First online: August 13, 2021
Last modified: August 13, 2021
Katsunori Kubo, ASRC, JAEA

Second quantization

In the following, we show the equivalence between the first quantization with the (anti-) symmetrized wave functions and the second quantization by checking the effects of operators.

Notation

We use the following abbreviations:

$$n_1(i)\, n_N = n_1 \cdots n_{i-1} n_{i+1} \cdots n_N,$$

$$n_1(i_1, i_2)\, n_N = \begin{cases} n_1 \cdots n_{i_1-1} n_{i_1+1} \cdots n_{i_2-1} n_{i_2+1} \cdots n_N & \text{for } i_1 < i_2 \\ n_1 \cdots n_{i_2-1} n_{i_2+1} \cdots n_{i_1-1} n_{i_1+1} \cdots n_N & \text{for } i_1 > i_2 \end{cases}.$$

Field operator

We define the field operator as

$$\Psi(x) \equiv \sum_i \phi_i(x) c_i.$$

Here, $\phi_1(x), \phi_2(x), \cdots$ are orthonormal basis functions. We assume the (anti-) commutation relations:

$$[c_i, c_j^\dagger]_\pm \equiv c_i c_j^\dagger \mp c_j^\dagger c_i = \delta_{ij},$$
$$[c_i, c_j]_\pm = 0.$$

The upper signs are for bosons and the lower signs are for fermions.

$$[\Psi(x), c_i^\dagger]_\pm = \sum_j \phi_j(x) [c_j, c_i^\dagger]_\pm = \phi_i(x).$$

$$[\Psi(x), \Psi^\dagger(x')]_\pm = \sum_i [\Psi(x), c_i^\dagger]_\pm \phi_i^*(x') = \sum_i \phi_i(x) \phi_i^*(x').$$

Since

$$\int dx' \sum_i \phi_i(x) \phi_i^*(x')\, \phi_j(x') = \phi_j(x),$$

for any $\phi_j(x')$, we obtain

$$[\Psi(x), \Psi^\dagger(x')]_\pm = \delta(x - x').$$

Basis wave function

We consider N-body states written as

$$|n_1 \cdots n_N\rangle \equiv c^\dagger_{n_1} \cdots c^\dagger_{n_N}|0\rangle.$$

$|0\rangle$ stands for the state without any particle (vacuum state). These are basis states for general N-body states. In general, this formula is not normalized for bosons, but we are not concerned about normalization in this note. We express an N-body state constructed from the field operator as

$$|x_1 \cdots x_N\rangle \equiv \Psi^\dagger(x_1)\cdots\Psi^\dagger(x_N)|0\rangle.$$

We define the N-body basis wave function by

$$\psi_{n_1\cdots n_N}(x_1,\cdots,x_N) = \langle x_1\cdots x_N|n_1\cdots n_N\rangle.$$

From this definition, the wave function is (anti-) symmetrized. For the calculation of a one-body operator and to show the completeness, we decompose the N-body basis wave function into one-body and $(N-1)$-body basis wave functions:

$$\begin{aligned}
\psi_{n_1\cdots n_N}(x_1,\cdots,x_N) &= \langle x_1\cdots x_N|n_1\cdots n_N\rangle \\
&= (\pm1)^{i+1}\langle x_1 (i)\, x_N|\Psi(x_i)c^\dagger_{n_1}\cdots c^\dagger_{n_N}|0\rangle \\
&= (\pm1)^{i+1}\langle x_1 (i)\, x_N|[\phi_{n_1}(x_i) \pm c^\dagger_{n_1}\Psi(x_i)]c^\dagger_{n_2}\cdots c^\dagger_{n_N}|0\rangle \\
&= (\pm1)^{i+1}\{\phi_{n_1}(x_i)\langle x_1 (i)\, x_N|n_2\cdots n_N\rangle \\
&\quad \pm \langle x_1 (i)\, x_N|c^\dagger_{n_1}[\phi_{n_2}(x_i) \pm c^\dagger_{n_2}\Psi(x_i)]c^\dagger_{n_3}\cdots c^\dagger_{n_N}|0\rangle\} \\
&= \sum_k (\pm1)^{i+k}\phi_{n_k}(x_i)\langle x_1 (i)\, x_N|n_1 (k)\, n_N\rangle.
\end{aligned}$$

