Homework 4, 620 Many body

December 12, 2022

1) The excitations spectra of the superconductor: Calculate the excitations spectra of quasiparticles as well as the real electrons in the BCS state wave function.
In class we derived the BCS Hamiltonian

$$H^{BCS} = \sum_{\mathbf{k}} \Psi^{\dagger}_{\mathbf{k}} \begin{pmatrix} \varepsilon_{\mathbf{k}} & -\Delta \\ -\Delta & -\varepsilon_{-\mathbf{k}} \end{pmatrix} \Psi_{\mathbf{k}} + \varepsilon_{-\mathbf{k}} \quad (1)$$

in which the $\Psi_{\mathbf{k}}$ spinor is

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c^{\dagger}_{-\mathbf{k},\downarrow}. \end{pmatrix} \quad (2)$$

The Hamiltonian is diagonalized with a unitary transformation in the form

$$\hat{U}_{\mathbf{k}} = \begin{pmatrix} \cos(\theta_{\mathbf{k}}) & \sin(\theta_{\mathbf{k}}) \\ \sin(\theta_{\mathbf{k}}) & -\cos(\theta_{\mathbf{k}}) \end{pmatrix} \quad (3)$$

where

$$\cos(\theta_{\mathbf{k}}) = \sqrt{\frac{1}{2}(1 + \frac{\varepsilon_{\mathbf{k}}}{\sqrt{\varepsilon_{\mathbf{k}} + \Delta^2}})} \quad (4)$$

$$\sin(\theta_{\mathbf{k}}) = -\sqrt{\frac{1}{2}(1 - \frac{\varepsilon_{\mathbf{k}}}{\sqrt{\varepsilon_{\mathbf{k}} + \Delta^2}})} \quad (5)$$

and the quasiparticle spinors are

$$\begin{pmatrix} \Phi_{\mathbf{k},\uparrow} \\ \Phi^{\dagger}_{-\mathbf{k},\downarrow} \end{pmatrix} = \hat{U}_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c^{\dagger}_{-\mathbf{k},\downarrow}. \end{pmatrix} \quad (6)$$

The diagonal BCS Hamiltonian has the form

$$H^{BCS} = \sum_{\mathbf{k}} \lambda_{\mathbf{k}} \Phi^{\dagger}_{\mathbf{k},s} \Phi_{\mathbf{k},s} - E_0 \quad (7)$$

with $E_0 = \sum_{\mathbf{k}} \lambda_{\mathbf{k}} - \varepsilon_{\mathbf{k}}$ and $\lambda_{\mathbf{k}} = \sqrt{\varepsilon^2_{\mathbf{k}} + \Delta^2}$

- Show that the quasiparticle Green's function $\widetilde{G}_{\mathbf{k}} = -\langle T_\tau \Phi_{\mathbf{k},s}(\tau)\Phi^\dagger_{\mathbf{k},s}(0)\rangle$ has a gap with the size Δ. What is the spectral function corresponding to this Green's function? Show that the corresponding densities of states has the form $D(\omega) \approx D_0\ \omega/\sqrt{\omega^2-\Delta^2}$, where D_0 is density of states at the Fermi level of the normal state.
- Compute the physical Green's function (measured in ARPES)

$$G_{\mathbf{k},s} = -\langle T_\tau c_{\mathbf{k},s}(\tau)c^\dagger_{\mathbf{k},s}(0)\rangle \tag{8}$$

  and its density of states. Show that the corresponding spectral function has the form

$$A_{\mathbf{k},s}(\omega) = \cos^2\theta_{\mathbf{k}}\ \delta(\omega-\lambda_{\mathbf{k}}) + \sin^2\theta_{\mathbf{k}}\ \delta(\omega+\lambda_{\mathbf{k}}) \tag{9}$$

  Sketch the bands and their weight, and sketch the density of states.

