SC ground state: What happens beyond the instability?

- we illustrate this using ATTRACTIVE Hubbard model

$$H = \sum_{\substack{i,j \\ \sigma}} t_{ij} c^{+}_{i\sigma} c_{j\sigma} - \mu \sum_{j\sigma} c^{+}_{j\sigma} c_{j\sigma} - V_0 \sum_{j} n_{j\uparrow} n_{j\downarrow} \, , \qquad V_0 > 0$$

- since we expect Cooper pair formation at low T we perform a "mean-field decoupling of the interaction term in the pairing channel", (or Bogoliubov decoupling)

$$- n_{j\uparrow} n_{j\downarrow} = - c^{+}_{j\uparrow} c_{j\uparrow} c^{+}_{j\downarrow} c_{j\downarrow} = + c^{+}_{j\uparrow} c^{+}_{j\downarrow} c_{j\uparrow} c_{j\downarrow}$$

$$\xrightarrow{MF} \langle c^{+}_{j\uparrow} c^{+}_{j\downarrow} \rangle c_{j\uparrow} c_{j\downarrow} + c^{+}_{j\uparrow} c^{+}_{j\downarrow} \langle c_{j\uparrow} c_{j\downarrow} \rangle - \langle \quad \rangle \langle \quad \rangle$$

Define pair amplitudes:

$$\Delta_j = V_0 \langle c_{j\uparrow} c_{j\downarrow} \rangle \qquad \Delta^{*}_{j} = V_0 \langle c^{+}_{j\downarrow} c^{+}_{j\uparrow} \rangle$$

$$\boxed{H_{MF} = \sum_{\substack{i,j \\ \sigma}} (t_{ij} - \mu \delta_{ij}) c^{+}_{i\sigma} c_{j\sigma} + \sum_{j} \left(\Delta_j c^{+}_{j\uparrow} c^{+}_{j\downarrow} + \Delta^{*}_{j} c_{j\downarrow} c_{j\uparrow} - \frac{1}{V_0} |\Delta_j|^2 \right)}$$

$\uparrow$ MF Bogoliubov - de Gennes Hamiltonian

Assume spatially uniform situation $\quad \Delta_j = \Delta = \frac{1}{N}\sum_j \Delta_j$

$$\Delta = \frac{1}{N}\sum_j V_0 \langle c_{j\uparrow} c_{j\downarrow}\rangle = \frac{V_0}{N}\sum_{k,k'} \underbrace{\frac{1}{N}\sum_j e^{i\vec{r}_j\cdot(\vec{k}+\vec{k}')}}_{\delta_{\vec{k}+\vec{k}'=0}} \langle c_{k\uparrow} c_{k'\downarrow}\rangle$$

$$= \frac{V_0}{N}\sum_k \langle c_{k\uparrow} c_{-k\downarrow}\rangle$$

Cooper pair $(k\uparrow, -k\downarrow)$

$$\boxed{H_{MF} = \sum_{k,\sigma}(\varepsilon_k - \mu)\, c^+_{k\sigma} c_{k\sigma} + \sum_k \left(\Delta\, c^+_{k\uparrow} c^+_{-k\downarrow} + h.c.\right) - \frac{N}{V_0}|\Delta|^2}$$

The Nambu notation: $\quad \Psi_k = \begin{pmatrix} c_{k\uparrow} \\ c^+_{-k\downarrow} \end{pmatrix}, \quad \Psi^+_k = (c^+_{k\uparrow}, c_{-k\downarrow})$

$$H_{MF} = \sum_k \Psi^+_k \begin{pmatrix} \varepsilon_k - \mu & \Delta \\ \Delta^* & -\varepsilon_k + \mu \end{pmatrix} \Psi_k + E_0$$

