}-\mathbf{r}_i) + \delta(\mathbf{r}-\mathbf{r}_i)\mathbf{v}_i\Big]. \tag{139}$$

Now recall $\mathbf{v}_i = \mathbf{p}_i/m = -i\nabla_i/m$. Consider again one-particle matrix element:

$$\begin{aligned}
(2m/e)\vec{J} &= \int dxdy\langle x|p_i\delta(r-r_i) + \delta(r-r_i)p_i|y\rangle\psi^\dagger(x)\psi(y) \\
&= \int dxdy\Big[\langle x|p_i\delta(r-y)|y\rangle\psi^\dagger(x)\psi(y) + \langle x|\delta(r-x)p_i|y\rangle\psi^\dagger(x)\psi(y)\Big] \\
&= \int dxdy\Big[\langle x|(-i\partial_y)\delta(r-y)|y\rangle\psi^\dagger(x)\psi(y) + \langle x|\delta(r-x)(-i\partial_x)_\leftarrow|y\rangle\psi^\dagger(x)\psi(y)\Big] \\
&= \int dxdy\Big[\delta(x-y)\psi^\dagger(x)(-i\partial_y)\psi(y))\delta(r-y) + \delta(x-y)(\psi^\dagger(x)(-i\partial_{x\leftarrow})\delta(r-x)\psi(y)\Big] \\
&= (-i)\Big[\psi^\dagger r\nabla_r\psi(r) - (\nabla_r\psi^\dagger(r))\psi(r)\Big].
\end{aligned} \tag{140}$$

In the last step a partial integration is assumed. On a more general basis

$$\psi(r) = \sum_\lambda c_\lambda\psi_\lambda(r), \quad \psi^\dagger(r) = \sum_\lambda c^\dagger_\lambda\psi^*_\lambda(r).$$

Then the current operator becomes

$$\mathbf{J}(\mathbf{q}) = \frac{e}{2mi}\sum_{\lambda,\eta} c^\dagger_\lambda c_\eta \int d^3re^{-i\mathbf{q}\cdot\mathbf{r}}\Big[\phi^*_\lambda(r)\nabla\phi_\eta(r) - \phi_\eta(r)\nabla\phi^*_\lambda(r)\Big]. \tag{141}$$

3.3 Tight-binding model

Consider a general hopping Hamiltonian.

$$H = \sum_{i\vec{\delta}}\Big[t_{i\vec{\delta}}|i\rangle\langle i+\vec{\delta}| + t^*_{i\vec{\delta}}|i+\vec{\delta}\rangle\langle i|\Big]. \tag{142}$$

The hopping amplitude can be evaluated in the following way.

$$\sum_{i,j}|i\rangle\langle i|\hat{T}|j\rangle\langle j|$$

The nature of hoppping Hamiltonian T is such that only $j = i+\vec{\delta}$, where $\vec{\delta}$ designates the vectors which connect the nearest (or next nearest) neighbors. Then we get

$$H = \sum_{i,\vec{\delta}}|i\rangle\langle i|T|i+\vec{\delta}\rangle\langle i+\vec{\delta}| + \text{H.C.} \tag{143}$$

Evaluating the matrix element $\langle i|T|i+\vec{\delta}\rangle$,

$$\begin{aligned}
t_{i\vec{\delta}} &= \int dxdy\langle i|x\sigma\rangle\langle x\sigma|T|y\sigma'\rangle\langle y\sigma'|i+\vec{\delta}\rangle \\
&= \int dxdy\psi^*(x-R_i)\langle x\sigma|T|y\sigma'\rangle\psi(y-R_{i+\vec{\delta}}).
\end{aligned} \tag{144}$$

The matrix element $\vec{\delta} = 0$ is called a site energy, and the elements $\vec{\delta} \neq 0$ are called the hopping energy, or just hopping integral. The second quantized Hamiltonian can be constructed easily.

$$\hat{H} = \sum_{i\vec{\delta}\sigma} \Big[t_{i\vec{\delta}} C^{\dagger}_{i\sigma} C_{i+\vec{\delta},\sigma} + t^{*}_{i\vec{\delta}} C^{\dagger}_{i+\vec{\delta}\sigma} C_{i\sigma} \Big]. \tag{145}$$

The above Hamiltonian can be solved by Fourier transform:

$$C_{j\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_j} C_{\mathbf{k}\sigma}. \tag{146}$$

