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Advanced Quantum Theory WS 2012 / 2013

Exercise Sheet 11

(To be handed in on 11. January and discussed on 14. and 15. January)

11.1 Further Properties of Coherent States (2 + 2 + 2 Points)

In this exercise we will continue our study of (bosonic) coherent states. We recall the definition of such a coherent state which was derived in the previous exercise sheet:

$$|\Phi\rangle = \sum_{n=0}^{\infty} \frac{(\phi a^\dagger)^n}{n!}|0\rangle, \tag{1}$$

where $\phi \in \mathbb{C}$ is the eigenvalue of the coherent state $|\Phi\rangle$

$$a|\Phi\rangle = \phi\,|\Phi\rangle. \tag{2}$$

a) Using knowledge from elementary quantum mechanics, calculate the probability $p(n)$ that there are n particles in the state $|\Phi\rangle$.

b) Using proper normalization of the coherent state $|\Phi\rangle$ ($\langle\Phi|\Phi\rangle = 1$) calculate the average particle number $\langle\hat{N}\rangle$, where $\hat{N} = a^\dagger a$

c) Using the result from part b), calculate now the variance of the average particle number $\sigma_N = \langle\hat{N}^2\rangle - \langle\hat{N}\rangle^2$

11.2 The Hartree-Fock Approximation (2 + 8 + 6 + 2 + 4 + 4 Points)

In this exercise we consider an approximation to describe the effects of 2-particle interactions. This method is based on the principle of the *mean-field*, or the assumption that the *fluctuations* of a quantity are small compared to its average. Specifically, we consider the a many-body system of electrons with mass m in free space, interacting via the Coulomb potential $V(\vec{r}_i - \vec{r}_j) = e^2/|\vec{r}_i - \vec{r}_j|$.

a) Using the results of exercise 8.3, show that the Hamiltonian of the system can be written in 2nd quantization as

$$H = \sum_{\vec{k},\sigma} \frac{\hbar^2 k^2}{2m} c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} + \frac{1}{2} \sum_{\substack{\vec{k},\vec{k}',\vec{q}\\ \sigma,\sigma'}}{}' V_{\vec{q}}\, c^\dagger_{\vec{k}+\vec{q},\sigma} c^\dagger_{\vec{k}'-\vec{q},\sigma'} c_{\vec{k}',\sigma'} c_{\vec{k},\sigma} = H_0 + H_{int}, \tag{3}$$

where $\sigma = \uparrow, \downarrow$ denotes spin,

$$V_{\vec{q}} = \frac{e^2}{V}\frac{4\pi}{q^2},$$

is the Fourier transform of the Coulomb potential and the prime symbol over the summation denotes exclusion of the $\vec{q} = 0$ term in the sum

Hint: To make the Fourier integral of the Coulomb potential convergent, introduce a convergence factor $e^{-\alpha r}$ and let $\alpha \to 0$ at the end of the calculation.

From the form of $V_{\vec{q}}$ you see that it diverges at $q = 0$. Physically, this divergence comes from the fact that the Coulomb interaction is a long-range one, and usually the presence of a positive ionic background charge compensates this divergency and provides a physically meaningful interpretation of $V_{\vec{q}}$. For our problem we will do the following redefinition: Set

$$V_{\vec{q}} = \begin{cases} \frac{e^2}{V}\frac{4\pi}{q^2}, & q \neq 0, \\ V_0, & q = 0 \end{cases} \tag{4}$$

where V_0 is a constant.

b) *Non-interacting many-body groundstate*

We first construct the groundstate of a system of non-interacting electrons, and calculate its energy with respect to the non-interacting Hamiltonian H_0. Denote the vacuum state (no particales present) by $|\, 0\,\rangle$. Argue that the groundstate $|\, \Phi_0\,\rangle$ of H_0 can be written as

$$|\, \Phi_0\,\rangle = \prod_{|\vec{k}|\leq k_F} c^\dagger_{\vec{k},\uparrow} c^\dagger_{\vec{k},\downarrow} |\, 0\,\rangle \tag{5}$$

Show that this is an eigenstate of the total particle number operator $N = \sum_{\vec{k},\sigma} c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma}$ and of the non-interacting Hamiltonian H_0. Give the corresponding particle number and energy eigenvalues N_0 and E_0, respectively, as sums over the momentum $\vec{k}$.

c) Show that $N_0 \propto k_F^3$ and $E_0 \propto k_F^5$.

Hint: use the relation

$$\sum_{\vec{k}} f(\vec{k}) = \frac{\mathcal{V}}{(2\pi)^3} \int d^3k\, f(\vec{k}), \tag{6}$$

valid for an arbitrary function f, with $\mathcal{V}$ the volume of the system.

d) *Mean-field approximation*

Let an arbitrary operator A be represented by its average ("mean field") $\langle A\rangle$ with respect to some state and the deviations ΔA as $A = \langle A\rangle + \Delta A$, and similarly for an operator B. Show that to first order in ΔA and ΔB the product AB reads,

$$AB = \langle A\rangle B + A\langle B\rangle - \langle A\rangle\langle B\rangle + O(\Delta A \Delta B). \tag{7}$$

e) *Hartree approximation*

In the Hamiltonian (3) choose the operators A and B such that

$$A = \sum_{\vec{k},\sigma} c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma} \tag{8}$$

$$B = \sum_{\vec{k}',\sigma'} c^\dagger_{\vec{k}'-\vec{q},\sigma'} c_{\vec{k}',\sigma'} \tag{9}$$

and use the mean-field approximation (7), with expectation values taken with respect to the non-interacting ground state, to transform H_{int} in (3) into an effective single-particle Hamiltonian,

$$H^{(Hartree)} = V_0 N \sum_{\vec{k},\sigma} c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} + \text{constant}, \tag{10}$$

where $V_0 \equiv V_{\vec{q}=0}$ and N is the total number of particles in the system (Hartree approximation), and the constant term is proportional to the square of the particle number (this term vanishes in the thermodynamic limit, and hence could be neglected).

