TFY4210 Quantum theory of many-particle systems, 2016: Solution to tutorial 2

1. Explicit connection between first and second quantization.

By our definition,

\[ |x_1, x_2\rangle = \frac{1}{\sqrt{2!}} \hat{\psi}^\dagger(x_1) \hat{\psi}^\dagger(x_2) |0\rangle \]  

and thus

\[ \langle x_1, x_2 | = \frac{1}{\sqrt{2!}} \langle 0 | \hat{\psi}(x_2) \hat{\psi}(x_1) \].

Furthermore,

\[ |\ldots, 1_\mu, \ldots, 1_\nu, \ldots\rangle = \hat{c}^\dagger_\mu \hat{c}^\dagger_\nu |0\rangle. \]

Here we used that \( \mu \) comes before \( \nu \) in the ordering of single-particle states (because \( \mu \) is to the left of \( \nu \) in the list of occupation numbers on the lhs), and so by our convention introduced in the lectures, \( \hat{c}^\dagger_\nu \) should act on the vacuum before \( \hat{c}^\dagger_\mu \) does. Thus we consider

\[ \langle x_1, x_2 | \ldots, 1_\mu, \ldots, 1_\nu, \ldots\rangle = \frac{1}{\sqrt{2!}} \langle 0 | \hat{\psi}(x_2) \hat{\psi}(x_1) \hat{c}^\dagger_\mu \hat{c}^\dagger_\nu |0\rangle \]

\[ = \frac{1}{\sqrt{2}} \sum_{\alpha, \beta} \phi_\alpha(x_2) \phi_\beta(x_1) \langle 0 | \hat{c}_\alpha \hat{c}_\beta \hat{c}^\dagger_\nu \hat{c}^\dagger_\mu |0\rangle \]

where we used \( \hat{\psi}(x) = \sum_\alpha \phi_\alpha(x) \hat{c}_\alpha \). We calculate the matrix element in (4) by using the anti-commutation relations to move the annihilation operators to the right until they are next to \( |0\rangle \) and then we use \( \hat{c}|0\rangle = 0 \) (also, by taking the adjoint of this relation one sees that creation operators standing next to \( \langle 0 | \) annihilate it: \( \langle 0 | \hat{c}^\dagger = 0 \)). This gives

\[ \langle 0 | \hat{c}_\alpha \hat{c}_\beta \hat{c}^\dagger_\nu \hat{c}^\dagger_\mu |0\rangle = \delta_{\beta\mu} \langle 0 | \hat{c}_\beta \hat{c}^\dagger_\nu \hat{c}^\dagger_\mu |0\rangle - \delta_{\beta\mu} \langle 0 | \hat{c}_\beta \hat{c}^\dagger_\nu \hat{c}^\dagger_\mu |0\rangle + \langle 0 | \hat{c}_\alpha \hat{c}_\beta \hat{c}^\dagger_\nu \hat{c}^\dagger_\mu |0\rangle \]

\[ = \delta_{\beta\mu} \delta_{\alpha\nu} - \delta_{\beta\nu} \delta_{\alpha\mu} \langle 0 |0\rangle + \delta_{\beta\nu} \langle 0 |0\rangle + \delta_{\beta\mu} \delta_{\alpha\nu} - \delta_{\beta\nu} \delta_{\alpha\mu}. \]

Thus

\[ \langle x_1, x_2 | \ldots, 1_i, \ldots, 1_j, \ldots\rangle = \frac{1}{\sqrt{2}} \sum_{\alpha, \beta} \phi_\alpha(x_2) \phi_\beta(x_1) (\delta_{\beta\mu} \delta_{\alpha\nu} - \delta_{\beta\nu} \delta_{\alpha\mu}) \]

\[ = \frac{1}{\sqrt{2}} \left( \phi_\nu(x_2) \phi_\mu(x_1) - \phi_\nu(x_2) \phi_\mu(x_1) \right) \]

| \phi_\mu(x_1) \phi_\mu(x_2) \phi_\nu(x_1) \phi_\nu(x_2) |. QED.
2. Density operators.

(a) The density operator $\hat{\rho}(x)$ is a single-particle operator. Expressed in terms of an arbitrary single-particle basis $\{|\alpha\rangle\}$, its second-quantized representation thus reads

$$\hat{\rho}(x) = \sum_{\alpha,\beta} \left( \int dx' \phi^*_\alpha(x')\delta(x-x')\phi_\beta(x') \right) \hat{c}^\dagger_\alpha \hat{c}_\beta$$  \hspace{1cm} (7)$$

$$= \sum_{\alpha,\beta} \phi^*_\alpha(x)\phi_\beta(x) \hat{c}^\dagger_\alpha \hat{c}_\beta.$$  \hspace{1cm} (8)