- Introduce the Nambu-Gorkov Green's function

$$\hat{G}(\vec{k}, t) = -i\langle T[\Psi_k(t)\, \Psi^+_k(0)]\rangle$$

$\leftarrow$ 2×2 matrix in "Nambu space"

or $\quad \hat{G}_{\alpha\beta}(\vec{k}, t) = -i\langle T[\psi_{k\alpha}(t)\, \psi^+_{k\beta}(0)]\rangle \qquad \alpha, \beta = 1, 2$

$$\Psi_k = \begin{pmatrix} \psi_{k1} \\ \psi_{k2} \end{pmatrix}$$

- Eq. of motion for $\hat{G}$:

$$\left[\begin{aligned} i\frac{\partial}{\partial t}\hat{G}_{\alpha\beta}(\vec{k},t) = \;& \delta_{\alpha\beta}\delta(t) + (\varepsilon_p-\mu)\left[\tau^3\hat{G}(\vec{k},t)\right]_{\alpha\beta} \\ & + \Delta\left[\tau^1\hat{G}(\vec{k},t)\right]_{\alpha\beta} \end{aligned}\right]$$

- we assumed $\Delta\in\mathbb{R}$ for simplicity and used

$$[\psi^+_{p\alpha}\psi_{p\beta},\psi_{p\gamma}] = -\delta_{\alpha\gamma}\psi_{p\beta} \qquad \text{(check!)}$$

$\{\tau^1,\tau^2,\tau^3\}$ are Pauli matrices in Nambu space

- Fourier transform in time $\quad \hat{G}(\vec{k},t)\to\hat{G}(\vec{k},\omega)$

$$(\omega-\xi_k\tau^3-\Delta\tau^1)\hat{G}(\vec{k},\omega) = \mathbb{1}\,, \qquad \xi_k\equiv\varepsilon_k-\mu$$

$$\boxed{\hat{G}(\vec{k},\omega) = (\omega-\xi_k\tau^3-\Delta\tau^1)^{-1} = \frac{\omega+\xi_k\tau^3+\Delta\tau^1}{\omega^2-\xi_k^2-\Delta^2+i\varepsilon}}$$

$\boxed{\varepsilon=0^+}$

↖ Nambu-Gorkov GF for a superconductor.

⇒ Poles at $\omega=\pm\sqrt{\xi_k^2+\Delta^2}$ represent EXCITATION energies in the SC state. For $|\Delta|>0$ the minimum excitation energy is $|\Delta|$ so the spectrum of a superconductor is GAPPED

→ major prediction of the BCS theory

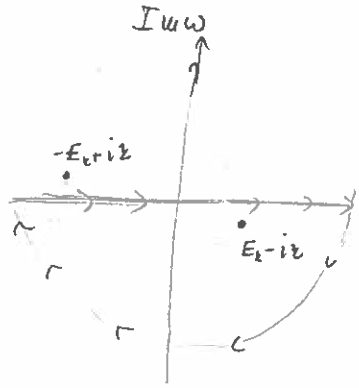
- The self-consistent gap equation

✓ check!

$$\Delta = \frac{V_0}{N}\sum_k \langle c_{k\uparrow} c_{-k\downarrow}\rangle = -i\,\frac{V_0}{N}\sum_k \frac{1}{2}\lim_{t\to 0^-} \mathrm{Tr}\left[\tau'\hat{G}(\vec{k},t)\right]$$

$$= -\frac{i}{2}\frac{V_0}{N}\sum_k \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\, e^{i\omega 0^-}\,\mathrm{Tr}\left[\tau'\,\hat{G}(\vec{k},\omega)\right]$$

$$= -\frac{i}{2}\frac{V_0}{N}\sum_k \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\, e^{i\omega 0^-}\,\frac{2\Delta}{\omega^2-\xi_k^2-\Delta^2+i\varepsilon}$$



$$= -i\,\frac{V_0}{N}\sum_k \frac{2\pi i}{2\pi}\,\frac{\Delta}{2\sqrt{\xi_k^2+\Delta^2}}$$

$$\boxed{\Delta = \frac{V_0}{2N}\sum_k \frac{\Delta}{\sqrt{\xi_k^2+\Delta^2}}}$$

← The BCS gap equation at $T=0$.

