Homework #10 — Phys625 — Spring 2002
Deadline: Tuesday, May 7, 2002.
Turn in homework in the class or put it in the box on the door of Phys 2314 by 10 a.m.

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Do not forget to write your name and the homework number!
Equation numbers with the period, like (3.25), refer to the equations of the textbook.
Equation numbers without period, like (5), refer to the equations of this homework.

This is the last homework

Superconductivity (Ch. V)

Because of limited time, in this homework we focus only on the many-body aspects of superconductivity. So, while it is recommended to read the whole Ch. V, pay particular attention to §39–44 and §51–54.

1. *Bogolyubov-de Gennes equations*

Let us consider the following model Hamiltonian:

$$\hat{H} = \int d^3r \left[\hat{\psi}^+_\uparrow(\mathbf{r})\,\hat{\xi}\,\hat{\psi}_\uparrow(\mathbf{r}) + \hat{\psi}^+_\downarrow(\mathbf{r})\,\hat{\xi}\,\hat{\psi}_\downarrow(\mathbf{r}) + g\,\hat{\psi}^+_\uparrow(\mathbf{r})\hat{\psi}^+_\downarrow(\mathbf{r})\hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r})\right]. \tag{1}$$

Here $\hat{\xi} = p^2/2m - \mu \approx v_F(p - p_F)$ is the operator of kinetic energy of electrons, and $g < 0$ is the interaction constant. Notice that we consider local interaction, thus, because of the Fermi statistics, only the electrons with opposite spins interact.

Suppose Cooper pairing takes place in the system, and the condensate $\langle\hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r})\rangle \neq 0$ is present. Here the average is taken over the thermodynamic equilibrium at finite or zero temperature. The original Hamiltonian (1) can be approximated by the following mean-field Hamiltonian:

$$\hat{H}_{MF} = \int d^3r \left[\hat{\psi}^+_\uparrow(\mathbf{r})\,\hat{\xi}\,\hat{\psi}_\uparrow(\mathbf{r}) + \hat{\psi}^+_\downarrow(\mathbf{r})\,\hat{\xi}\,\hat{\psi}_\downarrow(\mathbf{r}) + \Delta^*(\mathbf{r})\,\hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r}) + \Delta(\mathbf{r})\,\hat{\psi}^+_\uparrow(\mathbf{r})\hat{\psi}^+_\downarrow(\mathbf{r}) - \frac{|\Delta(\mathbf{r})|^2}{g}\right]. \tag{2}$$

Here we introduced an auxiliary complex function $\Delta(\mathbf{r})$, which should be determined by minimizing the energy of the system $\langle\hat{H}_{MF}\rangle$ with respect to $\Delta(\mathbf{r})$. We consider a general case where Δ may depend on coordinate $\mathbf{r}$, for example because of externally imposed boundary condition. However, in most common cases $\Delta(\mathbf{r}) = \Delta_0$ is a constant independent of $\mathbf{r}$.

(a) [**6 points**] By minimizing $\langle\hat{H}_{MF}\rangle$ with respect to $\Delta^*(\mathbf{r})$, show that

$$\Delta(\mathbf{r}) = g\langle\hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r})\rangle = -g\langle\hat{\psi}_\uparrow(\mathbf{r})\hat{\psi}_\downarrow(\mathbf{r})\rangle. \tag{3}$$

Here the second equation follows from Fermi statistics and demonstrates that the condensate is antisymmetric with respect to spin, i.e. the pairing is singlet.

By substituting Eq. (3) into Eq. (2), show that

$$\begin{aligned}\langle\hat{H}_{MF}\rangle &= \int d^3r \left[\langle\hat{\psi}^+_\uparrow(\mathbf{r})\,\hat{\xi}\,\hat{\psi}_\uparrow(\mathbf{r}) + \hat{\psi}^+_\downarrow(\mathbf{r})\,\hat{\xi}\,\hat{\psi}_\downarrow(\mathbf{r})\rangle + g\,\langle\hat{\psi}^+_\uparrow(\mathbf{r})\hat{\psi}^+_\downarrow(\mathbf{r})\rangle\langle\hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r})\rangle\right] \\ &= \int d^3r \left[\langle\hat{\psi}^+_\uparrow(\mathbf{r})\,\hat{\xi}\,\hat{\psi}_\uparrow(\mathbf{r}) + \hat{\psi}^+_\downarrow(\mathbf{r})\,\hat{\xi}\,\hat{\psi}_\downarrow(\mathbf{r})\rangle + \frac{|\Delta(\mathbf{r})|^2}{g}\right].\end{aligned} \tag{4}$$

Eq. (4) is in agreement with Eq. (1) with the average of the quartic term is replaced by the product of two bilinear averages.

