Second quantization for fermions

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Vladimir Aleksandrovich Fock (December 22, 1898 – December 27, 1974) was a Soviet physicist, who did foundational work on quantum mechanics and quantum electrodynamics. His primary scientific contribution lies in the development of quantum physics, although he also contributed significantly to the fields of mechanics, theoretical optics, theory of gravitation, physics of continuous media. In 1926 he derived the Klein–Gordon equation. He gave his name to Fock space, the Fock representation and Fock state, and developed the Hartree–Fock method in 1930. He made many subsequent scientific contributions, during the rest of his life. Fock developed the electromagnetic methods for geophysical exploration in a book *The theory of the study of the rocks resistance by the carottage method* (1933); the methods are called the well logging in modern literature. Fock made significant contributions to general relativity theory, specifically for the many body problems.
https://en.wikipedia.org/wiki/Vladimir_Fock

1. Introduction

What is the definition of the second quantization? In quantum mechanics, the system behaves like wave and like particle (duality). The first quantization is that particles behave like waves. For example, the wave function of electrons is a solution of the Schrödinger equation. Although electromagnetic waves behave like wave, they also behave like particle, as known as photon. This idea is known as second quantization; waves behave like particles.

Instead of traditional treatment of a wave function as a solution of the Schrödinger equation in the position representation or representation of some dynamical observable, we will now find a totally different basis formed by number states (or Fock states). This basis turns out to be a convenient and powerful tool to treat the systems of identical particles

2. Significance of the second quantization for many particle systems?

By convention, the original form of quantum mechanics is denoted first quantization, while quantum field theory is formulated in the language of second quantization. Second quantization greatly simplifies the discussion of many interacting particles. This approach merely reformulates the original Schrödinger equation. Nevertheless, it has the advantage that in second quantization operators incorporate the statistics, which contrasts with the more cumbersome approach of using symmetrized or anti-symmetrized products of single-particle wave functions.

The second quantization consists of the following three steps.

(a) One-particle Schrödinger equation

(**first quantization, wave-character**). The wave function is the eigenfunction of on-particle Hamiltonian.

$$\psi(x) = \sum_{\mu} a_{\mu}\phi_{\mu}(x), \qquad \psi^{*}(x) = \sum_{\mu} a_{\mu}{}^{*}\phi_{\mu}{}^{*}(x)$$

(b) Creation and annihilation operators (CAP's)

Commutation relation reflecting the symmetry of wave function (boson and fermion). Commutation relation (boson) and anti-commutation relation (fermion). Such commutation relations guarantee the symmetry of the wave function. *This means that we do not have to worry about the symmetry such as the Slater matrix for fermions.*

(c) Second quantization

By introducing the operators of creation and annihilation instead of the coefficients of the one particle wave function. The new operator for the wave function represents the character of particles.

$$\hat{\psi}(x) = \sum_{\mu} \hat{a}_{\mu} \phi_{\mu}(x), \qquad \hat{\psi}^{+}(x) = \sum_{\mu} \hat{a}_{\mu}^{+} \phi_{\mu}(x)$$

The state of many particles is represented by the occupation number state (the Fock space)

3. What is the advantage of second quantization?

From a practical point of view, the resulting equations for systems with many particles (the second quantization) are much simpler and more compact than the original many-particle Schrödinger equation. Indeed, the original scheme operates with a wave function of very many variables (the coordinates of all particles), which obeys a differential equation involving all these variables. In the framework of second quantization, we reduced this to an equation for an operator of one-single variable. Apart from the operator “hats,” it looks very much like the Schrödinger equation for a single particle, and is of the same level of complexity

$$i\hbar \frac{\partial}{\partial t} \psi(\boldsymbol{r}, t) = [-\frac{\hbar^2}{2m} \nabla^2 + V(\boldsymbol{r})] \psi(\boldsymbol{r}, t) \tag{2}$$

From an educational point of view, the advantage is enormous. To reveal it finally, let us take the expectation value of

$$i\hbar \frac{\partial}{\partial t} \hat{\psi}(\boldsymbol{r}, t) = [-\frac{\hbar^2}{2m} \nabla^2 + V(\boldsymbol{r})] \hat{\psi}(\boldsymbol{r}, t) \tag{1}$$

and introduce the (deliberately confusing) notation

$$\langle \hat{\psi}(r,t) \rangle = \psi(r,t),$$

Owing to the linearity of Eq.(1), the equation for the expectation value formally coincides with

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

However, let us put this straight: this equation is not for a wave function anymore. It is an equation for a *classical field*. Without noticing, we have thus got all the way from particles to fields and have understood that these concepts are just two facets of a single underlying concept: that of the quantum field.

4. Properties of the Slater determinant (fermions)

The slater determinant for the fermion systems is given by the Slater determinant

$$\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle$$
$$= \frac{1}{\sqrt{n!}} \begin{pmatrix} \langle x_1|\lambda^{(1)}\rangle & \langle x_1|\lambda^{(2)}\rangle & . & \langle x_1|\lambda^{(i-1)}\rangle & \langle x_1|\lambda^{(i)}\rangle & \langle x_1|\lambda^{(i+1)}\rangle & . & \langle x_1|\lambda^{(n)}\rangle \\ \langle x_2|\lambda^{(1)}\rangle & \langle x_2|\lambda^{(2)}\rangle & . & \langle x_2|\lambda^{(i-1)}\rangle & \langle x_2|\lambda^{(i)}\rangle & \langle x_2|\lambda^{(i+1)}\rangle & . & \langle x_2|\lambda^{(n)}\rangle \\ \langle x_3|\lambda^{(1)}\rangle & \langle x_3|\lambda^{(2)}\rangle & . & \langle x_3|\lambda^{(i-1)}\rangle & \langle x_3|\lambda^{(i)}\rangle & \langle x_3|\lambda^{(i+1)}\rangle & . & \langle x_3|\lambda^{(n)}\rangle \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ \langle x_n|\lambda^{(1)}\rangle & \langle x_n|\lambda^{(2)}\rangle & . & \langle x_n|\lambda^{(i-1)}\rangle & \langle x_n|\lambda^{(i)}\rangle & \langle x_n|\lambda^{(i+1)}\rangle & . & \langle x_n|\lambda^{(n)}\rangle \end{pmatrix} \quad (1)$$

$$\{n_1 = n_2 = ... = n_n = 1, n_{n+1} = n_{n+2} = ... = n_s = 0\} \qquad \text{(conventional form)}$$

with the number of occupation; $\{n_1, n_2, n_3, ..., n_{i-1}, n_i, n_{i+1}, ..., n_s\}$ for one-particle states $|\lambda^{(1)}\rangle$, $|\lambda^{(2)}\rangle$, $|\lambda^{(3)}\rangle$,…, which are different. Obviously, the fermion wave function changes sign when one exchanges the order of the occupancy. To prove this property we notice that the l.h.s. (left-hand side) of Eq.(1) corresponds to

$$\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_{i-1}, n_i, ..., n_s; n\rangle$$
$$= -\frac{1}{\sqrt{n!}} \begin{pmatrix} \langle x_1|\lambda^{(1)}\rangle & \langle x_1|\lambda^{(2)}\rangle & . & \langle x_1|\lambda^{(i)}\rangle & \langle x_1|\lambda^{(i-1)}\rangle & \langle x_1|\lambda^{(i+1)}\rangle & . & \langle x_1|\lambda^{(n)}\rangle \\ \langle x_2|\lambda^{(1)}\rangle & \langle x_2|\lambda^{(2)}\rangle & . & \langle x_2|\lambda^{(i)}\rangle & \langle x_2|\lambda^{(i-1)}\rangle & \langle x_2|\lambda^{(i+1)}\rangle & . & \langle x_2|\lambda^{(n)}\rangle \\ \langle x_3|\lambda^{(1)}\rangle & \langle x_3|\lambda^{(2)}\rangle & . & \langle x_3|\lambda^{(i)}\rangle & \langle x_3|\lambda^{(i-1)}\rangle & \langle x_3|\lambda^{(i+1)}\rangle & . & \langle x_3|\lambda^{(n)}\rangle \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ \langle x_n|\lambda^{(1)}\rangle & \langle x_n|\lambda^{(2)}\rangle & . & \langle x_n|\lambda^{(i)}\rangle & \langle x_n|\lambda^{(i-1)}\rangle & \langle x_n|\lambda^{(i+1)}\rangle & . & \langle x_n|\lambda^{(n)}\rangle \end{pmatrix}$$
$$= -\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, n_{i-1}, n_{i+1} ...., n_s; n\rangle$$

(2)

Because of the property of the determinant the sign changes when two columns are interchanged.

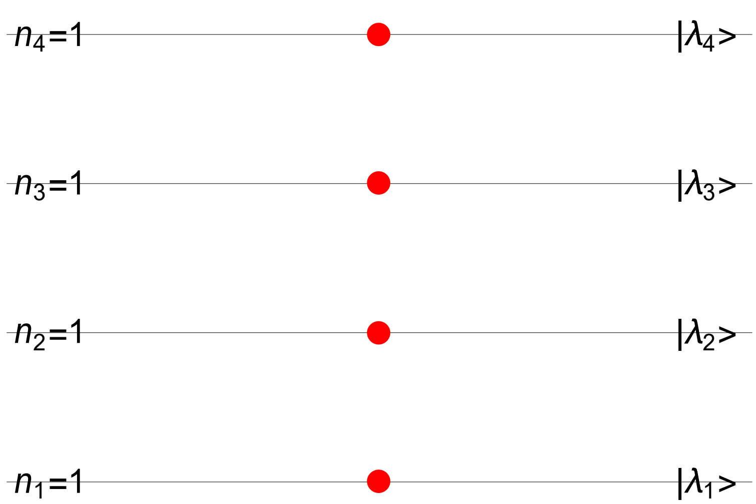
((**Example**))

Obviously, it is necessary to specify for a fermion wave function the order in which the single–particle states $\left|\lambda_j\right\rangle$ are occupied. For this purpose one must adhere to a strict convention: the labelling of single–particle states by indices *j* = 1, 2…, must be chosen once and for all at the beginning of a calculation and these states must be occupied always in the order of increasing indices. A proper example is the two particle fermion wave function

$$\left\langle x_1, x_2 \middle| n_1 = 1, n_2 = 1; n = 2\right\rangle = \frac{1}{\sqrt{2!}}\begin{vmatrix} \lambda_1(x_1) & \lambda_2(x_1) \\ \lambda_1(x_2) & \lambda_2(x_2) \end{vmatrix} \qquad \{ n_1 = 1, n_2 = 1, n_3 = n_4 = ... = 0\}$$

$$\left\langle x_1, x_2, x_3 \middle| n_1 = 1, n_2 = 1, n_3 = 1; n = 3\right\rangle = \frac{1}{\sqrt{3!}}\begin{vmatrix} \lambda_1(x_1) & \lambda_2(x_1) & \lambda_3(x_1) \\ \lambda_1(x_2) & \lambda_2(x_2) & \lambda_3(x_2) \\ \lambda_1(x_3) & \lambda_2(x_3) & \lambda_3(x_3) \end{vmatrix} \qquad \{ n_1 = 1, n_2 = 1, n_3 = 1, n_4 = n_5 = ... = 0\}$$

