SHANGHAI JIAO TONG UNIVERSITY
LECTURE 6
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BCS theory ($T = 0$)

Model: same as in Cooper problem. *i.e.* Sommerfeld model plus weak attraction,

$$V(r) = V_0 \delta(\boldsymbol{r}) \quad \text{(will be mostly interested in } V_0 < 0\text{)}$$

We keep the upper cutoff ϵ_c but now want to treat Fermi sea properly.

In Cooper problem, pair forms in spin singlet state with COM at rest, *i.e.* single-electron state $|\boldsymbol{k}, \uparrow\rangle$ is paired with $|-\boldsymbol{k}, \downarrow\rangle$. Let's assume this also holds in the realistic (many-body) case.

Crucial trick: work in terms not of behavior of individual electrons, but of occupation of states. Because of Pauli principle, the pair of states $(|\boldsymbol{k}\uparrow\rangle, |-\boldsymbol{k}\downarrow\rangle)$ has only four possible states of occupation: (4D Hilbert space)

$\lvert\mathbf{0},\mathbf{0}\rangle_k$	$\lvert\mathbf{1},\mathbf{1}\rangle_k$	$\lvert\mathbf{1},\mathbf{0}\rangle_k$	$\lvert\mathbf{0},\mathbf{1}\rangle_k$
↑	↑	↑	↑
both empty	both occupied	$\boldsymbol{k}\uparrow$ occupied, $-\boldsymbol{k}\downarrow$ empty	$\boldsymbol{k}\uparrow$ empty, $-\boldsymbol{k}\downarrow$ occupied

Guided by Cooper's solution, neglect for the moment $|1,0\rangle$ and $|0,1\rangle$. Then the wave function of the pair of states $|\boldsymbol{k}\uparrow, -\boldsymbol{k}, \downarrow\rangle$ is

$$\Phi_k = u_k|00\rangle_k + v_k|11\rangle_k \quad \text{with} \quad \underbrace{|u_k|^2 + |v_k|^2 = 1}_{\text{normalization}}$$

and the groundstate of the whole system is

$$\Psi = \prod_k \Phi_k$$

Note:

(a) The many-body wave function Ψ does not correspond to a definite total number of particles! In fact it is of the form

$$\Psi = \sum_N C_N \, \Psi_N$$

(However, possible to project off a definite$-N$ state if we need to).

In any case, we must choose the v_k's so that

$$\langle N \rangle = 2 \sum_k |v_k|^2 = N$$

⇐ actual number of electrons in system

(b) Normal GS is special case, with

$$u_k = 0, v_k = 1 \quad |\boldsymbol{k}| < k_F$$
$$u_k = 1, v_k = 0 \quad |\boldsymbol{k}| > k_F$$

(in this case N is definite)

(c) Can always take u_k real without loss of generality.

A useful way of visualizing BCS GSWF: Anderson "pseudospin" representation.

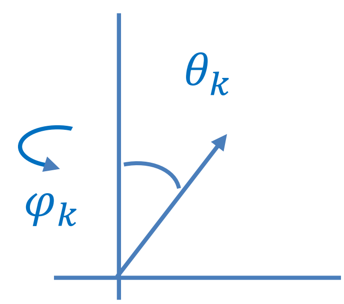
Consider specific pair of states $(\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow) \equiv \boldsymbol{k}$ and think of states $|11\rangle$ and $|00\rangle$ as analogous to 2 states $(\sigma_z = \pm 1)$ of a spin-1/2 particle. Then the superposition $\Phi_k \equiv |u_k\rangle|00\rangle + v_k|11\rangle$ corresponds to the "spin" being oriented (partially) in the xy-plane $\Rightarrow$ described by angles θ_k, φ_k.