(b) [**4 points**] Rewrite Hamiltonian (2) in the following form

$$\hat{H}_{MF} = \hat{H}_{BdG} - \int d^3r\,\frac{|\Delta(\mathbf{r})|^2}{g} + \sum_p \xi_p, \tag{5}$$

where the formal sum $\sum_p \xi_p$ is taken over all momenta and

$$\hat{H}_{BdG} = \int d^3r\,[\hat{\psi}^+_\uparrow(\mathbf{r}), \hat{\psi}_\downarrow(\mathbf{r})] \begin{pmatrix} \hat{\xi} & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -\hat{\xi} \end{pmatrix} \begin{pmatrix} \hat{\psi}_\uparrow(\mathbf{r}) \\ \hat{\psi}^+_\downarrow(\mathbf{r}) \end{pmatrix}. \tag{6}$$

Show that Hamiltonian $\hat{H}_{BdG}$ can be diagonalized by the Bogolyubov transformation

$$\begin{aligned} \hat{\psi}_\uparrow(\mathbf{r}) &= \sum_n \left[u_n(\mathbf{r})\,\hat{\gamma}_{n,1} + v_n^*(\mathbf{r})\,\hat{\gamma}^+_{n,2}\right], \\ \hat{\psi}^+_\downarrow(\mathbf{r}) &= \sum_n \left[u_n^*(\mathbf{r})\,\hat{\gamma}^+_{n,2} - v_n(\mathbf{r})\,\hat{\gamma}_{n,1}\right], \end{aligned} \tag{7}$$

where (u_n, v_n) are the eigenvectors of the Bogolyubov-de Gennes equation with the eigenvalues E_n:

$$\begin{pmatrix} \hat{\xi} & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & -\hat{\xi} \end{pmatrix} \begin{pmatrix} u_n(\mathbf{r}) \\ -v_n(\mathbf{r}) \end{pmatrix} = E_n \begin{pmatrix} u_n(\mathbf{r}) \\ -v_n(\mathbf{r}) \end{pmatrix}, \tag{8}$$

so that

$$\hat{H}_{BdG} = \sum_n (\hat{\gamma}^+_{n,1}, \hat{\gamma}_{n,2}) \begin{pmatrix} E_n & 0 \\ 0 & -E_n \end{pmatrix} \begin{pmatrix} \hat{\gamma}_{n,1} \\ \hat{\gamma}^+_{n,2} \end{pmatrix}. \tag{9}$$

Show by substituting Eq. (9) into Eq. (5) that

$$\hat{H}_{MF} = \sum_n E_n(\hat{\gamma}^+_{n,1}\hat{\gamma}_{n,1} + \hat{\gamma}^+_{n,2}\hat{\gamma}_{n,2}) + \sum_n(-E_n + \xi_n) - \int d^3r\,\frac{|\Delta(\mathbf{r})|^2}{g}. \tag{10}$$

In Eq. (10) the first term describes the Bogolyubov quasiparticle excitations, whereas the other terms represent the ground state energy.
Show that the difference between the ground energies of the superconducting and normal states is

$$E_0 = \sum_n(-E_n + \xi_n) - \int d^3r\,\frac{|\Delta(\mathbf{r})|^2}{g} - 2\sum_{\xi_n<0}\xi_n = \sum_n(-E_n + |\xi_n|) - \int d^3r\,\frac{|\Delta(\mathbf{r})|^2}{g}, \tag{11}$$

where the factor 2 comes from two spin orientations.

