Advanced Quantum Mechanics – Winter Term 2017/18

Problem Sheet 06 – due on January 31st

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Problem 6.1

In the lecture we have discussed how to write basis states in Fock space with creation operators for both, bosons as well as fermions. However, for the fermionic case the proof of some formulas is still missing.

Let $\widehat{a}_k^\dagger$ and $\widehat{a}_k$ be fermionic creation and annihilation operators. They obey anti-commutation relations, where the only non-trivial anti-commutators are $\{\widehat{a}_k, \widehat{a}_l^\dagger\} = \delta_{kl}$. The Fock basis states are given by

$$|n_1\, n_2\, ...\rangle \;=\; (\widehat{a}_1^\dagger)^{n_1}\,(\widehat{a}_2^\dagger)^{n_2}\,(\widehat{a}_3^\dagger)^{n_3}\,...\,|0\rangle\;, \tag{1}$$

with occupation number $n_k \in \{0,1\}$. Show the following relations:

$$\langle n_1'\, n_2'\, ...\,|\,n_1\, n_2\, ...\rangle \;=\; \delta_{n_1',n_1}\,\delta_{n_2',n_2}\,\cdots\;, \tag{2}$$

$$\widehat{a}_k^\dagger\,|n_1\, n_2\, ...\rangle \;=\; (1-n_k)\,(-1)^{\sum_{j<k} n_j}\,|n_1\, ...\, n_k+1\, ...\,\rangle\;, \tag{3}$$

$$\widehat{a}_k\,|n_1\, n_2\, ...\rangle \;=\; n_k\,(-1)^{\sum_{j<k} n_j}\,|n_1\, ...\, n_k-1\, ...\,\rangle\;, \tag{4}$$

$$\widehat{n}_k\,|n_1\, n_2\, ...\rangle \;=\; n_k\,|n_1\, n_2\, ...\rangle\;, \tag{5}$$

where $\widehat{n}_k \;=\; \widehat{a}_k^\dagger\,\widehat{a}_k$ is the number operator.

Problem 6.2

In the lecture we introduced the Hubbard model. Its Hamilton operator is given by

$$\widehat{H} \;=\; -t\sum_x\sum_{\mu=1}^{d}\sum_{\sigma=\pm}\Big[\widehat{a}_{x+\hat{\mu},\sigma}^\dagger\,\widehat{a}_{x,\sigma} \;+\; \widehat{a}_{x,\sigma}^\dagger\,\widehat{a}_{x+\hat{\mu},\sigma}\Big] \;+\; U\sum_x \widehat{n}_{x,+}\,\widehat{n}_{x,-}\;, \tag{6}$$

where $\widehat{a}_{x,\sigma}^\dagger$ and $\widehat{a}_{x,\sigma}$ are fermionic creation and annihilation operators for electrons at a site x of the d-dimensional lattice with spin up ($\sigma=+$) and spin down ($\sigma=-$) and $\widehat{n}_{x,\sigma}$ is the corresponding number operator. The terms in the first sum describe hopping of the electrons to neighboring sites, and the second term the Coulomb repulsion between electrons at the same site (due to the Pauli principle they must have opposite spin).

We now use the Hubbard model as a toy model for a ${H_3}^+$ ion. The protons are arranged at the corners of an equilateral triangle, and we label the three corresponding sites x where the electron may sit with $x = 1, 2, 3$. Thus we have 6 creation operators $\widehat{a}^\dagger_{x,\sigma}$ with $x = 1, 2, 3$ and $\sigma = \pm$ and the corresponding annihilators $\widehat{a}_{x,\sigma}$.

Since we describe a ${H_3}^+$ ion, we only need to consider all states with exactly two creation operators. For example a state $|\Phi_1\rangle$ with an electron with spin up at site 1 and an electron with spin down at site 2 is given by

$$|\Phi_1\rangle \;=\; \widehat{a}^\dagger_{1,+}\,\widehat{a}^\dagger_{2,-}\,|0\rangle\;, \tag{7}$$

while a state $|\Phi_2\rangle$ with two electrons at site 3 is given by

$$|\Phi_2\rangle \;=\; \widehat{a}^\dagger_{3,+}\,\widehat{a}^\dagger_{3,-}\,|0\rangle\;. \tag{8}$$

Make a complete list of all basis states $|\Phi_i\rangle$, $i = 1, \ldots N$ that are possible for our ${H_3}^+$ ion. What is their number N?

