§ 6 BCS ground state $|0\rangle \equiv |FS\rangle$

$$\boxed{|\Psi_{BCS}\rangle = \prod_k (u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow})|0\rangle}$$

normalization $u_k, v_k \in \mathbb{C}$ - trial parameters

$$1 = \langle \Psi_{BCS}|\Psi_{BCS}\rangle = \langle 0|\prod_k (u_k^* + v_k^* c_{-k\downarrow} c_{k\uparrow}) \prod_{k'} (u_{k'} + v_{k'} c^\dagger_{k'\uparrow} c^\dagger_{-k'\downarrow})$$

$$= \langle 0|\prod_k \Big(|u_k|^2 + u_k^* v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} + v_k^* u_k c_{-k\downarrow} c_{k\uparrow} + |v_k|^2 \overbrace{c_{-k\downarrow} c_{k\uparrow} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}}\Big)|0\rangle =$$

$$= \prod_k (|u_k|^2 + |v_k|^2) \rightarrow \boxed{|u_k|^2 + |v_k|^2 = 1}$$

occupations of $|k\uparrow\rangle$ and $|-k\downarrow\rangle$ are maximally correlated - entangled state

$|\Psi_{BCS}\rangle$ does not conserve number of particles

$$\rightarrow \langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\rangle_{BCS} \equiv \langle \Psi_{BCS}| c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}|\Psi_{BCS}\rangle =$$

$$= \langle 0|\prod_{k'} (u_{k'}^* + \underline{v_{k'}^* c_{-k'\downarrow} c_{k'\uparrow}})\, \underline{c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}} \prod_{k''} (u_{k''} + v_{k''} c^\dagger_{k''\uparrow} c^\dagger_{-k''\downarrow})|0\rangle$$

$$= \langle 0| u_k^* v_k^* \prod_{k' \neq k} \underbrace{(|u_{k'}|^2 + |v_{k'}|^2)}_{=1} |0\rangle = u_k^* v_k^* \neq 0$$

if $u_k \neq 0$ and $v_k \neq 0$ at the same time (not $|FS\rangle$)

Hamiltonian

$$H = \sum_{k\sigma} \xi_k c^\dagger_{k\sigma} c_{k\sigma} + V_{int}, \quad \xi_k = \varepsilon_k - \mu$$

$$V_{int} = \frac{1}{N} \sum_{kk'} V_{kk'} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow}$$

$$V_{kk'} = \begin{cases} -V_0 & |\xi_k| < \hbar\omega_D,\ |\xi_{k'}| < \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

For time symmetric case $\xi_k = \xi_{-k} \rightarrow u_k = u_{-k},\ v_k = v_{-k}$

$\langle \Psi_{BCS} | H | \Psi_{BCS} \rangle =$

$= \sum_{k\sigma} \xi_k \langle 0 | \prod_q (u_q^* + v_q^* c_{-q\downarrow} c_{q\uparrow}) c_{k\sigma}^\dagger c_{k\sigma} \prod_{q'} (u_{q'} + v_{q'} c_{q'\uparrow}^\dagger c_{-q'\downarrow}^\dagger) |0\rangle$

$+ \frac{1}{N} \sum_{kk'} V_{kk'} \langle 0 | \prod_q (u_q^* + v_q^* c_{-q\downarrow} c_{q\uparrow}) c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow} \prod_{q'} (u_{q'} + v_{q'} c_{q'\uparrow}^\dagger c_{-q'\downarrow}^\dagger) |0\rangle$

$= \sum_k \xi_k \langle 0 | |v_k|^2 c_{-k\downarrow} c_{k\uparrow} c_{k\uparrow}^\dagger c_{k\uparrow} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger |0\rangle +$

$+ \sum_k \xi_k \langle 0 | |v_{-k}|^2 c_{k\downarrow} c_{-k\uparrow} c_{k\downarrow}^\dagger c_{k\downarrow} c_{-k\uparrow}^\dagger c_{k\downarrow}^\dagger |0\rangle +$

$+ \frac{1}{N} \sum_{kk'} V_{kk'} \langle 0 | v_k^* u_{k'}^* u_k v_{k'} c_{-k\downarrow} c_{k\uparrow} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger c_{-k'\downarrow} c_{k'\uparrow} c_{k'\uparrow}^\dagger c_{-k'\downarrow}^\dagger |0\rangle =$

$= \sum_k 2 \xi_k |v_k|^2 + \frac{1}{N} \sum_{kk'} V_{kk'} v_k^* u_k u_{k'}^* v_{k'} \quad = E_{BCS}[u_k, v_k]$

$E_{BCS}[u_k, v_k] \in \mathbb{R} \rightarrow$ phase of $u_k$ and $v_k$ must be the same.