((**Fermions**)) Energy levels and states



Fermions

$$\langle x_1, x_2, x_3, x_4; n=4 | n_1=1, n_2=1, n_3=1, n_4=1; n=4\rangle_F$$

5. Co-factor of the Slater determinant

We now start with the Slater determinant

$$\langle x_1, x_2, x_3,..., x_n; n | n_1, n_2, n_3,..., n_i,...., n_s\rangle$$

$$= \frac{1}{\sqrt{n!}} \begin{pmatrix} \langle x_1|\lambda^{(1)}\rangle & \langle x_1|\lambda^{(2)}\rangle & . & \langle x_1|\lambda^{(i-1)}\rangle & \langle x_1|\lambda^{(i)}\rangle & \langle x_1|\lambda^{(i+1)}\rangle & . & \langle x_1|\lambda^{(n)}\rangle \\ \langle x_2|\lambda^{(1)}\rangle & \langle x_2|\lambda^{(2)}\rangle & . & \langle x_2|\lambda^{(i-1)}\rangle & \langle x_2|\lambda^{(i)}\rangle & \langle x_2|\lambda^{(i+1)}\rangle & . & \langle x_2|\lambda^{(n)}\rangle \\ \langle x_3|\lambda^{(1)}\rangle & \langle x_3|\lambda^{(2)}\rangle & . & \langle x_3|\lambda^{(i-1)}\rangle & \langle x_3|\lambda^{(i)}\rangle & \langle x_3|\lambda^{(i+1)}\rangle & . & \langle x_3|\lambda^{(n)}\rangle \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . \\ \langle x_n|\lambda^{(1)}\rangle & \langle x_n|\lambda^{(2)}\rangle & . & \langle x_n|\lambda^{(i-1)}\rangle & \langle x_n|\lambda^{(i)}\rangle & \langle x_n|\lambda^{(i+1)}\rangle & . & \langle x_n|\lambda^{(n)}\rangle \end{pmatrix}$$

Using the co-factor for the element $\langle x_1|\lambda^{(i)}\rangle$;

$$\langle x_2, x_3,..., x_{i-1}, x_i, x_{i+1},...; n-1 | n_1, n_2, n_3,..., n_{i-1}, n_i - 1, n_{i+1},...., n_s; n-1\rangle$$

$$= \frac{1}{\sqrt{(n-1)!}} \begin{pmatrix} \langle x_2|\lambda^{(1)}\rangle & \langle x_2|\lambda^{(2)}\rangle & . & \langle x_2|\lambda^{(i-1)}\rangle & \langle x_2|\lambda^{(i+1)}\rangle & & . & . & \langle x_2|\lambda^{(n)}\rangle \\ \langle x_3|\lambda^{(1)}\rangle & \langle x_3|\lambda^{(2)}\rangle & . & \langle x_3|\lambda^{(i-1)}\rangle & \langle x_3|\lambda^{(i+1)}\rangle & & . & . & \langle x_3|\lambda^{(n)}\rangle \\ \langle x_4|\lambda^{(1)}\rangle & \langle x_4|\lambda^{(2)}\rangle & . & \langle x_4|\lambda^{(i-1)}\rangle & \langle x_4|\lambda^{(i+1)}\rangle & & . & . & \langle x_4|\lambda^{(n)}\rangle \\ . & . & . & . & . & & . & . & . \\ . & . & . & . & . & & . & . & . \\ . & . & . & . & . & & . & . & . \\ . & . & . & . & . & & . & . & . \\ \langle x_n|\lambda^{(1)}\rangle & \langle x_n|\lambda^{(2)}\rangle & . & \langle x_n|\lambda^{(i-1)}\rangle & \langle x_n|\lambda^{(i+1)}\rangle & \langle x_n|\lambda^{(i+1)}\rangle & . & & \langle x_n|\lambda^{(n)}\rangle \end{pmatrix}$$

we have

$$\langle x_1, x_2, x_3,..., x_n; n | n_1, n_2, n_3,..., n_i,...., n_s; n\rangle$$
$$= \frac{1}{\sqrt{n}} \sum_{m=1}^{n} \langle x_1|\lambda^{(m)}\rangle (-1)^{m-1} \langle x_2, x_3,..., x_{m-1}, x_m, x_{m+1},...; n-1 | n_1, n_2, n_3, ..., n_{m-1}, n_m - 1, n_{m+1}, ..., n_s\rangle$$

or more formally,

$$\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle$$
$$= \frac{1}{\sqrt{n}} \sum_{i=1}^{\infty} \langle x_1 | \lambda^{(i)}\rangle n_i (-1)^{s_i} \langle x_2, x_3, ..., x_{i-1}, x_i, x_{i+1}, ...; n-1 | n_1, n_2, n_3, ..., n_{i-1}, n_i - 1, n_{i+1}, ..., n_s; n-1\rangle$$

((**Expansion formula**))

where

$$s_i = \sum_{k=1}^{i-1} n_k = n_1 + n_2 + n_3 + ... + n_{i-1}$$

is equal to the number of occupied states up to the i-th.

((**Note**))

$$s_i = i - 1$$

for the conventional case ($n_1 = n_2 = ... = n_{i-1} = 1$; occupied).

6. Creation and annihilation operator (fermions)

We now define the annihilation operator $\hat{a}_i$ by

$$\hat{a}_i | n_1, n_2, n_3, ..., n_{i-1}, n_i, n_{i+1}, ..., n_s; n\rangle = (-1)^{s_i} n_i | n_1, n_2, n_3, ..., n_{i-1}, n_i - 1, n_{i+1}, ..., n_s; n-1\rangle$$

The factors n_i guarantee that if the state $|\lambda_i\rangle$ is not occupied, no particle can be newly removed in that state. We also define the creation operator $\hat{a}_i^+$ by

$$\hat{a}_i^+ | n_1, n_2, n_3, ..., n_{i-1}, n_i, n_{i+1}, ..., n_s; n\rangle = (-1)^{s_i} (1 - n_i) | n_1, n_2, n_3, ..., n_{i-1}, n_i + 1, n_{i+1}, ..., n_s; n+1\rangle$$

The factors $(1 - n_i)$ guarantee that if the state $|\lambda_i\rangle$ is already occupied, a second particle cannot be put into that state. No state can have an occupation number greater than one.

The commutation rules are now verified to be

$$[\hat{a}_i, \hat{a}_j]_+ = [\hat{a}_i^+, \hat{a}_j^+]_+ = 0, \qquad [\hat{a}_i, \hat{a}_j^+]_+ = \hat{1}\delta_{i,j}$$

where

$$[\hat{A},\hat{B}]_+ = \hat{A}\hat{B}+\hat{B}\hat{A}, \quad \text{or} \quad \{\hat{A},\hat{B}\} = \hat{A}\hat{B}+\hat{B}\hat{A}$$

is the anti-commutator of $\hat{A}$ and $\hat{B}$. These relations can be proved as follows.

$$\begin{aligned}\hat{a}_i\hat{a}_i^{+}|n_1,n_2,n_3,...,n_{i-1},n_i,n_{i+1},....,n_s;n\rangle &= (-1)^{s_i}(1-n_i)\hat{a}_i|n_1,n_2,n_3,...,n_{i-1},n_i+1,n_{i+1},....,n_s;n+1\rangle \\ &= (-1)^{2s_i}(1-n_i)(n_i+1)|n_1,n_2,n_3,...,n_{i-1},n_i,n_{i+1},....,n_s;n\rangle\end{aligned}$$

$$\begin{aligned}\hat{a}_i^{+}\hat{a}_i|n_1,n_2,n_3,...,n_{i-1},n_i,n_{i+1},....,n_s;n\rangle &= (-1)^{s_i}n_i\hat{a}_i^{+}|n_1,n_2,n_3,...,n_{i-1},n_i-1,n_{i+1},....,n_s;n-1\rangle \\ &= (-1)^{2s_i}n_i(2-n_i)|n_1,n_2,n_3,...,n_{i-1},n_i,n_{i+1},....,n_s;n\rangle\end{aligned}$$

and

$$[\hat{a}_i,\hat{a}_i^{+}]_+|n_1,n_2,n_3,...,n_{i-1},n_i,n_{i+1},....,n_s;n\rangle = |n_1,n_2,n_3,...,n_{i-1},n_i,n_{i+1},....,n_s;n\rangle$$

or

$$[\hat{a}_i,\hat{a}_i^{+}]_+ = \hat{1}$$

since

$$(1-n_i)(n_i+1)+n_i(2-n_i) = 1-n_i^{2}+2n_i-n_i^{2} = 1$$

and

$$n_i^{2} = n_i.$$

Note that

$$\hat{a}_i^{2} = 0, \qquad \hat{a}_i^{+2} = 0,$$

since

$$\begin{aligned}\hat{a}_i\hat{a}_i|n_1,n_2,n_3,...,n_{i-1},n_i,n_{i+1},....,n_s\rangle &= (-1)^{s_i}n_i\hat{a}_i|n_1,n_2,n_3,...,n_{i-1},n_i-1,n_{i+1},....,n_s\rangle \\ &= (-1)^{2s_i}n_i(n_1-1)|n_1,n_2,n_3,...,n_{i-1},n_i,n_{i+1},....,n_s\rangle \\ &= 0\end{aligned}$$

$$\hat{a}_i^{+}\hat{a}_i^{+}\left|n_1, n_2, n_3, ..., n_{i-1}, n_i, n_{i+1}, ..., n_s\right\rangle = (-1)^{s_i}(1-n_i)\hat{a}_i^{+}\left|n_1, n_2, n_3, ..., n_{i-1}, n_i + 1, n_{i+1}, ..., n_s\right\rangle$$
$$= (-1)^{2s_i}(1-n_i)(-n_i)\left|n_1, n_2, n_3, ..., n_{i-1}, n_i 1, n_{i+1}, ..., n_s\right\rangle$$
$$= 0$$

and

$$\hat{a}_i^{+}\hat{a}_i^{+}\left|n_1, n_2, n_3, ..., n_{i-1}, n_i, n_{i+1}, ..., n_s\right\rangle = (-1)^{s_i}(1-n_i)\hat{a}_i^{+}\left|n_1, n_2, n_3, ..., n_{i-1}, n_i + 1, n_{i+1}, ..., n_s\right\rangle$$
$$= -(-1)^{2s_i} n_i (1-n_i)\left|n_1, n_2, n_3, ..., n_{i-1}, n_i 1, n_{i+1}, ..., n_s\right\rangle$$

((**Note**))

What is really strange about the definitions is that they are subjective. They explicitly depend on the way we have ordered the levels. We usually find it convenient to organize the levels in order of increasing energy, but we could also choose decreasing energy or any other order. The point is that the signs of the matrix elements of fermionic CAP's (creation and annihilation operators) are subjective indeed. Therefore, the CAP's do not purport to correspond on the choice of the level ordering. Therefore, the products correspond to physical quantities (**Nazarov and Danon**).

7. The number operator (fermions)

The number operator for the *i*-th state is defined by

$$\hat{N}_i = \hat{a}_i^{+}\hat{a}_i .$$

We note that

$$\hat{N}_i^2 = \hat{a}_i^{+}\hat{a}_i\hat{a}_i^{+}\hat{a}_i = \hat{a}_i^{+}(\hat{1} - \hat{a}_i^{+}\hat{a}_i)\hat{a}_i = \hat{a}_i^{+}\hat{a}_i - \hat{a}_i^{+}\hat{a}_i^{+}\hat{a}_i\hat{a}_i = \hat{N}_i$$

since $\hat{a}_i^2 = 0$, $\hat{a}_i^{+2} = 0$.

