Theoretical Physics V

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Assignment VIII **Due date 11.6.2014**

Prof. Dr. Wilhelm-Mauch http://qsolid.uni-saarland.de/?Lehre:TP_V

Problem 1 *Superconducting ground state*

This exercise goes through in detail certain key concepts describing a superconducting state. A superconductor can be described by a so-called reduced Hamiltonian that only takes into account interactions between pairs of electrons with vanishing momentum and angular momentum

$$\hat{H} = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k},\sigma} a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\sigma} V_{\mathbf{k},\mathbf{k}'} a^\dagger_{\mathbf{k},\sigma} a^\dagger_{-\mathbf{k},-\sigma} a_{-\mathbf{k}',-\sigma} a_{\mathbf{k}',\sigma}. \tag{1}$$

The first term describes the kinetic energy of the electrons. The interaction is characterized by the matrix element $V_{\mathbf{k},\mathbf{k}'} \equiv \langle 0 | a^\dagger_{-\mathbf{k},-\sigma} a^\dagger_{\mathbf{k},\sigma} \hat{V} a_{\mathbf{k}',\sigma} a_{-\mathbf{k}',-\sigma} | 0 \rangle < 0$ that is here assumed to be real, negative, and independent of the spin σ. Such *attractive* interaction can be mediated by phonons (lattice vibrations). The vacuum state is denoted by $|0\rangle$. Let us consider an Ansatz for the ground state

$$|\Psi\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_k a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow}) |0\rangle. \tag{2}$$

Here the so-far undetermined coefficients $u_{\mathbf{k}}, v_{\mathbf{k}} \in \mathbb{R}$, called *coherence factors*, can be found through variational methods.

a) Show that

$$u_k^2 + v_k^2 = 1. \tag{3}$$

(0.25 points)

Hint: The state vector $|\Psi\rangle$ has to be normalized. Use canonical commutation relations.

b) Calculate $\langle \Psi | a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} | \Psi \rangle$. You have to express it through coherence factors. Interpret the result. *(0.25 points)*

c) It turns out that with vectors $|\Psi\rangle$, the particle number is not fixed. Therefore, to find the ground state, rather than minimizing energy, one has to find coherence factors that minimize the quantity $\langle \Psi | \hat{H} - \hat{N}\mu | \Psi \rangle$. Here $\hat{N} = \sum_{\mathbf{k},\sigma} a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}$ is the particle number operator. Mathematically, the chemical potential μ plays the role of a Lagrange multiplier. The condition $\langle \hat{N} \rangle = N$ yields $\mu = E_F$, with E_F the Fermi energy. Show that

$$\langle \Psi | \hat{H} - \hat{N} E_F | \Psi \rangle = 2 \sum_{\mathbf{k}} \xi_{\mathbf{k}} v^2_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} u_{\mathbf{k}} v_{\mathbf{k}} u_{\mathbf{k}'} v_{\mathbf{k}'}, \tag{4}$$

where $\xi_k \equiv \varepsilon_{\mathbf{k}} - E_F$ is the kinetic energy counted from the Fermi surface. *(1 point)*

d) The *energy gap* can be defined by

$$\Delta_{\mathbf{k}'} \equiv -\sum_{k} V_{\mathbf{k}',\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}. \tag{5}$$

Show that for $|\Psi_0\rangle$ that minimizes (4) the coherence factors are

$$2u_{\mathbf{k}}v_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}}}, \quad v_{\mathbf{k}}^2 - u_{\mathbf{k}}^2 = -\frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}, \quad v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \quad u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\right), \tag{6}$$

where $E_{\mathbf{k}} \equiv \sqrt{\xi_{\mathbf{k}}^2 + \Delta_k^2}$ is *quasiparticle energy.* *(0.75 points)*
Hint: Remember that $u_{\mathbf{k}}$ *and* $v_{\mathbf{k}}$ *are not independent. It is convenient to introduce the parametrization* $u_{\mathbf{k}} \equiv \sin\theta_{\mathbf{k}}$, $v_{\mathbf{k}} \equiv \cos\theta_{\mathbf{k}}$ *that satisfies (3) by construction. To choose the signs, note that for very large positive* $\xi_{\mathbf{k}}$, *one has* $u_{\mathbf{k}} = 1$, $v_{\mathbf{k}} = 0$ *so that such states are unoccupied.*

e) Show that $\Delta_{\mathbf{k}}$ satisfies the gap equation

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2\sqrt{\xi_{\mathbf{k}'}^2 + \Delta_{\mathbf{k}'}^2}}. \tag{7}$$