3.4 Current operator in tight-binding model formalism

The trick is to use the equation of continuity which holds in general. Take polarization operator:

$$\mathbf{P} = \int d^3 r \vec{r} \rho(\vec{r}).$$

Then it follows that

$$\begin{aligned} \frac{\partial \mathbf{P}}{\partial t} &= \int d^3 r \vec{r} \frac{\partial \rho(\vec{r}, t)}{\partial t} \\ &= \int d^3 r \vec{r} (-1) \nabla \cdot \mathbf{j}(\vec{r}) = \int d^3 r \mathbf{j}(\vec{r}) \cdot \nabla(\vec{r}) = \int d^3 r \mathbf{j}(\vec{r}). \end{aligned} \tag{147}$$

To obtain the last expression we dumped a boundary terms. Now in the tight-binding model

$$\mathbf{P} = \sum_i \vec{R}_i n_i, \quad \mathbf{J} = \frac{\partial \mathbf{P}}{\partial t} = i[\hat{H}, \mathbf{P}] = i \sum_i [\hat{H}, n_i] \vec{R}_i.$$

Carrying out calculations assuming real hopping integral we get

$$\mathbf{J} = it \sum_{i,\vec{\delta}} (\vec{R}_i - \vec{R}_{i+\vec{\delta}}) c^{\dagger}_{i+\vec{\delta}} c_i = -it \sum_{i,\vec{\delta}} \vec{\delta} c^{\dagger}_{i+\vec{\delta}} c_i. \tag{148}$$

The energy current can be obtained along the similar line. We employ the continuity equation of energy flux.

$$\frac{\partial H}{\partial t} + \nabla \cdot \mathbf{j}_E = 0. \tag{149}$$

Defining

$$\mathbf{R}_E = \frac{1}{2} \int d^3 r \left[\vec{r} \mathcal{H}(\vec{r}) + \mathcal{H}(\vec{r}) \vec{r} \right]$$

it follows that

$$\frac{\partial \mathbf{R}_E}{\partial t} = \mathbf{J}_E.$$

For free system

$$\mathbf{J}_E = \sum_{\mathbf{p},\sigma} \vec{v}_{\mathbf{p}} \epsilon_{\mathbf{p}} c^{\dagger}_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma}. \tag{150}$$

The **Heat** current is given by

$$\mathbf{J}_Q = \mathbf{J}_E - \mu \mathbf{J}_{number}. \tag{151}$$

3.5 Derivation of Hubbard Model

The Coulomb interaction in Wannier basis is given by

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta}\sum_{ijml}(jm|V|il)\, c^{\dagger}_{j\beta}c^{\dagger}_{m\alpha}c_{l\alpha}c_{i\beta}. \tag{152}$$

The explicit expression of matrix element in position space is

$$\begin{aligned}(jm|V|il) &= (jm|xy)(xy|V|zw)(zw|il) \\ &= \int dxdydzdw(jm|xy)V(x-y)\delta(x-z)\delta(y-w)\,(zw|il) \\ &= \int dxdy\phi^*(x-R_j)\phi^*(y-R_m)\phi_(x-R_i)\phi_(y-R_l)\,\frac{e^2}{|x-y|}\end{aligned} \tag{153}$$

Evidently the configuration with the largest energy would be the one $i = j = l = m$. In this case the configuration $\alpha = \beta$ is not allowed, and the allowed configurations are $\alpha =\uparrow, \beta =\downarrow$ and $\alpha =\uparrow, \beta =\downarrow$. This gives a factor of two, cancelling the 1/2 in front. Then a simple algebra shows that this leading term can be expressed as

$$\hat{V}_{largest} = U\sum_i n_{i\uparrow}n_{i\downarrow}, \quad U = \int dxdy|\phi(x-R_i)|^2\frac{e^2}{|x-y|}|\phi(y-R_i)|^2. \tag{154}$$

Next one can try a configuration with $i = j, l = m, i \neq l$, the so-called direct term. Then the interaction can be reduced to

$$\hat{V}_{direct} = \frac{1}{2}\sum_{i\neq l}V_{il}n_in_l, \quad V_{il} = \int dxdy|\phi(x-R_i)|^2\frac{e^2}{|x-y|}\,|\phi(y-R_l)|^2. \tag{155}$$

Similary, the exchange terms can be constructed.