TFY4210, Quantum theory of many-particle systems, 2013: Tutorial 2

1. Explicit connection between first and second quantization.

An explicit connection between the basis states $|n\rangle \equiv |n_1, n_2, \ldots\rangle$ in second quantization and the basis wavefunctions $\Phi_n(x_1, \ldots, x_N)$ in first quantization can be established. Let

$$|x_1, x_2, \ldots, x_N\rangle \equiv \frac{1}{\sqrt{N!}} \hat{\psi}^\dagger(x_1) \ldots \hat{\psi}^\dagger(x_N)|0\rangle. \tag{1}$$

Then the (correctly normalized) basis wavefunctions are given by

$$\Phi_n(x_1, \ldots, x_N) = \langle x_1, \ldots, x_N|n\rangle. \tag{2}$$

As an example, consider a fermionic 2-particle basis state $|\ldots, 1_i, \ldots, 1_j, \ldots\rangle$, i.e. the single-particle states i and j are occupied and all others are empty. Evaluate the rhs of (2) to show that the wavefunction is indeed the correct Slater determinant,

$$\Phi(x_1, x_2) = \frac{1}{\sqrt{2!}} \begin{vmatrix} \phi_i(x_1) & \phi_i(x_2) \\ \phi_j(x_1) & \phi_j(x_2) \end{vmatrix}. \tag{3}$$

2. Density operators.

The density operator $\hat{\rho}(x)$ is in first quantization given by $\hat{\rho}(x) = \sum_{i=1}^N \delta(x - x_i)$.

(a) Show that in second quantization,

$$\hat{\rho}(x) = \hat{\psi}^\dagger(x)\hat{\psi}(x). \tag{4}$$

(b) Using second quantization, show that

$$\int dx \; \hat{\rho}(x) = \hat{N} \tag{5}$$

where $\hat{N}$ is the total number operator.

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

In first quantization a two-particle operator H_I takes the form

$$H_I = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} v(x_i, x_j). \tag{6}$$

(a) Show that this can be rewritten (with $\hat{\rho}(x)$ given by its first-quantization expression)

$$H_I = \frac{1}{2} \left[\int dx \int dx' \; v(x, x') \hat{\rho}(x) \hat{\rho}(x') - \int dx \; v(x, x) \hat{\rho}(x) \right]. \tag{7}$$

(b) Show that in second quantization H_I can be written (for both fermionic and bosonic systems)

$$H_I = \frac{1}{2} \int dx \int dx' \; v(x, x') \; \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') \hat{\psi}(x') \hat{\psi}(x). \tag{8}$$

(c) Use this to show that the second-quantized representation of H_I, expressed using the arbitrary basis $\{|\alpha\rangle\}$ for single-particle states, is given by

$$\hat{H}_I = \frac{1}{2} \sum_{\alpha,\beta,\gamma,\delta} \left(\int dx \int dx' \; \phi^*_\alpha(x) \phi^*_\beta(x') v(x, x') \phi_\delta(x') \phi_\gamma(x) \right) \; \hat{c}^\dagger_\alpha \hat{c}^\dagger_\beta \hat{c}_\delta \hat{c}_\gamma, \tag{9}$$

which is exactly of the form claimed in the lectures (the expression enclosed in parentheses is the matrix element denoted $\langle \alpha\beta | v | \gamma\delta \rangle$ in the lectures).