Since $E_{BCS}$ is invariant with $u_k \rightarrow u_k e^{i\varphi_k}$, $v_k \rightarrow v_k e^{i\varphi_k}$

we ~~to~~ can choose all $u_k, v_k \in \mathbb{R}$.

Normalization constrain

$$u_k^2 + v_k^2 = 1 \quad \rightarrow \quad u_k = \cos\theta_k, \quad v_k = \sin\theta_k$$

Then $E_{BCS} = \sum_k 2\xi_k \sin^2\theta_k + \frac{1}{N} \sum_{kk'} V_{kk'} \sin\theta_k \cos\theta_k \sin\theta_{k'} \cos\theta_{k'} =$

$$= \sum_k \xi_k (1 - \cos 2\theta_k) + \frac{1}{N} \sum_{kk'} \frac{V_{kk'}}{4} \sin 2\theta_k \sin 2\theta_{k'}$$

$\frac{\partial E_{BCS}}{\partial \theta_q} = 2\xi_q \sin 2\theta_q + \frac{1}{N} \sum_{k'} \frac{V_{qk'}}{2} \cos 2\theta_q \sin 2\theta_{k'} +$

$+ \frac{1}{N} \sum_k \frac{V_{kq}}{2} \sin 2\theta_k \cos 2\theta_q =$

$$= 2\xi_q \sin 2\theta_q + \frac{1}{N} \sum_{k'} V_{qk'} \cos 2\theta_q \sin 2\theta_{k'} = 0$$

Let $p \to k$, and parametrize by $\Delta_k$:

$$\sin 2\theta_k =: \frac{\Delta_k}{\sqrt{\xi_k^2+\Delta_k^2}}$$

$$\cos 2\theta_k =: \frac{\xi_k}{\sqrt{\xi_k^2+\Delta_k^2}}$$

[up to $\pm$ factor, but $-$ gives higher energy]

Hence

$$2\frac{\xi_k \Delta_k}{\sqrt{\xi_k^2+\Delta_k^2}} + \frac{1}{N}\sum_{k'} V_{kk'} \frac{\xi_k \Delta_{k'}}{\sqrt{\xi_k^2+\Delta_k^2}\sqrt{\xi_{k'}^2+\Delta_{k'}^2}} = 0$$

$$\Rightarrow \boxed{\Delta_k = -\frac{1}{N}\sum_{k'} V_{kk'} \frac{\Delta_{k'}}{2\sqrt{\xi_{k'}^2+\Delta_{k'}^2}}}$$

BCS - gap equation on $\Delta_k$ - order parameter. (see later)

From this we find

$$u_k^2 = \frac{1}{2}\left(1+\frac{\xi_k}{\sqrt{\xi_k^2+\Delta_k^2}}\right)$$

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

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

relative sign of $u_k$ and $v_k$ is the sign of $\Delta_k$. The absolute sign is irrelevant due to invariance of $E_{BCS}$ by a phase $e^{i\pi}=1$.

For BCS model

$$V_{kk'} = \begin{cases} -V_0 \\ 0 \end{cases}$$

$$\Delta_k = \begin{cases} -\frac{1}{N}\sum_{k'}^{|\xi_{k'}|<\omega_D} (-V_0)\frac{\Delta_{k'}}{2\sqrt{\xi_{k'}^2+\Delta_{k'}^2}} & |\xi_k|<\omega_D \\ 0 & \text{otherwise} \end{cases}$$

$$\Rightarrow \Delta_k = \begin{cases} \Delta_0 > 0 & \text{for } |\xi_k|<\omega_D \\ 0 & \text{otherwise} \end{cases}$$

$$\Delta_0 = \frac{V_0}{N} \sum_{\substack{k' \\ |\xi_{k'}|<\omega_D}} \frac{\Delta_0}{2(\xi_{k'}^2+\Delta_0^2)^{1/2}}$$

$$1 = V_0 \int_{-\omega_D}^{\omega_D} d\xi \, \rho(\xi+\mu) \frac{1}{2\sqrt{\xi^2+\Delta_0^2}}$$

