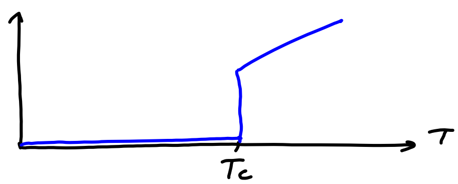
Superconductivity: Elements of BCS theory

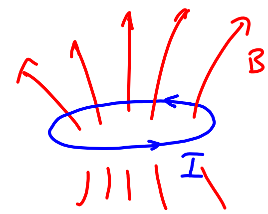
9.11.09 $\boxed{\text{BCS1}}$

Basic properties of superconductors

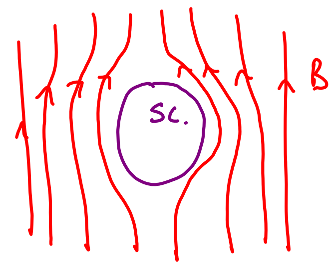


- Perfect conductivity

$\Rightarrow$ persistent current with "infinite" decay time ($> 10^5$ years)



- Perfect diamagnetism (Meissner-Effect)



$\Rightarrow$ large B-field destroys SC, when energy cost for excluding B-field exceeds energy gain from SC.

$\boxed{\text{BCS2}}$

History:

- discovery of zero resistance : Kammerling-Onnes (1911)
- discovery of Meissner effect : W. Meissner & R. Ochsenfeld, 1933
- F. London & H. London (1935) : phenomenological theory for electrodynamics of SC. (e.g. Meissner effect)
- Landau & Ginzburg (1951) : phenomenological theory of phase transition, in terms of complex order parameter $\psi = |\psi| e^{i\varphi}$

  (later identified as wave function of Cooper pairs)
- Bardeen, Cooper, Schrieffer (BCS), (1957) : microscopic theory in terms of pairing of electrons and condensation of Cooper pairs.

$\boxed{BCS3}$

Free electron gas (model for normal metals)

$$H = \sum_{k\sigma} \xi_k \, c^\dagger_{k\sigma} c_{k\sigma}$$

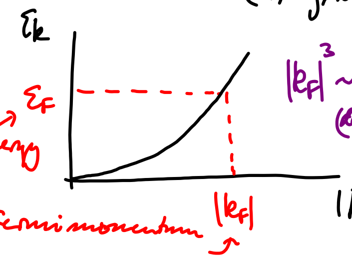
charges of background ions and mobile electrons neutralize each other $\Rightarrow$ free motion!

$c^\dagger_{k\sigma}$: creates electron with momentum k, spin σ

$k \equiv (k_x, k_y, k_z) \equiv \vec{k}$

Properties of H_0: $\quad \xi_k = \frac{k^2}{2m} - \mu$

("free" electrons)

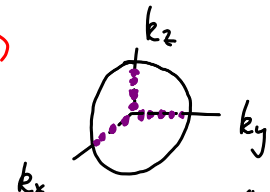


$|k_F|^3 \sim n$ (density)

Ground state of H_0: filled Fermi sea: $\quad |F\rangle = \prod_{|k_F|} c^\dagger_{k\uparrow} c^\dagger_{k\downarrow} |0\rangle$

states with $\xi_k < 0$: filled: $\quad c^\dagger_{k\sigma} |F\rangle = 0$

$\xi_k > 0$: empty: $\quad c_{k\sigma} |F\rangle = 0$

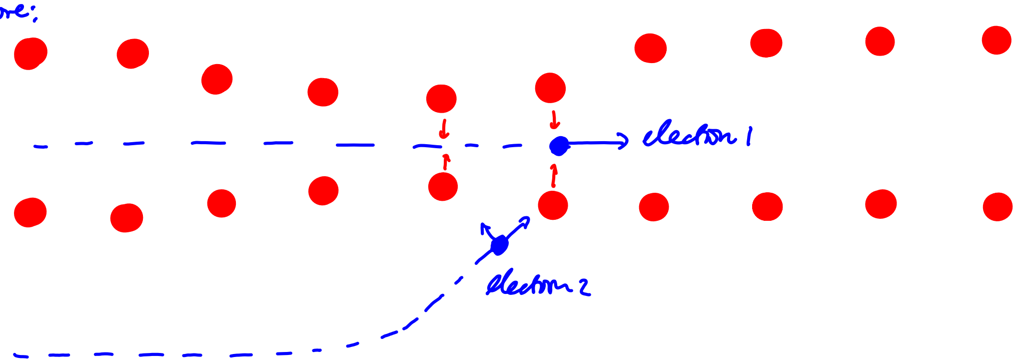


"Fermi sphere"

$\boxed{BCS4}$

Lattice ions ("phonons") yield retarded attractive e-e interaction

Before:



electron 1 moves through lattice, attracts ions (which react slowly), polarizing lattice, leaving behind excess positive charge which attracts electron 2 $\Big\}$ $\Rightarrow$ "phonon-induced electron-electron interaction"

Herbert Fröhlich, 1950 (PhD student of Arnold Sommerfeld, at LMU!)