For the calculation of a two-body operator, we decompose the N-body basis wave function into two-body and $(N-2)$-body basis wave functions. Provided $N \geq 2$ and $i_1 \neq i_2$,

$$\begin{aligned}
&\psi_{n_1\cdots n_N}(x_1,\cdots,x_N) \\
&= \langle x_1\cdots x_N|n_1\cdots n_N\rangle \\
&= (\pm1)^{i_1+i_2+\theta(i_2-i_1)}\langle x_1 (i_1,i_2)\, x_N|\Psi(x_{i_2})\Psi(x_{i_1})c^\dagger_{n_1}\cdots c^\dagger_{n_N}|0\rangle \\
&= \sum_{k_1\neq k_2}(\pm1)^{i_1+i_2+\theta(i_2-i_1)+k_1+k_2+\theta(k_2-k_1)}\phi_{n_{k_1}}(x_{i_1})\phi_{n_{k_2}}(x_{i_2})\langle x_1 (i_1,i_2)\, x_N|n_1 (k_1,k_2)\, n_N\rangle \\
&= \sum_{k_1\neq k_2}(\pm1)^{\alpha(i_1,i_2)+\alpha(k_1,k_2)}\phi_{n_{k_1}}(x_{i_1})\phi_{n_{k_2}}(x_{i_2})\langle x_1 (i_1,i_2)\, x_N|n_1 (k_1,k_2)\, n_N\rangle.
\end{aligned}$$

Here, $\theta(i)$ is the step function and we have introduced the notation $\alpha(i_1,i_2) = i_1 + i_2 + \theta(i_2 - i_1)$.

Completeness

$$\langle x|i\rangle = \langle 0|\Psi(x)c_i^\dagger|0\rangle = \phi_i(x).$$

$$\int dx\, |x\rangle\langle x|\, i\rangle = \int dx \sum_j \phi_j^*(x)c_j^\dagger|0\rangle\phi_i(x) = c_i^\dagger|0\rangle = |i\rangle.$$

Hence, for 1-body states,

$$\int dx\, |x\rangle\langle x| = 1.$$

If

$$\frac{1}{(N-1)!}\int dx_1\cdots dx_{N-1}|x_1\cdots x_{N-1}\rangle\langle x_1\cdots x_{N-1}|n_1\cdots n_{N-1}\rangle = |n_1\cdots n_{N-1}\rangle,$$

is satisfied for any $|n_1\cdots n_{N-1}\rangle$,

$$\begin{aligned}
&\frac{1}{N!}\int dx_1\cdots dx_N|x_1\cdots x_N\rangle\langle x_1\cdots x_N|n_1\cdots n_N\rangle \\
&= \frac{1}{N!}\int dx_1\cdots dx_N \sum_i \phi_i^*(x_1)c_i^\dagger|x_2\cdots x_N\rangle \sum_k (\pm 1)^{k+1}\phi_{n_k}(x_1)\langle x_2\cdots x_N|n_1(k)\, n_N\rangle \\
&= \frac{1}{N}\int dx_1 \sum_i \phi_i^*(x_1)c_i^\dagger \sum_k (\pm 1)^{k+1}\phi_{n_k}(x_1)|n_1(k)\, n_N\rangle \\
&= \frac{1}{N}\sum_k (\pm 1)^{k+1}c_{n_k}^\dagger|n_1(k)\, n_N\rangle \\
&= \frac{1}{N}\sum_k |n_1\cdots n_N\rangle \\
&= |n_1\cdots n_N\rangle.
\end{aligned}$$

Hence, for any N-body state,

$$\frac{1}{N!}\int dx_1\cdots dx_N|x_1\cdots x_N\rangle\langle x_1\cdots x_N| = 1.$$

The factor $N!$ appears for the following reason. In the two-body case, for example, both $|x_1x_2\rangle$ and $|x_2x_1\rangle$ are considered, but they are the same except for the sign. By using an integration region that avoids such over-counting, we can formulate without the factor $N!$.