Quantitatively:

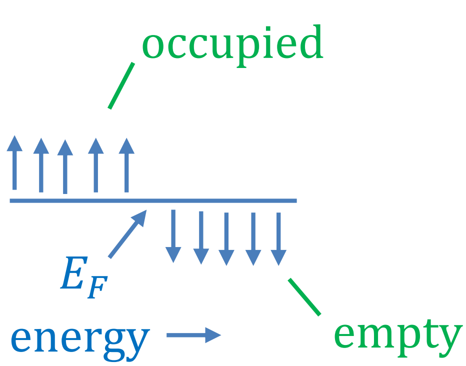
$$\langle\sigma_{zk}\rangle = |v_k|^2 - u_k^2 = \cos\theta_k$$

$$\langle\sigma_{xk}\rangle = 2Re(u_k v_k^*) = \sin\theta_k \cos\varphi_k$$

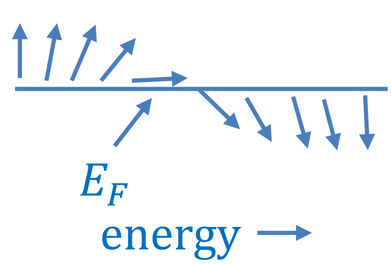
$$\langle\sigma_{yk}\rangle = 2Im(u_k v_k^*) = \sin\theta_k \sin\varphi_k$$



For simple BCS case in equilibrium, possible without loss of generality to choose all v_k as well as u_k real $\Rightarrow$ "spins" lie in xz-plane. ($\langle\sigma_{xk}\rangle = \sin\theta_k$)



N state
$(T = 0)$



S state

Q: what determines values of u_k, v_k for physical GS?

A: Energetics! Because N not definite, must minimize not $\langle \hat{H} \rangle$ but

$$\underset{\substack{\uparrow \\ \text{chemical potential}}}{\langle \hat{H} - \mu \hat{N} \rangle}$$

with μ fixed either by leads or by condition $\langle \hat{N} \rangle = N_{\text{true}}$

Kinetic energy contribution:

$$\langle \hat{T} \rangle = 2 \sum_k \underbrace{\left(\frac{\hbar^2 k^2}{2m} - \mu \right)}_{\epsilon_k} \hat{n}_k = \sum_k (2\epsilon_k |v_k|^2)$$

Potential energy: tricky!

Pauli principle $\Rightarrow$ can only scatter into pair state $\boldsymbol{k}$ if it is empty, *i.e.* $|0,0\rangle_k$, or out of it if it is full, $|1,1\rangle_k$. So for a given process $(\boldsymbol{k}\uparrow, -\boldsymbol{k}\downarrow) \Rightarrow |\boldsymbol{k}'\uparrow, -\boldsymbol{k}'\downarrow\rangle$ the contribution to $\langle \hat{V} \rangle$ is

$$\langle \hat{V} \rangle_{k \to k'} = \left(\psi_f, \hat{V} \psi_{in} \right) = V_0 \times \text{amplitude for } (|1,1\rangle_k; |0,0\rangle_{k'}) \times$$

$$\text{amplitude* for } (|0,0\rangle_k; |1,1\rangle_{k'})$$

$$= V_0 v_k u_{k'} \cdot u_k v_{k'}^* \equiv V_0 (u_k v_k) \cdot (u_{k'} v_{k'}^*)$$

Hence

$$\langle \hat{H} - \mu \hat{N} \rangle = \sum_k 2\epsilon_k |v_k|^2 + V_0 \sum_{kk'} (u_k v_k)(u_{k'} v_{k'}^*)$$

must minimize w.r.t. $\{u_k v_k\}$ subject to $|u_k|^2 + |v_k|^2 = 1$.

In Anderson pseudospin representation,

$$\langle \sigma_{zk} \rangle = 2|v_k|^2 - 1 \,,\, \langle \sigma_{xk} \rangle = 2 u_k v_k^*$$

$\Rightarrow$ apart from constant, $\left(\sum_k \epsilon_k \right)$

$$\langle \hat{H} - \mu \hat{N} \rangle = \sum_k \epsilon_k \langle \sigma_{zk} \rangle + \frac{1}{4} V_0 \sum_{kk'} \langle \sigma_{xk} \rangle \langle \sigma_{xk'} \rangle$$