"Reduced BCS Hamiltonian" $\boxed{BCS5}$

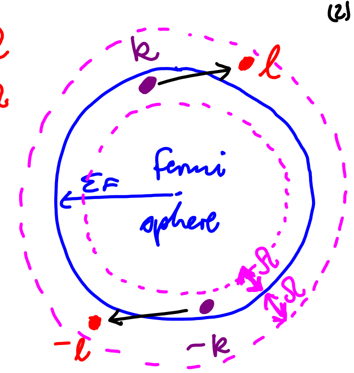
$$H_{red} = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{kl} V_{kl}\, c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} c_{-l\downarrow} c_{l\uparrow} \qquad (1)$$

$$= H_0 + H_1$$

reduced BCS interaction:

(2)

with: $$V_{kl} \begin{cases} = -V_0 \ (<0) \text{ for } & |\xi_k| < \Omega,\ |\xi_l| < \Omega \\ 0 & \text{otherwise} \end{cases}$$



V_{kl} scatters a pair of electrons with opposite momentum and spin $(l\uparrow, -l\downarrow)$, to another, similar pair $(k\uparrow, -k\downarrow)$.

[These are not the only processes possible for phonon-induced e-e interactions, but the ones with most phase space.]

Compact notation: "hard-core bosons" $\boxed{BCS6}$

define: $$b^\dagger_k \equiv c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}, \qquad b \equiv c_{-k\uparrow} c_{k\uparrow} \qquad (1)$$

"hardcore", since $b_k^2 = 0$, $b_k^{\dagger 2} = 0$ (2)

"bosons", since:

$$[b_k, b^\dagger_{k'}] \overset{\text{exercise!}}{=} \dots = \delta_{kk'}\left[1 - (c^\dagger_{k\uparrow} c_{k\uparrow} + c^\dagger_{-k\downarrow} c_{-k\downarrow})\right] \qquad (3)$$

when acting on states of the form $b^\dagger_{k_1} b^\dagger_{k_2} \dots |0\rangle$, this simplifies to

$$[b_k, b^\dagger_{k'}] = \delta_{kk'}\left[1 - 2 b^\dagger_k b_k\right] \qquad (4)$$

similarly: $$[b_k, b_{k'}] = [b^\dagger_k, b^\dagger_{k'}] = 0 \qquad (5)$$

$\Rightarrow$ b's are "bosonic" for $k \neq k'$ (4,5), but "hardcore" for equal k's (2).

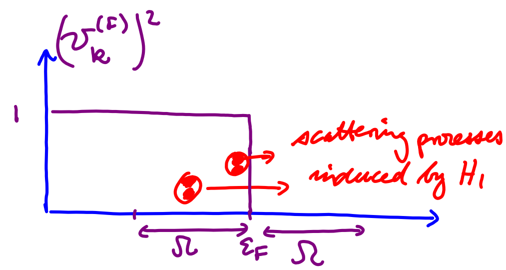
BCS7

Pair scattering for Fermi sea:

$$H_{red} = \sum_k 2\xi_k b_k^\dagger b_k + \sum_{kl} b_k^\dagger b_l$$

Fermi sea: $|F\rangle = \prod_{|k|<|k_F|} b_k^\dagger |0\rangle$

$$\left(v_k^{(F)}\right)^2 \equiv \langle F | b_k^\dagger b_k | F \rangle$$



But: $|F\rangle$ is not an eigenstate of H_1!

Also: $\langle F | b_k^\dagger b_l | F \rangle = \langle \equiv | b_k^\dagger b_l | \equiv \rangle = \langle \equiv | \equiv \rangle = 0$ if $k \neq l$.

$\Rightarrow$ Energy could be gained from H_1 by redistributing pairs!

The more pair scattering can occur, the better for lowering ground state energy. Hence, don't fill states strictly up to ε_F, but leave some space for pair scattering!

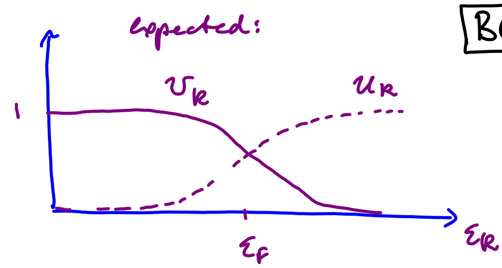
BCS8

BCS variational wave function

Bardeen, Cooper, Schrieffer, 1957

(PhD thesis of Schrieffer, 1957!

