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Theorie zu Magnetismus, Supraleitung und Elektronische Korrelation in Festkörpern

Sommersemester 2019

Blatt 11

(Abgabe: 02.07.2019)

Aufgabe 1 (**Solution of the BCS Hamiltonian**) (5=1+4 Punkte)

In the lecture we introduced the BCS Hamiltonian and its effective form in the mean-field approximation, given by

$$H_{eff} = \sum_{\vec{k}\sigma} \xi_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} - \Delta^* \sum_{\vec{k}} c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} - \Delta \sum_{\vec{k}} c^\dagger_{\vec{k}\uparrow} c^\dagger_{-\vec{k}\downarrow} + \frac{|\Delta|^2}{V}, \tag{1}$$

where

$$\xi_{\vec{k}} = \epsilon_{\vec{k}} - E_F \tag{2}$$

$$\Delta = V \sum_{\vec{k}'} \langle c_{-\vec{k}'\downarrow} c_{\vec{k}'\uparrow} \rangle \tag{3}$$

$$\Delta^* = V \sum_{\vec{k}'} \langle c^\dagger_{\vec{k}'\uparrow} c^\dagger_{-\vec{k}'\downarrow} \rangle. \tag{4}$$

In order to diagonalize the Hamiltonian, one introduces the Bogoliubov operators

$$\alpha_{\vec{k}} = u_{\vec{k}} c_{\vec{k}\uparrow} - v_{\vec{k}} c^\dagger_{-\vec{k}\downarrow} \tag{5}$$

$$\beta_{\vec{k}} = u_{\vec{k}} c_{-\vec{k}\downarrow} + v_{\vec{k}} c^\dagger_{\vec{k}\uparrow}. \tag{6}$$

a) Show that by demanding the Bogoliubov transformation to be canonical, i.e. it preserves the commutation relations

$$\{\alpha, \beta\} = \{\alpha, \beta^\dagger\} = 0 \tag{7}$$

$$\{\alpha, \alpha^\dagger\} = \{\beta, \beta^\dagger\} = 1, \tag{8}$$

it follows that $|u_{\vec{k}}|^2 + |v_{\vec{k}}|^2 = 1$.

b) Use the Bogoliubov transformation to diagonalize H_{eff}. This is done by inserting the substitution of the Bogoliubov operators into H_{eff} and requesting that the off-diagonal terms vanish. What is the dispersion of the Bogoliubov quasiparticles and the ground state energy?
Hint: You can choose $v_{\vec{k}}$ to be real. As you arrive at the equation

$$2u_{\vec{k}} v_{\vec{k}} \xi_{\vec{k}} - \Delta u^2_{\vec{k}} + \Delta^* v^2_{\vec{k}} = 0 \tag{9}$$

it may be helpful to multiply by $\frac{\Delta^*}{u^2_{\vec{k}}}$. Furthermore, you can use that $\frac{\Delta^* v_{\vec{k}}}{u_{\vec{k}}} > 0$.

Aufgabe 2 (**BCS variational ansatz**) (5=2+3 Punkte)

The BCS gap equation can also be obtained by a minimization approach. We define

$$b_{\vec{k}} := c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} \tag{10}$$

$$b^\dagger_{\vec{k}} := c^\dagger_{\vec{k}\uparrow} c^\dagger_{-\vec{k}\downarrow}, \tag{11}$$

and assume that all electrons form pairs, which allows us to write the BCS Hamiltonian as (check this)

$$H = \sum_{\vec{k}} 2\epsilon_{\vec{k}} b^\dagger_{\vec{k}} b_{\vec{k}} + \sum_{\vec{k}\vec{k}'} V_{\vec{k}\vec{k}'} b^\dagger_{\vec{k}'} b_{\vec{k}}. \tag{12}$$

We also consider the usual variational Eigenstate of H as

$$|\Psi\rangle = \prod_{\vec{k}} \left(u_{\vec{k}} + v_{\vec{k}} b^\dagger_{\vec{k}} \right) |0\rangle, \tag{13}$$

with variational parameters $u_{\vec{k}}, v_{\vec{k}}$.

a) Using the method of Lagrange multipliers, one can minimize the energy

$$E = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{14}$$

while keeping the number of particles constant

$$N = \frac{\langle\Psi| \sum_{\vec{k}\sigma} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} |\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi|2 \sum_{\vec{k}} b^\dagger_{\vec{k}} b_{\vec{k}} |\Psi\rangle}{\langle\Psi|\Psi\rangle}, \tag{15}$$

by introducing the Lagrange multiplier μ. With the constraint $u^2_{\vec{k}} + v^2_{\vec{k}} = 1$, the equation to minimize is then

$$W = E + \mu \left(N - \frac{\langle\Psi|2 \sum_{\vec{k}} b^\dagger_{\vec{k}} b_{\vec{k}} |\Psi\rangle}{\langle\Psi|\Psi\rangle} \right) + \lambda(u^2_{\vec{k}} + v^2_{\vec{k}} - 1). \tag{16}$$

Using $u^2_{\vec{k}} + v^2_{\vec{k}} = 1$, show that W can be written as (dropping constant terms)

$$W = \sum_{\vec{k}} 2(\epsilon_{\vec{k}} - \mu) v^2_{\vec{k}} + \sum_{\vec{k}\vec{k}'} V_{\vec{k}\vec{k}'} u_{\vec{k}'} v_{\vec{k}'} u_{\vec{k}} v_{\vec{k}} + \lambda(u^2_{\vec{k}} + v^2_{\vec{k}} - 1). \tag{17}$$

b) Minimize W with respect to $u_{\vec{k}}, v_{\vec{k}}$, using the definitions of

$$\Delta_{\vec{k}} := -\sum_{\vec{k}'} V_{\vec{k}\vec{k}'} u_{\vec{k}'} v_{\vec{k}'} \tag{18}$$

$$E_{\vec{k}} := \sqrt{(\epsilon_{\vec{k}} - \mu)^2 + \Delta^2_{\vec{k}}}, \tag{19}$$

and feel free to use a mathematic tool of your choice (Mathematica, Maple ...) to show that one arrives at the final self-consistent equation

$$\Delta_{\vec{k}} = -\sum_{\vec{k}'} V_{\vec{k}\vec{k}'} \frac{\Delta_{\vec{k}'}}{2E_{\vec{k}'}}. \tag{20}$$

Hint: Choose $u_{\vec{k}}, v_{\vec{k}}$ as real.