Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

Prof. Luis Gregório Dias
luisdias@if.usp.br

Today's class: *Introduction to BCS theory.*

- Cooper pairs.
- Microscopic BCS model
- Mean-field solution: Bogoliubov transformation.
- Mean-field solution: Matsubara GFs.
- Expression for the order parameter (gap).

Cooper pair wavefunction

$$\begin{cases} \hat{H}_0 = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} \\ \hat{H}_{\mathrm{CP}} = \hat{H}_0 + \hat{V}_{\mathrm{eff}} \end{cases}$$

Cooper pair wave function:

$$\begin{cases} |\mathrm{CP}\ \mathbf{k}\rangle = \sum_{|\mathbf{k}|>k_F} a_{\mathbf{k}} \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow} |\Phi_0\rangle \\ \hat{H}_{\mathrm{CP}} |\mathrm{CP}\ \mathbf{k}\rangle = E_{\mathrm{CP}} |\mathrm{CP}\ \mathbf{k}\rangle \end{cases}$$

$$\epsilon_{\mathbf{k}} \equiv k^2/2m - \mu$$

$$\langle \mathrm{CP}\ \mathbf{k}' | \hat{V}_{\mathrm{eff}} | \mathrm{CP}\ \mathbf{k} \rangle \equiv V_{\mathbf{k},\mathbf{k}'} = -V w_{\mathbf{k}'} w_{\mathbf{k}} \quad \begin{cases} w_{\mathbf{k}} = 1 \ \text{ if } |\epsilon_{\mathbf{k}}| < \omega_D \\ w_{\mathbf{k}} = 0 \ \text{ if } |\epsilon_{\mathbf{k}}| > \omega_D \end{cases}$$

(Assignment)

$$V\rho(\epsilon_F) \ll 1$$

$$E_{\mathrm{CP}} = -2\omega_D \left(e^{2/(V\rho(\epsilon_F)))} - 1 \right)^{-1} \quad \Rightarrow \quad \boxed{|E_{\mathrm{CP}}| \approx 2\omega_D e^{-2/(V\rho(\epsilon_F)))}}$$

Microscopic model and mean field

$$\hat{H}_{\mathrm{BCS}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \hat{c}^{\dagger}_{\mathbf{k},\uparrow} \hat{c}^{\dagger}_{-\mathbf{k},\downarrow} \hat{c}_{-\mathbf{k}',\downarrow} \hat{c}_{\mathbf{k}',\uparrow}$$

$$V_{\mathbf{k},\mathbf{k}'} = -V w_{\mathbf{k}'} w_{\mathbf{k}}$$

Mean-field approximation

$$\Delta_{\mathbf{k}} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \left\langle \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} \right\rangle$$

Gap parameter or order parameter

$$\hat{H}^{\mathrm{MF}}_{\mathrm{BCS}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} - \sum_{\mathbf{k}} \Delta_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\uparrow} \hat{c}^{\dagger}_{-\mathbf{k},\downarrow} - \Delta^{*}_{\mathbf{k}} \hat{c}_{-\mathbf{k},\downarrow} \hat{c}_{\mathbf{k},\uparrow}$$

