8.512 Recitation 5

Today: 1) BCS mean-field theory
2) Quasiparticle excitations
3) Gap equation at finite-T
4) Critical temperature T_c

Ref: "Theory of Superconductivity" by C. Timm, Ch. 10

1) BCS Hamiltonian

$$H_{BCS} = \sum_{k,\sigma=\uparrow,\downarrow} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,k'} U_{kk'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} - \mu$$

- Mean-field approximation: for any ops. A, B consider small fluctuations about GS exp. values

$$(A - \langle A \rangle)(B - \langle B \rangle) \approx 0$$
$$\Rightarrow AB \approx \langle A \rangle B + \langle B \rangle A - \langle A \rangle \langle B \rangle$$

- Let $A = c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}$, $B = c_{-k'\downarrow} c_{k'\uparrow}$

and define $\Delta_k \equiv -\sum_{k'} U_{kk'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle = -\sum_{k'} U_{kk'} \langle c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow} \rangle$

$$\Rightarrow H_{BCS} = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} - \sum_k \Delta_k \Big(c_{-k\downarrow} c_{k\uparrow} + c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} - \underbrace{\langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle}_{\text{const.}} \Big)$$

- H_{BCS} is particle non-conserving; diagonalize w/ Bogoliubov transform

$$\begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^\dagger_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & -v_k \\ v_k & u_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}$$

- γ should satisfy anti-commutation relation:

$$1 = \{\gamma_{k\uparrow}, \gamma^\dagger_{k\uparrow}\} = u_k^2 \underbrace{\{c_{k\uparrow}, c^\dagger_{k\uparrow}\}}_{=1} - u_k v_k \underbrace{\{c_{k\uparrow}, c_{-k\downarrow}\}}_{=0}$$

$$- v_k u_k \underbrace{\{c^\dagger_{-k\downarrow}, c^\dagger_{k\uparrow}\}}_{=0} + v_k^2 \underbrace{\{c^\dagger_{-k\downarrow}, c_{-k\downarrow}\}}_{=1}$$

$$= u_k^2 + v_k^2$$

$$\Rightarrow \boxed{u_k^2 + v_k^2 = 1}$$

- Inverse transform $\begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^\dagger_{-k\downarrow} \end{pmatrix}$

$$H_{BCS} = \sum_k \Big[\left(\varepsilon_k (u_k^2 - v_k^2) + 2\Delta_k u_k v_k\right)\left(\gamma^\dagger_{k\uparrow}\gamma_{k\downarrow} + \gamma^\dagger_{-k\downarrow}\gamma_{-k\downarrow}\right)$$

$$+ \left(2\varepsilon_k u_k v_k - \Delta_k (u_k^2 - v_k^2)\right)\left(\gamma_{k\uparrow}\gamma^\dagger_{-k\downarrow} + \gamma_{-k\downarrow}\gamma_{k\uparrow}\right)$$

$$+ \underbrace{2\varepsilon_k v_k^2 - 2\Delta_k u_k v_k + \Delta_k \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\rangle}_{\text{const.}} \Big]$$

Define $E_{BCS} = \sum_k \left(2\varepsilon_k v_k^2 - 2\Delta_k u_k v_k + \Delta_k \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\rangle \right)$

- To diagonalize Hamiltonian, choose

$$\begin{cases} 2\varepsilon_k u_k v_k - \Delta_k (u_k^2 - v_k^2) = 0 \\ u_k^2 + v_k^2 = 1 \end{cases} \iff \boxed{\begin{aligned} u_k^2 &= \frac{1}{2}\left(1 + \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2+\Delta_k^2}}\right) \\ v_k^2 &= \frac{1}{2}\left(1 - \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2+\Delta_k^2}}\right) \end{aligned}}$$

$$\Rightarrow u_k v_k = \frac{\Delta_k}{2\sqrt{\varepsilon_k^2+\Delta_k^2}}$$

$$H_{BCS} = \sum_k \sqrt{\varepsilon_k^2+\Delta_k^2}\left(\gamma_{k\uparrow}^\dagger \gamma_{k\uparrow} + \gamma_{-k\downarrow}^\dagger \gamma_{-k\downarrow}\right) + E_{BCS}$$

