Phys 726 – Lecture 23

<u>Recap</u>: We derived the BCS Hamiltonian as a mean field decomposition (in the "pairing channel") of the attractive Hubbard model

$$\to \quad \hat{H} = \sum_{\vec{k},\alpha} \varepsilon_{\vec{k}} c^\dagger_{k\alpha} c_{k\alpha} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \qquad (U<0)$$

$$= \sum_{\vec{k},\alpha} \varepsilon_{\vec{k}} c^\dagger_{k\alpha} c_{k\alpha} - |U| \hat{A}^\dagger \hat{A}$$

where $\hat{A} = \sum_{\vec{k}} c_{+k,\downarrow} c_{-k,\uparrow}$

$$\hat{A}^\dagger = \sum_{\vec{k}} c^\dagger_{-\vec{k},\uparrow} c^\dagger_{+k,\downarrow}$$

→ Approximating the interaction by

$$-|U| \hat{A}^\dagger \hat{A} \simeq -|U| \left(\hat{A}^\dagger \langle \hat{A} \rangle + \langle \hat{A} \rangle^* \hat{A} - \langle \hat{A} \rangle \right)$$

$$= \Delta \hat{A}^{+} + \Delta^{*} \hat{A} + \frac{|\Delta|^2}{|U|}$$

and the self-consistency condition $\Delta = -|U| \langle \hat{A} \rangle$.

→ Leads to

$$\hat{H}_{BCS} = \sum_k \Big\{ \varepsilon_k c^{\dagger}_{k\uparrow} c_{k\uparrow} + \varepsilon c^{\dagger}_{k\downarrow} c_{k\downarrow} + \Delta^{*} c_{k\downarrow} c_{-k\uparrow} + \Delta c^{\dagger}_{-k\uparrow} c^{\dagger}_{k\downarrow} + \text{const} \Big\} - \mu \hat{N}$$

$$= \sum_k \begin{pmatrix} c^{\dagger}_{k\uparrow} & c_{-k\downarrow} \end{pmatrix} \begin{pmatrix} \varepsilon_k - \mu & \Delta \\ \Delta^{*} & \mu - \varepsilon_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^{\dagger}_{-k\downarrow} \end{pmatrix} + \text{const.}$$

↑ 2×2 structure

$$= (\varepsilon_k - \mu)\sigma^z + (\mathrm{Re}\,\Delta)\sigma^x + (\mathrm{Im}\,\Delta)\sigma^y$$

$$= \sum_k \begin{pmatrix} c^{\dagger}_{k\uparrow} & c_{-k\downarrow} \end{pmatrix} \underbrace{(\varepsilon_k - \mu, \mathrm{Re}\,\Delta, \mathrm{Im}\,\Delta) \cdot \vec{\sigma}}_{\text{"Isospin" representation}} \begin{pmatrix} c_{k\uparrow} \\ c^{\dagger}_{-k\downarrow} \end{pmatrix}$$

$$= \sum_k E_k \begin{pmatrix} c^\dagger_{k\uparrow} & c_{-k\downarrow} \end{pmatrix} \left(\frac{\varepsilon_k - \mu}{E_k}, \frac{\mathrm{Re}\,\Delta}{E_k}, \frac{\mathrm{Im}\,\Delta}{E_k} \right) \cdot \vec{\sigma} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}$$

define unit vector $\vec{l}_k$

with $E_k = \sqrt{(\varepsilon_k - \mu)^2 + (\mathrm{Re}\,\Delta)^2 + (\mathrm{Im}\,\Delta)^2}$

$$= \sqrt{(\varepsilon_k - \mu) + |\Delta|^2}$$

$$= \sum_k E_k \begin{pmatrix} c^\dagger_{k\uparrow} & c_{-k\downarrow} \end{pmatrix} \vec{l}_k \cdot \vec{\sigma} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}$$

diagonalizing this requires that we perform a rotation in spin space that aligns the matrix with σ_z