Approach 1: Bogoliubov transformation

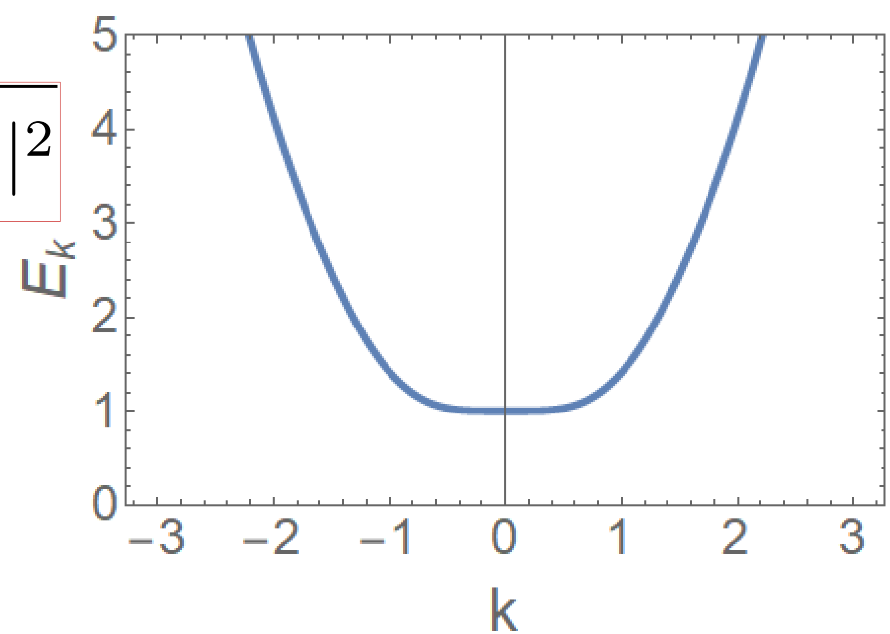
$$\hat{H}^{\mathrm{MF}}_{\mathrm{BCS}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} - \sum_{\mathbf{k}} \Delta_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\uparrow} \hat{c}^{\dagger}_{-\mathbf{k},\downarrow} - \Delta^{*}_{\mathbf{k}} \hat{c}_{-\mathbf{k},\downarrow} \hat{c}_{\mathbf{k},\uparrow}$$

(see Assignment 6!)

$$\begin{pmatrix} \hat{\gamma}_{\mathbf{k},\uparrow} \\ \hat{\gamma}^{\dagger}_{-\mathbf{k},\downarrow} \end{pmatrix} = \begin{pmatrix} u^{*}_{\mathbf{k}} & v_{\mathbf{k}} \\ -v^{*}_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k},\uparrow} \\ \hat{c}^{\dagger}_{-\mathbf{k},\downarrow} \end{pmatrix} \Rightarrow \hat{H}^{\mathrm{MF}}_{\mathrm{BCS}} = \sum_{\mathbf{k},\sigma} E_{\mathbf{k}} \, \hat{\gamma}^{\dagger}_{\mathbf{k},\sigma} \hat{\gamma}_{\mathbf{k},\sigma} + \text{ const.}$$

$$\begin{cases} |u_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \\ |v_{\mathbf{k}}|^2 = \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \end{cases}$$

$$E_{\mathbf{k}} = \sqrt{\epsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}$$



Self-consistency:

[redacted] $$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} u_{\mathbf{k}'} v_{\mathbf{k}'} \left(1 - 2n_F(E_{\mathbf{k}})\right)$$

Approach 2: Matsubara GFs

$$\hat{H}^{\mathrm{MF}}_{\mathrm{BCS}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} - \sum_{\mathbf{k}} \Delta_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k},\uparrow} \hat{c}^{\dagger}_{-\mathbf{k},\downarrow} - \Delta^{*}_{\mathbf{k}} \hat{c}_{-\mathbf{k},\downarrow} \hat{c}_{\mathbf{k},\uparrow}$$

$$\begin{cases} \mathcal{G}_{\uparrow\uparrow}(\mathbf{k},\tau) = -\left\langle \mathcal{T}_{\tau} \left(\hat{c}_{\mathbf{k}\uparrow}(\tau) \hat{c}^{\dagger}_{\mathbf{k}\uparrow}(0) \right) \right\rangle \\ \mathcal{F}_{\downarrow\uparrow}(\mathbf{k},\tau) = -\left\langle \mathcal{T}_{\tau} \left(\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}(\tau) \hat{c}^{\dagger}_{\mathbf{k}\uparrow}(0) \right) \right\rangle \end{cases}$$

In frequency domain:

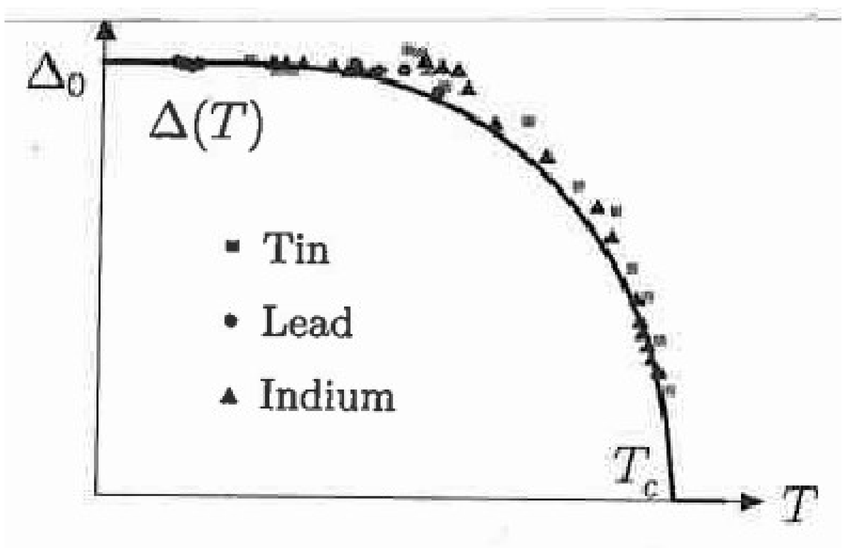
[redacted]