$$= \sum_{k,\sigma} E_k \gamma_{k\sigma}^\dagger \gamma_{k\sigma} + E_{BCS} \qquad (\Delta_k = \Delta_{-k})$$

with $\boxed{E_k = \sqrt{\varepsilon_k^2+\Delta_k^2}}$

2) GS is given by $\gamma_{k\sigma}|0\rangle_{BCS} = 0$

Ex: Check that trial wavefunction

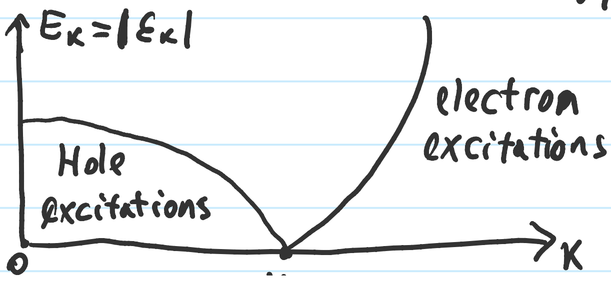
$$|\psi_{BCS}\rangle = \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger)|0\rangle$$

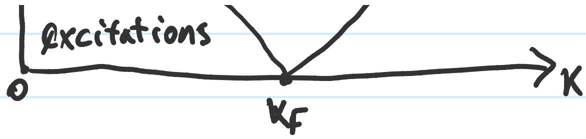
is indeed a GS!

- For a normal metal $\Delta_k \to 0$ so

$$u_k^2 = \begin{cases} 0 & \text{if } \varepsilon_k < 0 \\ 1 & \text{if } \varepsilon_k > 0 \end{cases} \qquad v_k^2 = \begin{cases} 1 & \text{if } \varepsilon_k < 0 \\ 0 & \text{if } \varepsilon_k > 0 \end{cases}$$

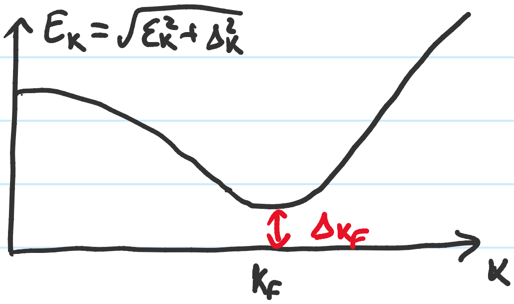
$\Rightarrow$ Quasiparticles are holes below Fermi energy $(\varepsilon_k<0)$ and electrons above Fermi energy $(\varepsilon_k>0)$

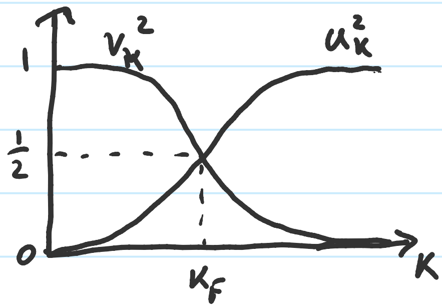




- SC has a gap $\Delta_{k_F} > 0$, $0 < v_k^2, u_k^2 < 1$

$\Rightarrow$ Quasiparticles are superpositions of particles and holes!





3) Gap is determined self-consistantly:

$$\Delta_k = -\sum_{k'} U_{kk'} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle$$

- Effective $e^- - e^-$ interaction is attractive due to phonons and is larger than Coulomb interaction when $E_k - E_{k'} < \hbar\omega_D$

Hence we can approximate the potential

$$U_{kk'} = \begin{cases} -U_0 & \text{if } |\varepsilon_{k'}|, |\varepsilon_k| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

$$\Rightarrow \Delta_k = U_0 \sum_{-\hbar\omega_D < \varepsilon_{k'} < \hbar\omega_D} \langle c_{-k'\downarrow} c_{k'\uparrow} \rangle \equiv \Delta_0$$

(k-independent)