One-body operator

We define a one-body operator in the second quantization as

$$\hat{T} \equiv \int dy\, \Psi^\dagger(y) T(y) \Psi(y).$$

The wave function of the state $|n_1 \cdots n_N\rangle$ multiplied by this operator is

$$\begin{aligned}
&\langle x_1 \cdots x_N | \hat{T} | n_1 \cdots n_N \rangle \\
&= \int dy \frac{1}{N!} \int dx'_1 \cdots dx'_N \langle x_1 \cdots x_N | \Psi^\dagger(y) T(y) \Psi(y) | x'_1 \cdots x'_N \rangle \langle x'_1 \cdots x'_N | n_1 \cdots n_N \rangle.
\end{aligned}$$

$$\begin{aligned}
\Psi(y)|x'_1 \cdots x'_N\rangle &= \Psi(y)\Psi^\dagger(x'_1) \cdots \Psi^\dagger(x'_N)|0\rangle \\
&= [\delta(x'_1 - y) \pm \Psi^\dagger(x'_1)\Psi(y)]\Psi^\dagger(x'_2) \cdots \Psi^\dagger(x'_N)|0\rangle \\
&= \delta(x'_1 - y)|x'_2 \cdots x'_N|0\rangle \\
&\quad \pm \Psi^\dagger(x'_1)[\delta(x'_2 - y) \pm \Psi^\dagger(x'_2)\Psi(y)]\Psi^\dagger(x'_3) \cdots \Psi^\dagger(x'_N)|0\rangle \\
&= \sum_j (\pm 1)^{j+1} \delta(x'_j - y)|x'_1 (j)\, x'_N\rangle.
\end{aligned}$$

$$\langle x_1 \cdots x_N | \Psi^\dagger(y) T(y) \Psi(y) | x'_1 \cdots x'_N \rangle = \sum_{ij} (\pm 1)^{i+j} \delta(x_i - y) T(y) \delta(x'_j - y) \langle x_1 (i)\, x_N | x'_1 (j)\, x'_N \rangle.$$

$$\begin{aligned}
&\langle x_1 \cdots x_N | \hat{T} | n_1 \cdots n_N \rangle \\
&= \int dy \frac{1}{N!} \int dx'_1 \cdots dx'_N \sum_{ij} (\pm 1)^{i+j} \delta(x_i - y) T(y) \delta(x'_j - y) \langle x_1 (i)\, x_N | x'_1 (j)\, x'_N \rangle \\
&\quad \times \sum_k (\pm 1)^{j+k} \phi_{n_k}(x'_j) \langle x'_1 (j)\, x'_N | n_1 (k)\, n_N \rangle \\
&= \sum_{ijk} \frac{1}{N} (\pm 1)^{i+k} \int dy \int dx'_j\, \delta(x_i - y) T(y) \delta(x'_j - y) \phi_{n_k}(x'_j) \langle x_1 (i)\, x_N | n_1 (k)\, n_N \rangle \\
&= \sum_{ijk} \frac{1}{N} (\pm 1)^{i+k} \int dy\, \delta(x_i - y) T(y) \phi_{n_k}(y) \langle x_1 (i)\, x_N | n_1 (k)\, n_N \rangle \\
&= \sum_{ik} (\pm 1)^{i+k} \int dy\, \delta(x_i - y) T(y) \phi_{n_k}(y) \langle x_1 (i)\, x_N | n_1 (k)\, n_N \rangle \\
&= \sum_{ik} (\pm 1)^{i+k} T(x_i) \phi_{n_k}(x_i) \langle x_1 (i)\, x_N | n_1 (k)\, n_N \rangle \\
&= \sum_i T(x_i) \psi_{n_1 \cdots n_N}(x_1, \cdots, x_N) = T(x_1, \cdots, x_N) \psi_{n_1 \cdots n_N}(x_1, \cdots, x_N).
\end{aligned}$$

Here, we have defined $T(x_1, \cdots, x_N) = \sum_i T(x_i)$.

