Second quantization for bosons

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Here we discuss the second quantization for boson, which is similar to that for fermion. The wavefunction should be symmetric under the exchange of position of two particles.

1. Fock space representation (boson)

The symmetric wave function for the bosons is given by

$$\langle x_1, x_2, x_3,..., x_n; n | n_1, n_2, n_3,..., n_i,...., n_s; n\rangle$$
$$= \sqrt{\frac{n!}{n_1!n_2!n_3!...n_i!..}} \frac{1}{n!}\sum_P P[\langle x_1|\lambda^{(1)}\rangle\langle x_2|\lambda^{(2)}\rangle\langle x_3|\lambda^{(3)}\rangle...]$$

where P is the permutation operator which interchanges the label of x's and the summation runs over all $n!$ permutation of the n labels. Note that

$$n = \sum_{i=1} n_i$$

$|n_1, n_2, n_3,..., n_i,..; n\rangle$ is the Fock state with

n_1 particles in the state $|\lambda_1\rangle$
n_2 particles in the state $|\lambda_2\rangle$
……………………………..
n_i particles in the state $|\lambda_i\rangle$
……………………………..

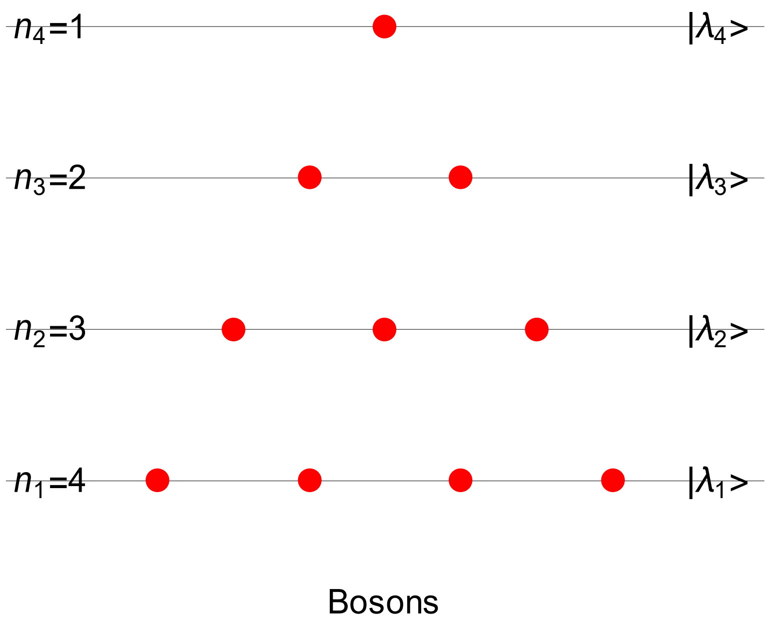
((The expansion formula))

The expansion formula is given by Schweber as

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

((**Example**)) Boson systems

Energy levels and states for bosons



$$\langle x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}; n=10 | n_1 = 4, n_2 = 3, n_3 = 2, n_4 = 1; n=10 \rangle_B$$

$$4|\lambda_1\rangle, 3|\lambda_2\rangle, 2|\lambda_3\rangle, 1|\lambda_4\rangle$$

2. Creation and annihilation operator for bosons

We now introduce the annihilation operator $\hat{b}_i$ for boson, which is defined as

$$\hat{b}_i|n_1, n_2, ..., n_i, ...\rangle = \sqrt{n_i}|n_1, n_2, ..., n_i - 1, ...\rangle$$

The creation operator $\hat{b}_i^+$ is defined by

$$\hat{b}_i^+|n_1, n_2, ..., n_i, ...\rangle = \sqrt{n_i + 1}|n_1, n_2, ..., n_i + 1, ...\rangle$$

We note that

$$\begin{aligned}\hat{b}_i^+\hat{b}_i|n_1, n_2, ..., n_i, ...\rangle &= \sqrt{n_i}\hat{b}_i^+|n_1, n_2, ..., n_i - 1, ...\rangle \\ &= n_i|n_1, n_2, ..., n_i, ...\rangle\end{aligned}$$

$$\hat{b}_i\hat{b}_i^+|n_1,n_2,...,n_i,...\rangle = \sqrt{n_i+1}\hat{b}_i|n_1,n_2,...,n_i+1,...\rangle$$
$$= (n_i+1)|n_1,n_2,...,n_i,...\rangle$$