The total number operator is defined by

$$\hat{N} = \sum_{i=1}^{\infty} \hat{N}_i$$

The number of operators belonging to different states commute,

$$[\hat{N}_i, \hat{N}_j] = \hat{N}_i\hat{N}_j - \hat{N}_j\hat{N}_i = 0$$

Consequently functions can be found that are simultaneously eigenfunctions of all these number operators. It can be shown that

$$[\hat{N}_i, \hat{a}_j] = -\delta_{ij}\hat{a}_i$$

and

$$[\hat{N}_i, \hat{a}_j^{+}] = \delta_{ij}\hat{a}_i^{+}.$$

((**Proof**))

$$\begin{aligned}[\hat{N}_i, \hat{a}_j] &= \hat{a}_i^{+}\hat{a}_i\hat{a}_j - \hat{a}_j\hat{a}_i^{+}\hat{a}_i \\ &= -\hat{a}_i^{+}\hat{a}_j\hat{a}_i - \hat{a}_j\hat{a}_i^{+}\hat{a}_i \\ &= -[\hat{a}_i^{+}, \hat{a}_j]_{+}\hat{a}_i \\ &= -\delta_{ij}\hat{a}_i\end{aligned}$$

$$\begin{aligned}[\hat{N}_i, \hat{a}_j^{+}] &= \hat{a}_i^{+}\hat{a}_i\hat{a}_j^{+} - \hat{a}_j^{+}\hat{a}_i^{+}\hat{a}_i \\ &= \hat{a}_i^{+}\hat{a}_i\hat{a}_j^{+} + \hat{a}_i^{+}\hat{a}_j^{+}\hat{a}_i \\ &= \hat{a}_i^{+}[\hat{a}_i, \hat{a}_j^{+}]_{+} \\ &= \delta_{ij}\hat{a}_i^{+}\end{aligned}$$

8. Anti-commutation relation for fermion operator: simple case

((**Schiff**))

Find two matrices $\hat{a}$ and $\hat{a}^{+}$ that satisfy the following equations;

$$\hat{a}^2 = 0, \qquad \hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a} = \hat{1}, \qquad \hat{N} = \hat{a}^{+}\hat{a}$$

Show that $\hat{N}^2 = \hat{N}$. Obtain explicit expressions for $\hat{a}$ and $\hat{N}$ in a representation in which $\hat{N}$ is diagonal, assuming that it is nondegenerate. Can $\hat{a}$ be diagonalized in any representation?

((**Solution**))

$$\hat{N} = \hat{a}^{+}\hat{a}\,, \qquad \hat{a}^{2} = 0$$

$$\hat{a}\hat{a}^{+} + \hat{a}^{+}\hat{a} = \hat{1}$$

Using these relations, we get

$$\hat{N}^{2} = \hat{a}^{+}\hat{a}\hat{a}^{+}\hat{a} = \hat{a}^{+}(\hat{1} - \hat{a}^{+}\hat{a})\hat{a} = \hat{a}^{+}\hat{a} - \hat{a}^{+}\hat{a}\hat{a} = \hat{a}^{+}\hat{a} = \hat{N}$$

We also note that

$$[\hat{N}, \hat{a}] = -\hat{a}\,, \qquad [\hat{N}, \hat{a}^{+}] = \hat{a}^{+}.$$

((**Proof**))
(i)

$$\begin{aligned}
[\hat{N}, \hat{a}] &= \hat{a}^{+}\hat{a}\hat{a} - \hat{a}\hat{a}^{+}\hat{a} \\
&= -\hat{a}\hat{a}^{+}\hat{a} \\
&= -(\hat{1} - \hat{a}^{+}\hat{a})\hat{a} \\
&= -\hat{a}
\end{aligned}$$

since $\hat{a}^{2} = 0$.

(ii)

$$\begin{aligned}
[\hat{N}, \hat{a}^{+}] &= \hat{a}^{+}\hat{a}\hat{a}^{+} - \hat{a}^{+}\hat{a}^{+}\hat{a} \\
&= \hat{a}^{+}\hat{a}\hat{a}^{+} \\
&= \hat{a}^{+}(-\hat{a}^{+}\hat{a} + \hat{1}) \\
&= \hat{a}^{+} - \hat{a}^{+}\hat{a}^{+}\hat{a}) \\
&= \hat{a}^{+}
\end{aligned}$$

since $\hat{a}^{2} = 0$.

Eigenket

$$\hat{N}|N\rangle = N|N\rangle$$

$$\hat{N}^2|N\rangle = \hat{N}|N\rangle$$

leading to the result,

$$N^2 = N$$

or

$N = 1$, or 0.   (eigenvalues)

This is satisfied only for $N = 0$ and $N = 1$. Thus these are the eigenvalues of the number operator $\hat{N} = \hat{a}^+\hat{a}$. We see that at most one particle can occupy the state $|N\rangle$. These particles obey the Fermi-Dirac statistics.

We need the matrix elements of $\hat{a}$ and $\hat{a}^+$.We now consider the eigenvalue problem

$$(\hat{N}\hat{a} - \hat{a}N|N\rangle = -\hat{a}|N\rangle$$

or

$$\hat{N}\hat{a}|N\rangle = (N-1)\hat{a}|N\rangle$$

So $\hat{a}|N\rangle$ is the eigenket of $\hat{N}$ with the eigenvalue $(N-1)$,

$$\hat{a}|N\rangle = c|N-1\rangle$$

The constant *c* is determined as follows,

$$\hat{a}|N\rangle = c|N-1\rangle, \qquad \langle N|\hat{a}^+ = c^*\langle N-1|$$

or

$$\langle N|\hat{a}^+\hat{a}|N\rangle = |c|^2 = N$$

or

$$|c|^2 = N$$

Thus we have

$$\hat{a}^{+}|N\rangle = \sqrt{N}|N-1\rangle$$

except for a phase factor of modulus unity. We note that

$$\hat{a}^{+}|N\rangle = N|N-1\rangle$$

since $N^2 = N$. Similarly, we get

$$(\hat{N}\hat{a}^{+} - \hat{a}^{+}\hat{N}|N\rangle = \hat{a}^{+}|N\rangle.$$

or

$$(\hat{N}\hat{a}^{+}|N\rangle = (N+1)\hat{a}^{+}|N\rangle,$$

So $\hat{a}^{+}|N\rangle$ is the eigenket of $\hat{N}$ with the eigenvalue $(N+1)$,

$$\hat{a}^{+}|N\rangle = c'|N+1\rangle$$

Since $\langle N|\hat{a} = \langle N+1|c'^{*}$, we get

$$\langle N|\hat{a}\hat{a}^{+}|N\rangle = \langle N|\hat{1} - \hat{a}^{+}\hat{a}|N\rangle = 1 - N = |c'|^2$$

or

$$|c'| = \sqrt{1-N}$$

Then we have

$$\hat{a}^{+}|N\rangle = \sqrt{1-N}|N+1\rangle$$

We note that

$$\hat{a}^{+}|N\rangle = (1-N)|N+1\rangle$$

since $(1-N)^2 = 1-N$.

Under the basis of $\{|0\rangle$ and $|1\rangle\}$, we get the matrix element of $\hat{a}$ and $\hat{a}^{+}$,

$$\hat{a}|1\rangle = |0\rangle, \qquad \hat{a}|0\rangle = 0, \qquad \hat{a}^{+}|1\rangle = 0, \qquad \hat{a}^{+}|0\rangle = |1\rangle$$

the matrix representation of $\hat{a}$, $\hat{a}^{+}$, and $\hat{N}$ is given by

$$\hat{a} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{a}^{+} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad \hat{N} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$\hat{N}$ is a diagonal matrix, while $\hat{a}$ and $\hat{a}^{+}$ are not non-diagonal. The state vector is expressed by

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Can $\hat{a}$ be diagonalized in any representation? Suppose that we have an eigenstate such that

$$\hat{a}|a'\rangle = a'|a'\rangle$$

Then we have

$$\hat{a}^2|a'\rangle = a'^2|a'\rangle = 0$$

since $\hat{a}^2 = 0$. So we have $\hat{a}|a'\rangle = 0$.

Since $\hat{a}^{+}\hat{a} + \hat{a}\hat{a}^{+} = \hat{1}$ we have

$$\langle a'|\hat{a}^{+}\hat{a} + \hat{a}\hat{a}^{+}|a'\rangle = \langle a'|a'\rangle = 1,$$

or

$$\langle a'|\hat{a}\hat{a}^{+}|a'\rangle = 1.$$

However, this result contradicts with the relation

$$\langle a'|\hat{a}\hat{a}^{+}|a'\rangle = \sum_{a''}\langle a'|\hat{a}|a''\rangle\langle a''|\hat{a}^{+}|a'\rangle = 0,$$

since

$$\langle a'|\hat{a}|a''\rangle = 0.$$

9. Comparison between two formula for the CAP's relation

Two expressions (a) the formula-I and (b) the formula II are compared.

(a) **Formula-I (general definition)**

$$\hat{a}_i|n_1, n_2, n_3, ..., n_{i-1}, n_i, n_{i+1}, ..., n_s\rangle = (-1)^{s_i} n_i |n_1, n_2, n_3, ..., n_{i-1}, n_i - 1, n_{i+1}, ..., n_s\rangle$$

$$\hat{a}_i^{+}|n_1, n_2, n_3, ..., n_{i-1}, n_i, n_{i+1}, ..., n_s\rangle = (-1)^{s_i}(1-n_i)|n_1, n_2, n_3, ..., n_{i-1}, n_i + 1, n_{i+1}, ..., n_s\rangle$$

(b) **Formula-II (simple case)**

$$\hat{a}|N\rangle = N|N-1\rangle, \qquad \hat{a}^{+}|N\rangle = (1-N)|N+1\rangle$$

with $N^2 = N$.

These expressions for the formula I and formula II are the same as those reported by Schiff.