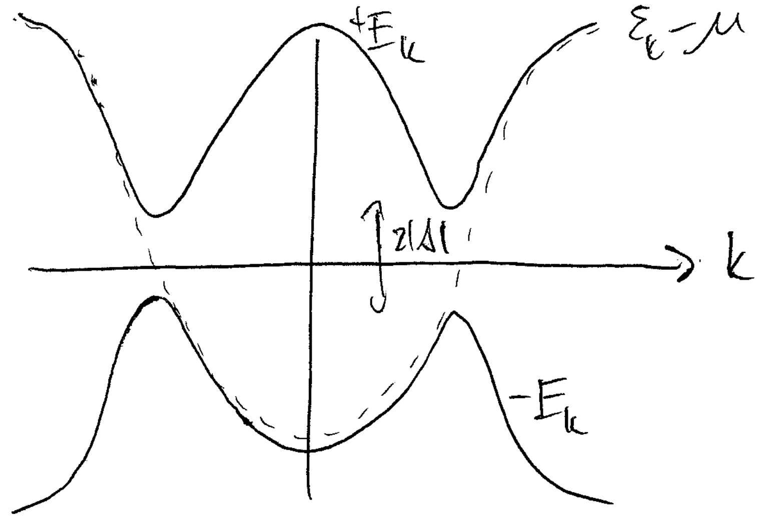
i.e. let $\begin{pmatrix} \gamma_{k+} \\ \gamma_{k-} \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}$

k-dependent unitary transformation

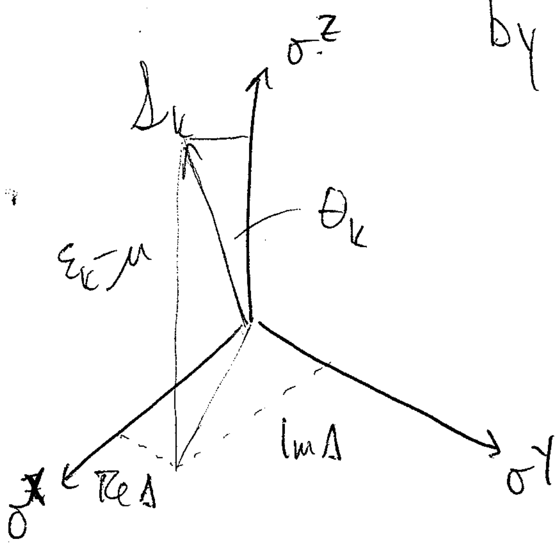
$$= \sum_k E_k \begin{pmatrix} \gamma^\dagger_{k+} & \gamma^\dagger_{k-} \end{pmatrix} \underbrace{U^\dagger_k \vec{l}_k U_k}\cdot \vec{\sigma} \begin{pmatrix} \gamma_{k+} \\ \gamma_{k-} \end{pmatrix}$$

$$= \sum_k E_k \left(\gamma_{k+}^\dagger \gamma_{k+} - \gamma_{k-}^\dagger \gamma_{k-} \right)$$

$$= \sum_k \sum_{n=\pm} n E_k \gamma_{kn}^\dagger \gamma_{kn}$$



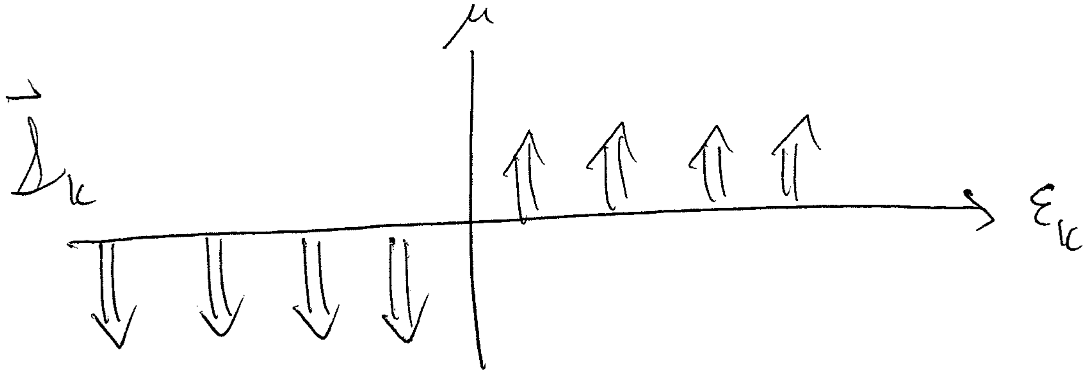
* The isospin direction is tilted away from σ^z by an angle $\theta_k = \cos^{-1} \frac{\varepsilon_k - \mu}{E_k}$