which leads to

$$[\hat{b}_i,\hat{b}_i]|n_1,n_2,...,n_i,...\rangle = 1|n_1,n_2,...,n_i-1,...\rangle$$

or

$$[\hat{b}_i,\hat{b}_i^+] = \hat{1} \qquad \text{(commutation relation)}$$

where

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

For $i > j$, we have

$$\hat{b}_i\hat{b}_j^+|n_1,n_2,...,n_i,...\rangle = \sqrt{n_j+1}\hat{b}_i|n_1,n_2,...,n_i,..,n_j+1,...\rangle$$
$$= \sqrt{n_i}\sqrt{n_j+1}|n_1,n_2,...,n_i-1,..,n_j+1,...\rangle$$

and

$$\hat{b}_j^+\hat{b}_i|n_1,n_2,...,n_i,...\rangle = \sqrt{n_i}\hat{b}_j^+|n_1,n_2,...,n_i-1,..,n_j,...\rangle$$
$$= \sqrt{n_i}\sqrt{n_j+1}|n_1,n_2,...,n_i-1,..,n_j+1,...\rangle$$

which leads to the commutation relation

$$[\hat{b}_i,\hat{b}_j^+] = 0.$$

Combining two relations, we have

$$[\hat{b}_i,\hat{b}_j^+] = \hat{1}\delta_{i,j}.$$

using the Krnocker delta. Similarly we have

$$[\hat{b}_i,\hat{b}_j] = 0, \qquad [\hat{b}_i^+,\hat{b}_j^+] = 0$$

3. Quantum field operator for bosons (I)

We introduce the field operators for boson which are defined by

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

where $\langle x | \lambda_k \rangle = \phi_k(x)$ is the eigenfunction of the single particle. These field operators satisfy the commutation relations

$$\begin{aligned}
[\hat{\psi}(x), \hat{\psi}^+(x')] &= \sum_{k,k'} [\hat{b}_k, \hat{b}_{k'}{}^+] \phi_k(x) \phi_{k'}{}^*(x') \\
&= \sum_{k,k'} \delta_{k,k'} \phi_k(x) \phi_{k'}{}^*(x') \\
&= \sum_k \phi_k(x) \phi_k{}^*(x') \\
&= \sum_k \langle x | \phi_k \rangle \langle \phi_k | x' \rangle \\
&= \langle x | x' \rangle \\
&= \delta(x - x')
\end{aligned}$$

and

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

The total number operator is defined by

$$\begin{aligned}
\hat{N} &= \int dx \hat{\psi}^+(x) \hat{\psi}(x) \\
&= \int dx \sum_{k,k'} \hat{b}_{\boldsymbol{k}}{}^+ \hat{b}_{\boldsymbol{k}'} \langle \phi_{\boldsymbol{k}} | x \rangle \langle x | \phi_{\boldsymbol{k}'} \rangle \\
&= \sum_{k,k'} \hat{b}_k{}^+ \hat{b}_{k'} \langle \phi_{\boldsymbol{k}} | \phi_{\boldsymbol{k}'} \rangle \\
&= \sum_{k,k'} \hat{b}_k{}^+ \hat{b}_{k'} \delta_{k,k'} \\
&= \sum_k \hat{b}_{\boldsymbol{k}}{}^+ \hat{b}_k
\end{aligned}$$

4. Second quantization for boson

Using the quantum field operator and the annihilation operator, the expansion formula can be rewritten as

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

By induction we have

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

or

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

where *S* denotes the anti-symmetrizing operator.

In general case, we have

$$
\begin{aligned}
\langle x_1, x_2, ..., x_n | x_1', x_2', ..., x_m' \rangle_B &= \frac{1}{n!} \langle 0 | \hat{\psi}(x_1) \hat{\psi}(x_2) ... \hat{\psi}(x_n) \hat{\psi}^+(x_n') ... \hat{\psi}^+(x_2') \hat{\psi}^+(x_1') | 0 \rangle \\
&= \delta_{n,m} \frac{1}{n} \sum_{\{P\}} \delta(x_1' - x_1) \delta(x_2' - x_2) .... \delta(x_n' - x_n)
\end{aligned}
$$

where the index *B* denotes the boson.

$$
\begin{aligned}
&\langle x_1, x_2, x_3, ..., x_n; n | \Psi \rangle \\
&= \int dx_1' \int dx_2' ... \int dx_n' \langle x_1, x_2, x_3, ..., x_n; n | x_1', x_2', x_3', ..., x_n'; n \rangle \langle x_1', x_2', x_3', ..., x_n'; n | \Psi \rangle \\
&= \frac{1}{n!} \int dx_1' \int dx_2' ... \int dx_n' \langle 0 | \hat{\psi}(x_1) \hat{\psi}(x_2) .. \hat{\psi}(x_n) \hat{\psi}^+(x_n) ... \hat{\psi}^+(x_2') \hat{\psi}^+(x_1') | 0 \rangle \langle x_1', x_2', x_3', ..., x_n'; n | \Psi \rangle
\end{aligned}
$$

((**Example**)) We consider the simple case.

