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Advanced Quantum Theory WS 2012 / 2013

Exercise Sheet 9

(To be handed in on 14. December and discussed on 17. and 18. December)

9.1 Hamiltonian of the One-Dimensional Hubbard Model (6 Points)

N electrons with spin quantum number $\sigma = \pm 1/2$ are placed in orbitals located at discrete sites x_i, $i = 1, 2, \ldots$, separated by distance a on an infinitely long one-dimensional chain. The electronic Hamiltonian can be written in 2nd quantization in the form

$$H_0 = -t \sum_{i=1}^{N} \sum_{\sigma} (c_\sigma^\dagger(x_i) c_\sigma(x_i + a) + c_\sigma^\dagger(x_i) c_\sigma(x_i - a)),$$

where the two terms describe movement of the electrons by one site to the left and right, respectively. The operators $c(x_i)$ fulfill the canonical anticommutation relation $\{c_\sigma(x_i), c_{\sigma'}^\dagger(x_j)\} = \delta_{\sigma,\sigma'} \delta_{x_i,x_j}$.

a) Show that H_0 can be written in the following form

$$H_0 = -\frac{1}{2\pi} \sum_{\sigma} \int dk\, \varepsilon(k) c_\sigma^\dagger(k) c_\sigma(k),$$

in momentum representation. Write down the explicit form of the dispersion relation $\varepsilon(k)$. In the limit of an infinitely long chain, use the discrete Fourier transformation $c_\sigma(k) = \frac{1}{N} \sum_i e^{-ikx_i} c_\sigma(x)$ and $c_\sigma(x_i) = \frac{1}{2\pi} \int dk\, e^{ikx} c_\sigma(k)$.

b) Consider now the additional interaction term (what physical meaning does it carry?)

$$H' = \frac{U}{2} \sum_{i,\sigma} c_\sigma^\dagger(x_i) c_\sigma(x_i) c_{-\sigma}^\dagger(x_i) c_{-\sigma}(x_i).$$

Show that $M_\sigma = \sum_i c_\sigma^\dagger(x_i) c_\sigma(x_i)$ are good quantum numbers corresponding to the total Hamiltonian $H = H_0 + H'$. What is the meaning of M_σ?

c) The spin operators for site i are defined via by the expression

$$\vec{S}_i = \frac{\hbar}{2} \sum_{\sigma,\sigma'} c_\sigma^+(x_i) \vec{\sigma}_{\sigma\sigma'} c_{\sigma'}(x_i),$$

where the $\vec{\sigma}$ are Pauli matrices. Show that these operators fulfill the angular momentum commutation relations. Why do spin operators on different sites commute?

9.2 The Hartree-Fock Approximation (6 Points)

In this exercise we introduce a simple but often-used approximation to deal with the effects of 2-particle interactions. This method is based on the principle of the *mean-field*, or the assumption that *fluctuations* are small relative to some average quantity. In generic terms, this can be quantified in the following manner: given an "interaction" term that is a simple product of 2 operators A and B

$$H_{int} = AB,$$

the mean-field approximation allows us to approximate it as follows

$$H_{int}^{MF} = A\,\langle B\rangle + \langle A\rangle\, B - \langle A\rangle\,\langle B\rangle\,, \tag{1}$$

where the average $\langle \dots \rangle$ is performed with respect to the noninteracting Hamiltonian. We have seen in the previous exercise sheet that the Hamiltonian corresponding to a system of interacting electrons can be written in momentum space as follows

$$\begin{aligned} H &= \sum_{\vec{k},\sigma} \frac{\hbar^2 k^2}{2m} a^\dagger_{\vec{k},\sigma} a_{\vec{k},\sigma} + \frac{e^2}{2V} \sum_{\substack{\vec{k},\vec{k}',\vec{q}\\ \sigma,\sigma'}}{}' V_{\vec{q}}\, a^\dagger_{\vec{k}+\vec{q},\sigma} a^\dagger_{\vec{k}'-\vec{q},\sigma'} a_{\vec{k}',\sigma'} a_{\vec{k},\sigma}, \\ &= \mathcal{H}_0 + \mathcal{H}_{int} \end{aligned} \tag{2}$$

where we have omitted the potential term, and the prime symbol over the summation denotes exclusion of the $\vec{q} = 0$ term in the sum (Note that the Coulomb interaction is momentum dependent!).