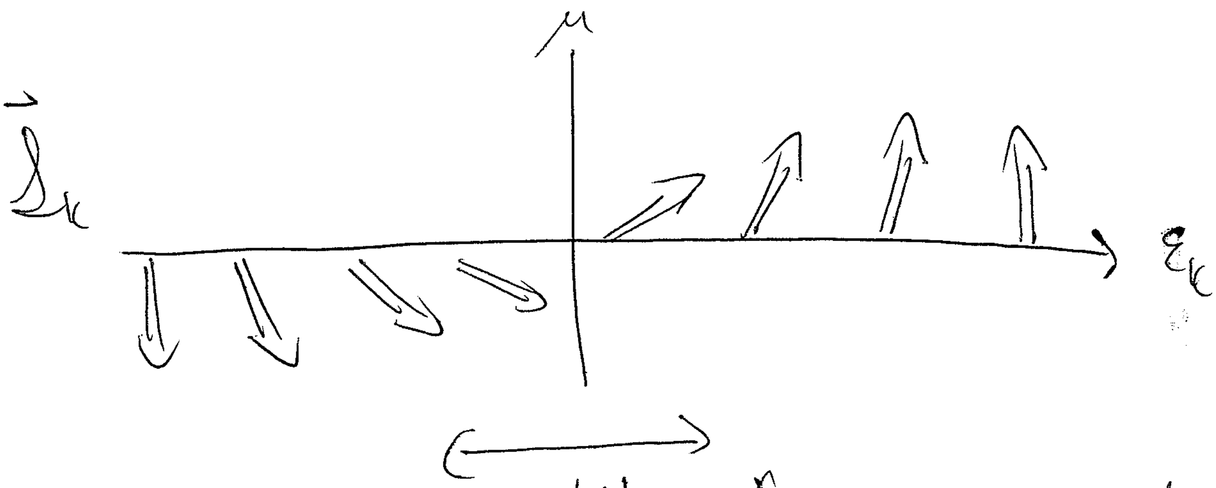
→ if we choose Δ real then

$$\vec{s}_k = (\sin\theta_k, 0, \cos\theta_k),$$

which is a vector that slowly switches sign across the chemical potential



when $\Delta = 0$ (conventional metal) there is an abrupt reversal in the pseudospin across the Fermi surface



in a superconductor this reversal is smeared out

→ what does this mean? Let's go back to the Hamiltonian

$$\hat{H}_{BCS} = \sum_k E_k \left(c^\dagger_{k\uparrow} \;\; c_{-k\downarrow} \right) \vec{S}_k \cdot \vec{\sigma} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}$$

$$= \sum_k E_k \vec{\hat{d}}_k \cdot (c^\dagger_{k\uparrow} \; c_{-k\downarrow}) \vec{\sigma} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}$$

$$= - \sum_k \vec{B}_k \cdot \hat{\psi}^\dagger_k \vec{\sigma} \hat{\psi}_k$$

This is just the model of a "spin" $\hat{\psi}^\dagger_k \vec{\sigma} \hat{\psi}_k$ Zeeman coupled to a (k-dependent) field $B_k = -E_k \hat{d}_k$. So the ground state $|\psi_{BCS}\rangle$ must be the fully polarized state

$$\langle \psi_{BCS} | \hat{\psi}^\dagger_k \vec{\sigma} \hat{\psi}_k | \psi_{BCS} \rangle \equiv \langle \hat{\psi}_k \vec{\sigma} \psi_k \rangle = - \vec{\hat{d}}_k$$

i.e. $$\left\langle (c^\dagger_{k\uparrow} \; c_{-k\downarrow}) \vec{\sigma} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} \right\rangle = - (\sin\theta_k , 0 , \cos\theta_k)$$

$$= - \left(\frac{\mathrm{Re}\,\Delta}{\sqrt{(\varepsilon_k - \mu)^2 + |\Delta|^2}} , 0 , \frac{\varepsilon_k - \mu}{\sqrt{(\varepsilon_k - \mu)^2 + |\Delta|^2}} \right)$$