Two-body operator

We define a two-body operator in the second quantization as

$$\hat{V} \equiv \frac{1}{2}\int dy_1 dy_2 \Psi^\dagger(y_1)\Psi^\dagger(y_2)V(y_1, y_2)\Psi(y_2)\Psi(y_1).$$

Provided $N \geq 2$, the wave function of the state $|n_1 \cdots n_N\rangle$ multiplied by this operator is

$$\begin{aligned}
&\langle x_1 \cdots x_N|\hat{V}|n_1 \cdots n_N\rangle \\
&= \frac{1}{2}\int dy_1 dy_2 \frac{1}{N!}\int dx'_1 \cdots dx'_N \, \langle x_1 \cdots x_N|\Psi^\dagger(y_1)\Psi^\dagger(y_2)V(y_1, y_2)\Psi(y_2)\Psi(y_1)|x'_1 \cdots x'_N\rangle \\
&\quad \times \langle x'_1 \cdots x'_N|n_1 \cdots n_N\rangle
\end{aligned}$$

$$\begin{aligned}
\Psi(y_2)\Psi(y_1)|x'_1 \cdots x'_N\rangle &= \Psi(y_2)\Psi(y_1)\Psi^\dagger(x'_1) \cdots \Psi^\dagger(x'_N)|0\rangle \\
&= \sum_{j_1 \neq j_2} (\pm 1)^{j_1+j_2+\theta(j_2-j_1)}\delta(x'_{j_1} - y_1)\delta(x'_{j_2} - y_2)|x'_1(j_1, j_2)\, x'_N\rangle \\
&= \sum_{j_1 \neq j_2} (\pm 1)^{\alpha(j_1,j_2)}\delta(x'_{j_1} - y_1)\delta(x'_{j_2} - y_2)|x'_1(j_1, j_2)\, x'_N\rangle.
\end{aligned}$$

$$\begin{aligned}
&\langle x_1 \cdots x_N|\Psi^\dagger(y_1)\Psi^\dagger(y_2)V(y_1, y_2)\Psi(y_2)\Psi(y_1)|x'_1 \cdots x'_N\rangle \\
&= \sum_{i_1 \neq i_2, j_1 \neq j_2} (\pm 1)^{\alpha(i_1,i_2)+\alpha(j_1,j_2)} \\
&\quad \times \delta(x_{i_1} - y_1)\delta(x_{i_2} - y_2)V(y_1, y_2)\delta(x'_{j_1} - y_1)\delta(x'_{j_2} - y_2)\langle x_1(i_1, i_2)\, x_N|x'_1(j_1, j_2)\, x'_N\rangle.
\end{aligned}$$