(c) [**6 points**] Show that the transformation inverse to (7) is

$$\begin{aligned} \hat{\gamma}_{n,1} &= \int d^2r\left[u_n^*(\mathbf{r})\,\hat{\psi}_\uparrow(\mathbf{r}) - v_n^*(\mathbf{r})\,\hat{\psi}^+_\downarrow(\mathbf{r})\right], \\ \hat{\gamma}^+_{n,2} &= \int d^2r\left[u_n(\mathbf{r})\,\hat{\psi}^+_\downarrow(\mathbf{r}) + v_n(\mathbf{r})\,\hat{\psi}_\uparrow(\mathbf{r})\right]. \end{aligned} \tag{12}$$

Show that the coefficients u and v must satisfy the following relations:

$$\begin{aligned} &\sum_n [u_n(\mathbf{r})u_n^*(\mathbf{r}') + v_n(\mathbf{r})v_n^*(\mathbf{r}')] = \delta(\mathbf{r}) - \mathbf{r}'), \\ &\sum_n [u_n(\mathbf{r})v_n^*(\mathbf{r}') - u_n(\mathbf{r}')v_n^*(\mathbf{r})] = 0, \\ &\int d^3r\,[u_n(\mathbf{r})u_{n'}^*(\mathbf{r}) + v_n(\mathbf{r})v_{n'}^*(\mathbf{r})] = \delta_{n-n'}, \\ &\int d^3r\,[u_n(\mathbf{r})v_{n'}(\mathbf{r}) - u_{n'}(\mathbf{r})v_n^*(\mathbf{r})] = 0. \end{aligned}$$

2. *BCS theory*

Now let us specialize to the spatially uniform case, the index n is simply the momentum, and $u_n(\mathbf{r})$ and $v_n(\mathbf{r})$ are plain waves.

(a) [**2 points**] Using representation $\hat{\psi}(\mathbf{r}) = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\hat{a}_{\mathbf{k}}$, show that Eqs. (7) and (12) become

$$\begin{aligned} \hat{a}_{\mathbf{k},\uparrow} &= u_{\mathbf{k}}\,\hat{\gamma}_{\mathbf{k},1} + v_{\mathbf{k}}\,\hat{\gamma}^{+}_{-\mathbf{k},2}, \\ \hat{a}^{+}_{-\mathbf{k},\downarrow} &= u_{\mathbf{k}}\,\hat{\gamma}^{+}_{-\mathbf{k},2} - v_{\mathbf{k}}\,\hat{\gamma}^{+}_{\mathbf{k},1}, \end{aligned} \tag{13}$$

$$\begin{aligned} \hat{\gamma}_{\mathbf{k},1} &= u_{\mathbf{k}}\,\hat{a}_{\mathbf{k},\uparrow} - v_{\mathbf{k}}\,\hat{a}^{+}_{-\mathbf{k},\downarrow}, \\ \hat{\gamma}^{+}_{-\mathbf{k},2} &= u_{\mathbf{k}}\,\hat{a}^{+}_{-\mathbf{k},\downarrow} + v_{\mathbf{k}}\,\hat{a}_{\mathbf{k},\uparrow}. \end{aligned} \tag{14}$$

(b) [**4 points**] Show that the Bogolyubov-de Gennes equation (8) becomes

$$\begin{pmatrix} \xi_{\mathbf{k}} & \Delta \\ \Delta^* & -\xi_{-\mathbf{k}} \end{pmatrix}\begin{pmatrix} u_{\mathbf{k}} \\ -v_{\mathbf{k}} \end{pmatrix} \approx \begin{pmatrix} v_F(k-k_F) & \Delta \\ \Delta^* & -v_F(k-k_F) \end{pmatrix}\begin{pmatrix} u_{\mathbf{k}} \\ -v_{\mathbf{k}} \end{pmatrix} = E_{\mathbf{k}}\begin{pmatrix} u_{\mathbf{k}} \\ -v_{\mathbf{k}} \end{pmatrix}. \tag{15}$$

Find the eigenvalues and eigenfunctions of Eq. (15) compare the answers with the textbook.