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

$$\langle x_1, x_2|\Psi\rangle$$
$$= \int dx_1' \int dx_2' \langle x_1, x_2|x_1', x_2'\rangle\langle x_1', x_2'|\Psi\rangle$$
$$= \frac{1}{2}\int dx_1' \int dx_2' \langle 0|\hat{\psi}(x_1)\hat{\psi}(x_2)\hat{\psi}^+(x_2')\hat{\psi}^+(x_1')|0\rangle\langle x_1', x_2'|\Psi\rangle$$
$$= \frac{1}{2}\int dx_1' \int dx_2' [\delta(x_2 - x_2')\delta(x_1 - x_1') + \delta(x_2 - x_1')\delta(x_1 - x_2')]\langle x_1', x_2'|\Psi\rangle$$
$$= \frac{1}{2}[\langle x_1, x_2|\Psi\rangle + \langle x_2, x_1|\Psi\rangle]$$

(symmetric function)

5. Hamiltonian

The Hamiltonian can be expressed by

$$\hat{H}_0 = \int dr[\frac{\hbar^2}{2\mu}\nabla\hat{\psi}^+(\mathbf{r},t)\cdot\nabla\hat{\psi}(\mathbf{r},t) + V(\mathbf{r})\hat{\psi}^+(\mathbf{r},t)\hat{\psi}(\mathbf{r},t)]$$
$$= \int dr\,\hat{\psi}^+(\mathbf{r},t)[-\frac{\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})]\hat{\psi}(\mathbf{r},t)$$

Using the quantum field operator

$$\hat{\psi}(\mathbf{r},t) = \sum_{\mathbf{k}}\hat{b}_{\mathbf{k}}\phi_{\mathbf{k}}(\mathbf{r})\exp(-\frac{i\varepsilon_k t}{\hbar})$$

we have

$$\begin{aligned}\hat{H}_0 &= \sum_{\mathbf{k},\mathbf{k}'}\int d\mathbf{r}[\frac{\hbar^2}{2\mu}\nabla\phi_{\mathbf{k}}^*(\mathbf{r})\cdot\nabla\phi_{\mathbf{k}'}(\mathbf{r})+\phi_{\mathbf{k}}^*(\mathbf{r})V(\mathbf{r})\phi_{\mathbf{k}'}(\mathbf{r})]\hat{a}_{\mathbf{k}}{}^+\hat{a}_{\mathbf{k}'}\exp[\frac{i}{\hbar}(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'})t] \\
&= \sum_{\mathbf{k},\mathbf{k}'}\int d\mathbf{r}\phi_{\mathbf{k}}^*(\mathbf{r})[-\frac{\hbar^2}{2\mu}\nabla^2+V(\mathbf{r})]\phi_{\mathbf{k}'}(\mathbf{r})\hat{b}_{\mathbf{k}}{}^+\hat{b}_{\mathbf{k}'}\exp[\frac{i}{\hbar}(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'})t] \\
&= \sum_{\mathbf{k},\mathbf{k}'}\int d\mathbf{r}\phi_{\mathbf{k}}^*(\mathbf{r})\phi_{\mathbf{k}'}(\mathbf{r})\varepsilon_{\mathbf{k}'}\hat{b}_{\mathbf{k}}{}^+\hat{b}_{\mathbf{k}'}\exp[\frac{i}{\hbar}(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'})t] \\
&= \sum_{\mathbf{k},\mathbf{k}'}\delta_{\mathbf{k},\mathbf{k}'}\varepsilon_{\mathbf{k}'}\hat{b}_{\mathbf{k}}{}^+\hat{b}_{\mathbf{k}'}\exp[\frac{i}{\hbar}(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'})t] \\
&= \sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}\hat{b}_{\mathbf{k}}{}^+\hat{b}_{\mathbf{k}}\end{aligned}$$