→ In the normal metal ($\Delta = 0$)

$$\left\langle (c^{\dagger}_{k\uparrow}\ c_{-k\downarrow})\,\vec{\sigma}\begin{pmatrix} c_{k\uparrow} \\ c^{\dagger}_{-k\downarrow}\end{pmatrix}\right\rangle = -\left(0,\ 0,\ \frac{\varepsilon_k - \mu}{|\varepsilon_k - \mu|}\right)$$

$$= -\left(0,\ 0,\ \mathrm{sgn}(\varepsilon_k - \mu)\right)$$

Only the third component survives:

$$\left\langle (c^{\dagger}_{k\uparrow}\ c_{-k\downarrow})\,\sigma^z\begin{pmatrix} c_{k\uparrow} \\ c^{\dagger}_{-k\downarrow}\end{pmatrix}\right\rangle = \langle c^{\dagger}_{k\uparrow} c_{k\uparrow} - c_{-k\downarrow} c^{\dagger}_{-k\downarrow}\rangle$$

$$= \langle c^{\dagger}_{k\uparrow} c_{k\uparrow}\rangle + \langle c^{\dagger}_{k\downarrow} c_{k\downarrow}\rangle - 1 = \begin{cases} +1 & \varepsilon_k < \mu \\ -1 & \varepsilon_k > \mu \end{cases}$$

$$\Rightarrow \quad \langle \hat{n}_{k\uparrow}\rangle + \langle \hat{n}_{k\downarrow}\rangle = \begin{cases} 2 & \text{if } \varepsilon_k < \mu \\ 0 & \text{if } \varepsilon_k > \mu \end{cases}$$

a sharp Fermi surface, as expected.

But in a superconductor $2\langle n_k\rangle = 1 - \dfrac{\varepsilon_k - \mu}{\sqrt{(\varepsilon_k - \mu)^2 + |\Delta|^2}}$

BCS Ground State

* Let's make use of the isospin notation

$$|\Downarrow_k\rangle = |n_k = 0\rangle \quad \text{(angle zero)}$$

$$|\Uparrow_k\rangle = |n_k = 2\rangle = c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} |0\rangle \quad \text{(angle } \pi\text{)}$$

→ Intermediate angles are produced by rotation

$$|\theta_k\rangle = e^{-i\frac{\theta_k}{2}\hat{\psi}^{\dagger}_k \sigma^y \psi_k} |\Downarrow_k\rangle$$

$$= \left(\cos\frac{\theta_k}{2} - i\sin\frac{\theta_k}{2}\hat{\psi}^{\dagger}_k \sigma^y \hat{\psi}_k\right)|\Downarrow_k\rangle$$

$$= \cos\frac{\theta_k}{2}|\Downarrow_k\rangle - \sin\frac{\theta_k}{2}|\Uparrow_k\rangle$$

where $\cos^2\frac{\theta_k}{2} = \frac{1}{2}\left(1 + \cos\frac{\theta_k}{2}\right) = \frac{1}{2}\left(1 + \frac{\epsilon_k - \mu}{E_k}\right)$

and $\sin^2\frac{\theta_k}{2} = \frac{1}{2}\left(1 - \cos\frac{\theta_k}{2}\right) = \frac{1}{2}\left(1 - \frac{\epsilon_k - \mu}{E_k}\right)$

→ Alternatively, we can write

$$|\theta_k\rangle = \left(\cos\frac{\theta_k}{2} - \sin\frac{\theta_k}{2}\, c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|vac\rangle$$

$$\sim \left(1 - \tan\frac{\theta_k}{2}\, c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|vac\rangle$$

so that the (unnormalized) wave function is

$$|\Psi_{BCS}\rangle = \prod_k |\theta_k\rangle = \prod_k \left(1 + \tan\frac{\theta_k}{2}\, c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|vac\rangle$$