(c) [**4 points**] Calculate the energy (11) of the system per unit volume at zero temperature

$$\frac{E_0}{V} = \int \frac{d^3k}{(2\pi)^3}\left(-E_k + |\xi_k|\right) - \frac{|\Delta_0|^2}{g}, \tag{16}$$

By minimizing E_0 with respect to Δ_0, find Δ_0 at zero temperature. Express the condensation energy E_0/V at zero temperature in terms of Δ_0. Compare the answer with the textbook. (Remember that in our notation $g<0$.) This calculation is similar to the Peierls Problem 2 of HW 6.

(d) [**2 points**] Show that Hamiltonian (10) (counted from the normal ground-state energy) becomes

$$\hat{H}_{MF} = V\int \frac{d^3k}{(2\pi)^3}\,E_k(\hat{\gamma}^{+}_{\mathbf{k},1}\hat{\gamma}_{\mathbf{k},1} + \hat{\gamma}^{+}_{\mathbf{k},2}\hat{\gamma}_{\mathbf{k},2}) + E_0. \tag{17}$$

Show that at a finite temperature the energy of the system is

$$\frac{E}{V} = \int \frac{d^3k}{(2\pi)^3}\left\{[2f(E_k)-1]E_k + |\xi_k|\right\} - \frac{|\Delta|^2}{g}, \tag{18}$$

where $f(E_k)$ is the Fermi distribution function. By minimizing (18) with respect to Δ with the fixed occupation numbers $f(E_k)$, obtain an equation for Δ. Compare with the textbook.

(e) [**4 points**] Show that the wave function $|\Psi\rangle$ of the ground state of Hamiltonian (17) can be written as

$$|\Psi\rangle = \prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}}\hat{a}^{+}_{\mathbf{k},\uparrow}a^{+}_{-\mathbf{k},\downarrow})|0\rangle, \tag{19}$$

where $|0\rangle$ is a completely empty state without any particles.

You need to show that $\hat{\gamma}_{\mathbf{k},1,2}|\Psi\rangle = 0$, and $\hat{\gamma}^{+}_{\mathbf{k},1,2}|\Psi\rangle$ are the eigenstates of Hamiltonian (17) with the eigenvalues E_k.

3. [**4 points**] Using the Landau criterion (23.3), determine the critical velocity of flow and the critical current density for a superconductor with the gap Δ at zero temperature. Sketch what happens to the spectrum of excitations at the critical velocity.

4. *Electrodynamic response*

In the presence of vector potential $\mathbf{A}(\mathbf{r}) = \mathbf{A}_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}$, the kinetic energy of the system becomes $(\mathbf{p} - e\mathbf{A}/c)^2/2m$. Thus, the Hamiltonian (2) experiences the following perturbation:

$$\hat{H}_1 = -\frac{e}{mc}\sum_{\mathbf{k},\sigma}\mathbf{A}_{\mathbf{q}}\cdot\mathbf{k}\,\hat{a}^{+}_{\mathbf{k}+\mathbf{q},\sigma}\hat{a}_{\mathbf{k},\sigma}, \qquad \hat{H}_2 = \mathbf{A}^2_{\mathbf{q}}\frac{e^2}{2mc^2}\sum_{\mathbf{k},\sigma}\hat{a}^{+}_{\mathbf{k},\sigma}\hat{a}_{\mathbf{k},\sigma}. \tag{20}$$

The current $\mathbf{j} = -\delta\langle\hat{H}\rangle/\delta\mathbf{A}$ consists of two terms, corresponding to the two terms in Eq. (20):

$$\mathbf{j}^{(1)}_{\mathbf{q}} = \frac{e}{mc}\sum_{\mathbf{k},\sigma}\mathbf{k}\langle\hat{a}^{+}_{\mathbf{k}+\mathbf{q},\sigma}\hat{a}_{\mathbf{k},\sigma}\rangle, \qquad \hat{\mathbf{j}}^{(2)}_{\mathbf{q}} = -\mathbf{A}_{\mathbf{q}}\frac{e^2\rho}{mc^2}, \tag{21}$$

where we consider static response at the wave vector $\mathbf{q}$, ρ is the total concentration of electrons, and σ is the spin index. The average in $\mathbf{j}^{(1)}_{\mathbf{q}}$ must be calculated using $\hat{H}_1$ as the perturbation.

