

TFY4210, Quantum theory of many-particle systems, 2014:

Tutorial 2

1. Explicit connection between first and second quantization.

An explicit connection between the basis states $|n\rangle \equiv |n_1, n_2, \dots\rangle$ with $\sum_{\nu} n_{\nu} = N$ in second quantization and the basis wavefunctions $\Phi_n(x_1, \dots, x_N)$ in first quantization can be established. Let

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

Then the (correctly normalized) basis wavefunctions are given by

$$\Phi_n(x_1, \dots, x_N) = \langle x_1, \dots, x_N | n \rangle. \quad (2)$$

As an example, consider a fermionic 2-particle basis state $|\dots, 1_{\mu}, \dots, 1_{\nu}, \dots\rangle$ in which the single-particle states μ and ν are occupied and all others are empty. Evaluate the rhs of (2) to show that the wavefunction is indeed the correct Slater determinant,

$$\Phi(x_1, x_2) = \frac{1}{\sqrt{2!}} \begin{vmatrix} \phi_{\mu}(x_1) & \phi_{\mu}(x_2) \\ \phi_{\nu}(x_1) & \phi_{\nu}(x_2) \end{vmatrix}. \quad (3)$$

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,

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

(b) Using second quantization, show that

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

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

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

In first quantization a two-particle operator \hat{H}_I takes the form

$$\hat{H}_I = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N v(x_i, x_j). \quad (6)$$

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

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

(b) Show that in second quantization \hat{H}_I can be written (for both fermionic and bosonic systems)

$$\hat{H}_I = \frac{1}{2} \int dx \int dx' v(x, x') \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x') \hat{\psi}(x') \hat{\psi}(x). \quad (8)$$

(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

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

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).