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

1. Explicit connection between first and second quantization.

By our definition,

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

and thus

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

Furthermore,

$$|\ldots, 1_\mu, \ldots, 1_\nu, \ldots\rangle = \hat{c}_\mu^\dagger \hat{c}_\nu^\dagger |0\rangle. \tag{3}$$

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

$$\begin{aligned}\langle x_1, x_2|\ldots, 1_\mu, \ldots, 1_\nu, \ldots\rangle &= \frac{1}{\sqrt{2!}}\langle 0|\hat{\psi}(x_2)\hat{\psi}(x_1)\hat{c}_\mu^\dagger\hat{c}_\nu^\dagger|0\rangle \\ &= \frac{1}{\sqrt{2}}\sum_{\alpha,\beta}\phi_\alpha(x_2)\phi_\beta(x_1)\langle 0|\hat{c}_\alpha\hat{c}_\beta\hat{c}_\mu^\dagger\hat{c}_\nu^\dagger|0\rangle\end{aligned} \tag{4}$$

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

$$\begin{aligned}\langle 0|\hat{c}_\alpha \underbrace{\hat{c}_\beta\hat{c}_\mu^\dagger}_{\delta_{\beta\mu}-\hat{c}_\mu^\dagger\hat{c}_\beta} \hat{c}_\nu^\dagger|0\rangle &= \delta_{\beta\mu}\langle 0|\underbrace{\hat{c}_\alpha\hat{c}_\nu^\dagger}_{\delta_{\alpha\nu}-\hat{c}_\nu^\dagger\hat{c}_\alpha}|0\rangle - \langle 0|\hat{c}_\alpha\hat{c}_\mu^\dagger\underbrace{\hat{c}_\beta\hat{c}_\nu^\dagger}_{\delta_{\beta\nu}-\hat{c}_\nu^\dagger\hat{c}_\beta}|0\rangle \\ &= \delta_{\beta\mu}\delta_{\alpha\nu}\underbrace{\langle 0|0\rangle}_{1} - \delta_{\beta\mu}\underbrace{\langle 0|\hat{c}_\nu^\dagger}_{0}\underbrace{\hat{c}_\alpha|0\rangle}_{0} - \delta_{\beta\nu}\langle 0|\underbrace{\hat{c}_\alpha\hat{c}_\mu^\dagger}_{\delta_{\alpha\mu}-\hat{c}_\mu^\dagger\hat{c}_\alpha}|0\rangle + \langle 0|\hat{c}_\alpha\hat{c}_\mu^\dagger\hat{c}_\nu^\dagger\underbrace{\hat{c}_\beta|0\rangle}_{0} \\ &= \delta_{\beta\mu}\delta_{\alpha\nu} - \delta_{\beta\nu}\delta_{\alpha\mu}\langle 0|0\rangle + \delta_{\beta\nu}\underbrace{\langle 0|\hat{c}_\mu^\dagger}_{0}\underbrace{\hat{c}_\alpha|0\rangle}_{0} = \delta_{\beta\mu}\delta_{\alpha\nu} - \delta_{\beta\nu}\delta_{\alpha\mu}.\end{aligned} \tag{5}$$

Thus

$$\begin{aligned}\langle x_1, x_2|\ldots, 1_i, \ldots, 1_j, \ldots\rangle &= \frac{1}{\sqrt{2}}\sum_{\alpha,\beta}\phi_\alpha(x_2)\phi_\beta(x_1)(\delta_{\beta\mu}\delta_{\alpha\nu} - \delta_{\beta\nu}\delta_{\alpha\mu}) \\ &= \frac{1}{\sqrt{2}}(\phi_\nu(x_2)\phi_\mu(x_1) - \phi_\mu(x_2)\phi_\nu(x_1)) \\ &= \frac{1}{\sqrt{2!}}\begin{vmatrix}\phi_\mu(x_1) & \phi_\mu(x_2) \\ \phi_\nu(x_1) & \phi_\nu(x_2)\end{vmatrix}. \quad \text{QED.}\end{aligned} \tag{6}$$

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

$$\hat{\rho}(x) = \sum_{\alpha\beta} \left(\int dx' \; \phi_\alpha^*(x')\delta(x-x')\phi_\beta(x') \right) \hat{c}_\alpha^\dagger \hat{c}_\beta \tag{7}$$

$$= \sum_{\alpha,\beta} \phi_\alpha^*(x)\phi_\beta(x) \; \hat{c}_\alpha^\dagger \hat{c}_\beta. \tag{8}$$