$$\frac{1}{N}\sum_k \longrightarrow \int\frac{d^3k}{(2\pi)^3} \longrightarrow \int_{-k_B\theta_D}^{k_B\theta_D} d\xi\,\mathcal{N}(\xi) \simeq \mathcal{N}(0)\int_{-k_B\theta_D}^{k_B\theta_D} d\xi$$

$$\boxed{\Delta = \frac{1}{2}V_0\,\mathcal{N}(0)\int_{-k_B\theta_D}^{k_B\theta_D} d\xi\,\frac{\Delta}{\sqrt{\xi^2+\Delta^2}}}$$

This has 2 solutions:

(i) $\Delta = 0$ "normal metal"

(ii) $\Delta \neq 0$ superconductor

integrate to obtain $\Delta \neq 0$:

$$\rightarrow \quad \mathcal{N}(0)\,V_0\,\mathrm{arcsinh}\left(\frac{k_B\theta_D}{\Delta}\right) = 1$$

$$\mathrm{arcsinh}\,x = \ln\left(x+\sqrt{x^2+1}\right) \simeq \ln 2x \quad \text{for } x \gg$$

$$\boxed{\Delta \simeq 2k_B\theta_D\, e^{-1/\mathcal{N}(0)V_0}}$$

- ## Gap equation at non-zero temperature

- We could have equally well developed the theory in terms of Matsubara GF

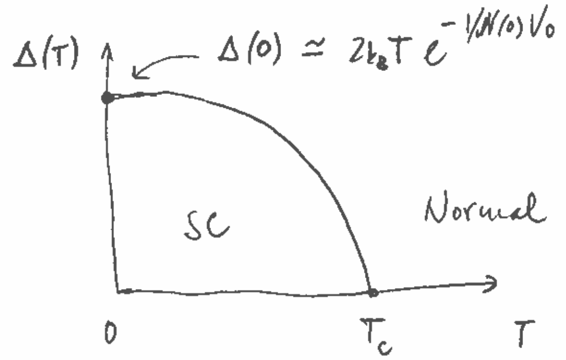
$$\hat{g}(\vec{k},\omega_n) = (i\omega_n - \xi_k \tau^3 - \Delta\tau^1)^{-1} = -\frac{i\omega_n + \xi_k\tau^3 + \Delta\tau^1}{\omega_n^2 + \xi_k^2 + \Delta^2}$$

→ gap equation at $T \neq 0$:

$$\boxed{\Delta = \frac{V_0}{2N\beta}\sum_k \sum_{\omega_n} \frac{\Delta}{\omega_n^2 + \xi_k^2 + \Delta^2} = \frac{V_0}{2}\int \frac{d^3k}{(2\pi)^3}\frac{\Delta}{E_k}\tanh\left(\tfrac{1}{2}\beta E_k\right)}$$

$$\beta = \frac{1}{k_B T}, \quad E_k = \sqrt{\xi_k^2 + \Delta^2}$$

- The gap eq can be solved numerically at arbitrary T



- We can determine the critical temperature T_c analyticaly
- at $T \to T_c^-$ we have $\Delta \to 0$, just below T_c we thus have

$$1 = V_0 \int_0^{k_B\Theta_D} d\xi \, \frac{N(\xi)}{\xi}\tanh\left(\tfrac{1}{2}\beta\xi\right)$$

$$\simeq N(0)V_0 \int_0^{k_B\Theta_D} \frac{d\xi}{\xi}\tanh\left(\tfrac{1}{2}\beta\xi\right)$$

but this is the same eq we obtained for T_c previously!

$$\rightarrow \quad \boxed{T_c \simeq 1.14\, \theta_D\, e^{-1/N(0)V_0}}$$

- It is instructive to take a ratio

$$\boxed{\frac{\Delta(0)}{k_B T_c} \simeq 1.76 \qquad \text{"the universal BCS ratio"}}$$

Observed values in simple metals:

Cd	Al	Sn	Pb
1.6	1.3-2.1	1.6	2.2

} BCS-like superconductors

high-T_c cuprates $\quad \frac{\Delta(0)}{k_B T_c} \simeq 3-6 \quad$ non-BCS

- From the gap equation one can also extract behavior of $\Delta(T)$ close to T_c:

$$\boxed{\Delta(T) \simeq 3.06\, k_B T_c \sqrt{1 - \frac{T}{T_c}}}$$