$$\begin{cases} \mathcal{G}_{\uparrow\uparrow}(\mathbf{k}, ik_n) = \dfrac{ik_n + \epsilon_{\mathbf{k}}}{(ik_n)^2 - (\epsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2)} \\ \mathcal{F}_{\downarrow\uparrow}(\mathbf{k}, ik_n) = \dfrac{-\Delta^{*}_{\mathbf{k}}}{(ik_n)^2 - (\epsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2)} \end{cases}$$

Self-consistency equation for the gap

$$\Delta_{\mathbf{k}} \equiv -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \langle \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} \rangle \quad \Rightarrow \quad \Delta_{\mathbf{k}} = +V \sum_{\mathbf{k}'}^{|\epsilon_{\mathbf{k}'}|<\omega_D} \mathcal{F}^*_{\downarrow\uparrow}(\mathbf{k}', \tau = 0^+)$$

Isotropic case (s-wave pairing): $\Delta_{\mathbf{k}} = \Delta(T)$



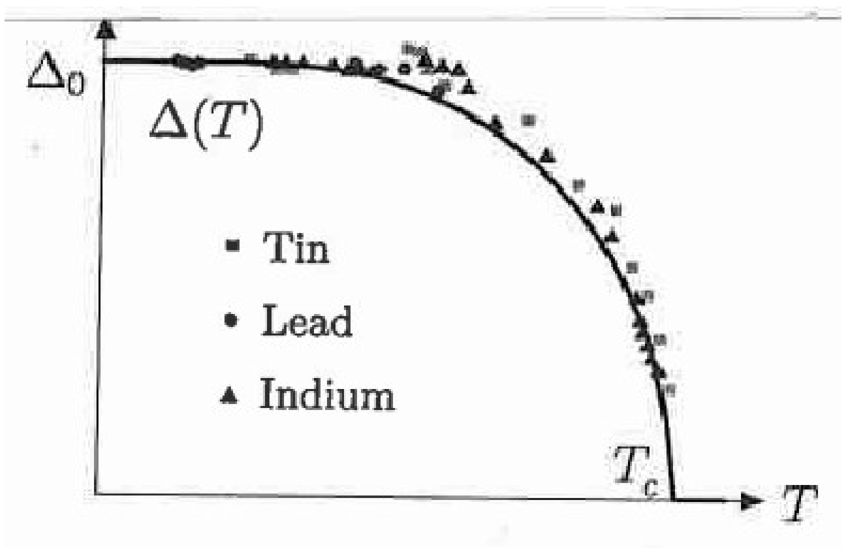
Gap equation: [redacted]

$$1 = +V\rho(\epsilon_F) \int_0^{\omega_D} d\epsilon \frac{\tanh\left(\frac{\beta}{2}\sqrt{\epsilon^2 + \Delta^2}\right)}{\sqrt{\epsilon^2 + \Delta^2}}$$

Useful limits and energy scales.

$$\left.\begin{array}{l} T \to 0 \\ V\rho(\epsilon_F) \ll 1 \end{array}\right\} \quad \Delta(T \to 0) = \Delta_0 \approx 2\omega_D e^{-1/(V\rho(\epsilon_F)))}$$

Critical temperature: $\Delta(T \to T_c) = 0^+ \qquad k_B T_c = \frac{e^\gamma}{\pi}\Delta_0 \to \frac{2\Delta_0}{k_B T_c} = 3.53$



Metal	$2\Delta_0/k_B T_c$
Tin	3.46
Lead	4.29
Indium	3.63