Here $\Delta_{\mathbf{k}}$ must be solved *self-consistently.* In general it can not be expressed in closed form but has to be calculated iteratively and numerically. However, for simple enough $V_{\mathbf{k},\mathbf{k}'}$ a closed-form solution exists, cf. item (g). *(0.25 points)*

f) In the reduced Hamiltonian potential energy is described by the operator

$$\hat{H}_{int} \equiv \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\sigma} V_{\mathbf{k},\mathbf{k}'} a_{\mathbf{k},\sigma}^\dagger a_{-\mathbf{k},-\sigma}^\dagger a_{-\mathbf{k}',-\sigma} a_{\mathbf{k}',\sigma}. \tag{8}$$

Show that if the interaction is not repulsive, $V_{\mathbf{k},\mathbf{k}'} \leq 0$, potential energy is not positive

$$\langle\Psi_0|\hat{H}_{int}|\Psi_0\rangle \leq 0. \tag{9}$$

(0.5 points)

g) Let us now consider a model where

$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -|V| & \text{if } |\xi_{\mathbf{k}}|, |\xi_{\mathbf{k}'}| \leq \hbar\omega_D \\ 0, & \text{otherwise.} \end{cases} \tag{10}$$

The cut-off frequency ω_D is called the Debye frequency. Show that

$$\begin{aligned} \Delta_{\mathbf{k}} &= 0 \quad \text{if } |\xi_{\mathbf{k}}| > \hbar\omega_{\mathrm{D}}, \\ \Delta_{\mathbf{k}} &= \Delta \text{ (independent of } \mathbf{k}) \quad \text{if } |\xi_{\mathbf{k}}| < \hbar\omega_{\mathrm{D}}. \end{aligned} \tag{11}$$

Items (h), (i), and (k) below assume this model. *(0.25 points)*
Hint: Use the gap equation.

h) Show that

$$\Delta = \frac{\hbar\omega_D}{\sinh\left(\frac{1}{N(0)|V|}\right)} \tag{12}$$

and in the *weak coupling limit* $N(0)|V| \ll 1$

$$\Delta = 2\hbar\omega_D e^{\frac{-1}{N(0)|V|}}. \tag{13}$$

Here $N(0)$ is the density of states per unit energy at the Fermi level $\xi_{\mathbf{k}} = 0$ in the normal (non-superconducting) state for a given spin direction. *(0.5 points)*
Hint: Use the gap equation. On the energy interval $-\hbar\omega_D < \xi_{\mathbf{k}} < \hbar\omega_D$ the density of states is approximately constant $N(\xi_{\mathbf{k}}) \approx N(0)$.

i) Show that in the state $|\Psi_0\rangle$ the potential energy corresponding to the operator (8) is

$$\langle\Psi_0|\hat{H}_{int}|\Psi_0\rangle = \frac{-\Delta^2}{|V|}. \tag{14}$$

(0.5 points)

Hint: Note that the last term in Eq. (4) corresponds to potential energy.

j) Prove the integration formula

$$\int_{x_1}^{x_2} \frac{x^2}{\sqrt{1+x^2}} dx = \frac{1}{2}\Big/_{x_1}^{x_2} \left[x^2\sqrt{1+\frac{1}{x^2}} - \text{arcsinh}(x)\right]. \tag{15}$$

(1 point)

k) Kinetic energy counted from the Fermi surface is described by the operator

$$\hat{H}_{kin} - E_F\hat{N} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k},\sigma} a^\dagger_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma}. \tag{16}$$

Show that in the state $|\Psi_0\rangle$ we have

$$\langle\Psi_0|\hat{H}_{kin} - E_F\hat{N}|\Psi_0\rangle = 2\sum_{k<k_F} \xi_{\mathbf{k}} + \frac{\Delta^2}{|V|} - \frac{N(0)\Delta^2}{2}. \tag{17}$$

(1.75 points)

Hint: Use Eqs. (4), (6), (12), (13), and (15). Note that

$$\sum_{\xi_k} = \sum_{\xi_{\mathbf{k}}<-\hbar\omega_D} + \sum_{-\hbar\omega_D<\xi_{\mathbf{k}}<\hbar\omega_D} + \sum_{\xi_{\mathbf{k}}>\hbar\omega_D}. \tag{18}$$