Note that the basis states $|\Phi_i\rangle$, $i = 1, \ldots N$ are not the physical eigenstates $|\Psi\rangle$ of the system. To determine these one needs to solve the time independent Schrödinger equation $\widehat{H}|\Psi\rangle = E\,|\Psi\rangle$. For this step we expand the physical states $|\Psi\rangle$ in our basis states:

$$|\Psi\rangle \;=\; \sum_{j=1}^{N} a_j\;|\Phi_j\rangle\;, \tag{9}$$

where the a_j are the coefficients we need to determine. Insert this series in the Schrödinger equation and multiply from left with a basis state $\langle\Phi_i|$ and show that the coefficients a_j obey the following eigenvalue problem

$$\sum_{j=1}^{N} H_{ij}\,a_j \;=\; E\,a_i\;,\quad \text{with } H_{ij} \;=\; \langle\Phi_i|\widehat{H}|\Phi_j\rangle\;. \tag{10}$$

In vector/matrix notation the eigenvalue problem has the form $H\,\vec{a} \;=\; E\,\vec{a}$. Since the operator $\widehat{H}$ is hermitian the $N \times N$ matrix H is hermitian and the eigenvalues E are real. Solving the eigenvalue problem gives rise to N eigenvectors $\vec{a}^{(n)}$, $n = 1, \ldots N$ with eigenvalues $E^{(n)}$. The physical eigenstates $|\Psi^{(n)}\rangle$ with energy eigenvalues $E^{(n)}$ are then given by

$$|\Psi^{(n)}\rangle \;=\; \sum_{j=1}^{N} a^{(n)}_j\,|\Phi_j\rangle\;. \tag{11}$$

The eigenvalue problem (10) is typically very large and has to be solved numerically. However, the matrix elements have to be known in closed form. Thus as last part of this problem determine all matrix elements $H_{ij} = \langle\Phi_i|\widehat{H}|\Phi_j\rangle$ for your basis states $|\Phi_j\rangle$. Use the fact that H is a hermitian matrix – this essentially cuts the amount of work in half.

Problem 6.3

In the lecture we discussed the Fock space representation for free bosons in an $L \times L \times L$ box with periodic boundary conditions. They are described by bosonic annihilation and creation operators $\widehat{a}_{\vec{k}}$ and $\widehat{a}^\dagger_{\vec{k}}$ which are labelled by the wave vectors $\vec{k} = \frac{2\pi}{L}(n_1, n_2, n_3)$ with $n_i \in \mathbb{Z}$. The corresponding free Hamilton operator is given by

$$\widehat{H}_0 \;=\; \sum_{\vec{k}} \frac{\hbar^2\, \vec{k}^2}{2m}\, \widehat{n}_{\vec{k}}\;, \tag{12}$$

where $\widehat{n}_{\vec{k}} = \widehat{a}^\dagger_{\vec{k}}\, \widehat{a}_{\vec{k}}$ is the number operator.

Now we would like to construct a repulsion of the bosons at short distances ("hard core bosons"). A crude but simple way to model this interaction is to add to the Hamiltonian $\widehat{H}_0$ an interaction term of the form ($U > 0$),

$$\widehat{H}_I \;=\; U \int_V d^3x\, \widehat{n}_{\vec{x}}\, (\widehat{n}_{\vec{x}} - 1)\;, \tag{13}$$

where $\widehat{n}_{\vec{x}}$ is the operator for the number of particles at position $\vec{x}$. Obviously the energy goes up when the occupation numbers $n_{\vec{x}}$ at a position $\vec{x}$ become larger than 1.

Find the form of this interaction for the representation in terms of creation and annihilation operators $\widehat{a}^\dagger_{\vec{k}}$ and $\widehat{a}_{\vec{k}}$ for quanta labelled with wave vectors $\vec{k}$.

Hint: Try to represent the number operator $\widehat{n}_{\vec{x}}$ through the $\widehat{n}_{\vec{k}}$ via inverse Fourier transformation.