Let's define a quantity

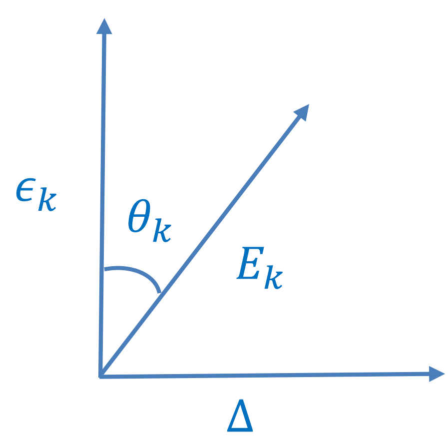
$$\Delta \equiv V_0 \sum_{k'} \langle \sigma_{xk'} \rangle / 2$$

then spin k sits in "magnetic field"

$$\mathcal{H} = -\epsilon_k \hat{\boldsymbol{z}} + \Delta \hat{\boldsymbol{x}}$$

of magnitude

$$E_k \equiv \left(\epsilon_k^2 + |\Delta|^2 \right)^{1/2}$$



Since in equilibrium the spin points along the (total) field, this gives

$$v_k^2 - u_k^2 = \cos\theta_k = -\epsilon_k/E_k\ ,$$

$$u_k v_k = \frac{1}{2}\sin\theta_k = \Delta/2E_k \quad (\text{and } u_k^2 + v_k^2 = 1)$$

with the solution

$$u_k = \left(\frac{1}{2}(1+\epsilon_k/E_k)\right)^{1/2} \qquad v_k = \left(\frac{1}{2}(1-\epsilon_k/E_k)\right)^{1/2}$$

We still have to fix Δ. Since $\langle\sigma_{xk\prime}\rangle = \sin\theta_{k\prime} = \Delta/E_{k\prime}$, df. of Δ gives

$$\Delta = -V_0 \sum_{k\prime} \Delta/2E_{k\prime}$$

or in the more general case when matrix element for scattering $(k\uparrow, -k\downarrow) \to (k'\uparrow, -k'\downarrow)$ is $V_{kk\prime}$,

$$\Delta_k = -\sum_{k\prime} V_{kk\prime}\,\Delta_{k\prime}/2E_{k\prime} \qquad \left(E_k \equiv \epsilon_k^2 + |\Delta_k|^2\right)^{1/2}$$

↑

BCS gap equation

In original BCS model ($V_{kk'} = V_O$, with cutoff $\pm\,\epsilon_c$), gap equation reduces to

$$1 = -\frac{1}{2} V_O \sum_k \left(\epsilon_k^2 + |\Delta|^2\right)^{-1} = -\tfrac{1}{4} V_O \tfrac{dn}{d\epsilon} \int_{-\epsilon_c}^{\epsilon_c} \frac{d\epsilon'}{\left(\epsilon'^2 + |\Delta|^2\right)^{1/2}}$$

which has no solution for $V_O > 0$ (repulsion). For $V_O < 0$ (attraction)

$$1 = \frac{1}{2} |V_O| \frac{dn}{d\epsilon} \sinh^{-1}(\epsilon_c/\Delta) \Longrightarrow \Delta = \epsilon_c / \sinh\left(\frac{1}{2}|V_O|\left(\frac{dn}{d\epsilon}\right)\right)^{-1}$$

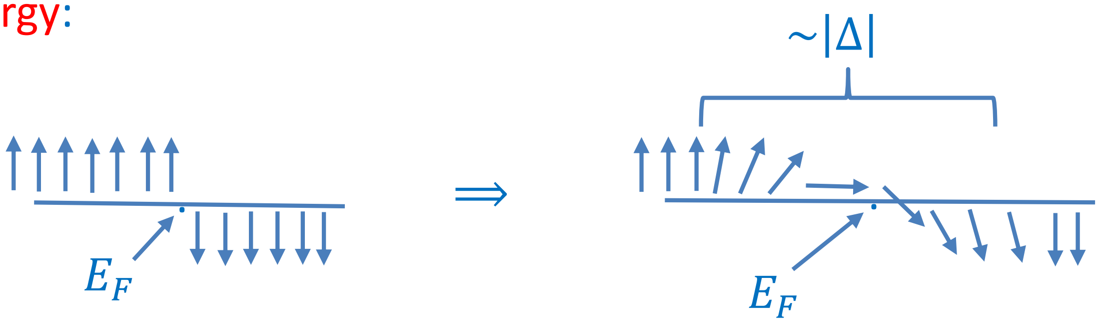
$$\approx 2\epsilon_c exp - 1/\frac{1}{2}|V_O|\frac{dn}{d\epsilon}$$