$\hat{b}_{\mathbf{k}}{}^+\hat{b}_{\mathbf{k}}$ is the number operator. The eigenket of $\hat{H}_0$ is given by

$$|n_1,n_2,n_3,...\rangle$$

with the eigenvalue

$$\sum_i \varepsilon_i n_i$$

Note that

$$\hat{H}_0|n_1,n_2,n_3,...\rangle = \sum_i \varepsilon_i \hat{b}_i{}^+\hat{b}_i|n_1,n_2,n_3,...\rangle$$

Field operator:

$$\begin{aligned}\hat{\psi}(\mathbf{r},t) &= \sum_{\mathbf{k}}\hat{b}_{\mathbf{k}}\phi_{\mathbf{k}}(\mathbf{r},t) \\
&= \sum_{\mathbf{k}}\hat{b}_{\mathbf{k}}\phi_{\mathbf{k}}(\mathbf{r})\exp(-\frac{i\varepsilon_k t}{\hbar})\end{aligned}$$

Commutation relation:

$$[\hat{b}_k,\hat{b}_{k'}{}^+]=\hat{1}\delta_{k,k'}, \qquad [\hat{b}_k,\hat{b}_{k'}]=[\hat{b}_k{}^+,\hat{b}_{k'}{}^+]=0$$

$$[\hat{b}_{\mathbf{k}},\hat{N}_{\mathbf{k}'}]=\hat{b}_{\mathbf{k}}\delta_{\mathbf{k},\mathbf{k}'}$$

6. Proof of the expression $i\hbar\frac{\partial}{\partial t}\hat{\psi}(x,t) = H_0(x)\hat{\psi}(x,t)$

We show the relation of $i\hbar\frac{\partial}{\partial t}\hat{\psi}(x,t) = H_0(x)\hat{\psi}(x,t)$

((**Proof**))
We start with

$$\hat{\psi}(x,t) = \sum_k \hat{b}_k \phi_k(x,t) = \sum_k \hat{b}_k \phi_k(x)\exp(-\frac{i\varepsilon_k t}{\hbar})$$

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(x,t) = \sum_k \hat{b}_{\mathbf{k}} \phi_{\mathbf{k}}(x) i\hbar\frac{\partial}{\partial t}\exp(-\frac{i\varepsilon_k t}{\hbar}) = \sum_k \varepsilon_k \hat{b}_{\mathbf{k}} \phi_{\mathbf{k}}(x)\exp(-\frac{i\varepsilon_k t}{\hbar})$$

$$H_0\hat{\psi}(x,t) = \sum_k \hat{b}_k [H_0\phi_k(\mathbf{r})]\exp(-\frac{i\varepsilon_k t}{\hbar}) = \sum_k \varepsilon_k \hat{b}_k \phi_k(x)\exp(-\frac{i\varepsilon_k t}{\hbar})$$

leading to

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(x,t) = H_0(x)\hat{\psi}(x,t)$$

7. Heisenberg's equation of motion

$$[\hat{\psi}(x,t), \hat{H}_0] = \sum_k [\hat{b}_k, \hat{H}_0]\phi_{\mathbf{k}}(x)\exp(-\frac{i\varepsilon_k t}{\hbar})$$
$$= \sum_k [\hat{b}_k, \hat{H}_0]\phi_k(x)\exp(-\frac{i\varepsilon_k t}{\hbar})$$
$$= \sum_k \varepsilon_k \hat{b}_k \phi_k(x)\exp(-\frac{i\varepsilon_k t}{\hbar})$$
$$= i\hbar\frac{\partial}{\partial t}\hat{\psi}(x,t)$$

or

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(x,t)=[\hat{\psi}(x,t),\hat{H}_0]$$

with

$$[\hat{b}_k,\hat{N}_{k'}]=\hat{b}_k\delta_{k,k'}.$$

8. The commutation relation of quantum field operator

When we discuss the quantum mechanics of *n*-particle system, instead of using the Schrödinger equation for the *n* particle system, we use the field operator $\hat{\psi}(x,t)$.