Use Eq. (6) to evaluate the coherence factors in different regions of summation. It is possible to cast $\langle\Psi_0|\hat{H}_{kin} - E_F\hat{N}|\Psi_0\rangle$ to the form

$$\langle\Psi_0|\hat{H}_{kin} - E_F\hat{N}|\Psi_0\rangle = 2\sum_{k<k_F} \xi_{\mathbf{k}} + 2\sum_{0<\xi_k<\hbar\omega_D} \left(\xi_{\mathbf{k}} - \frac{\xi^2_{\mathbf{k}}}{E_{\mathbf{k}}}\right). \tag{19}$$

l) Let us now consider noninteracting electron gas described by the state vector

$$|\tilde{\Psi}_0\rangle = \prod_{k<k_F} a^\dagger_{\mathbf{k},\uparrow} a^\dagger_{-\mathbf{k},\downarrow}|0\rangle. \tag{20}$$

Find the coherence factors u_k and v_k and $\Delta_\mathbf{k}$ for this state. *(0.25 points)*
Hint: Use Eqs. (2) and (5).

m) Show that

$$\langle\tilde{\Psi}_0|\hat{H} - E_F\hat{N}|\tilde{\Psi}_0\rangle = 2\sum_{k<k_F} \xi_\mathbf{k}. \tag{21}$$

(0.25 points)

Hint: Use the results of item (l) and Eq. (4).

n) One of the states $|\Psi_0\rangle$, $|\tilde{\Psi}_0\rangle$ is actually the true ground state of the Hamiltonian (1). Which one? Why? Calculate the *condensation energy*

$$E_c \equiv \langle\Psi_0|\hat{H} - E_F\hat{N}|\Psi_0\rangle - \langle\tilde{\Psi}_0|\hat{H} - E_F\hat{N}|\tilde{\Psi}_0\rangle. \tag{22}$$

(0.5 points)

Hint: Consider the results of items (i), (k), and (m).

Problem 2 *Anderson model*

The Anderson Impurity Model is used to describe systems of heavy fermions (e.g. electrons) in a lattice which contain impurities. For a single impurity, the Hamiltonian in $1D$ takes the form $H = H_0 + H_T$, with

$$H_0 = \epsilon_d \sum_\sigma d^\dagger_\sigma d_\sigma + U n_{d_\uparrow} n_{d_\downarrow} + \sum_{k_a\sigma} \epsilon_{k_a} c^\dagger_{k_a\sigma} c_{k_a\sigma}, \tag{23}$$

$$H_T = \sum_{k_a\sigma}\left[t_{k_a} c^\dagger_{k_a\sigma} d_\sigma + t^*_{k_a} c_{k_a\sigma} d^\dagger_\sigma\right], \tag{24}$$

where d_σ is the annihilation operator of an impurity electron with spin state σ and $c_{k_a\sigma}$ corresponds to the annihilation operator for a electron in the conduction band of the lattice, either on the left ($a = L$) or on the right ($a = R$) of the impurity. The onsite Coulomb repulsion is U is usually the dominant energy scale, where $n_{d_\uparrow}(n_{d_\downarrow})$ is the number operator for an impurity spin up (down) state, and t_{k_a} is the coupling matrix between the impurity and the conducting band. In this exercise we will use the techniques of quasi-degenerate perturbation theory discussed in previous lectures (and assignments) to show that this coupling matrix is allows electrons in a lattice to tunnel through the impurity.

a) Use the canonical (Schrieffer-Wolff) transformation $\bar{H} = e^S H e^{-S}$ studied in previous assignments and show that the anti-Hermitian operator satisfying $[S, H_0] = -H_T$ is given by $S = S_1 - S_1^\dagger$ where

$$S_1 \equiv \sum_{k_a\sigma}\left[\frac{t_{k_a}}{\epsilon_{k_a} - \epsilon_d - U} n_{d_\downarrow} c^\dagger_{k_a\sigma} d_\sigma + \frac{t_{k_a}}{\epsilon_{k_a} - \epsilon_d}(1 - n_{d_\downarrow}) c^\dagger_{k_a\sigma} d_\sigma\right]. \tag{25}$$

(3 point)

b) In order to account for second-order processes in H_T, evaluate the next-leading order contribution to $\bar{H}$ given by $[S, H_T]/2$. Show that $\bar{H}$ decomposes into $\bar{H} = H_0 + H_{dir} + H_{ex} + H_{pair} + H_0'$, where H_{dir} contains a direct tunneling of electrons from one side of the impurity to the other. H_{ex} describes the tunneling mediated by exchange of electrons with the impurity. H_{pair} represents the tunneling of a pair of electrons from the conduction band into the impurity states (and vice-versa) and finally H_0' is a mere shift of the energy levels. *(3 point)*