* The BCS state is <u>not</u> a state of definite particle number; it's clearly not an eigenstate of

$$\hat{N} = \sum_{i\alpha} c^\dagger_{i\alpha} c_{i\alpha} = \sum_k \left(c^\dagger_{k\uparrow} c_{k\uparrow} + c^\dagger_{k\downarrow} c_{k\downarrow}\right)$$

→ $|\Psi_{BCS}\rangle$ is an example of what we call a <u>coherent state</u>

→ Note that the pair creation operator cannot act twice

$$(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow})^2 = c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}$$

$$= -\cancel{(c^\dagger_{k\uparrow})^2}^{\,0} \cancel{(c^\dagger_{-k\downarrow})^2}^{\,0}$$

So we can write

$$1 + \tan\frac{\theta_k}{2} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} = \exp\left(\tan\frac{\theta_k}{2} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)$$

and

$$|\psi_{BCS}\rangle = \prod_k \left(1 + \tan\frac{\theta_k}{2} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\right)|vac\rangle$$

$$= \exp\Big(\underbrace{\sum_k \tan\frac{\theta_k}{2} c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}}_{b^\dagger}\Big)|vac\rangle$$

$b^\dagger$ = bosonic pair operator that condenses in the superconducting state

→ BCS state has an indefinite number of particles; it's a linear combination

$$|\psi_{BCS}\rangle = e^{b^\dagger}|vac\rangle$$
$$= \sum_{n=0}^{\infty} \frac{1}{n!} \underbrace{(b^\dagger)^n |vac\rangle}_{\text{state with } n \text{ Cooper pairs}}$$

→ In the ground state it costs no energy to add an electron pair

* Let's return to our assumption that Δ is real

→ recall that $\Delta = -|U| \sum_k \langle c_{k\downarrow} c_{-k\uparrow} \rangle$,

so if we perform a phase rotation (global)

$c^\dagger_{k\alpha} \to e^{i\theta} c^\dagger_{k\alpha}$ then $\sum_\alpha c^\dagger_{k\alpha} c_{k\alpha}$ is invariant but $\Delta \to e^{-2i\theta}\Delta$.

→ the BCS state changes according to

$$|\psi_{BCS}\rangle = \prod_k \left(1 + e^{i2\theta} \tan\frac{\theta_k}{2} c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger\right) |vac\rangle$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} e^{i2n\theta} (b^\dagger)^n |vac\rangle$$

number of electron pairs

→ the number operator acting on this gives

$$\hat{N} |\psi_{BCS}\rangle = \sum_n \frac{1}{n!} (2n) e^{i2n\theta} (b^\dagger)^n |vac\rangle$$

$$= \sum_n \frac{1}{n!} \left(-i \frac{d}{d\theta}\right) (b^\dagger)^n |vac\rangle$$

$$= -i \frac{d}{d\theta} |\psi_{BCS}\rangle$$

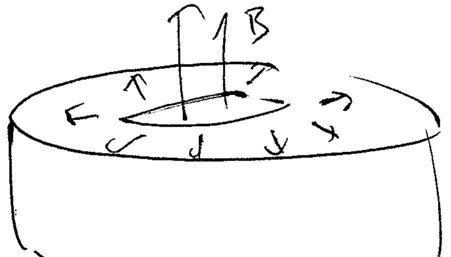
* In this context, we identify the number operator as $N = -i\frac{d}{d\theta}$,

which is to same that particle number and the phase angle are complementary variables

→ $[N, \theta] = 1$ in exactly the way that $[x, p] = \hbar$ is simple quantum mechanics

→ We have an uncertainty relation
$\Delta\theta \Delta N \gtrsim 1$

→ The BCS state is one of well-defined phase but indeterminate number
$(\Delta\theta \to 0, \Delta N \to \infty)$



This phase coherence manifests itself in many ways: e.g. flux quantization