Department of Physics, NTNU

Homework 9
TFY4210/FY8302 Quantum theory of solids
Spring 2021.

Problem 1

In class, we have introduced new operators $\eta_{\mathbf{k}}, \gamma_{\mathbf{k}}$ to diagonalize the mean-field BCS-Hamiltonian using transformation coefficients $(u_{\mathbf{k}}, v_{\mathbf{k}})$ that are real. Let us generalize this to the case where $(u_{\mathbf{k}}, v_{\mathbf{k}})$ can be complex. As in class, we choose $V_{\mathbf{k},\mathbf{k}'}$ to be a constant within a thin shell around the Fermi surface. We will use the following transformation

$$\begin{pmatrix} \eta_{\mathbf{k}} \\ \gamma_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ -v^*_{\mathbf{k}} & u^*_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c^\dagger_{-\mathbf{k},\downarrow} \end{pmatrix}$$

a) Show that preservation of anti-commutation relations gives the constraint

$$|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1$$

b) We next want to diagonalize the problem such that only terms of the form $\gamma^\dagger_{\mathbf{k}}\gamma_{\mathbf{k}}$ and $\eta^\dagger_{\mathbf{k}}\eta_{\mathbf{k}}$ appear in the Hamiltonian. Show that the condition for this is given by

$$-2(\varepsilon_{\mathbf{k}} - \mu)u_{\mathbf{k}}v_{\mathbf{k}} = u^2_{\mathbf{k}}\Delta - v^2_{\mathbf{k}}\Delta^*$$
$$-2(\varepsilon_{\mathbf{k}} - \mu)u^*_{\mathbf{k}}v^*_{\mathbf{k}} = (u^*_{\mathbf{k}})^2\Delta^* - (v^*_{\mathbf{k}})^2\Delta$$

c) Show that the coefficient of $\gamma^\dagger_{\mathbf{k}}\gamma_{\mathbf{k}}$ is given by

$$E_{\mathbf{k}} = (\varepsilon_{\mathbf{k}} - \mu)\left(|v_{\mathbf{k}}|^2 - |u_{\mathbf{k}}|^2\right) + \Delta v^*_{\mathbf{k}}u_{\mathbf{k}} + \Delta^* v_{\mathbf{k}}u^*_{\mathbf{k}}$$

and that the corresponding coefficient of $\eta^\dagger_{\mathbf{k}}\gamma_{\mathbf{k}}$ is given by $-E_{\mathbf{k}}$.

d) We next parametrize $u = \cos\chi\ e^{i\phi_u}$, $v = \sin\chi\ e^{i\phi_v}$, $\Delta = |\Delta|e^{i\phi}$. Use the constraint in **b** to find constraints on the phases ϕ_u, ϕ_v, ϕ. Conclude from this that $E_{\mathbf{k}}$ is real.

e) Use the definition of Δ as given in class to show that in this case, the phase of the gap may be cancelled out of the self-consistent equation for Δ. Hence, in this case, we can consider Δ to be real and positive without loss of generality.

Problem 2

In this problem, we will consider a generalization of the BCS-theory to a situation where electrons originating with two energy-bands can participate in superconductivity. Such a situation arises in transition metal elements, where scattering of electrons in s- and d-orbitals constributes to the resistivity in the normal state. The generalization of the BCS-reduced Hamiltonian to this case is straightforward. We denote the single-particle excitation energies of the electrons on the s- and d-bands as $\varepsilon_{\mathbf{k}s}$ and $\varepsilon_{\mathbf{k}d}$, respectively.

The BCS-reduced Hamiltonian for this case is given by

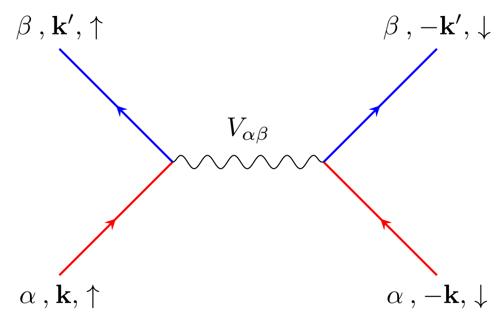
$$
\begin{aligned}
H = & \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}s} - \mu) \; c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}d} - \mu) \; d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} \\
& - V_{ss} \sum_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}',\uparrow} c^\dagger_{-\mathbf{k}',\downarrow} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} - V_{dd} \sum_{\mathbf{k},\mathbf{k}'} d^\dagger_{\mathbf{k}',\uparrow} d^\dagger_{-\mathbf{k}',\downarrow} d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} \\
& - V_{sd} \sum_{\mathbf{k},\mathbf{k}'} \left[d^\dagger_{\mathbf{k}',\uparrow} d^\dagger_{-\mathbf{k}',\downarrow} c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} + c^\dagger_{\mathbf{k}',\uparrow} c^\dagger_{-\mathbf{k}',\downarrow} d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} \right]
\end{aligned}
$$