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(x,t)=\hat{H}_0\hat{\psi}(x,t),$$

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(x,t)=[\hat{\psi}(x,t),\hat{H}_0],$$

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}^+(x,t)=[\hat{\psi}^+(x,t),\hat{H}_0]$$

The commutation relations hold

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

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

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

where

$$\begin{aligned}\hat{H}_0&=\int dr[\frac{\hbar^2}{2\mu}\nabla\hat{\psi}^+(x,t)\cdot\nabla\hat{\psi}(x,t)+V(x)\hat{\psi}^+(x,t)\hat{\psi}(x,t)]\\&=\int dr\,\hat{\psi}^+(x,t)[-\frac{\hbar^2}{2\mu}\nabla^2+V(x)]\hat{\psi}(x,t)\end{aligned}$$

We note that the condition

$$N = \sum_i n_i$$

is not included in these expressions,

9. Proof of $[\hat{H}_0, \hat{\psi}^+(x_i)] = H_0(x_i)\hat{\psi}^+(x_i)$

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

$$\begin{aligned}
H_0 \hat{\psi}^+(x_i) &= H_0(x_i) \sum_k \hat{b}_k^+ \phi_k^*(x_i)] \\
&= \sum_k \varepsilon_k \phi_k^*(x_i)\hat{b}_{k'}^+
\end{aligned}$$

where

$$[\hat{N}_k, \hat{b}_{k'}^+] = \hat{b}_k^+ \delta_{k,k'}, \qquad H_0(x_i)\phi_k^*(x_i) = \varepsilon_{\mathbf{k}} \phi_{\mathbf{k}}^*(x_i)$$

Then we have

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

10. One-particle Hamiltonian $\hat{H}_0$ in the Schrödinger equation

Schrödinger equation:

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

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

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

Number operator:

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

Note that $\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_1)|0\rangle$ 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

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

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

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

with

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

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

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

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

In general, we have

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

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

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

11. Interaction Hamiltonian between two particles in the Schrödinger equation

The interaction Hamiltonian is given by

$$H_1=\sum_{i<j}V(x_i,x_j)=\frac{1}{2}\sum_{\substack{i,j\\ i\neq j}}V(x_i,x_j)$$

The corresponding operator is

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

We now consider the Schrödinger equation for the state vector

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

The n-particle state $\Psi^{(n)}(x_1,x_2,...,x_n;t)$ can be represented by the function

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

We consider

$$\begin{aligned}\hat{H}_0\left|\Psi^{(n)}(t)\right\rangle &= \frac{1}{\sqrt{n!}}\int dx_1.....\int dx_n\Psi^{(n)}(x_1,x_2,...,x_n;t)\hat{H}_0\hat{\psi}^+(x_n)\hat{\psi}^+(x_{n-1})...\hat{\psi}^+(x_1)\left|0\right\rangle \\ &= \int dx_1.....\int dx_n\hat{H}_0\left|x_1,x_2,...,x_n\right\rangle\left\langle x_1,x_2,...,x_n\right|\Psi^{(n)}(t)\rangle\end{aligned}$$

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

$$= \int dx_1 .....\int dx_n \left\langle x_1, x_2,..., x_n \left| \hat{H}_0 \right| x_1', x_2',..., x_n' \right\rangle \left\langle x_1', x_2',..., x_n' \right| \Psi^{(n)}(t) \right\rangle$$

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

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

First we consider the following term

$$\hat{\psi}(x) \left| x_1, x_2,..., x_n \right\rangle = \hat{\psi}(x) \frac{1}{\sqrt{n!}} \hat{\psi}^+(x_n) \hat{\psi}^+(x_{n-1}) ... \hat{\psi}^+(x_1) \left| 0 \right\rangle$$

$$= \{[\hat{\psi}(x), \hat{\psi}^+(x_n)] + \hat{\psi}^+(x_n) \hat{\psi}(x)\} \hat{\psi}^+(x_{n-1}) ... \hat{\psi}^+(x_1) \left| 0 \right\rangle$$

$$= \delta(x - x_n) \hat{\psi}^+(x_{n-1}) ... \hat{\psi}^+(x_1) \left| 0 \right\rangle$$

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

$$= \delta(x - x_n) \hat{\psi}^+(x_{n-1}) ... \hat{\psi}^+(x_1) \left| 0 \right\rangle$$

$$+ \hat{\psi}^+(x_n) \{[\hat{\psi}(x), \hat{\psi}^+(x_{n-1})] + \hat{\psi}^+(x_{n-1}) \hat{\psi}(x) ... \hat{\psi}^+(x_1) \left| 0 \right\rangle$$

$$= \delta(x - x_n) \hat{\psi}^+(x_{n-1}) ... \hat{\psi}^+(x_1) \left| 0 \right\rangle + \delta(x - x_{n-1}) \hat{\psi}^+(x_n) \hat{\psi}^+(x_{n-2}) ... \hat{\psi}^+(x_1) \left| 0 \right\rangle + ..$$