$$
\begin{aligned}
&\langle x_1 \cdots x_N|\hat{V}|n_1 \cdots n_N\rangle \\
&= \frac{1}{2}\int dy_1 dy_2 \, \frac{1}{N!}\int dx'_1 \cdots dx'_N \sum_{i_1\neq i_2, j_1\neq j_2} (\pm 1)^{\alpha(i_1,i_2)+\alpha(j_1,j_2)} \\
&\quad \times \delta(x_{i_1}-y_1)\delta(x_{i_2}-y_2)V(y_1,y_2)\delta(x'_{j_1}-y_1)\delta(x'_{j_2}-y_2)\langle x_1(i_1,i_2)\, x_N|x'_1(j_1,j_2)\, x'_N\rangle \\
&\quad \times \sum_{k_1\neq k_2} (\pm 1)^{\alpha(j_1,j_2)+\alpha(k_1,k_2)}\phi_{n_{k_1}}(x'_{j_1})\phi_{n_{k_2}}(x'_{j_2})\langle x'_1(j_1,j_2)\, x'_N|n_1(k_1,k_2)\, n_N\rangle \\
&= \frac{1}{2}\sum_{i_1\neq i_2, j_1\neq j_2, k_1\neq k_2} \frac{1}{N(N-1)}(\pm 1)^{\alpha(i_1,i_2)+\alpha(k_1,k_2)} \int dy_1 dy_2 \int dx'_{j_1} dx'_{j_2} \\
&\quad \times \delta(x_{i_1}-y_1)\delta(x_{i_2}-y_2)V(y_1,y_2)\delta(x'_{j_1}-y_1)\delta(x'_{j_2}-y_2)\phi_{n_{k_1}}(x'_{j_1})\phi_{n_{k_2}}(x'_{j_2}) \\
&\quad \times \langle x_1(i_1,i_2)\, x_N|n_1(k_1,k_2)\, n_N\rangle \\
&= \frac{1}{2}\sum_{i_1\neq i_2, j_1\neq j_2, k_1\neq k_2} \frac{1}{N(N-1)}(\pm 1)^{\alpha(i_1,i_2)+\alpha(k_1,k_2)} \int dy_1 dy_2 \\
&\quad \times \delta(x_{i_1}-y_1)\delta(x_{i_2}-y_2)V(y_1,y_2)\phi_{n_{k_1}}(y_1)\phi_{n_{k_2}}(y_2)\langle x_1(i_1,i_2)\, x_N|n_1(k_1,k_2)\, n_N\rangle \\
&= \frac{1}{2}\sum_{i_1\neq i_2, k_1\neq k_2} (\pm 1)^{\alpha(i_1,i_2)+\alpha(k_1,k_2)} \int dy_1 dy_2 \\
&\quad \times \delta(x_{i_1}-y_1)\delta(x_{i_2}-y_2)V(y_1,y_2)\phi_{n_{k_1}}(y_1)\phi_{n_{k_2}}(y_2)\langle x_1(i_1,i_2)\, x_N|n_1(k_1,k_2)\, n_N\rangle \\
&= \frac{1}{2}\sum_{i_1\neq i_2, k_1\neq k_2} (\pm 1)^{\alpha(i_1,i_2)+\alpha(k_1,k_2)} V(x_{i_1},x_{i_2})\phi_{n_{k_1}}(x_{i_1})\phi_{n_{k_2}}(x_{i_2})\langle x_1(i_1,i_2)\, x_N|n_1(k_1,k_2)\, n_N\rangle \\
&= \frac{1}{2}\sum_{i_1\neq i_2} V(x_{i_1},x_{i_2})\psi_{n_1\cdots n_N}(x_1,\cdots,x_N) \\
&= V(x_1,\cdots,x_N)\psi_{n_1\cdots n_N}(x_1,\cdots,x_N).
\end{aligned}
$$

Here, we have defined $V(x_1,\cdots,x_N) = \frac{1}{2}\sum_{i_1\neq i_2} V(x_{i_1},x_{i_2})$.

General wave function

Any N-body state can be written by a superposition of $\{|n_1 \cdots n_N\rangle\}$. Here, we write a such N-body state as $|\psi\rangle$ and its wave function as $\langle x_1 \cdots x_N|\psi\rangle = \psi(x_1, \cdots, x_N)$.

$$\langle x_1 \cdots x_N|\hat{T}|\psi\rangle = T(x_1, \cdots, x_N)\psi(x_1, \cdots, x_N),$$
$$\langle x_1 \cdots x_N|\hat{V}|\psi\rangle = V(x_1, \cdots, x_N)\psi(x_1, \cdots, x_N).$$

Expectation value of an operator

$$\begin{aligned}
\langle\psi|\hat{O}|\psi\rangle &= \frac{1}{N!}\int dx_1 \cdots dx_N \langle\psi|x_1 \cdots x_N\rangle\langle x_1 \cdots x_N|\hat{O}|\psi\rangle \\
&= \frac{1}{N!}\int dx_1 \cdots dx_N\, \psi^*(x_1, \cdots, x_N) O(x_1, \cdots, x_N)\psi(x_1, \cdots, x_N), \\
\langle\psi|\psi\rangle &= \frac{1}{N!}\int dx_1 \cdots dx_N \langle\psi|x_1 \cdots x_N\rangle\langle x_1 \cdots x_N|\psi\rangle \\
&= \frac{1}{N!}\int dx_1 \cdots dx_N\, \psi^*(x_1, \cdots, x_N)\psi(x_1, \cdots, x_N).
\end{aligned}$$

$$\frac{\langle\psi|\hat{O}|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\int dx_1 \cdots dx_N\, \psi^*(x_1, \cdots, x_N) O(x_1, \cdots, x_N)\psi(x_1, \cdots, x_N)}{\int dx_1 \cdots dx_N\, \psi^*(x_1, \cdots, x_N)\psi(x_1, \cdots, x_N)}.$$