10. Examples for two and three fermions

The fermions obey the Pauli's exclusion principle. We consider two fermions occupying either the state $|0\rangle$ or state $|1\rangle$. There are four possible states;

$$|0,0\rangle = |0\rangle_1 \otimes |0\rangle_2, |0,1\rangle = |0\rangle_1 \otimes |1\rangle_2, \ |1,0\rangle = |1\rangle_1 \otimes |0\rangle_2, |1,1\rangle = |1\rangle_1 \otimes |1\rangle_2,$$

We introduce the creation and annihilation operators $\{\hat{a}_1, \hat{a}_1^{+}, \hat{a}_2, \hat{a}_2^{+}\}$, such that

$$\hat{a}_1^{\ +}|0,0\rangle = |1,0\rangle, \qquad \hat{a}_1^{\ +}|0,1\rangle = |1,1\rangle$$

$$\hat{a}_1^{\ +}|1,0\rangle = 0, \qquad \hat{a}_1^{\ +}|1,1\rangle = 0$$

$$\hat{a}_1|0,0\rangle = 0, \qquad \hat{a}_1|0,1\rangle = 0$$

$$\hat{a}_1|1,0\rangle = |0,0\rangle, \qquad \hat{a}_1|1,1\rangle = |0,1\rangle$$

$$\hat{a}_2^{\ +}|0,0\rangle = |0,1\rangle, \qquad \hat{a}_2^{\ +}|0,1\rangle = 0$$

$$\hat{a}_2^{\ +}|1,0\rangle = |1,1\rangle, \qquad \hat{a}_2^{\ +}|1,1\rangle = 0$$

$$\hat{a}_2|0,0\rangle = 0, \qquad \hat{a}_2|0,1\rangle = |0,0\rangle$$

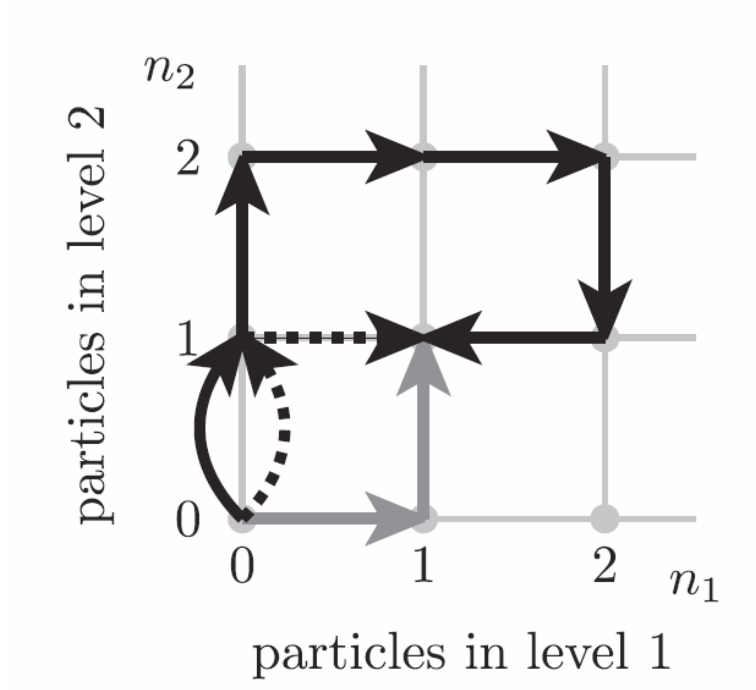
$$\hat{a}_2|1,0\rangle = 0, \qquad \hat{a}_2|1,1\rangle = |1,0\rangle$$

We consider the interchange of particles.

$$\hat{a}_2|1,1\rangle = |1,0\rangle$$

$$\hat{a}_2^{\ +}\hat{a}_1|1,0\rangle = \hat{a}_2^{\ +}|0,0\rangle = |0,1\rangle$$

$$\hat{a}_1^{\ +}\hat{a}_2^{\ +}\hat{a}_1\hat{a}_2|1,1\rangle = \hat{a}_1^{\ +}\hat{a}_2^{\ +}|0,0\rangle = \hat{a}_1^{\ +}|0,1\rangle$$



There are many different ways to create the state $|1,1\rangle$ from the state $|0,0\rangle$ using creation and annihilation operators: $\hat{a}_2^{\,+}\hat{a}_1^{\,+}$ (gray arrows), $\hat{a}_1^{\,+}\hat{a}_2^{\,+}$ (dotted arrows), and $\hat{a}_1\hat{a}_2\hat{a}_1^{\,+}\hat{a}_1^{\,+}\hat{a}_2^{\,+}\hat{a}_2^{\,+}$ (black arrows).

11. Quantum field operator for fermion

We define the quantum field operator by

$$\hat{\psi}(x) = \sum_i \langle x | \lambda^{(i)} \rangle \hat{a}_i$$

and

$$\hat{\psi}^+(x) = \sum_i \langle x | \lambda^{(i)} \rangle^* \hat{a}_i^{\,+}$$

These satisfy the following anti-commutation relations

$$[\hat{\psi}(x), \hat{\psi}^+(x')]_+ = \hat{1}\,\delta(x - x')$$

$$[\hat{\psi}(x), \hat{\psi}(x')]_+ = [\hat{\psi}^+(x), \hat{\psi}^+(x')]_+ = 0$$

The first rule can be proved as follows.

$$\begin{aligned}[\hat{\psi}(x),\hat{\psi}^{+}(x')]_{+} &= \sum_{i,j}[\hat{a}_i,\hat{a}_j^{+}]_{+}\langle x|\lambda^{(i)}\rangle\langle x'|\lambda^{(j)}\rangle^{*} \\ &= \sum_{i,j}\delta_{i,j}\langle x|\lambda^{(i)}\rangle\langle \lambda^{(j)}|x'\rangle \\ &= \sum_{i}\langle x|\lambda^{(i)}\rangle\langle \lambda^{(i)}|x'\rangle \\ &= \langle x|x'\rangle \\ &= \delta(x-x')\end{aligned}$$

((**Note**))
Physical meaning of $\hat{\psi}^{+}(x)|0\rangle$ (R.A. Jishi)

$\hat{\psi}^{+}(x)$ is defined as the operator that create a particle at the position *x*.

$$\begin{aligned}\hat{\psi}^{+}(x)|0\rangle &= \sum_{i}\langle x|\lambda^{(i)}\rangle^{*}\hat{a}_i^{+}|0\rangle \\ &= \sum_{i}\hat{a}_i^{+}|0\rangle\langle x|\lambda^{(i)}\rangle^{*} \\ &= \sum_{i}|\lambda^{(i)}\rangle\langle x|\lambda^{(i)}\rangle^{*} \\ &= \sum_{i}|\lambda^{(i)}\rangle\langle \lambda^{(i)}|x\rangle \\ &= |x\rangle\end{aligned}$$

or

$$\hat{\psi}^{+}(x)|0\rangle = |x\rangle$$

where

$$\hat{a}_i^{+}|0\rangle = |\lambda^{(i)}\rangle$$

12. Second quantization based on the quantum field operator
(a) The expansion formula I of Slater determinant

$$\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, ..., n_s; n \rangle$$
$$= \frac{1}{\sqrt{n}} \sum_{i=1}^{\infty} \langle x_1 | \lambda^{(i)} \rangle n_i (-1)^{s_i} \langle x_2, x_3, ..., x_{i-1}, x_i, x_{i+1}, ...; n-1 | n_1, n_2, n_3, ..., n_{i-1}, n_i - 1, n_{i+1}, ..., n_s; n-1 \rangle$$

(b) Annihilation operator

$$\hat{a}_i | n_1, n_2, n_3, ..., n_{i-1}, n_i, n_{i+1}, ..., n_s; n \rangle = (-1)^{s_i} n_i | n_1, n_2, n_3, ..., n_{i-1}, n_i - 1, n_{i+1}, ..., n_s; n-1 \rangle$$

(c) Quantum field operator

$$\hat{\psi}(x) = \sum_i \langle x | \lambda^{(i)} \rangle \hat{a}_i$$

(d) Second quantization:

From the above equations we can calculate

$$\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, ..., n_s; n \rangle$$
$$= \frac{1}{\sqrt{n}} \sum_{i=1}^{\infty} \langle x_1 | \lambda^{(i)} \rangle n_i (-1)^{s_i} \langle x_2, x_3, ..., x_{i-1}, x_i, x_{i+1}, ...; n-1 | n_1, n_2, n_3, ..., n_{i-1}, n_i - 1, n_{i+1}, ..., n_s; n-1 \rangle$$
$$= \frac{1}{\sqrt{n}} \sum_{i=1} \langle x_2, x_3, ..., x_{i-1}, x_i, x_{i+1}, ...; n-1 | \langle x_1 | \lambda^{(i)} \rangle n_i (-1)^{s_i} | n_1, n_2, n_3, ..., n_{i-1}, n_i - 1, n_{i+1}, ..., n_s; n-1 \rangle$$
$$= \frac{1}{\sqrt{n}} \sum_{i=1} \langle x_2, x_3, ..., x_{i-1}, x_i, x_{i+1}, ...; n-1 | \langle x_1 | \lambda^{(i)} \rangle \hat{a}_i | n_1, n_2, n_3, ..., n_i, ..., n_s; n \rangle$$
$$= \frac{1}{\sqrt{n}} \langle x_2, x_3, ..., x_{i-1}, x_i, x_{i+1}, ...; n-1 | \hat{\psi}(x_1) | n_1, n_2, n_3, ..., n_i, ..., n_s; n \rangle$$

In other words, we have

$$\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, ..., n_s; n \rangle$$
$$= \frac{1}{\sqrt{n}} \langle x_2, x_3, ..., x_{i-1}, x_i, x_{i+1}, ...; n-1 | \hat{\psi}(x_1) | n_1, n_2, n_3, ..., n_i, ..., n_s; n \rangle$$

Similarly, we have

$$\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, ..., n_s; n \rangle$$
$$= \frac{1}{\sqrt{n(n-1)}} \langle x_3, ..., x_{i-1}, x_i, x_{i+1}, ...; n-1 | \hat{\psi}(x_2) \hat{\psi}(x_1) | n_1, n_2, n_3, ..., n_i, ..., n_s; n \rangle$$

$$\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle$$
$$= \frac{1}{\sqrt{n(n-1)(n-2)}} \langle x_4, ..., x_{i-1}, x_i, x_{i+1}, ...; n-1 | \hat{\psi}(x_3)\hat{\psi}(x_2)\hat{\psi}(x_1) | n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle$$

……………………………………………………………………………..

By induction, we have

$$\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle$$
$$= \frac{1}{\sqrt{n!}} \langle 0 | \hat{\psi}(x_n)\hat{\psi}(x_{n-1})...\hat{\psi}(x_2)\hat{\psi}(x_1) | n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle$$

or

$$\hat{A} | x_1, x_2, x_3, ..., x_n; n\rangle = \frac{1}{\sqrt{n!}} \hat{\psi}(x_1)\hat{\psi}(x_2)...\hat{\psi}(x_n) | 0\rangle$$

where A denotes the anti-symmetrizing operator. The Fox state can be expressed by

$$| n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle = \int dx_1 ... \int dx_n | x_1, x_2, x_3, ..., x_n; n\rangle\langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle$$
$$= \int dx_1 ... \int dx_n \Psi^{(n)}(x_1, x_2, x_3, ..., x_n; n) | x_1, x_2, x_3, ..., x_n; n\rangle$$

where we use the closure relation $\int dx_1 ... \int dx_n | x_1, x_2, x_3, ..., x_n; n\rangle\langle x_1, x_2, x_3, ..., x_n; n | = \hat{1}$. We will show that

$$\Psi^{(n)}(x_1, x_2, x_3, ..., x_n; n) = \langle x_1, x_2, x_3, ..., x_n; n | n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle$$

satisfies the Schrödinger equation of many-particle system. So the method of second quantization is an appropriate method for discussing the many-body problem.