(a) **[4 points]** Show that $\hat{H}_1$ can be expressed in terms of the Bogolyubov operators in the following way

$$\begin{aligned}\hat{H}_1 \quad = -\tfrac{e}{mc}\textstyle\sum_{\mathbf{k},\sigma}\mathbf{A}_{\mathbf{q}}\cdot\mathbf{k} \quad & [(u_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}} + v_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}})(\hat{\gamma}^{+}_{\mathbf{k}+\mathbf{q},1}\hat{\gamma}_{\mathbf{k},1} - \hat{\gamma}^{+}_{\mathbf{k}+\mathbf{q},2}\hat{\gamma}_{\mathbf{k},2}) \\ & + (v_{\mathbf{k}}u_{\mathbf{k}+\mathbf{q}} - u_{\mathbf{k}}v_{\mathbf{k}+\mathbf{q}})(\hat{\gamma}^{+}_{\mathbf{k}+\mathbf{q},1}\hat{\gamma}^{+}_{\mathbf{k},2} - \hat{\gamma}_{\mathbf{k}+\mathbf{q},2}\hat{\gamma}_{\mathbf{k},1})]\end{aligned} \tag{22}$$

Show that the so-called coherence factor of case II are

$$(uu' + vv')^2 = \frac{1}{2}\left(1 + \frac{\xi\xi' + \Delta^2}{EE'}\right), \qquad (uv' - vu')^2 = \frac{1}{2}\left(1 - \frac{\xi\xi' + \Delta^2}{EE'}\right). \tag{23}$$

(b) **[4 points]** Let us consider the case $q \to 0$. Then, $\hat{H}_1 = -\frac{e}{mc}\sum_{\mathbf{k},\sigma}\mathbf{A}_0\cdot\mathbf{k}[(\hat{\gamma}^{+}_{\mathbf{k},1}\hat{\gamma}_{\mathbf{k},1} - \hat{\gamma}^{+}_{\mathbf{k},2}\hat{\gamma}_{\mathbf{k},2})]$, i.e.

$$E_{\mathbf{k},1} \to E_{\mathbf{k},1} - \frac{e}{mc}\mathbf{A}_0\cdot\mathbf{k}, \qquad E_{\mathbf{k},2} \to E_{\mathbf{k},2} + \frac{e}{mc}\mathbf{A}_0\cdot\mathbf{k}. \tag{24}$$

Show that the current is

$$\mathbf{j}^{(1)}_0 = \frac{e}{mc}\sum_{\mathbf{k}}\mathbf{k}\left(\langle\hat{\gamma}^{+}_{\mathbf{k},1}\hat{\gamma}_{\mathbf{k},1}\rangle - \langle\hat{\gamma}^{+}_{\mathbf{k},2}\hat{\gamma}_{\mathbf{k},2}\rangle\right) \approx -\frac{2e^2}{m^2c^2}\sum_{\mathbf{k}}\mathbf{k}\left[\mathbf{A}_0\cdot\mathbf{k}\right]\frac{\partial f}{\partial E_{\mathbf{k}}}, \tag{25}$$

where f is the Fermi distribution function.
Thus, show that

$$\mathbf{j}_0 = -\mathbf{A}_{\mathbf{q}}\frac{e^2\rho_s}{mc^2}, \tag{26}$$

where the superfluid density is $\rho_s = \rho - \rho_n$ and the normal density is

$$\rho_n = -\frac{1}{3\pi^2 m}\int dk\, k^4\frac{\partial f}{\partial E_k}, \qquad \frac{\rho_n}{\rho} \approx -2\int_0^\infty d\xi\,\frac{\partial f}{\partial E}. \tag{27}$$

Describe qualitatively the behavior of ρ_s and ρ_n at $T \to 0$ and $T \to T_c$.

(c) **[4 points]** Using Eq. (22) as a perturbation, obtain an a relation between $\mathbf{j}_{\mathbf{q}}$ and $\mathbf{A}_{\mathbf{q}}$ for $q \neq 0$. Describe qualitatively how this expression can be obtained also from the Feynman diagrams for a superconducting system.