- First consider $T=0$ $\Rightarrow$ BCS ground state

$$\langle c_{-k'\downarrow} c_{k'\uparrow} \rangle = \langle c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow} \rangle = u_k v_k$$

$$\Rightarrow \quad 1 = \frac{1}{2} U_0 \sum_{\substack{k' \\ |\varepsilon_{k'}| < \hbar\omega_D}} \frac{1}{\sqrt{|\varepsilon_{k'}|^2 + \Delta_0^2}}$$

$$\Leftrightarrow \quad 1 = \frac{1}{2} U_0 \int_{-\hbar\omega_D}^{\hbar\omega_D} d\varepsilon \; \underset{\substack{\uparrow \\ \text{density of} \\ \text{states}}}{g(\varepsilon)} \; \frac{1}{\sqrt{\varepsilon^2 + \Delta_0^2}}$$

$\hbar\omega_D \ll \varepsilon_F = \mu$ $\Rightarrow$ integral is over a narrow window close to Fermi surface!

$$g(\varepsilon) \simeq g(\varepsilon_F) = \text{const.}$$

$$\Rightarrow \quad 1 = \frac{1}{2} U_0 g(\varepsilon_F) \cdot 2 \sinh^{-1}\left(\frac{\hbar\omega_D}{\Delta_0}\right)$$

$$\boxed{\Delta_0 = \frac{\hbar\omega_D}{\sinh\left(\frac{1}{U_0 g(\varepsilon_F)}\right)}} \qquad (T=0)$$

- In the weak coupling limit $U_0 g(\varepsilon_F) \ll 1$

$$\boxed{\Delta_0 \simeq 2\hbar\omega_D \, e^{-\frac{1}{U_0 g(\varepsilon_F)}}} \qquad (T=0)$$

- The BCS GS energy is given by

$$E_{BCS} = \sum_k \left(2\varepsilon_k v_k^2 - 2\Delta_k u_k v_k + \Delta_k \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \rangle \right)$$

$$= \sum_{k}^{\hbar\omega_D} \left(\varepsilon_k - \frac{\varepsilon_k^2}{\sqrt{\varepsilon_k^2 + \Delta_k^2}} - \frac{1}{2} \frac{\Delta_k^2}{\sqrt{\varepsilon_k^2 + \Delta_k^2}} \right)$$

$$= \sum_k \left(\epsilon_k - \frac{\epsilon_k^2}{\sqrt{\epsilon_k^2+\Delta_k^2}} - \frac{1}{2}\frac{\Delta_k^2}{\sqrt{\epsilon_k^2+\Delta_k^2}} \right)$$

$$\approx \int_{-\hbar\omega_D}^{\hbar\omega_D} d\epsilon\, g(\epsilon) \left(\epsilon - \frac{\epsilon^2}{\sqrt{\epsilon^2+\Delta_0^2}} - \frac{1}{2}\frac{\Delta_0^2}{\sqrt{\epsilon^2+\Delta_0^2}} \right)$$

- The GS energy of a normal metal is

$$E_N = 2\sum_{k<k_F} \epsilon_k = 2\int_0^{\epsilon_F} d\epsilon\, g(\epsilon)$$

If $\Delta_0 << \hbar\omega_D$ (weak coupling), then

$$E_{BCS} - E_N \approx -\frac{1}{2} g(\epsilon_F)\Delta_0^2 < 0$$

$\Rightarrow$ SC is energetically favorable!

- Recall that for type-I SC we have a critical field above which SC is destoyed

$$E_{BCS} - E_N = -\frac{H_c^2}{8\pi}$$

$$\Rightarrow \boxed{H_c = \sqrt{4\pi g(\epsilon_F)}\ \Delta_0}$$

$\Rightarrow H_c \sim \Delta_0 \sim \hbar\omega_D \sim \frac{1}{\sqrt{M}}$ ← atomic mass of SC element

This is called the "isotope effect" and it relates a macroscopic parameter H_c to the microscopic atomic mass M!

Can be used to check that SC is indeed mediated by phonons.