2) In class we derived the BCS action, which takes the form

$$S = \int_0^\beta d\tau \int d^3\mathbf{r}\Psi^\dagger(\mathbf{r})\begin{pmatrix} \frac{\partial}{\partial\tau} - \mu + \frac{(i\nabla+e\vec{A})^2}{2m} + ie\phi & -\Delta \\ -\Delta^\dagger & \frac{\partial}{\partial\tau} + \mu - \frac{(i\nabla-e\vec{A})^2}{2m} - ie\phi \end{pmatrix}\Psi(\mathbf{r}) + s_0 \tag{10}$$

where $s_0 = \int_0^\beta d\tau \int d^3\mathbf{r}\frac{|\Delta|^2}{g}$

Show that the action can also be expressed by

$$S = s_0 + \mathrm{Tr}\log(-G) \tag{11}$$

where

$$G^{-1} = \begin{pmatrix} i\omega_n + \mu - \frac{(\mathbf{p}-e\mathbf{A})^2}{2m} - ie\phi, \Delta & \\ \Delta^\dagger & i\omega - \mu + \frac{(\mathbf{p}+e\mathbf{A})^2}{2m} + ie\phi \end{pmatrix} \tag{12}$$

Show that the transformation $UG^{-1}U^\dagger$, where U is

$$U = \begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix} \tag{13}$$

leads to the following change of the quantities

$$\Delta \rightarrow e^{-2i\theta}\Delta \tag{14}$$

$$\mathbf{A} \rightarrow \mathbf{A} + \frac{1}{e}\nabla\theta \tag{15}$$

$$\phi \rightarrow \phi - \frac{1}{e}\dot{\theta} \tag{16}$$

and otherwise the same form of the action. Argue that since this corresponds to the change of the EM gauge, the phase of Δ is arbitrary in BCS theory, and can always be changed. Moreover, the phase can not be experimentally measurable quantity.

In the absence of the EM field, derive the saddle point equations in field Δ, which are often written as $\Delta = gG_{12}$, and cam be expressed as

$$\frac{1}{g} = -\frac{1}{V\beta}\sum_{\mathbf{k},n}\frac{1}{(i\omega_n)^2-\lambda_{\mathbf{k}}^2}. \tag{17}$$

Show that the same equation can also be expressed as

$$\frac{1}{g} = \frac{1}{V}\sum_{\mathbf{k}}\frac{1-2f(\lambda_{\mathbf{k}})}{2\lambda_{\mathbf{k}}} \tag{18}$$

and with D_0 being the density of the normal state at the Fermi level, it can also be expressed as

$$\frac{1}{g} \approx D_0\int_0^{\frac{\omega_D}{2T}} dx\frac{\tanh(\sqrt{x^2+\kappa^2})}{\sqrt{x^2+\kappa^2}} \tag{19}$$

where $x = \varepsilon/(2T)$ and $\kappa = \Delta/(2T)$.

Next, derive the critical temperature by taking the limit $\Delta \to 0$ ($\kappa \to 0$). Assuming that $\omega_D/(2T) \gg 1$, break the integral into two parts $[0,\Lambda]$, and $[\Lambda, \frac{\omega}{2T}]$. Here $\Lambda \gg 1$. In the second part set $\tanh(x) = 1$, as x is large. Using numerical integration (in Mathematica or similar tool) verify that

$$\lim_{\Lambda\to\infty}\int_0^{\Lambda} dx\frac{\tanh(x)}{x} - \log(\Lambda) \approx \log(2\times 1.13) \tag{20}$$

Next, show that T_c is determined by

$$\frac{1}{gD_0} \approx \log(2\times 1.13) + \log(\frac{\omega_D}{2T_c}) \tag{21}$$

and consequently

$$T_c \approx 1.13\,\omega_D e^{-1/(gD_0)}$$

Using Eq. 19 compute the size of the gap at $T = 0$. Show that to the leading order in Δ/ω_D the gap size is

$$\Delta(T=0) = 2\omega_D e^{-1/(gD_0)} \tag{22}$$

Finally, show that within BCS there is universal ration $\Delta(T=0)/(2T_c) \approx 1/1.13 \approx 0.88$.

3) Starting from action Eq. 10 derive the effective action for small EM field A, ϕ. Show that for a constant and time independent phase, the action takes the form

$$S_{eff} = \mathrm{Tr}\log(-G_{A=0,\phi=0}) + \mathrm{Tr}(\frac{|\Delta|^2}{g}) + e^2\int_0^{\beta} d\tau\int d^3\mathbf{r}\left[D_0(\phi(\mathbf{r},\tau))^2 + \frac{n_s}{2m}\left[\mathbf{A}(\mathbf{r},\tau)\right]^2\right] \tag{23}$$

Note that using EM gauge transformation, we arrive at an equivalent action

$$S_{eff} = S_0 + e^2\int_0^{\beta} d\tau\int d^3\mathbf{r}\left[D_0(\phi(\mathbf{r},\tau)+\dot{\theta})^2 + \frac{n_s}{2m}\left[\mathbf{A}(\mathbf{r},\tau)-\nabla\theta\right]^2\right] \tag{24}$$

Below we summarize the steps to derive this effective action.