(often written
$\Delta = 2\epsilon_c exp - 1/N(0)|V|$

$\equiv \frac{1}{2}\frac{dn}{d\epsilon}$)

So: in S state at $T = O$, Anderson pseudospins are

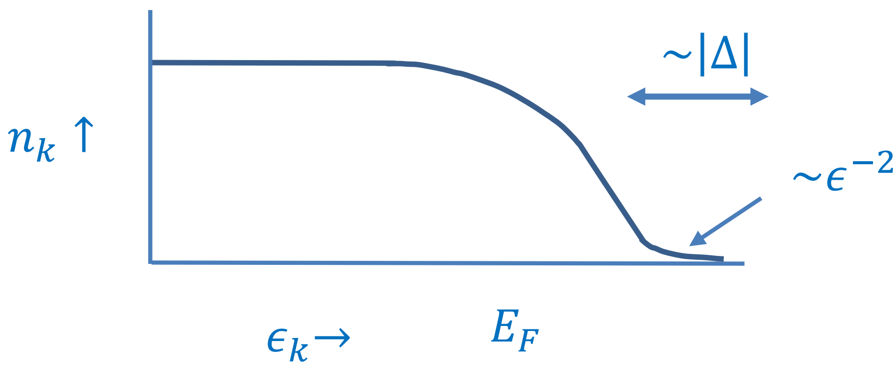
tilted away from *z*-axis over an energy range $\sim|\Delta|$ around Fermi energy:



i.e. state of pair ($k\uparrow$, $-k\downarrow$) is a coherent quantum superposition of $|0, 0\rangle_k$ and $|1, 1\rangle_k$

Two important quantities:

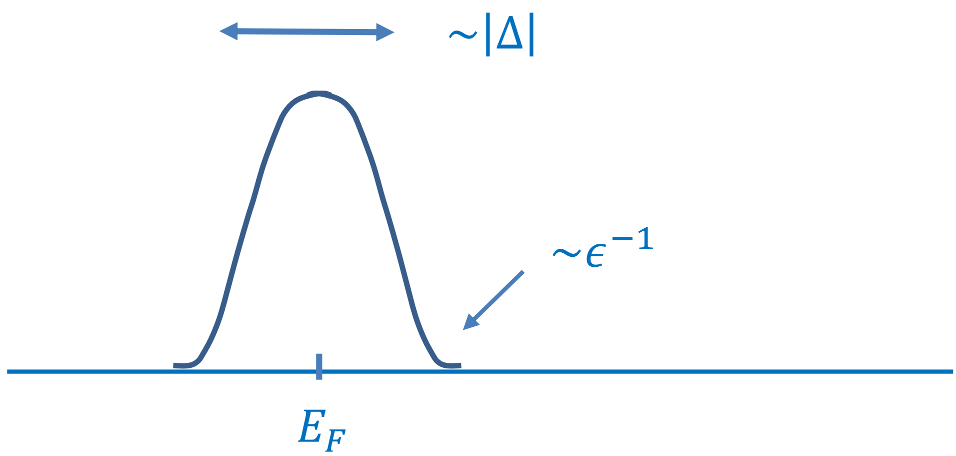
(a) Occupation of single-electron states:



(note similarity to thermal smearing – but tails more extensive $\sim\epsilon^{-2}$)