a) 2-*particle interaction in momentum space*
Starting from the Coulomb interaction in position space

$$V(\vec{r}_i - \vec{r}_j) = \frac{e^2}{|\vec{r}_i - \vec{r}_j|},$$

show that

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

where V is the volume of the system
Hint: Due to the long-range nature of the Coulomb interaction the initial integral does not converge; use the trick of supposing that the potential decays like $r^{-1}e^{-\alpha r}$ and setting $\alpha \to 0$ at the end of the calculation.

b) *Construction of N-particle groundstate wavefunction.*
In this exercise we will construct the groundstate wavefunction of a system of noninteracting electrons, and use it to calculate the energy of the *interacting* system to 1st order in the interaction.

i) Start from the vacuum state $|\,0\,\rangle$. Argue that the N-particle noninteracting state $|\,\Phi_0\,\rangle$ can be written as

$$|\,\Phi_0\,\rangle = \left(\prod_{i=1}^{N} c^\dagger_{\vec{k}_i,\uparrow}\right)\left(\prod_{i=1}^{N} c_{\vec{k}_i,\downarrow}\right)|\,0\,\rangle \tag{3}$$

and show that (3) is an eigenfunction of the occupation number operator and hence of the noninteracting Hamiltonian

$$\mathcal{H}_0\,|\,\Phi_0\,\rangle = \sum_{i=1}^{N} \mathcal{E}_{\vec{k}_i}\,|\,\Phi_0\,\rangle\,,$$

where $\mathcal{E}_{\vec{k}_i} = \frac{\hbar^2 \vec{k}_i^2}{2m}$

ii) We can now calculate the groundstate energy of the noninteracting system. The energy is defined in the usual form in perturbation theory as

$$E^{(0)} = \langle\, \Phi_0 \,|\, \mathcal{H}_0 \,|\, \Phi_0 \,\rangle \tag{4}$$

We denote the wavevector corresponding to the highest energy state k_F ("Fermi wavevector"). Show that $E^{(0)}$ is proportional to k_F^5.
Hint: To evaluate (4) *use the relation*

$$\sum_{\vec{k}} f(\vec{k}) = \frac{V}{(2\pi)^3} \int d^3k\, f(\vec{k}). \tag{5}$$

iii) We can now calculate the energy of the interaction perturbatively to 1st order. For this use the same wavefunction that you constructed in part (i) and the form of the interaction term $\mathcal{H}_{int}$ in (2). Argue that, in order for $E^{(1)} = \langle\, \Phi_0 \,|\, \mathcal{H}_{int} \,|\, \Phi_0 \,\rangle$ to be different from zero, the condition $\vec{k}' = \vec{k} + \vec{q}$ has to be fulfilled. Calculate $E^{(1)}$ using the same hint as in part (ii).

c) *Effective one-particle Hamiltonian from the Hartree-Fock approximation.*
Using the explanation of the mean-field as given in this exercise we can rewrite the full interacting Hamiltonian (2) as an *effective one-particle* Hamiltonian. Using the fact that $\langle\, a^\dagger_{\vec{k},\sigma} a_{\vec{k}',\sigma'} \,\rangle = \langle\, \hat{n}_{\vec{k},\sigma} \,\rangle\, \delta_{\vec{k}\vec{k}'}\delta_{\sigma\sigma'}$, where $\hat{n}_{\vec{k},\sigma}$ is the occupation number operator, perform the averaging procedure as described in (1) on $\mathcal{H}_{int}$ of (2) and show that one obtains an effective one-particle Hamiltonian, in which the free electron dispersion $\varepsilon_0(\vec{k}) = \frac{\hbar^2\vec{k}^2}{2m}$ gets renormalized by a term

$$\varepsilon_{HF}(\vec{k}) = -\frac{e^2}{V} {\sum_{\vec{q}}}' \frac{4\pi}{q^2} \langle\, \hat{n}_{\vec{k}+\vec{q},\sigma} \,\rangle \tag{6}$$

9.3 The Residual Theorem (6 Points)

The residual theorem states: If a function $f(z)$ has n simple poles in a closed curve C, then the relation

$$\oint_c f(z)dz = 2\pi i \sum_{k=1}^{n} a_{-1}(z_k)$$

holds, where a_{-1} are the residues of the function $f(z)$. Show the following with the help of the residue theorem:

a)

$$\oint_{|z|=3} \frac{1}{z^4 + z^3 - 2z^2} dz = 0$$

b)

$$\int_0^\infty \frac{1}{(x^2+1)^2} dx = \frac{\pi}{4}$$