4) Now consider finite $T \neq 0$

$$\langle c_{-k'\downarrow} c_{k'\uparrow} \rangle = -v_{k'}u_{k'} \underbrace{\langle \gamma^{\dagger}_{k'\uparrow} \gamma_{k'\uparrow} \rangle}_{= n_F(E_{k'})} - v_{k'}^2 \underbrace{\langle \gamma^{\dagger}_{k'\uparrow} \gamma^{\dagger}_{-k'\downarrow} \rangle}_{=0}$$

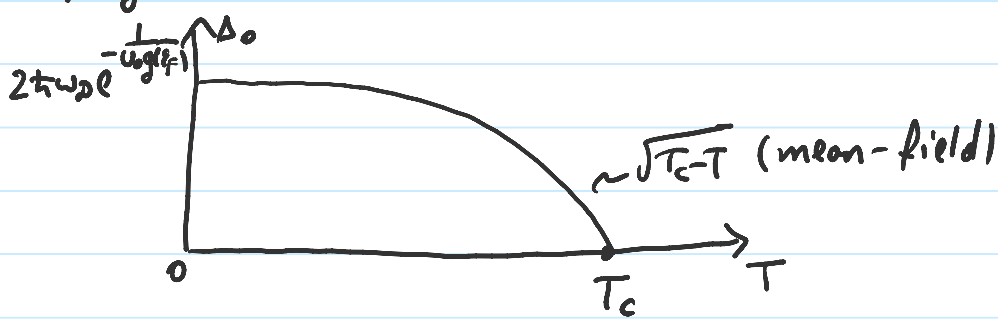
$$+ u_{k'}^2 \underbrace{\langle \gamma_{-k'\downarrow} \gamma_{k'\uparrow} \rangle}_{=0} + v_{k'}u_{k'} \underbrace{\langle \gamma_{-k'\downarrow} \gamma^{\dagger}_{-k'\uparrow} \rangle}_{= 1 - n_F(E_{k'})}$$

$$= v_{k'}u_{k'} \left(1 - 2 n_F(E_{k'}) \right) = v_{k'}u_{k'} \tanh\left(\frac{\beta E_{k'}}{2}\right)$$

where $n_F(E_{k'}) = \dfrac{1}{1 + e^{\beta E_{k'}}}$

- Gap equation: $1 = \frac{1}{2} U_0 g(\varepsilon_F) \displaystyle\int_{-\hbar\omega_D}^{\hbar\omega_D} d\varepsilon \, \frac{\tanh\left(\frac{\beta}{2}\sqrt{\varepsilon^2 + \Delta_0^2}\right)}{\sqrt{\varepsilon^2 + \Delta_0^2}}$

Integral can be evaluated numerically



- Phase transition to normal at $\Delta_0 = 0$, $T = T_c$.

$$1 = U_0 g(\varepsilon_F) \int_0^{\hbar\omega_D} \frac{d\varepsilon}{\varepsilon} \tanh\left(\frac{\varepsilon}{2k_B T_c}\right)$$

$x = \dfrac{\varepsilon}{2k_B T_c}$ $\Rightarrow$ $\displaystyle\int_0^{\hbar\omega_D/2k_B T_c} dx \, \frac{\tanh(x)}{x} = \frac{1}{U_0 g(\varepsilon_F)}$

Integrate LHS by parts

$$\ln\left(\frac{\hbar\omega_D}{2k_BT_c}\right)\tanh\left(\frac{\hbar\omega_D}{2k_BT_c}\right) - \int_0^{\hbar\omega_D/2k_BT_c} dx\, \frac{\ln(x)}{\cosh^2(x)} \simeq$$

weak coupling $\hbar\omega_D \gg k_BT_c$

$$\approx \ln\left(\frac{\hbar\omega_D}{2k_BT_c}\right)\cdot 1 - \underbrace{\int_0^{\infty} dx\, \frac{\ln x}{\cosh^2(x)}}_{\ln\frac{\pi}{4}-\gamma}$$

where Euler $\gamma \simeq 0.577$

$$\Rightarrow \quad \frac{1}{U_0\, g(\varepsilon_F)} = \ln\left(\frac{2\hbar\omega_D}{\pi k_BT_c}e^{\gamma}\right)$$

$$\Rightarrow \boxed{k_BT_c = \frac{2e^{\gamma}}{\pi}\hbar\omega_D\, e^{-\frac{1}{U_0 g(\varepsilon_F)}} = \frac{e^{\gamma}}{\pi}\Delta_0(T=0)}$$

$$\boxed{2\Delta_0(T=0) \simeq 3.52\, k_BT_c}$$

Ex: For tin (Sn), one finds experimentally

$$2\Delta_0(T=0) \approx 3.46\, k_BT_c$$