13. Expressions of $\langle x_1, x_2, ..., x_n | x_1', x_2', ..., x_n'\rangle$

In general, we have

$$\hat{A} | x_1, x_2, x_3, ..., x_n\rangle = \frac{1}{\sqrt{n!}} \hat{\psi}^+(x_n).....\hat{\psi}^+(x_1) | 0\rangle$$

and

$$\langle x_1, x_2, ..., x_n | x_1', x_2', ..., x_n' \rangle = \frac{1}{n!} \langle 0 | \hat{\psi}(x_1) ...... \hat{\psi}(x_n) \hat{\psi}^+(x_n') ...... \hat{\psi}^+(x_1') | 0 \rangle$$

Suppose that

$$|x_1, x_2, x_3\rangle = \frac{1}{\sqrt{3!}} \hat{\psi}^+(x_3) \hat{\psi}^+(x_2) \hat{\psi}^+(x_1) |0\rangle$$

$$\begin{aligned} |x_1, x_3, x_2\rangle &= \frac{1}{\sqrt{3!}} \hat{\psi}^+(x_2) \hat{\psi}^+(x_3) \hat{\psi}^+(x_1) |0\rangle \\ &= -\frac{1}{\sqrt{3!}} \hat{\psi}^+(x_3) \hat{\psi}^+(x_2) \hat{\psi}^+(x_1) |0\rangle \qquad \text{(antisymmetric)} \\ &= -|x_1, x_2, x_3\rangle \end{aligned}$$

$$\begin{aligned} |x_1, x_2\rangle &= \frac{1}{\sqrt{2!}} \hat{\psi}^+(x_2) \hat{\psi}^+(x_1) |0\rangle \\ &= \frac{1}{\sqrt{2}} \frac{1}{V} \sum_{k_1, k_2} e^{-ik_2 \cdot x_2} e^{-ik_1 \cdot x_1} \hat{b}_{k_2}{}^+ \hat{b}_{k_1}{}^+ |0\rangle \end{aligned}$$

$$\langle x_1, x_2| = \frac{1}{\sqrt{2}} \frac{1}{V} \sum_{k_1, k_2} e^{ix_2 \cdot x_2} e^{ix_1 \cdot x_1} \langle 0| \hat{b}_{k_1} \hat{b}_{k_2}$$

$$\begin{aligned} \langle x_1 | x_1' \rangle &= \langle 0 | \hat{\psi}(x_1) \hat{\psi}^+(x_1') | 0 \rangle \\ &= \langle 0 | -\hat{\psi}^+(x_1') \hat{\psi}(x_1) + \delta(x_1 - x_1') | 0 \rangle \\ &= \delta(x_1 - x_1') \langle 0 | 0 \rangle \\ &= \delta(x_1 - x_1') \end{aligned}$$

$$\langle x_1,x_2|x_1',x_2'\rangle = \frac{1}{2!}\langle 0|\hat{\psi}(x_2)\hat{\psi}(x_1)\hat{\psi}^+(x_1')\hat{\psi}^+(x_2')|0\rangle$$
$$= \frac{1}{2}\langle 0|\hat{\psi}(x_2)\{-\hat{\psi}^+(x_1')\hat{\psi}(x_1)+\delta(x_1-x_1')\}\hat{\psi}^+(x_2')|0\rangle$$
$$= -\frac{1}{2}\langle 0|\hat{\psi}(x_2)\hat{\psi}^+(x_1')\hat{\psi}(x_1)\hat{\psi}^+(x_2')|0\rangle + \frac{1}{2}\langle 0|\hat{\psi}(x_2)\hat{\psi}^+(x_2')|0\rangle\delta(x_1-x_1')$$
$$= -\frac{1}{2}\langle 0|\hat{\psi}(x_2)\hat{\psi}^+(x_1')\{-\hat{\psi}^+(x_2')\hat{\psi}(x_1)+\delta(x_1-x_2')\}|0\rangle$$
\
$$+\frac{1}{2}\langle 0|\hat{\psi}(x_2)\hat{\psi}^+(x_2')|0\rangle\delta(x_1-x_1')$$
$$= -\frac{1}{2}\delta(x_1-x_2')\langle 0|\hat{\psi}(x_2)\hat{\psi}^+(x_1')|0\rangle + \frac{1}{2}\langle 0|\hat{\psi}(x_2)\hat{\psi}^+(x_2')|0\rangle\delta(x_1-x_1')$$
$$= \frac{1}{2}[-\delta(x_1-x_2')\delta(x_2-x_1')+\delta(x_1-x_1')\delta(x_2-x_2')]$$

and

$$\langle x_1,x_2|\Psi\rangle = \int dx_1'\int dx_2'\langle x_1,x_2|x_1',x_2'\rangle\langle x_1',x_2'|\Psi\rangle$$
$$= \int dx_1'\int dx_2'\langle x_1',x_2'|\Psi\rangle[\frac{1}{2}[-\delta(x_1-x_2')\delta(x_2-x_1')$$
$$+\delta(x_1-x_1')\delta(x_2-x_2')]$$
$$= \frac{1}{2}[\langle x_1,x_2|\Psi\rangle - \langle x_2,x_1|\Psi\rangle]$$

In general (lemma), we have

$$\langle x_1,x_2,...,x_n|x_1',x_2',...,x_m'\rangle = \langle 0|\hat{\psi}(x_1)...\hat{\psi}(x_n)\hat{\psi}^+(x_n')...\hat{\psi}^+(x_1')|0\rangle$$
$$= \sum_{P_n}\text{sgn}(P_n)\delta(x_1-x_1')\delta(x_2-x_2').......\delta(x_n-x_n')$$

where the sum is to be taken over all permutations P_n of the co-ordinates $x_1,x_2,...,x_n$, $\text{sgn}(P_n)$ is the sign of the permutation. For bosons, $\text{sgn}(P_n)=1$. For fermions, $\text{sgn}(P_n)=1$ if the permutation is even and $\text{sgn}(P_n)=-1$ if it is odd (**Merzbacher**, Quantum Mechanics).

14. One-particle state and two-particle state using the quantum field operator

The occupation operator is defined by

$$\hat{N} = \int dx\,\hat{\psi}^+(x)\hat{\psi}(x)$$

This can be rewritten as

$$\begin{aligned}\hat{N} &= \sum_{k,l} \hat{a}_k{}^+ \hat{a}_l \int dx \langle \phi_k | x \rangle \langle x | \phi_k \rangle \\ &= \sum_{k,l} \hat{a}_k{}^+ \hat{a}_l \delta_{k,l} \\ &= \sum_{k} \hat{a}_k{}^+ \hat{a}_k \\ &= \sum_{k} \hat{N}_k\end{aligned}$$

and

$$\begin{aligned}\hat{N}|n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle &= \sum_k \hat{N}_k |n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle \\ &= \sum_k n_k |n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle \\ &= N|n_1, n_2, n_3, ..., n_i, ..., n_s; n\rangle\end{aligned}$$

So the definition of the operator $\hat{N}$ is appropriate.
The commutation relations (but not the anti-commutation relation) are given by

$$[\hat{N}, \hat{\psi}^+(x)] = \hat{\psi}^+(x), \qquad [\hat{N}, \hat{\psi}(x)] = -\hat{\psi}(x)$$

((**Proof**))

$$\begin{aligned}[\hat{N}, \hat{\psi}^+(x)] &= \int dx' [\hat{\psi}^+(x')\hat{\psi}(x'), \hat{\psi}^+(x)] \\ &= \int dx' \delta(x - x')\hat{\psi}^+(x') \\ &= \hat{\psi}^+(x)\end{aligned}$$

since

$$\begin{aligned}[\hat{\psi}^+(x')\hat{\psi}(x'), \hat{\psi}^+(x)] &= \hat{\psi}^+(x')\hat{\psi}(x')\hat{\psi}^+(x) - \hat{\psi}^+(x)\hat{\psi}^+(x')\hat{\psi}(x') \\ &= \hat{\psi}^+(x')\hat{\psi}(x')\hat{\psi}^+(x) + \hat{\psi}^+(x')\hat{\psi}^+(x)\hat{\psi}(x') \\ &= \hat{\psi}^+(x')[\hat{\psi}(x'), \hat{\psi}^+(x)]_+ \\ &= \delta(x - x')\hat{\psi}^+(x')\end{aligned}$$

Similarly,

$$[\hat{N},\hat{\psi}(x)] = \int dx'[\hat{\psi}^+(x')\hat{\psi}(x'),\hat{\psi}(x)]$$
$$= -\int dx'\delta(x-x')\hat{\psi}(x')$$
$$= -\hat{\psi}(x)$$

since

$$[\hat{\psi}^+(x')\hat{\psi}(x'),\hat{\psi}(x)] = \hat{\psi}^+(x')\hat{\psi}(x')\hat{\psi}(x) - \hat{\psi}(x)\hat{\psi}^+(x')\hat{\psi}(x')$$
$$= -\hat{\psi}^+(x')\hat{\psi}(x)\hat{\psi}(x') - \hat{\psi}(x)\hat{\psi}^+(x')\hat{\psi}(x')$$
$$= -[\hat{\psi}(x),\hat{\psi}^+(x')]_+\hat{\psi}(x')$$
$$= -\delta(x-x')\hat{\psi}(x')$$

Thus we get

$$[\hat{N},\hat{\psi}^+(x)]|0\rangle = \hat{\psi}^+(x)|0\rangle$$

or

$$\hat{N}\hat{\psi}^+(x)]|0\rangle = \hat{\psi}^+(x)|0\rangle$$

since

$$\hat{N}|0\rangle = 0$$

So $\hat{\psi}^+(x)|0\rangle$ is the eigenket of $\hat{N}$ with the eigenvalue 1. It is the one-particle state. Similarly

$$\hat{\psi}^+(x_1)\hat{\psi}^+(x_2)|0\rangle$$

is a two-particle state. In general,

$$\frac{1}{\sqrt{n!}}\hat{\psi}^+(x_1)\hat{\psi}^+(x_2)...\hat{\psi}^+(x_n)|0\rangle$$

is the *n*-particle ket state. In other words,

$$\frac{1}{\sqrt{n!}}\langle 0|\hat{\psi}(x_n)\hat{\psi}(x_{n-1})...\hat{\psi}(x_1)$$

is the n-particle bra state.

15. Representation of operators

We consider the matrix representation of the operator $\hat{F}$

$$\langle x_1', x_2',,..., x_n'|\hat{F}|x_1, x_2,,..., x_n\rangle = \delta(x_1 - x_1')\delta(x_2 - x_2')........\delta(x_n - x_n')F(x_1, x_2,,..., x_n)$$

Using the basis,

$$\hat{A}|x_1, x_2,....;n\rangle = \frac{1}{\sqrt{n!}}\hat{\psi}^+(x_1)\hat{\psi}^+(x_2).....\hat{\psi}^+(x_n)|0\rangle_F \qquad \text{(fermions)}$$

the above matrix element can be rewritten as

$$\begin{aligned}
\langle n_1', n_2',...|\hat{F}|n_1, n_2,...\rangle &= \int dx_1.....\int dx_n \int dx_1'.....\int dx_n' \langle n_1', n_2',...|x_1', x_2',,..., x_n'\rangle \\
&\quad \times \langle x_1', x_2',,..., x_n'|\hat{F}|x_1, x_2,,..., x_n\rangle\langle x_1, x_2,,..., x_n|n_1, n_2,...\rangle \\
&= \int dx_1.....\int dx_n \langle n_1', n_2',...|x_1, x_2,,..., x_n\rangle F(x_1, x_2,,..., x_n)\langle x_1, x_2,,..., x_n|n_1, n_2,...\rangle \\
&= \frac{1}{n!}\int dx_1.....\int dx_n \langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1}).....\hat{\psi}^+(x_1) \\
&\quad F(x_1, x_2,,..., x_n)\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1, n_2,...\rangle \\
&= \frac{1}{n!}\int dx_1.....\int dx_n \langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1}).....\hat{\psi}^+(x_1)|0\rangle \\
&\quad F(x_1, x_2,,..., x_n)\langle 0|\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1, n_2,...\rangle
\end{aligned}$$

where $n_1 + n_2 + ... = n_1' + n_2'' + ... = n$, and $\hat{\psi}(x_n)\hat{\psi}(x_{n-1}).....\hat{\psi}(x_1)|n_1, n_2,...\rangle$ has a non-vanishing component only on the no-particle state $|0\rangle$. Note that

$$\langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1}).....\hat{\psi}^+(x_1)F(x_1,x_2,,...,x_n)\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1,n_2,...\rangle$$
$$= \sum_{k'}\langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1}).....\hat{\psi}^+(x_1)F(x_1,x_2,,...,x_n)|k_1',k_2',...\rangle\langle k_1',k_2',...|\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1,n_2,...\rangle$$
$$= \langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1}).....\hat{\psi}^+(x_1)F(x_1,x_2,,...,x_n)|0\rangle\langle 0|\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1,n_2,...\rangle$$
$$= \langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1}).....\hat{\psi}^+(x_1)|0\rangle F(x_1,x_2,,...,x_n)\langle 0|\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1,n_2,...\rangle$$