We start by splitting G^{-1} in Eq.12 into $G_{A=0,\phi=0} \equiv G^0$ and terms linear and quadratic in EM-fields, i.e,

$$G^{-1} = \left(G^0\right)^{-1} - X_1 - X_2$$

where

$$X_1 = ie\phi\,\sigma_3 + \frac{ie}{2m}[\nabla, A]_+ I \tag{25}$$

$$X_2 = \frac{e^2}{2m}\mathbf{A}^2\,\sigma_3 \tag{26}$$

and σ_3, σ_1 are Pauli matrices. Show that action 11 can then be expressed as

$$S = s_0 + \mathrm{Tr}\log(-G^0) - \mathrm{Tr}\log(I - G^0(X_1 + X_2)) \tag{27}$$

$$\approx S_0 + \mathrm{Tr}(G^0 X_1) + \mathrm{Tr}(G^0 X_2) + \frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1) + O(X^3) \tag{28}$$

where $S_0 = s_0 + \mathrm{Tr}\log(-G^0)$ (which vanishes at T_c), and the second term, which is linear in fields, while third and fourth are quadratic.

Next show that the form of G^0 is

$$G^0_{\mathbf{p}n,\mathbf{p}'n'} = \delta_{\mathbf{p},\mathbf{p}'}\delta_{nn'}\left(i\omega_n I - \left(\frac{p^2}{2m} - \mu\right)\sigma_3 + \Delta\,\sigma_1\right)^{-1} \tag{29}$$

where the inverse is in the 2×2 space only, while G^0 is diagonal in frequency& momentum space. We will use $(\mathbf{p}, n) = p$ for short notation. Similarly, show that X_1 is

$$(X_1)_{p_1,p_2} = (ie\phi\,\sigma_3 + \frac{ie}{2m}[\nabla, A]_+ I)_{p_1,p_2} = ie\phi_{p_2-p_1}\sigma_3 - \frac{e}{2m}(\mathbf{p}_1 + \mathbf{p}_2)\mathbf{A}_{p_2-p_1} \tag{30}$$

Show that

$$\mathrm{Tr}(G^0 X_1) = \frac{1}{\beta}\sum_{\omega_n,\mathbf{p}} \mathrm{Tr}_{2\times 2}(G^0_{\mathbf{p}}(i\omega_n)[ie\phi_{\mathbf{q}=0}\sigma_3 - \frac{e}{m}\mathbf{p}\mathbf{A}_{\mathbf{q}=0}]).$$

Argue that the second term vanishes when inversion symmetry is present, as it is odd in $\mathbf{p}$ (with $G^0_{\mathbf{p}}$ even function). The first term than becomes $nie\phi_{\mathbf{q}=0,\omega=0}$ (n is total density), which describes the electron density in uniform electric field, which should cancel with the action between negative ions and the external field.

Next show that

$$\mathrm{Tr}(G^0 X_2) = \frac{e^2}{2m}\frac{1}{\beta}\sum_{\omega_n,\mathbf{p}} \mathrm{Tr}_{2\times 2}(G^0_{\mathbf{p}}(i\omega_n)\mathbf{A}^2_{q=0}\sigma_3) = \frac{e^2}{2m} n \sum_{\mathbf{q}} \mathbf{A}_{\mathbf{q}}\mathbf{A}_{-\mathbf{q}}$$

is standard diamagnetic term, which will be used later.

Finally, we address the term $\frac{1}{2}\mathrm{Tr}(G^0X_1G^0X_1)$. We find

$$\frac{1}{2}\mathrm{Tr}(G^0X_1G^0X_1) = \frac{1}{2}\sum_{p_1,p_2}\mathrm{Tr}_{2\times2}\left(G^0_{p_1}(X_1)_{p_1,p_2}G^0_{p_2}(X_1)_{p_2,p_1}\right) \quad (31)$$

$$\frac{1}{2}\sum_{p,q}\mathrm{Tr}_{2\times2}\left(G^0_{p-q/2}(X_1)_{p-q/2,p+q/2}G^0_{p+q/2}(X_1)_{p+q/2,p-q/2}\right) \quad (32)$$

