Universität Bonn 30.11.2012
Physikalisches Institut
Prof. Dr. J. Kroha, Zhong Yuan Lai, Ammar Nejati
www.uni-bonn.de/kroha/teaching/lectures-and-seminars/ws2012/aqt

Advanced Quantum Theory WS 2012 / 2013

Exercise Sheet 8

(To be handed in on 7. December and discussed on 10. and 11. December)

8.1 Many-Particle Hamiltonian in Second Quantization (6 Points)

We consider the Hamilton operator of a many-particle system with kinetic energy T, potential energy $U(\vec{x})$ and a two-particle interaction $V(\vec{x}_i, \vec{x}_j)$,

$$H = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + U(\vec{x}) + \frac{1}{2}\sum_{i\neq j} V(x_i, x_j). \tag{1}$$

Show that in 2nd quantization the Hamiltonian takes the form,

$$H = \sum_{\alpha,\beta}(t_{\alpha\beta} + U_{\alpha\beta})a_\alpha^\dagger a_\beta + \frac{1}{2}\sum_{\alpha,\beta,\gamma\delta} V_{\alpha,\beta,\delta,\gamma} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \tag{2}$$

where the matrix elements are,

$$t_{\alpha,\beta} = \langle\alpha|t|\beta\rangle$$

$$U_{\alpha,\beta} = \langle\alpha|U(\vec{x})|\beta\rangle$$

$$V_{\alpha,\beta,\delta,\gamma} = \langle\alpha,\beta|V(\vec{x}_i,\vec{x}_j)|\gamma,\delta\rangle = \int d^3x_i \int d^3x_j\ \phi_\alpha^*(\vec{x}_i)\phi_\beta^*(\vec{x}_j)V(\vec{x}_i,\vec{x}_j)\phi_\gamma(\vec{x}_i)\phi_\delta(\vec{x}_j)$$

and $\{|\alpha\rangle\}$ is a complete one-particle basis and $a_\alpha^\dagger$, a_α are the corresponding creation and annihilation operators, respectively.

8.2 The Field Operator Representation (6 Points)

The field operators in position representation are defined as follows:

$$\Psi(\vec{x}) = \sum_\alpha \phi_\alpha(\vec{x})a_\alpha$$
$$\Psi^\dagger(\vec{x}) = \sum_\alpha \phi_\alpha^*(\vec{x})a_\alpha^\dagger$$

where $\phi_\alpha(\vec{x})$ is the wavefunction corresponding to single-particle state α. It has been shown in the lecture that these operators create and destroy a particle at position $\vec{x}$, respectively. Show that the following representation of the many-particle Hamiltonian in terms of field operators holds:

$$H = \frac{h^2}{2m}\int d^3x\ \Big(\nabla\Psi^\dagger(\vec{x})\nabla\Psi(\vec{x}) + U(\vec{x})\Psi^\dagger(\vec{x})\Psi(\vec{x})\Big) + \frac{1}{2}\int d^3x \int d^3x'\ \Psi^\dagger(\vec{x})\Psi^\dagger(\vec{x}')V(\vec{x},\vec{x}')\Psi(\vec{x}')\Psi(\vec{x}).$$

8.3 Momentum representation (6 Points)

For translationally invariant systems it is useful to work with momentum states as the single-particle basis. We define the normalized momentum eigenfunction in the following manner:

$$\phi_{\vec{k}}(\vec{x}) = \frac{1}{\sqrt{(2\pi)^3}} e^{i\vec{k}\cdot\vec{x}} \tag{3}$$

The eigenfunctions fulfill the following orthonormality relation

$$\int d^3x \; \phi^*_{\vec{k}}(\vec{x}) \phi_{\vec{k}'}(\vec{x}) = \delta^3(\vec{k}' - \vec{k}) \tag{4}$$

Show that the following representation of the many-particle Hamiltonian in the momentum representation holds:

$$H = \sum_{\vec{k}} \frac{(\hbar k)^2}{2m} a^\dagger_{\vec{k}} a_{\vec{k}} + \sum_{\vec{k},\vec{k}'} \frac{1}{(2\pi)^3} U_{\vec{k}'-\vec{k}} a^\dagger_{\vec{k}'} a_{\vec{k}} + \sum_{\vec{q},\vec{p},\vec{k}} \frac{1}{2(2\pi)^3} V_{\vec{q}} \, a^\dagger_{\vec{p}+\vec{q}} a^\dagger_{\vec{k}-\vec{q}} a_{\vec{k}} a_{\vec{p}} \tag{5}$$

where $U_{\vec{k}'-\vec{k}}$ and $V_{\vec{q}}$ are the Fourier-transformed one- and two particle potentials, respectively. Note that in the translationally invariant system $V(\vec{x}_i, \vec{x}_j) = V(|\vec{x}_i - \vec{x}_j|)$ holds.

8.4 Orthonormality of the Many-Particle Basis State (3 Points)

Using properties of the single-particle basis states as described in the lecture, show the orthonormality property of the many-particle basis state:

$$\langle m_1, m_2, \ldots, m_k \ldots | n_1, n_2, \ldots, n_k \ldots \rangle = \delta_{m_1,n_1} \delta_{m_2,n_2} \cdots = \prod_{k=1}^{\infty} \delta_{m_k,n_k}$$