Note that we used $x'$ as an integration variable in the integral in the matrix element here (the expression enclosed in the parentheses), since $x$ was already “taken” as $\hat{\rho}(x)$ depends on $x$ as a parameter. [Alternatively, if you want to start from the more basic expression $\langle \alpha | \hat{h} | \beta \rangle$ for the matrix element, we have here $\hat{h} = \delta(\hat{x} - x)$ where the operator $\hat{x}$ and the parameter $x$ should not be confused with each other. This gives, upon inserting two copies of the identity operator resolved as $I = \int dx'|x'|\langle x' | x' \rangle$ and using $f(\hat{x})|x'\rangle = f(x')|x'\rangle$, that

$$\langle \alpha | \delta(\hat{x} - x) | \beta \rangle = \int dx' \int dx'' (\alpha | x' \rangle \langle x' | \delta(\hat{x} - x) | x'' \rangle \langle x'' | \beta \rangle$$

$$= \int dx' \int dx'' (\alpha | x' \rangle \delta(x'' - x') \langle x' | \beta \rangle)$$

$$= \int dx' \phi^*_\alpha(x')\delta(x' - x) \phi_\beta(x'),$$  \hspace{1cm} (9)

which is identical to the integral in (7).] Using $\hat{\psi}(x) = \sum_\alpha \phi_\alpha(x)\hat{c}_\alpha$ and its adjoint, we see that the above expression for $\hat{\rho}(x)$ can be written as

$$\hat{\rho}(x) = \hat{\psi}^\dagger(x)\hat{\psi}(x).$$  \hspace{1cm} (10)

Alternatively, we could have used the position-spin basis directly to write

$$\hat{\rho}(x) = \int dx' \hat{\psi}^\dagger(x')\delta(x - x')\hat{\psi}(x') = \hat{\psi}^\dagger(x)\hat{\psi}(x).$$  \hspace{1cm} (11)

(b) Using Eq. (8) we get

$$\int dx \hat{\rho}(x) = \sum_{\alpha,\beta} \hat{c}^\dagger_\alpha \hat{c}_\beta \int dx \phi^*_\alpha(x)\phi_\beta(x) = \sum_\alpha \hat{c}^\dagger_\alpha \hat{c}_\alpha = \sum_\alpha \hat{n}_\alpha = \hat{N}.$$  \hspace{1cm} (12)

Note that the basis $\{|\alpha\rangle\}$ used here is arbitrary, i.e. $\hat{N}$ takes the same form regardless of which basis one uses to express it. If the basis states are not countable and therefore must be labeled by a continuous variable, the sum over $\alpha$ is replaced by an integral, and $\hat{n}_\alpha$ then becomes a density operator. This is an alternative way of seeing that

$$\hat{N} = \int dx \hat{\rho}(x) = \int dx \hat{\psi}^\dagger(x)\hat{\psi}(x).$$  \hspace{1cm} (13)

(a) Let us start from the expression

\[
\frac{1}{2} \left[ \int dx \int dx' v(x, x') \hat{\rho}(x) \hat{\rho}(x') - \int dx v(x, x) \hat{\rho}(x) \right].
\]

(14)

Insert \( \hat{\rho}(x) = \sum_i \delta(x - x_i) \) to get

\[
\frac{1}{2} \left[ \int dx \int dx' v(x, x') \sum_i \delta(x - x_i) \sum_j \delta(x' - x_j) - \int dx v(x, x) \sum_i \delta(x - x_i) \right]
= \frac{1}{2} \sum_{i \neq j} v(x_i, x_j) = \hat{H}_I.
\]

(15)

(b) In second quantization we have \( \hat{\rho}(x) = \hat{\psi}^\dagger(x) \hat{\psi}(x) \). This gives

\[
\hat{H}_I = \frac{1}{2} \left[ \int dx \int dx' v(x, x') \hat{\psi}^\dagger(x) \hat{\psi}(x') \hat{\psi}(x) \hat{\psi}^\dagger(x') - \int dx v(x, x) \hat{\psi}^\dagger(x) \hat{\psi}(x) \right]
= \frac{1}{2} \left[ \int dx \int dx' v(x, x') \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}^\dagger(x') \hat{\psi}(x') \right. \text{ rewrite}
\left. - \int dx v(x, x) \hat{\psi}^\dagger(x) \hat{\psi}(x) \right]
\]

(16)

Now we use that

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

(17)

where \( \zeta = \pm 1 \) for fermionic/bosonic field operators. Therefore

\[
\hat{\psi}(x) \hat{\psi}^\dagger(x') = -\zeta \hat{\psi}^\dagger(x') \hat{\psi}(x) + \delta(x - x').
\]

(18)

We insert this for the product labeled “rewrite” in (16) and do the \( x' \) integration in the term with the Dirac delta function. This gives

\[
\hat{H}_I = \frac{1}{2} \left[ -\zeta \int dx \int dx' v(x, x') \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}^\dagger(x') \hat{\psi}(x') \right. \text{ rewrite}
\left. + \int dx v(x, x) \hat{\psi}^\dagger(x) \hat{\psi}(x) - \int dx v(x, x) \hat{\psi}^\dagger(x) \hat{\psi}(x) \right]
\]

\[
= -\frac{1}{2} \zeta \int dx \int dx' v(x, x') \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}^\dagger(x') \hat{\psi}(x') \hat{\psi}(x) - \zeta \hat{\psi}(x') \hat{\psi}(x)
\]

\[
= \frac{1}{2} \int dx \int dx' v(x, x') \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') \hat{\psi}(x') \hat{\psi}(x)
\]

(19)
where we used $(-\zeta)^2 = 1$.

(c) Starting from the previous expression and using $\hat{\psi}(x) = \sum_\alpha \phi_\alpha(x)\hat{c}_\alpha$ and its adjoint gives

$$\hat{H}_I = \frac{1}{2} \sum_{\alpha, \beta, \gamma, \delta} \int dx \int dx' v(x, x') \phi^*_\alpha(x) \phi^*_\beta(x') v(x, x') \phi_\delta(x') \phi_\gamma(x) \hat{c}^\dagger_\alpha \hat{c}^\dagger_\beta \hat{c}_\delta \hat{c}_\gamma,$$

(20)