Here, $(V_{ss}, V_{dd}, V_{sd}) > 0$ are attractive interactions operative provided both $\mathbf{k}, \mathbf{k}'$ both are located within a thin shell around the Fermi-surface of the s- and d-bands. The c- and d-operators are fermionic creation- and destruction operators of the s and d-bands, respectively. Note that the Hamiltonian decouples into two independent single-band problems if $V_{sd} = 0$.

The V_{ss}- and V_{dd}-terms are intra-band scattering processes on the s- and d-bands, respectively. The V_{sd}-term is an inter-band scattering between the s- and the d-band.

The summations of $\mathbf{k}, \mathbf{k}'$ are close to the Fermi-surface both for the s- and the d-band, so the regions in $\mathbf{k}$-space will be quite different in the two cases. Furthermore, we will denote the single-particle densities of states on the Fermi-surface in the s- and d-bands as N_s and N_d, respectively.

The Feynman-diagram illustrating the various scattering processes is given below.



a) We next perform a mean-field approximation along the same lines that we did in class for the single-band case. Introduce mean-field expectation values

$$
\begin{aligned}
b_{\mathbf{k},s} &= \langle c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} \rangle \\
b_{\mathbf{k},d} &= \langle d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} \rangle
\end{aligned}
$$

and write

$$
\begin{aligned}
c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} &= b_{\mathbf{k},s} + \delta b_{\mathbf{k},s} \\
d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} &= b_{\mathbf{k},d} + \delta b_{\mathbf{k},d}
\end{aligned}
$$

and discard terms $\mathcal{O}(\delta b_{\mathbf{k},s})^2$ and $\mathcal{O}(\delta b_{\mathbf{k},s})^2$. Show that the mean-field Hamiltonian may be written on form

$$
\begin{aligned}
H = & \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}s} - \mu)\ c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}d} - \mu)\ d^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} \\
& - V_{ss} \sum_{\mathbf{k},\mathbf{k}'} \left[b^\dagger_{\mathbf{k}',s}\ c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} + h.c. \right] - V_{dd} \sum_{\mathbf{k},\mathbf{k}'} \left[b^\dagger_{\mathbf{k}',d}\ d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} + h.c. \right] \\
& - V_{sd} \sum_{\mathbf{k},\mathbf{k}'} \left[b^\dagger_{\mathbf{k}',d}\ c_{-\mathbf{k},\downarrow} c_{\mathbf{k},\uparrow} + h.c. + b^\dagger_{\mathbf{k}',s}\ d_{-\mathbf{k},\downarrow} d_{\mathbf{k},\uparrow} + h.c. \right] \\
& + V_{ss} \sum_{\mathbf{k},\mathbf{k}'} b^\dagger_{\mathbf{k}',s}\ b_{\mathbf{k},s} + V_{dd} \sum_{\mathbf{k},\mathbf{k}'} b^\dagger_{\mathbf{k}',d}\ b_{\mathbf{k},d} + V_{sd} \sum_{\mathbf{k},\mathbf{k}'} \left[b^\dagger_{\mathbf{k}',d}\ b_{\mathbf{k},s} + b^\dagger_{\mathbf{k}',s}\ b_{\mathbf{k},d} \right]
\end{aligned}
$$

b) Introduce the two quantities Δ_1 and Δ_2 (to be dermined selfconsistently)

$$
\begin{aligned}
\Delta_1 &\equiv V_{ss} \sum_{\mathbf{k}} b_{\mathbf{k},s} + V_{sd} \sum_{\mathbf{k}} b_{\mathbf{k},d} \\
\Delta_2 &\equiv V_{sd} \sum_{\mathbf{k}} b_{\mathbf{k},s} + V_{dd} \sum_{\mathbf{k}} b_{\mathbf{k},d}
\end{aligned}
$$