$\uparrow$ DOS per spin, per unit cell

$$1 = V_0 \, \rho(\varepsilon_F) \, \frac{1}{2} \int_{-\omega_D}^{\omega_D} \frac{d\xi}{\sqrt{\xi^2+\Delta_0^2}} = V_0 \, \rho(\varepsilon_F) \, \mathrm{arcsinh}\left(\omega_D/\Delta_0\right)$$

$$\Rightarrow \boxed{\Delta_0 = \omega_D \frac{1}{\sinh\left(\frac{1}{V_0 \rho(\varepsilon_F)}\right)} \simeq 2\omega_D \, e^{-\frac{1}{V_0 \rho(\varepsilon_F)}}}$$

~~...~~ the same as binding energy for Cooper pair

$$E_b = \cancel{\ldots} 2\omega_D \, e^{-\frac{1}{V_0 \rho(\varepsilon_F)}}$$

## Ground state energy

$$E_{BCS} = \sum_k 2\xi_k \frac{1}{2}\left(1 - \frac{\xi_k}{\sqrt{\xi_k^2+\Delta_k^2}}\right) + \frac{1}{N}\sum_{kk'} V_{kk'} \frac{\Delta_k \Delta_{k'}}{4\sqrt{\xi_k^2+\Delta_k^2}\sqrt{\xi_{k'}^2+\Delta_{k'}^2}} =$$

$$= N \int_{-\infty}^{-\omega_D} d\xi \, \rho(\mu+\xi) \, 2\xi + N \int_{-\omega_D}^{\omega_D} d\xi \, \rho(\mu+\xi) \, \xi \left(1 - \frac{\xi}{\sqrt{\xi^2+\Delta_0^2}}\right) +$$

$$+ N \int_{\omega_D}^{\infty} d\xi \, \rho(\mu+\xi) \, 0 + N \int_{-\omega_D}^{\omega_D} d\xi \int_{-\omega_D}^{\omega_D} d\xi' \, \rho(\mu+\xi) \rho(\mu+\xi') (-V_0) \frac{\Delta_0^2}{\sqrt{\xi^2+\Delta_0^2}\sqrt{\xi'^2+\Delta_0^2}}$$

$$\simeq 2N \int_{-\infty}^{-\omega_D} d\xi \, \rho(\mu+\xi) \, \xi + N \rho(\varepsilon_F) \left(-\omega_D \sqrt{\omega_D^2+\Delta_0^2} + \Delta_0^2 \, \mathrm{arcsinh}\, \omega_D/\Delta_0\right) -$$

$$- N V_0 \, \rho^2(\varepsilon_F) \, \Delta_0^2 \, \mathrm{arcsinh}^2 \, \omega_D/\Delta_0$$

with the gap equation $\quad 1 = V_0 \, \rho(\varepsilon_F) \, \mathrm{arcsinh}\, \omega_D/\Delta_0$

we get

$$E_{BCS} \simeq 2N \int_{-\infty}^{-\omega_D} d\xi\, \rho(\mu+\xi)\,\xi - N\rho(\xi_F)\,\omega_D\sqrt{\omega_D^2+\Delta_0^2}$$

Condensation energy

$$\Delta E_{BCS} = E_{BCS} - \lim_{\Delta_0\to 0} E_{BCS} = -N\rho(\xi_F)\,\omega_D\sqrt{\omega_D^2+\Delta_0^2} + N\rho(\xi_F)\,\omega_D^2 \underset{\Delta_0 \ll \omega_D}{\simeq}$$

$$\simeq -N\rho(\xi_F)\,\omega_D^2\sqrt{1+\left(\Delta_0/\omega_D\right)^2} + N\rho(\xi_F)\,\omega_D^2 \simeq -\frac{1}{2}N\rho(\xi_F)\,\Delta_0^2 < 0$$

For type I SC we get $H_c \simeq \sqrt{4\pi \frac{N}{V}\rho(\xi_F)}\,\Delta_0$