(a) Suppose that $F(x_1,x_2,,...,x_n)$ is given by the form

$$F(x_1,x_2,,...,x_n) = \sum_{i=1}^{n} f(x_i)$$

Then we get

$$\langle n_1', n_2',...|\hat{F}|n_1,n_2,...\rangle = \frac{1}{n!}\int dx_1.....\int dx_n\langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1}).....\hat{\psi}^+(x_1)$$
$$\sum_{i=1}^{n} f(x_i)\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1,n_2,...\rangle$$

Now we consider the term given by

$$\int dx_1.....\int dx_n\langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_1)\, f(x_n)\hat{\psi}^+(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1,n_2,...\rangle$$

which can be simplified since the integration yields the number operator $\hat{N}$. The integration over x_1 yields

$$\int dx_1\hat{\psi}^+(x_1)\hat{\psi}(x_1) = \hat{N}\,.$$

Using this, we have the integrant after the integration over x_1,

$$\int dx_2.....\int dx_n\langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_2)\, f(x_n)\hat{N}\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1,n_2,...\rangle$$
$$= \int dx_2.....\int dx_n\langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_2)\, f(x_n)\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1,n_2,...\rangle$$

since $\hat{N}\hat{\psi}(x_2).....\hat{\psi}(x_n)|n_1,n_2,...\rangle$ is the one-particle state. The integration over x_2 leads to the number operator

$$\int dx_2\hat{\psi}^+(x_2)\hat{\psi}(x_2) = \hat{N}\,.$$

Using this, we get

$$\int dx_3.....\int dx_n \langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_3) f(x_n)\hat{N}\hat{\psi}(x_3).....\hat{\psi}(x_n)|n_1, n_2,...\rangle$$
$$= 2\langle n_1', n_2',...|\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_3) f(x_n)\hat{\psi}(x_3).....\hat{\psi}(x_n)|n_1, n_2,...\rangle$$

since $\hat{N}\hat{\psi}(x_3).....\hat{\psi}(x_n)|n_1, n_2,...\rangle$ is the two-particle state. After integrating over the variables x_1, x_2, …, x_{n-1}, we get

$$(n-1)!\int dx_n \langle n_1', n_2',...|\hat{\psi}^+(x_n) f(x_n)\hat{\psi}(x_n)|n_1, n_2,...\rangle$$

which leads to

$$\langle n_1', n_2',...|\hat{F}|n_1, n_2,...\rangle = \frac{1}{n}\sum_{i=1}^{n}\langle n_1', n_2',...|\int dx_1\hat{\psi}^+(x_i) f(x_i)\hat{\psi}(x_i)|n_1, n_2,...\rangle$$
$$= \langle n_1', n_2',...|\int dx\hat{\psi}^+(x) f(x)\hat{\psi}(x)|n_1, n_2,...\rangle$$

or

$$\hat{F} = \int dx\hat{\psi}^+(x) f(x)\hat{\psi}(x)$$

(b) Suppose that F is given by the form

$$F(x_1, x_2,..., x_n) = \sum_{i<j} V(x_i, x_j) = \frac{1}{2}\sum_{\substack{i,j \\ i\neq j}} V(x_i, x_j)$$

The matrix element:

$$\langle n_1', n_2',...|\hat{F}|n_1, n_2,...\rangle = \frac{1}{n(n-1)}\langle n_1', n_2',...|\sum_{i<j}\int dx_i\int dx_j\hat{\psi}^+(x_i)\hat{\psi}^+(x_j)V(x_i, x_j)\hat{\psi}(x_j)\hat{\psi}(x_i)|n_1, n_2,...\rangle$$
$$= \langle n_1', n_2',...|\frac{1}{2}\int dx'\int dx\hat{\psi}^+(x')\hat{\psi}^+(x)V(x, x')\hat{\psi}(x)\hat{\psi}(x')|n_1, n_2,...\rangle$$

So that

$$\hat{F} = \frac{1}{2}\int dx'\int dx \hat{\psi}^+(x')\hat{\psi}^+(x)V(x,x')\hat{\psi}(x)\hat{\psi}(x').$$

The order of $\hat{\psi}^+(x')\hat{\psi}^+(x)\hat{\psi}(x)\hat{\psi}(x')$ is of importance since it implies that there is no self-interaction [i.e., there is not form such as $V(x_i, x_i)$]. This form guarantees the hermiticity of the operator F in the Fock space.

Then the Hamiltonian in the Fock space is given by

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

with

$$\hat{H}_0 = \int dx \hat{\psi}^+(x)[-\frac{\hbar^2}{2\mu}\nabla^2 + V(x)]\hat{\psi}(x)$$

$$\hat{H}_1 = \frac{1}{2}\int dx'\int dx \hat{\psi}^+(x')\hat{\psi}^+(x)V(x,x')\hat{\psi}(x)\hat{\psi}(x')$$

16. Simultaneous eigenket of $\hat{H}$ and $\hat{N}$

Since

$$[\hat{H}, \hat{N}] = 0$$

we have a simultaneous eigenket; $\left|\Psi^{(n)}(t)\right\rangle = \left|n_1, n_2, ..., t\right\rangle$

$$\hat{H}\left|\Psi^{(n)}(t)\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\Psi^{(n)}(t)\right\rangle,$$

$$\hat{N}\left|\Psi^{(n)}(t)\right\rangle = N\left|\Psi^{(n)}(t)\right\rangle$$

Note that

$$\begin{aligned}\left|\Psi^{(n)}(t)\right\rangle &= \int dx_1.....\int dx_n \left|x_1, x_2,..., x_n\right\rangle\left\langle x_1, x_2,..., x_n\right| n_1, n_2,..;t\rangle \\ &= \int dx_1.....\int dx_n \Psi^{(n)}(x_1, x_2,..., x_n, t)\left|x_1, x_2,..., x_n\right\rangle \\ &= \frac{1}{\sqrt{n!}}\int dx_1.....\int dx_n \Psi^{(n)}(x_1, x_2,..., x_n; t)[\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_1)\left|0\right\rangle]\end{aligned}$$

where

$$\begin{aligned}\Psi^{(n)}(x_1, x_2,..., x_n; t) &= \left\langle x_1, x_2,..., x_n \right| n_1, n_2,.., t\rangle \\ &= \left\langle x_1, x_2,..., x_n \right|\Psi^{(n)}(t)\rangle \\ &= \frac{1}{\sqrt{n!}}\left\langle 0\right|\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)\left|\Psi^{(n)}(t)\right\rangle\end{aligned}$$

((**Note**))

$$\begin{aligned}&\frac{1}{\sqrt{n!}}\left\langle 0\right|\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)\left|\Psi^{(n)}(t)\right\rangle \\ &= \frac{1}{n!}\int dx_1'.....\int dx_n'\Psi^{(n)}(x_1', x_2',..., x_n'; t)\left\langle 0\right|\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)\hat{\psi}^+(x_n')\hat{\psi}^+(x_{n-1}')...\hat{\psi}^+(x_1)\left|0\right\rangle.\end{aligned}$$

We need to calculate

$$\left\langle 0\right|\hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n)\hat{\psi}^+(x_n')\hat{\psi}^+(x_{n-1}')...\hat{\psi}^+(x_1)\left|0\right\rangle$$

For example, we consider the simple case (for fermions)

$$\begin{aligned}\frac{1}{\sqrt{2!}}\left\langle 0\right|\hat{\psi}(x_1)\hat{\psi}(x_2)\left|\Psi(t)\right\rangle &= \frac{1}{\sqrt{2!}}\left\langle 0\right|\hat{\psi}(x_1)\hat{\psi}(x_2)\frac{1}{\sqrt{2!}}\int dx_1'\int dx_2'\Psi^{(2)}(x_1', x_2')\hat{\psi}^+(x_2')\hat{\psi}^+(x_1')\left|0\right\rangle \\ &= \frac{1}{2!}\int dx_1'\int dx_2'\Psi^{(2)}(x_1', x_2')\left\langle 0\right|\hat{\psi}(x_1)\hat{\psi}(x_2)\hat{\psi}^+(x_2')\hat{\psi}^+(x_1')\left|0\right\rangle \\ &= \frac{1}{2!}\int dx_1'\int dx_2'\Psi^{(2)}(x_1', x_2')[\delta(x_2 - x_2')\delta(x_1 - x_1') - \delta(x_2 - x_1')\delta(x_1 - x_2')] \\ &= \frac{1}{2!}[\Psi^{(2)}(x_1, x_2) - \Psi^{(2)}(x_2, x_1)]\end{aligned}$$

which corresponds to the antisymmetric wave function for fermions, where

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2!}}\int dx_1'\int dx_2'\Psi^{(2)}(x_1',x_2')\hat{\psi}^+(x_2')\hat{\psi}^+(x_1')|0\rangle.$$

and

$$\begin{aligned}
\langle 0|\hat{\psi}(x_1)\hat{\psi}(x_2)\hat{\psi}^+(x_2')\hat{\psi}^+(x_1')|0\rangle &= \langle 0|\hat{\psi}(x_1)\{[\hat{\psi}(x_2),\hat{\psi}^+(x_2')]_+ - \hat{\psi}^+(x_2')\hat{\psi}(x_2)\}\hat{\psi}^+(x_1')|0\rangle \\
&= \langle 0|\hat{\psi}(x_1)\{\delta(x_2 - x_2') - \hat{\psi}^+(x_2')\hat{\psi}(x_2)\}\hat{\psi}^+(x_1')|0\rangle \\
&= \delta(x_2 - x_2')\langle 0|\hat{\psi}(x_1)\hat{\psi}^+(x_1')|0\rangle - \langle 0|\hat{\psi}(x_1)\hat{\psi}^+(x_2')\hat{\psi}(x_2)\hat{\psi}^+(x_1')|0\rangle \\
&= \delta(x_2 - x_2')\langle 0|\{[\hat{\psi}(x_1),\hat{\psi}^+(x_1')]_+ - \hat{\psi}^+(x_1')\hat{\psi}(x_1)\}|0\rangle \\
&\quad - \langle 0|\hat{\psi}(x_1)\hat{\psi}^+(x_2')\{[\hat{\psi}(x_2),\hat{\psi}^+(x_1')] - \hat{\psi}^+(x_1')\hat{\psi}(x_2)|0\rangle \\
&= \delta(x_2 - x_2')\delta(x_1 - x_1') - \delta(x_2 - x_1')\langle 0|\hat{\psi}(x_1)\hat{\psi}^+(x_2')|0\rangle \\
&= \delta(x_2 - x_2')\delta(x_1 - x_1') - \delta(x_2 - x_1')\langle 0|\{[\hat{\psi}(x_1)\hat{\psi}^+(x_2')]_+ - \hat{\psi}^+(x_2')\hat{\psi}(x_1)\}|0\rangle \\
&= \delta(x_2 - x_2')\delta(x_1 - x_1') - \delta(x_2 - x_1')\delta(x_1 - x_2')
\end{aligned}$$

In general case

$$\langle x_1, x_2, ..., x_n | x_1', x_2', ..., x_m' \rangle_F = \delta_{n,m}\frac{1}{n}\sum_{\{P\}}\text{sgn}(P)\delta(x_1' - x_1)\delta(x_2' - x_2)....\delta(x_n' - x_n)$$

(fermion)

where the index F denotes the fermion. $\text{sgn}(P)$ is equal to 1 for even permutation and is equal to -1 for odd permutation.