Hint: Separate H_{int} into a part with $q = 0$ and $q \neq 0$ and consider these 2 cases separately. Show that in the case of $\vec{q} \neq 0$ in the Hartree approximation the interaction correction to the energy vanishes. Use also the homogeneity restriction: $\langle c^\dagger_{\vec{k},\sigma} c_{\vec{k}',\sigma'}\rangle = \langle \hat{n}_{\vec{k},\sigma}\rangle \delta_{\vec{k}\vec{k}'} \delta_{\sigma\sigma'}$

f) *Fock approximation*

In the Hamiltonian (3) choose the operators A and B in a different way.

$$A = c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k}',\sigma'} \tag{11}$$

$$B = c^\dagger_{\vec{k}'-\vec{q},\sigma'} c_{\vec{k},\sigma}. \tag{12}$$

Commute the operators of the interaction term appropriately and then use the mean-field approximation (7) to transform H_{int} into an effective single-particle operator,

$$H^{(Fock)} = -\sum_{\substack{\vec{k},\vec{k}'\\ \sigma}} V(|\vec{k}-\vec{k}'|) n_{\vec{k},\sigma} c^\dagger_{\vec{k}',\sigma} c_{\vec{k}',\sigma} + \text{constant}.$$

(Fock approximation) and the constant term is again proportional to the square of the particle number. This term is called the "exchange term". From the form of this Hamiltonian read off that in the Hartee-Fock approximation the effect of the interaction is that the bare energy of a single elctron, $\varepsilon_0(\vec{k}) = \frac{(\hbar k)^2}{2m}$, is shifted by

$$\varepsilon_{HF}(\vec{k}, \sigma) = -\sum_{\vec{k}'} \frac{4\pi e^2}{|\vec{k} - \vec{k}'|^2} n_{\vec{k},\sigma}.$$

11.3 Equation of motion for the Greens function with local pair interaction (5 + 5 + 8 Points)

If one considers an electron gas with a local pair interaction between two electrons, the noninteracting Hamiltonian and the interaction terms in position representation in 2nd quantization looks like the following:

$$H_0 = \frac{\hbar^2}{2m} \sum_{\sigma} \int d^3x \nabla \Psi_\sigma^\dagger(x) \nabla \Psi_\sigma(x) \tag{13}$$

and

$$V = \frac{1}{2} \sum_{\sigma\sigma'} \int d^3x \, d^3x' v(x, x') \Psi_\sigma^\dagger(x) \Psi_{\sigma'}^\dagger(x') \Psi_{\sigma'}(x') \Psi_\sigma(x), \tag{14}$$

respectively, where the pair interaction is given by $v(x, x') = (2\pi)^3 V_0 \delta(x - x')$. In a real system, the local pair interaction can thought of as a strongly screened Coulomb interaction.

a) Transform the free and interaction terms in the Hamiltonian, (13) and (14), to momentum space and show that:

$$H = H_0 + V = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{1}{2} V_0 \sum_{\substack{kpq \\ \sigma\sigma'}} c_{k+q\sigma}^\dagger c_{p-q\sigma'}^\dagger c_{p\sigma'} c_{k\sigma} \tag{15}$$

b) Derive in analogy to the lecture the equation of motion of the retarded Greens function for the Hamiltonian H:

$$i\partial_t G_{k\sigma}^R(t, t') = \delta(t - t') + \varepsilon_k G_{k\sigma}^R(t, t') - i\theta(t - t') \langle [[c_{k\sigma}, V]_-(t), c_{k\sigma}^\dagger(t')]_+ \rangle$$

where we have set $\hbar = 1$. Write down the equation of motion for the Hamiltonian of part a) and show that the interaction term depends on the "higher" Greens function

$$\chi_{pqk}^{\sigma\sigma'} = -i\theta(t - t') \langle [(c_{p+q\sigma}^\dagger c_{p\sigma} c_{k+q\sigma'})(t), c_{k\sigma'}^\dagger(t')]_+ \rangle \tag{16}$$

c) Recall the mean field approximation which we have derived in problem 11.2: $AB = \langle A \rangle B + \langle B \rangle A - \langle A \rangle \langle B \rangle$. Use this approximation again with the same definitions as in exercise 11.2 to obtain the Hartree and Fock terms and hence show the retarded Green function for the Hamiltonian of (13) and (14) in the momentum space can be approximated as:

$$G_{k\tau}^R(\omega) = \frac{1}{\omega - \epsilon_k - \Sigma(\omega) + i\eta}$$

Write down the form of $\Sigma(\omega)$ and discuss this result.