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 $I = \int dx'|x'\rangle\langle x'|$ and using $f(\hat{x})|x'\rangle = f(x')|x'\rangle$, that

$$\begin{aligned}
\langle\alpha|\delta(\hat{x}-x)|\beta\rangle &= \int dx' \int dx'' \langle\alpha|x'\rangle\langle x'|\delta(\hat{x}-x)|x''\rangle\langle x''|\beta\rangle \\
&= \int dx' \int dx'' \langle\alpha|x'\rangle\delta(x''-x) \underbrace{\langle x'|x''\rangle}_{\delta(x'-x'')}\langle x''|\beta\rangle \\
&= \int dx' \; \phi_\alpha^*(x')\delta(x'-x)\phi_\beta(x'),
\end{aligned} \tag{9}$$

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

$$\hat{\rho}(x) = \hat{\psi}^\dagger(x)\hat{\psi}(x). \tag{10}$$

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

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

(b) Using Eq. (8) we get

$$\int dx \; \hat{\rho}(x) = \sum_{\alpha,\beta} \hat{c}_\alpha^\dagger \hat{c}_\beta \underbrace{\int dx \; \phi_\alpha^*(x)\phi_\beta(x)}_{\delta_{\alpha\beta}} = \sum_\alpha \hat{c}_\alpha^\dagger \hat{c}_\alpha = \sum_\alpha \hat{n}_\alpha = \hat{N}. \tag{12}$$

Note that the basis $\{|\alpha\}$ 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 α is replaced by an *integral*, and $\hat{n}_\alpha$ then becomes a *density* operator. This is an alternative way of seeing that

$$\hat{N} = \int dx \; \hat{\rho}(x) = \int dx \; \hat{\psi}^\dagger(x)\hat{\psi}(x). \tag{13}$$

3. Proof of the second-quantized representation of two-particle operators.

(a) Let us start from the expression

$$\frac{1}{2}\left[\int dx \int dx' v(x,x')\hat{\rho}(x)\hat{\rho}(x') - \int dx\ v(x,x)\hat{\rho}(x)\right]. \tag{14}$$

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

$$\begin{aligned}
&\frac{1}{2}\left[\int dx \int dx'\ v(x,x') \sum_i \delta(x-x_i) \sum_j \delta(x'-x_j) - \int dx\ v(x,x) \sum_i \delta(x-x_i)\right] \\
&= \frac{1}{2}\left[\sum_i \sum_j v(x_i,x_j) - \sum_i v(x_i,x_i)\right] = \frac{1}{2}\sum_{\substack{i,j \\ i\neq j}} v(x_i,x_j) = \hat{H}_I.
\end{aligned} \tag{15}$$

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

$$\begin{aligned}
\hat{H}_I &= \frac{1}{2}\left[\int dx \int dx'\ v(x,x')\hat{\rho}(x)\hat{\rho}(x') - \int dx\ v(x,x)\hat{\rho}(x)\right] \\
&= \frac{1}{2}\left[\int dx \int dx'\ v(x,x')\hat{\psi}^\dagger(x)\underbrace{\hat{\psi}(x)\hat{\psi}^\dagger(x')}_{\text{rewrite}}\hat{\psi}(x') - \int dx\ v(x,x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\right]
\end{aligned} \tag{16}$$

Now we use that

$$[\hat{\psi}(x), \hat{\psi}^\dagger(x')]_\zeta = \delta(x - x') \tag{17}$$

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

$$\hat{\psi}(x)\hat{\psi}^\dagger(x') = -\zeta\hat{\psi}^\dagger(x')\hat{\psi}(x) + \delta(x - x'). \tag{18}$$

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

$$\begin{aligned}
\hat{H}_I &= \frac{1}{2}\Bigg[-\zeta \int dx \int dx'\ v(x,x')\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')\hat{\psi}(x)\hat{\psi}(x') \\
&\quad + \underbrace{\int dx\ v(x,x)\hat{\psi}^\dagger(x)\hat{\psi}(x) - \int dx\ v(x,x)\hat{\psi}^\dagger(x)\hat{\psi}(x)}_{0}\Bigg] \\
&= -\frac{1}{2}\zeta \int dx \int dx'\ v(x,x')\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')\underbrace{\hat{\psi}(x)\hat{\psi}(x')}_{-\zeta\hat{\psi}(x')\hat{\psi}(x)} \\
&= \frac{1}{2}\int dx \int dx'\ v(x,x')\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')\hat{\psi}(x')\hat{\psi}(x)
\end{aligned} \tag{19}$$

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

$$\hat{H}_I = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \int dx \int dx' \; v(x,x')\phi^*_\alpha(x)\phi^*_\beta(x')v(x,x')\phi_\delta(x')\phi_\gamma(x) \; \hat{c}^\dagger_\alpha \hat{c}^\dagger_\beta \hat{c}_\delta \hat{c}_\gamma. \tag{20}$$