17. Commutation relation: $[\hat{H}_0, \hat{\psi}^+(x)] = H_i\hat{\psi}^+(x_i)$

We use the notation

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

for the commutation relation. We show that

$$[\hat{H}_0, \hat{\psi}^+(x_i)] = H_i\hat{\psi}^+(x_i)$$

((**Proof**))

$$[\hat{H}_0, \hat{\psi}^+(x_i)] = [\sum_k \varepsilon_k \hat{N}_k, \sum_{k'} \hat{a}_{k'}{}^+ \phi_{k'}{}^*(x_i)]$$
$$= \sum_{k,k'} \varepsilon_k \phi_{k'}{}^*(x_i)[\hat{N}_k, \hat{a}_{k'}{}^+]$$
$$= \sum_{k,k'} \varepsilon_k \phi_{k'}{}^*(x_i)\hat{a}_k{}^+ \delta_{k,k'}$$
$$= \sum_k \varepsilon_k \phi_k{}^*(x_i)\hat{a}_k{}^+$$

$$H_i(x_i)\hat{\psi}^+(x_i) = H_i(x_i)\sum_k \hat{a}_k{}^+ \phi_k{}^*(x_i)$$
$$= \sum_k \varepsilon_k \phi_k{}^*(x_i)\hat{a}_{k'}{}^+$$

where

$$H_i(x_i)\phi_k{}^*(x_i) = \varepsilon_k \phi_k{}^*(x_i)$$

$$[\hat{N}_k, \hat{a}_{k'}{}^+] = \hat{a}_k{}^+ \delta_{k,k'}, \qquad [\hat{N}_k, \hat{a}_{k'}] = -\hat{a}_k \delta_{k,k'}$$

((**Note**)) The proof of the following commutation relations are given before.

$$[\hat{N}, \hat{a}] = -\hat{a}, \qquad [\hat{N}, \hat{a}^+] = \hat{a}^+.$$

((**Proof-1**))

$$[\hat{N}_k, \hat{a}_{k'}{}^+] = \hat{a}_k{}^+ \hat{a}_k \hat{a}_{k'}{}^+ - \hat{a}_{k'}{}^+ \hat{a}_k{}^+ \hat{a}_k$$
$$= \hat{a}_k{}^+(-\hat{a}_{k'}{}^+ \hat{a}_k + \delta_{k,k'}) - \hat{a}_{k'}{}^+ \hat{a}_k{}^+ \hat{a}_k$$
$$= -\hat{a}_k{}^+ \hat{a}_{k'}{}^+ \hat{a}_k - \hat{a}_{k'}{}^+ \hat{a}_k{}^+ \hat{a}_k + \hat{a}_k{}^+ \delta_{k,k'}$$
$$= -[\hat{a}_k{}^+, \hat{a}_{k'}{}^+]_+ \hat{a}_k + \hat{a}_k{}^+ \delta_{k,k'}$$
$$= \hat{a}_k{}^+ \delta_{k,k'}$$

((**Proof-2**))

$$
\begin{aligned}
[\hat{N}_k, \hat{a}_{k'}] &= \hat{a}_k{}^+ \hat{a}_k \hat{a}_{k'} - \hat{a}_{k'} \hat{a}_k{}^+ \hat{a}_k \\
&= \hat{a}_k{}^+ \hat{a}_k \hat{a}_{k'} - (-\hat{a}_k{}^+ \hat{a}_{k'} + \delta_{k,k'}) \hat{a}_k \\
&= \hat{a}_k{}^+ \hat{a}_k \hat{a}_{k'} + \hat{a}_k{}^+ \hat{a}_{k'} \hat{a}_k - \hat{a}_k \delta_{k,k'} \\
&= \hat{a}_k{}^+ [\hat{a}_k, \hat{a}_{k'}{}^+] - \hat{a}_k \delta_{k,k'} \\
&= -\hat{a}_k \delta_{k,k'}
\end{aligned}
$$

Using this relation,

$$
[\hat{H}_0, \hat{\psi}^+(x_i)] = H_i \hat{\psi}^+(x_i)
$$

we can calculate the following term

$$
\begin{aligned}
\hat{H}_0 \hat{\psi}^+(x_1) \hat{\psi}^+(x_2) \hat{\psi}^+(x_3) |0\rangle &= \{[\hat{H}_0, \hat{\psi}^+(x_1)] + \hat{\psi}^+(x_1) \hat{H}_0\} \hat{\psi}^+(x_2) \hat{\psi}^+(x_3) |0\rangle \\
&= \{H_0(x_1) \hat{\psi}^+(x_1) + \hat{\psi}^+(x_1) \hat{H}_0\} \hat{\psi}^+(x_2) \hat{\psi}^+(x_3) |0\rangle \\
&= H_0(x_1) \hat{\psi}^+(x_1) \hat{\psi}^+(x_2) \hat{\psi}^+(x_3) |0\rangle \\
&\quad + \hat{\psi}^+(x_1) \hat{H}_0 \hat{\psi}^+(x_2) \hat{\psi}^+(x_3) |0\rangle
\end{aligned}
$$

The second term of this equation can be rewritten as

$$
\begin{aligned}
\hat{\psi}^+(x_1) \hat{H}_0 \hat{\psi}^+(x_2) \hat{\psi}^+(x_3) |0\rangle &= \hat{\psi}^+(x_1) \{[\hat{H}_0, \hat{\psi}^+(x_2)] + \hat{\psi}^+(x_2) \hat{H}_0\} \hat{\psi}^+(x_3) |0\rangle \\
&= \hat{\psi}^+(x_1) \{H_0(x_2) \hat{\psi}^+(x_2) + \hat{\psi}^+(x_2) \hat{H}_0\} \hat{\psi}^+(x_3) |0\rangle \\
&= \hat{\psi}^+(x_1) H_0(x_2) \hat{\psi}^+(x_2) \hat{\psi}^+(x_3) |0\rangle \\
&\quad + \hat{\psi}^+(x_1) \hat{\psi}^+(x_2) \hat{H}_0 \hat{\psi}^+(\mathbf{r}_3) |0\rangle
\end{aligned}
$$

Again the second term of this equation is

$$
\begin{aligned}
\hat{\psi}^+(x_1) \hat{\psi}^+(x_2) \hat{H}_0 \hat{\psi}^+(x_3) |0\rangle &= \hat{\psi}^+(x_1) \hat{\psi}^+(x_2) \{[\hat{H}_0, \hat{\psi}^+(x_3)] + \hat{\psi}^+(x_3) \hat{H}_0\} |0\rangle \\
&= \hat{\psi}^+(x_1) \hat{\psi}^+(x_2) H_0(x_3) \hat{\psi}^+(x_3) |0\rangle \\
&\quad + \hat{\psi}^+(x_1) \hat{\psi}^+(x_2) \hat{\psi}^+(x_3) \hat{H}_0 |0\rangle \\
&= \hat{\psi}^+(x_1) \hat{\psi}^+(x_2) H_0(x_3) \hat{\psi}^+(x_3) |0\rangle
\end{aligned}
$$

since $\hat{H}_0 |0\rangle = 0$. Thus we have

$$\hat{H}_0\hat{\psi}^+(x_1)\hat{\psi}^+(x_2)\hat{\psi}^+(x_3)\left|0\right\rangle = H_0(x_1)\hat{\psi}^+(x_1)\hat{\psi}^+(x_2)\hat{\psi}^+(x_3)\left|0\right\rangle$$
$$+\hat{\psi}^+(x_1)H_0(x_2)\hat{\psi}^+(x_2)\hat{\psi}^+(x_3)\left|0\right\rangle$$
$$+\hat{\psi}^+(x_1)\hat{\psi}^+(x_2)H_0(x_3)\hat{\psi}^+(x_3)\left|0\right\rangle$$
$$=\sum_{i=1}^{3}H_0(x_i)\hat{\psi}^+(x_1)\hat{\psi}^+(x_2)\hat{\psi}^+(x_3)\left|0\right\rangle$$

In general we have

$$\hat{H}_0\hat{\psi}^+(x_1)\hat{\psi}^+(x_2)....\hat{\psi}^+(x_n)\left|0\right\rangle = \sum_{i=1}^{n}H_0(x_i)\hat{\psi}^+(x_1)\hat{\psi}^+(x_2)...\hat{\psi}^+(x_n)\left|0\right\rangle$$

where

$$H_0(x_i) = -\frac{\hbar^2}{2m}\nabla_i^{\ 2} + V(x_i)\,.$$

Schrödinger equation for n-particle system;

$$i\hbar\frac{\partial}{\partial t}\psi(x_1, x_2,..., x_n;t) = H_{on}\psi(x_1, x_2,..., x_n;t)\,,$$

where

$$H_{on} = \sum_{i=1}^{n}H_0(x_i)$$

18. Application of $\hat{H}_0$ operator on Schrödinger equation

Schrödinger equation

$$\hat{H}\left|\Psi(t)\right\rangle = i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle, \qquad \hat{N}\left|\Psi(t)\right\rangle = N\left|\Psi(t)\right\rangle$$

$$\hat{H}\left|\Psi(t)\right\rangle = \frac{1}{\sqrt{n!}}\int dx_1.....\int dx_n\hat{H}\Psi^{(n)}(x_1, x_2,..., x_n;t)\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_1)\left|0\right\rangle.$$

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = \frac{1}{\sqrt{n!}}\int dx_1.....\int dx_n i\hbar\frac{\partial}{\partial t}\Psi^{(n)}(x_1,x_2,...,x_n;t)\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_1)\left|0\right\rangle.$$

Number operator:

$$\hat{N}\left|\Psi(t)\right\rangle = \frac{1}{\sqrt{n!}}\int dx_1.....\int dx_n \Psi^{(n)}(x_1,x_2,...,x_n;t)\hat{N}\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_1)\left|0\right\rangle.$$

Note that $\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_1)\left|0\right\rangle$ is the *n*-particle state.