$$= \frac{1}{2}\sum_{p,q}\mathrm{Tr}_{2\times2}\left(G^0_{p-q/2}\left(ie\phi_q\sigma_3 - \frac{e}{m}\mathbf{pA_q}\right)G^0_{p+q/2}\left(ie\phi_{-q}\sigma_3 - \frac{e}{m}\mathbf{pA_{-q}}\right)\right) \quad (33)$$

$$= \frac{1}{2}\sum_{p,q}\left(-e^2\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\mathrm{Tr}_{2\times2}\left(G^0_{p-q/2}\sigma_3G^0_{p+q/2}\sigma_3\right) + \frac{e^2}{m^2}(\mathbf{pA_q})(\mathbf{pA_{-q}})\mathrm{Tr}_{2\times2}\left(G^0_{p-q/2}G^0_{p+q/2}\right)\right) \quad (34)$$

In the last line we dropped the cross-terms, which are odd in $\mathbf{p}$ and vanish.

For any rotationally invariant function $R(\mathbf{p}^2)$, the following identity is satisfied

$$\sum_{\mathbf{p}}(\mathbf{pA_q})(\mathbf{pA_{-q}})R(\mathbf{p}^2) = \mathbf{A_qA_{-q}}\sum_{\mathbf{p}}\frac{\mathbf{p}^2}{3}R(\mathbf{p}^2). \quad (35)$$

We are interested in slowly varying fields (small q), hence $p \pm q/2 \approx p$. We therefore arrive at

$$\frac{1}{2}\mathrm{Tr}(G^0X_1G^0X_1) = \frac{e^2}{2}\sum_{p,q}\left(-\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\mathrm{Tr}_{2\times2}\left(G^0_p\sigma_3G^0_p\sigma_3\right) + \mathbf{A_qA_{-q}}\frac{\mathbf{p}^2}{3m^2}\mathrm{Tr}_{2\times2}\left(G^0_pG^0_p\right)\right) \quad (36)$$

Next, show that

$$\mathrm{Tr}_{2\times2}\left(G^0_p\sigma_3G^0_p\sigma_3\right) = 2\frac{(i\omega_n)^2 + \lambda^2_{\mathbf{p}} - 2\Delta^2}{\left((i\omega_n)^2 - \lambda^2_{\mathbf{p}}\right)^2} \quad (37)$$

$$\mathrm{Tr}_{2\times2}\left(G^0_pG^0_p\right) = 2\frac{(i\omega_n)^2 + \lambda^2_{\mathbf{p}}}{\left((i\omega_n)^2 - \lambda^2_{\mathbf{p}}\right)^2} \quad (38)$$

Next, carry out the frequency summations, and show that

$$\frac{1}{\beta}\sum_{\omega_n}\frac{(i\omega_n)^2 + \lambda^2_{\mathbf{p}} - 2\Delta^2}{\left((i\omega_n)^2 - \lambda^2_{\mathbf{p}}\right)^2} = f'(\lambda_{\mathbf{p}})(1 - \frac{\Delta^2}{\lambda^2_{\mathbf{p}}}) + (2\,f(\lambda_{\mathbf{p}}) - 1)\frac{\Delta^2}{2\lambda^3_{\mathbf{p}}} \approx -\frac{\Delta^2}{2\lambda^3_{\mathbf{p}}} \quad (39)$$

$$\frac{1}{\beta}\sum_{\omega_n}\frac{(i\omega_n)^2 + \lambda^2_{\mathbf{p}}}{\left((i\omega_n)^2 - \lambda^2_{\mathbf{p}}\right)^2} = f'(\lambda_{\mathbf{p}}) \quad (40)$$

Here $f'(\lambda_{\mathbf{p}}) = df(\lambda_{\mathbf{p}})/d\lambda_{\mathbf{p}}$ and we took only the leading terms at low temperature.