(b) The quantity

$$F_k \equiv u_k v_k^* = \frac{1}{2}\langle\sigma_{xk}\rangle = \Delta/2E_k$$



Significance of F_k(or its Fourier transform $F(\boldsymbol{r})$):

consider more general model, so that

$$\langle V \rangle_{BCS} = \sum_{kk'} V_{kk'} F_k F^*_{k'}$$

If we define $F.T.$ by

$$F(\boldsymbol{r}) \equiv \frac{1}{\sqrt{V}} \sum_k F_k \exp i\boldsymbol{k} \cdot \boldsymbol{r}$$

then

$$\langle V \rangle_{BCS} = \int V(r) |F(\boldsymbol{r})|^2 \boldsymbol{dr}$$

Compare for problem of 2 particles in free space

$$\langle V \rangle_{2p} = \int V(r) |\psi(r)|^2 dr$$

Hence, at least for the purposes of considering effects of pairing

$F(\boldsymbol{r})$ plays role of Cooper-pair wave function

(and the quantity

$$\int |F(r)|^2 dr = \sum_k |F_k|^2 \sim \frac{dn}{d\epsilon} \int d\epsilon\, |\Delta|^2/(\epsilon^2 + |\Delta|^2) \sim N\, \Delta/E_F$$

plays the role of "number of Cooper-pairs".)

General structure of $F(\boldsymbol{r})$:

$$F(r) \sim \Delta \sum_k (2E_k)^{-1} \exp i\boldsymbol{k}\cdot\boldsymbol{r}$$

If we smooth the cutoff at $\pm\epsilon_c$, then for $r \gg k_F^{-1}, v_F/\epsilon_c$, the form of F is

$$F(r) \cong \frac{1}{2}\Delta\frac{dn}{d\epsilon}\cdot\frac{\sin k_F r}{k_F r} exp - r/\xi' \qquad \xi' \equiv \frac{\hbar v_F}{2^{1/2}|\Delta|}$$

wave function of 2 free particles at Fermi energy

Thus, pair wave function is "bound" in coordinate space, with "radius" $\sim\hbar v_F/|\Delta|$ (thus exponentially large for $|V_0| \to 0$)

in practice, $\xi' \sim 10^3 - 10^4$ Å for "classical" superconductors hence, $\sim 10^9$ electrons within pair radius – strongly collective effect.

Condensation energy of BCS state ($T = 0$):
using above formulae, can calculate for arbitrary Δ

$$\langle \hat{T} \rangle = N(0)\Delta^2 \left(\ell n \left(\frac{2\epsilon_c}{\Delta} \right) - \frac{1}{2} \right)$$

$$\left(N(0) \equiv \frac{1}{2} \left(\frac{dn}{d\epsilon} \right) \right)$$

$$\langle \hat{V} \rangle = -V_0 N^2(0) \Delta^2 \ell n^2 (2\epsilon_c / \Delta)$$

Differentiation with respect to Δ of $\langle \hat{T} \rangle + \langle \hat{V} \rangle$ gives back gap equation, and substituting this value gives a condensation energy relative to the normal ground state of

$$E_{cond} = -\frac{1}{2} N(0) \Delta^2$$

Note this is a fraction $\sim(\Delta/E_F)^2 \sim 10^{-8}$ of N ground state energy!

Alternative (handwaving) derivation: in S state, energies of Anderson pseudo spins perturbed by amount $\sim\Delta$ over an energy range itself $\sim\Delta$ around Fermi surface, which contains $\sim N(0)\Delta$ states. Hence, total $S - N$ energy difference $\sim N(0)\Delta^2$

(↑: doesn't address cancellation of high-energy divergences.)

Summary of lecture 6

In a Sommerfeld model with weak attraction $-|V_0|\delta(\boldsymbol{r})$ collective bound state formed, with "characteristic energy" $\Delta \sim exp - -1/N(0|V_0|)$ and radius $\sim \hbar \mathrm{v}_F/\Delta$. Most of the "disturbance" to the normal ground state is confined to an energy region of width $\sim\Delta$ around Fermi surface: Number of pairs occupying bound state is $\sim N(\Delta/E_F)$, and condensation energy is $\sim N(0)\Delta^2 \sim N(\Delta^2/E_F)$.