Here we show that

$$i\hbar\frac{\partial}{\partial t}\Psi^{(n)}(x_1,x_2,...,x_n;t) = H_{0n}\Psi^{(n)}(x_1,x_2,...,x_n;t)$$

((**Simple case**))

The Hamiltonian $\hat{H}$ is defined by

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

with

$$\hat{H}_0 = \int dx\hat{\psi}^+(x)[-\frac{\hbar^2}{2\mu}\nabla^2 + V(x)]\hat{\psi}(x)$$

and

$$H_0(x) = -\frac{\hbar^2}{2\mu}\nabla^2 + V(x)$$

and

$$\hat{H}_1\left|\Psi(t)\right\rangle = \frac{1}{\sqrt{2!}}\int dx_1\int dx_2\Psi^{(2)}(x_1,x_2;t)\hat{H}_1\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle.$$

Using the relation

$$[\hat{H}_0, \hat{\psi}^+(x_1)] = \hat{H}_0\hat{\psi}^+(x_1) - \hat{\psi}^+(x_1)\hat{H}_0 = H_0(x_1)\hat{\psi}^+(x_1)$$

we have

$$\begin{aligned}\hat{H}_0\hat{\psi}^+(x_3)\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle &= \{[\hat{H}_0, \hat{\psi}^+(x_3)] + \hat{\psi}^+(x_3)\hat{H}_0\}\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle \\ &= [H_0(x_3)\hat{\psi}^+(x_3) + \hat{\psi}^+(x_3)\hat{H}_0]\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle \\ &= H_0(x_3)\hat{\psi}^+(x_3)\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle \\ &\quad + \hat{\psi}^+(x_3)\hat{H}_0\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle\end{aligned}$$

with

$$\begin{aligned}\hat{\psi}^+(x_3)\hat{H}_0\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle &= \hat{\psi}^+(x_3)\{[\hat{H}_0, \hat{\psi}^+(x_2)] + \hat{\psi}^+(x_2)\hat{H}_0\}\hat{\psi}^+(x_1)\left|0\right\rangle \\ &= \hat{\psi}^+(x_3)[H_0(x_2)\hat{\psi}^+(x_2) + \hat{\psi}^+(x_2)\hat{H}_0]\hat{\psi}^+(x_1)\left|0\right\rangle \\ &= \hat{\psi}^+(x_3)H_0(x_2)\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle \\ &\quad + \hat{\psi}^+(x_3)\hat{\psi}^+(x_2)\hat{H}_0\hat{\psi}^+(x_1)\left|0\right\rangle\end{aligned}$$

$$\begin{aligned}\hat{\psi}^+(x_3)\hat{\psi}^+(x_2)\hat{H}_0\hat{\psi}^+(x_1)\left|0\right\rangle &= \hat{\psi}^+(x_3)\hat{\psi}^+(x_2)\{[\hat{H}_0, \hat{\psi}^+(x_1)] + \hat{\psi}^+(x_1)\hat{H}_0\}\left|0\right\rangle \\ &= \hat{\psi}^+(x_3)\hat{\psi}^+(x_2)H_0(x_1)\hat{\psi}^+(x_1)\left|0\right\rangle \\ &\quad + \hat{\psi}^+(x_3)\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\hat{H}_0\left|0\right\rangle \\ &= \hat{\psi}^+(x_3)\hat{\psi}^+(x_2)H_0(x_1)\hat{\psi}^+(x_1)\left|0\right\rangle\end{aligned}$$

since $\hat{H}_0\left|0\right\rangle = 0$. Thus we have

$$\hat{H}_0\hat{\psi}^+(x_3)\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle = \sum_{i=1}^{3} H_{0i}(x_i)\hat{\psi}^+(x_3)\hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle$$

In general we have

$$\hat{H}_0\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})....\hat{\psi}^+(x_1)\left|0\right\rangle = \sum_{i=1}^{n} H_0(x_i)\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})....\hat{\psi}^+(x_1)\left|0\right\rangle$$

where

$$H_0(x_i) = -\frac{\hbar^2}{2m}\nabla_i{}^2 + V(x_i)$$

For *n* particle system, we have

$$\begin{aligned}
\hat{H}_0\left|\Psi^{(n)}(t)\right\rangle &= \frac{1}{\sqrt{n!}}\int dx_1 ... \int dx_n \Psi^{(n)}(x_1, x_2, ..., x_n; t)\hat{H}_0 \hat{\psi}^+(x_n) .... \hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle \\
&= \frac{1}{\sqrt{n!}}\int dx_1 ... \int dx_n \Psi^{(n)}(x_1, x_2, ..., x_n; t)\sum_{i=1}^{n} H_0(x_i)\hat{\psi}^+(x_n) .... \hat{\psi}^+(x_2)\hat{\psi}^+(x_1)\left|0\right\rangle \\
&= \frac{1}{\sqrt{n!}}\sum_{i=1}^{n}\int dx_1 ... \int dx_n \Psi^{(n)}(x_1, x_2, ..., x_n; t) H_0(x_i)\hat{\psi}^+(x_n) .... \hat{\psi}^+(x_i) ... \hat{\psi}^+(x_1)\left|0\right\rangle \\
&= \frac{1}{\sqrt{n!}}\sum_{i=1}^{n}\int dx_1 ... \int dx_n \Psi^{(n)}(x_1, x_2, ..., x_n; t)[-\frac{\hbar^2}{2m}\nabla_i{}^2 + V(x_i)]\hat{\psi}^+(x_n) .... \hat{\psi}^+(x_i) ... \hat{\psi}^+(x_1)\left|0\right\rangle \\
&= \frac{1}{\sqrt{n!}}\sum_{i=1}^{n}\int dx_1 ... \int dx_n [-\frac{\hbar^2}{2m}\nabla_i{}^2 + V(x_i)]\Psi^{(n)}(x_1, x_2, ..., x_n; t)\hat{\psi}^+(x_n) .... \hat{\psi}^+(x_i) ... \hat{\psi}^+(x_1)\left|0\right\rangle
\end{aligned}$$

by partial integral with respect to variable x_i such that

$$\begin{aligned}
&\int dx_i \Psi^{(n)}(x_1, x_2, ..., x_n; t)[-\frac{\hbar^2}{2m}\nabla_i{}^2 + V(x_i)]\hat{\psi}^+(x_i) \\
&= \int dx_i \{[-\frac{\hbar^2}{2m}\nabla_i{}^2 + V(x_i)]\Psi^{(n)}(x_1, x_2, ..., x_n; t)\}\hat{\psi}^+(x_i)
\end{aligned}$$

Finally we get

$$\hat{H}_0\left|\Psi(t)\right\rangle = \frac{1}{\sqrt{n!}}\sum_{i=1}^{n}\int dx_1 ... \int dx_n \sum_{i=1}^{n} H_0(x_i)\Psi^{(n)}(x_1, x_2, ..., x_n; t)\hat{\psi}^+(x_n) .... \hat{\psi}^+(x_i) ... \hat{\psi}^+(x_1)\left|0\right\rangle$$

On the other hand,

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = \frac{1}{\sqrt{n!}}\int dx_1 ..... \int dx_n i\hbar\frac{\partial}{\partial t}\Psi^{(n)}(x_1, x_2, ..., x_n; t)\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1}) ... \hat{\psi}^+(x_1)\left|0\right\rangle.$$

Then we find that $\Psi^{(n)}(x_1, x_2, ..., x_n; t)$ satisfies the Schrödinger equation for *n*-particle system;

$$i\hbar\frac{\partial}{\partial t}\Psi^{(n)}(x_1,x_2,...,x_n;t)=H_{0n}\Psi^{(n)}(x_1,x_2,...,x_n;t),$$

where

$$H_{0n}=\sum_{i=1}^{n}H_0(x_i).$$

19. Conclusion

The second quantization is very useful method for the many-particle (boson and fermion). We do not have to solve the Schrödinger equation for many-particle systems directly. Instead of that, we need to solve the Schrödinger equation for one-particle systems. The quantum field operator can be obtained from the one-particle solution with the creation and annihilation operators (CAP's) depending on the nature of particles, boson or fermion. The quantum state for the many particle system can be uniquely determined by the combinations of quantum field operators which is acted on the Fox state (vacuum state).

((One-particle state))

$\psi(\boldsymbol{r})$ is the wave-function for on-particle state (first quantization)

$$\psi(x)=\sum_k a_k\phi_k(x),\qquad \psi^*(x)=\sum_{\boldsymbol{k}} a_k{}^*\phi_k{}^*(x)$$

where $\phi_k(x)$ is the one-particle Schrödinger solution and a_k is co-efficients.

((**Quantum state**))

The quantum field operator is

$$\hat{\psi}(x)=\sum_k \hat{a}_k\phi_k(x),\qquad \hat{\psi}^+(x)=\sum_{\boldsymbol{k}} \hat{a}_k{}^+\phi_k{}^*(x)$$

where $\hat{c}_k$ and $\hat{c}_k{}^+$ are the annihilation and creation operators;

$$[\hat{a}_k,\hat{a}_{k'}{}^+]_+=\hat{1}\delta_{k,k'},\qquad [\hat{a}_k,\hat{a}_{k'}]_+=[\hat{a}_k{}^+,\hat{a}_{k'}{}^+]_+=0\qquad \text{for fermions}$$

The quantum state of the many-particle can be expressed by the Fock state

$$\left|\Psi^{(n)}(t)\right\rangle = \left|n_1, n_2, n_3, ..., n_i, ..\right\rangle$$
$$= \int dx_1 ... \int dx_n \left|x_1, x_2, x_3, ..., x_n; n\right\rangle \left\langle x_1, x_2, x_3, ..., x_n; n \middle| n_1, n_2, n_3, ..., n_i, ..\right\rangle .$$
$$= \int dx_1 ... \int dx_n \Psi^{(n)}(x_1, x_2, ..., x_n; t) \left|x_1, x_2, x_3, ..., x_n; n\right\rangle$$

with

$$\Psi^{(n)}(x_1, x_2, ..., x_n; t) = \left\langle x_1, x_2, x_3, ..., x_n; n \middle| n_1, n_2, n_3, ..., n_i, ..\right\rangle$$
$$= \frac{1}{\sqrt{n!}} \left\langle 0 \middle| \hat{\psi}(x_1)\hat{\psi}(x_2).....\hat{\psi}(x_n) \middle| \Psi^{(n)}(t)\right\rangle$$

$\Psi^{(n)}(x_1, x_2, ..., x_n; t)$ satisfies the Schrodinger equation for the *n*-particle system

$$i\hbar \frac{\partial}{\partial t} \Psi^{(n)}(x_1, x_2, ..., x_n; t) = H\Psi^{(n)}(x_1, x_2, ..., x_n; t)$$

where $H = H_0 + H_1$ is the Hamiltonian of the many particle system. *The many-body problem in quantum mechanics is equivalent to the quantum field theory above described.* Using the quantum field operator, the Hamiltonian is given by

$$\hat{H}_0 = \int dx \hat{\psi}^+(x)[-\frac{\hbar^2}{2\mu}\nabla^2 + V(x)]\hat{\psi}(x)$$

$$\hat{H}_1 = \frac{1}{2}\int dx' \int dx \hat{\psi}^+(x)\hat{\psi}^+(x')U(x - x')\hat{\psi}(x')\hat{\psi}(x) .$$

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APPENDIX Second quantization

Sin-itiro Tomonaga (Nobe Prize Laureate, 1965, with Julian Schwinger and Richard Feynman), from the book titled as The Theory of Spin (University of Chicago, 1997).

In the above book by Prof. Tomonaga, I found his surprising comment (of Prof. Tomonaga) when he had the first encounter with two papers concerning on the second quantization.

"A little bit later, I met with Yukawa (Prof. Hideki Yukawa, Nobel Laureate, prediction of meson, 1949) in the library (Kyoto University), where he opened on a table the issues of Zeitschrift für Physik in which the Jordan-Klein paper and the Jordan-Wigner paper were published and informed me that there was this surprising work that, if ψ in the three-dimensional space is quantized by the canonical commutation relation or anticommutation relation, then we could obtain exactly the same conclusion as when we took the symmetric or antisymmetric wave function using ψ in configuration space. Thus I also read those papers right away and found that the murky problem of three dimensional wave versus multidimensional wave had been completely and elegantly answered."

P. Jordan and O. Klein, Z. Phys. **45**, 752 (1927).
P. Jordan and E.P. Wigner, Z. Phys. **47**, 631 (1928).