Combining all we learned so far, we get

$$\frac{1}{2}\mathrm{Tr}(G^0X_1G^0X_1) = e^2\sum_{q,\mathbf{p}}\left(\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\left(\frac{\Delta^2}{2\lambda^3_{\mathbf{p}}}\right) + \mathbf{A_qA_{-q}}\frac{\mathbf{p}^2}{3m^2}f'(\lambda_{\mathbf{p}})\right) \quad (41)$$

Next we combine this result with the diamagnetic term, derived before, and we obtain

$$\mathrm{Tr}(G^0X_2) + \frac{1}{2}\mathrm{Tr}(G^0X_1G^0X_1) = e^2\sum_{q,\mathbf{p}}\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\left(\frac{\Delta^2}{2\lambda_{\mathbf{p}}^3}\right) + \mathbf{A}_{\mathbf{q}}\mathbf{A}_{-\mathbf{q}}\left(\frac{n}{2m} + \frac{\mathbf{p}^2}{3m^2}f'(\lambda_{\mathbf{p}})\right) \tag{42}$$

Next we show that

$$\sum_{\mathbf{p}}\frac{\Delta^2}{2\lambda_{\mathbf{p}}^3} = \int d\varepsilon D(\varepsilon)\frac{\Delta^2}{2(\varepsilon^2+\Delta^2)^{3/2}} \approx D_0 \tag{43}$$

$$f'(\lambda_{\mathbf{p}}) = -\beta f(\lambda_{\mathbf{p}})f(-\lambda_{\mathbf{p}}) \tag{44}$$

hence $S_{eff} \equiv \mathrm{Tr}(G^0X_2) + \frac{1}{2}\mathrm{Tr}(G^0X_1G^0X_1)$ becomes

$$S_{eff} = e^2\sum_q \phi_{\mathbf{q}}\phi_{-\mathbf{q}}D_0 + \mathbf{A}_{\mathbf{q}}\mathbf{A}_{-\mathbf{q}}\left(\frac{n}{2m} - \beta\sum_{\mathbf{p}}\frac{\mathbf{p}^2}{3m^2}f(\lambda_{\mathbf{p}})f(-\lambda_{\mathbf{p}})\right) \tag{45}$$

Finally, we will prove that

$$\left(\frac{n}{2m} - \beta\sum_{\mathbf{p}}\frac{\mathbf{p}^2}{3m^2}f(\lambda_{\mathbf{p}})f(-\lambda_{\mathbf{p}})\right) \equiv \frac{n_s}{2m} \tag{46}$$

where n_s is superfluid density.

We see that

$$\frac{n_s}{2m} = \frac{n}{2m} - \beta\sum_{\mathbf{p}}\frac{2}{3m}(\varepsilon_{\mathbf{p}}+\mu)f(\lambda_{\mathbf{p}})f(-\lambda_{\mathbf{p}}) \tag{47}$$

$$= \frac{n}{2m} - \beta\frac{1}{2}\int d\varepsilon D(\varepsilon)\frac{2}{3m}(\varepsilon+\mu)f(\lambda_\varepsilon)f(-\lambda_\varepsilon) \tag{48}$$

$$\approx \frac{n}{2m} - \frac{D_0\mu}{3m}\int d\varepsilon\beta f(\lambda_\varepsilon)f(-\lambda_\varepsilon) \tag{49}$$

Note that here we used $D(\omega) = 2\sum_{\mathbf{p}}\delta(\omega - \varepsilon_{\mathbf{p}})$, where 2 is due to spin. This is essential because n contains the spin degeneracy as well. It is straightforward to prove that $\mu D_0 = \frac{3}{2}n$ in our approximation, because

$$D_0 = 2\sum_{\mathbf{p}}\delta(\mu - \frac{p^2}{2m}) = c\sqrt{\mu} \tag{50}$$

$$n = 2\sum_{\mathbf{p}}\theta(\mu - \frac{p^2}{2m}) = c(2/3)\mu^{3/2}. \tag{51}$$

We thus conclude that

$$\frac{n_s}{2m} = \frac{n}{2m}\left(1 - \int d\varepsilon\beta f(\sqrt{\varepsilon^2+\Delta^2})f(-\sqrt{\varepsilon^2+\Delta^2})\right) \tag{52}$$

At low temperature $f(\sqrt{\varepsilon^2 + \Delta^2}) \approx 0$, hence $n_s = n$ and all electrons contribute to the superfluid density. Above T_c we have

$$\int d\varepsilon \beta f(\varepsilon) f(-\varepsilon) = 1$$

and therefore $n_s = 0$ as expected. We interpret that n_s is the fraction of electrons that are parred up in superfluid, i.e., superfluid density, as promised.

We just proved that

$$S_{eff} = e^2 \sum_q \phi_{\mathbf{q}} \phi_{-\mathbf{q}} D_0 + \mathbf{A}_{\mathbf{q}} \mathbf{A}_{-\mathbf{q}} \frac{n_s}{2m}, \tag{53}$$

which is equivalent to Eq. 23.