Express the mean-field Hamiltonian in terms of Δ_1 and Δ_2 instead of $b_{\mathbf{k},s}$ and $b_{\mathbf{k},d}$. Try to give a physical interpretation of Δ_1 and Δ_2. (Hint: Try to infer what Δ_1 and Δ_2 mean based on how they appear in the Hamiltonian).

c) To diagonalize the mean-field problem, we will introduce new fermionic operators $e_{\mathbf{k},\sigma}$ and $f_{\mathbf{k},\sigma}$ as follows

$$
\begin{aligned}
c_{\mathbf{k},\uparrow} &= \cos(\theta_{\mathbf{k}}) e_{\mathbf{k},\uparrow} + \sin(\theta_{\mathbf{k}}) e^\dagger_{-\mathbf{k},\downarrow} \\
c_{\mathbf{k},\downarrow} &= \cos(\theta_{\mathbf{k}}) e_{\mathbf{k},\downarrow} - \sin(\theta_{\mathbf{k}}) e^\dagger_{-\mathbf{k},\uparrow} \\
d_{\mathbf{k},\uparrow} &= \cos(\phi_{\mathbf{k}}) f_{\mathbf{k},\uparrow} + \sin(\phi_{\mathbf{k}}) f^\dagger_{-\mathbf{k},\downarrow} \\
d_{\mathbf{k},\downarrow} &= \cos(\phi_{\mathbf{k}}) f_{\mathbf{k},\downarrow} - \sin(\phi_{\mathbf{k}}) f^\dagger_{-\mathbf{k},\uparrow}
\end{aligned}
$$

The parameters $\theta_{\mathbf{k}}$ and $\phi_{\mathbf{k}}$ are determined by substituting these expressions into H and equating the coefficients of terms $e^\dagger e^\dagger$ and ee to zero, and likewise for the f-operators. Show that this procedure yields the following equations determining $\theta_{\mathbf{k}}$ and $\phi_{\mathbf{k}}$

$$
\begin{aligned}
\varepsilon_{\mathbf{k}s} \sin(2\theta_{\mathbf{k}}) + D_s \cos(2\theta_{\mathbf{k}}) &= 0 \\
\varepsilon_{\mathbf{k}d} \sin(2\phi_{\mathbf{k}}) + D_d \cos(2\phi_{\mathbf{k}}) &= 0
\end{aligned}
$$

and give expressions for D_s and D_d.

d) Find the excitation energies of the Bogoliubov quasiparticles (e, f) defined above.

d) Find an expression for the free energy of the system.

e) Minimize the free energy w.r.t the quantities Δ_1 and Δ_2 and show that the coupled equations for these two quantities may be written

$$
\begin{aligned}
\Delta_\alpha &= \sum_{\beta=1}^{2} V_{\alpha\beta} \Delta_\beta\ \chi_\beta; \alpha = (1, 2) \\
\chi_\beta &\equiv \sum_{\mathbf{k}} \frac{1}{2E_{\beta\mathbf{k}}} \tanh\left(\frac{\beta E_{\beta\mathbf{k}}}{2} \right)
\end{aligned}
$$

f) With the real transformation coefficients we have used so far, Δ_α will be real. Imagine that we had used complex transformation coefficients instead, like in Problem 1. We would then get the same equations for Δ_α as above, but with the possibility of complex gaps, $\Delta_\alpha = |\Delta_\alpha| e^{i\phi_\alpha}$. We may thus cancel out an overall phase from the gap-equations, and be left with *one and only one* relative phase $\phi_{12} = \phi_1 - \phi_2$. Show, using the gap-equations, that $\phi_{12} = (0, \pi) \mod (2\pi)$. Therefore, the gaps again may both be taken to be real, but they may have opposite signs. What is the criterion for Δ_1 and Δ_2 having equal or opposite signs?

Note: This sort of simplification in general is not possible when one has more than two bands involved in the superconductivity. This leads to qualitatively new effects. Important examples of N-band superconductors with $N \geq 3$ are the iron-pnictide high-T_c superconductors currently of considerable interest.

g) Find an expression for the critical temperature of the system using the same technique that we used in class for the single-band case.