$$= \sum_{i=1}^{n} \frac{1}{\sqrt{n}} \delta(x - x_i) \frac{1}{\sqrt{(n-1)!}} \hat{\psi}^+(x_n) .. \hat{\psi}^+(x_{i-1}) \hat{\psi}^+(x_{i+1}) ... \hat{\psi}^+(x_1) \left| 0 \right\rangle$$

$$= \sum_{i=1}^{n} \frac{1}{\sqrt{n}} \delta(x - x_i) \left| x_1, x_2,.., x_{i-1}. x_{i+1},.., x_n \right\rangle$$

Similarly we have

$$\hat{\psi}(x') \hat{\psi}(x) \left| x_1, x_2,..., x_n \right\rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{\sqrt{n(n-1)}} \delta(x - x_i) \delta(x' - x_j) \left| x_1, x_2,..., x_{i-1}, x_{i+1},.., x_{j-1}, x_{j+1} ..., x_n \right\rangle$$

where the terms with $i = j$ are not included. Here we note that

$$\left\langle x_1, x_2,..., x_n \right| \hat{\psi}^+(x) \hat{\psi}^+(x') = \sum_{k=1}^{n} \sum_{l=1}^{n} \frac{1}{\sqrt{n(n-1)}} \delta(x - x_k) \delta(x' - x_l) \left\langle x_1, x_2,..., x_{k-1}, x_{k+1},.., x_{l-1}, x_{l+1} ..., x_n \right|$$

Using this we get the matrix element

$$\langle x_1, x_2, ..., x_n | \hat{\psi}^+(x)\hat{\psi}^+(x')\hat{\psi}(x')\hat{\psi}(x) | x_1', x_2', ..., x_n' \rangle$$
$$= \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n} \delta(x - x_i')\delta(x' - x_j')\delta(x - x_k)\delta(x' - x_l)\frac{1}{n(n-1)}$$
$$\times \langle x_1, x_2, ..., x_{k-1}, x_{k+1}, ..., x_{l-1}, x_{l+1} ..., x_n | x_1', x_2', ..., x_{i-1}', x_{i+1}', ..., x_{j-1}', x_{j+1}' ..., x_n' \rangle$$

$$\langle x_1, x_2, ..., x_n | \hat{\psi}^+(x)\hat{\psi}^+(x')\hat{\psi}(x')\hat{\psi}(x) | x_1', x_2', ..., x_n' \rangle$$
$$= \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n} \delta(x - x_k)\delta(x' - x_l)\delta(x - x_i')\delta(x' - x_j')\frac{1}{n(n-1)}$$
$$\times \frac{1}{(n-2)!}\sum_{(P)} \delta(x_1 - x_1')....\delta(x_n - x_n')$$

where $\sum_{(P)} \delta(x_1 - x_1')....\delta(x_n - x_n')$ is all the combination of

one choice from $\{x_1, x_2, ..., x_{k-1}, x_{k+1}, ..., x_{l-1}, x_{l+1} ..., x_n\}$,

and the other choice from $\{x_1', x_2', ..., x_{i-1}', x_{i+1}', .., x_{j-1}', x_{j+1}' ..., x_n\}$

We finally find out that $\Psi^{(n)}(x_1, x_2, ..., x_n; t)$ satisfy the Schrödinger equation given by

$$i\hbar\frac{\partial}{\partial t}\Psi^{(n)}(x_1, x_2, ..., x_n; t) = H_{0n}\Psi^{(n)}(x_1, x_2, ..., x_n; t) + \frac{1}{2}\sum_{k \neq l}^{n} V(|x_k - x_l|)\Psi^{(n)}(x_1, x_2, ..., x_n; t)$$

for the system with the Hamiltonian with $\hat{H} = \hat{H}_0 + \hat{H}_1$.

12. Summary

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 on-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

$$\psi(x) = \sum_k b_k \phi_k(x), \qquad \psi^*(x) = \sum_{\boldsymbol{k}} b_k^* \phi_k^*(x) \qquad \text{(first quantization)}$$

where $\phi_k(x)$ is the one-particle Schrödinger solution and b_k is coefficients.

((**Quantum field operator**))

The quantum field operator is

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

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

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

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

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

with

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

$\Psi^{(n)}(x_1, x_2, ..., x_n; t)$ satisfies the Schrödinger 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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