(Nobel prize 1972)



Variational wave function: allow more phase space for pair scattering! (1)

Ansatz: $$|BCS\rangle = \prod_{\text{all } k} (u_k + v_k b_k^\dagger)|0\rangle$$

[Schrieffer, had this idea on New York subway...]

v_k: amplitude that k-pair is occupied.
u_k: " " " empty.
$\Rightarrow |u_k|^2 + |v_k|^2 = 1$ (2)

u_k and v_k are <u>variational</u> parameters, to be chosen such that

$$\langle BCS | H_{red} | BCS \rangle = \text{minimum}$$

Normalization: $\boxed{\text{BCS9}}$

$=0$, since $\langle 0|b_k|0\rangle = \langle 0|b_{k'}^\dagger|0\rangle = 0$

$$\langle BCS|BCS\rangle = \prod_{k}\prod_{k'} \langle 0|(u_k^* + v_k^* b_k)(u_{k'} + v_{k'} b_{k'}^\dagger)|0\rangle$$

$$= \prod_{kk'} \delta_{kk'} \underbrace{(|u_k|^2 + |v_k|^2)}_{(8.2)\ =1} = 1 \quad \checkmark$$

$|BCS\rangle$ is not eigenstate of number operator: $\hat{N} = \sum_k 2 b_k^\dagger b_k$

Explicitly: $|BCS\rangle = \sum_N \lambda_N |\psi_N\rangle$, with $\hat{N}|\psi_N\rangle = N|\psi_N\rangle$

$\Rightarrow \quad \hat{N}|BCS\rangle \neq N|BCS\rangle$, although $[\hat{H}, \hat{N}] = 0$!

Using a non-number-eigenstate is a mathematical trick which makes calculations <u>very</u> much simpler.

Justification: <u>Number fluctuations are small in thermodynamic limit:</u> $\boxed{\text{BCS10}}$

Average: $\bar{N} = \langle BCS|\hat{N}|BCS\rangle \quad (1)$

$=0 \qquad \delta_{\ell k} \qquad =0 \qquad \delta_{\ell k'}$

$$= \prod_{kk'} \langle Vac|(u_k^* + v_k^* b_k)\Big(\sum_\ell 2 b_\ell^\dagger b_\ell\Big)(u_{k'} + v_{k'} b_{k'}^\dagger)|Vac\rangle \quad (2)$$

$$= \sum_\ell 2|v_\ell|^2 \quad (3)$$

$= \sim$ Volume, since the number of ℓ-states scales with volume $\quad (4)$

Fluctuations:

$$(\delta N)^2 = \langle BCS|(\hat{N} - \bar{N})^2|BCS\rangle \overset{\text{exercise!}}{=} 4\sum_k u_\ell^2 v_\ell^2 \neq 0$$

$\sim$ Vol (since each $\sum_\ell \sim$ Vol) $\Big\{$ would $=0$ only if for each k, either $u_\ell = 0$ or $v_\ell = 0$

$$\Rightarrow \frac{\delta N}{\bar{N}} \sim \frac{Vol^{1/2}}{Vol} \sim Vol^{-1/2} \rightarrow 0 \text{ in thermodynamic limit of } Vol \to \infty$$

<u>Variational minimization of ground state energy</u>

BCS11

$$E_{BCS}(\{v_k\}) = \langle BCS | \hat{H}_{red} | BCS \rangle \tag{1}$$

μ has role of Lagrange multiplier, to fix average particle #.

$$= \prod_{kk'} \langle 0 | (u_k^* + v_k^* b_k) \Big[\underbrace{\sum_l 2\xi_l \, b_l^\dagger b_l}_{\delta_{lk}} + \underbrace{\sum_{ll'} V_{ll'} b_l^\dagger b_{l'}}_{\delta_{lk'}} \Big] (u_k + v_k b_{k'}^\dagger) | 0 \rangle \tag{2}$$

analogous to (10.4)

$$= \sum_l 2\xi_l |v_l|^2 + \sum_{ll'} V_{ll'} (u_l v_l^*)(u_{l'}^* v_{l'}) \tag{3}$$

[don't worry about $l = l'$ terms; they are smaller by a factor $V\mathcal{L}^{-1/2}$]

we get contributions only if $k = l$, $k' = l'$, or $k = l'$; $k' = l$: e.g.

$$\langle 0 | \underbrace{(u_l^* + v_l^* b_l)(u_{l'}^* + v_{l'}^* b_{l'})}_{v_l^* u_{l'}^*} b_l^\dagger b_{l'} \underbrace{(u_l + v_l b_l^\dagger)(u_{l'} + v_{l'} b_{l'}^\dagger)}_{u_l v_{l'}} | 0 \rangle \tag{4}$$

$$\sim (u_l v_l^*)(u_{l'}^* v_{l'})$$

BCS12

Minimize E_{BCS} w.r.t. to v_k, under constraint $|u_k|^2 + |v_k|^2 \overset{(8.2)}{=} 1$

To this end, write $u_k = \sin\theta_k$ and $v_k = e^{-i\phi_k}\cos\theta_k$ (1)

relative phase.

$$2|v_k|^2 = 2\cos^2\theta_k = 1 + \cos 2\theta_k \tag{2}$$

$$u_k v_k^* = \tfrac{1}{2}\sin 2\theta_k \, e^{i\phi_k} \tag{3}$$

$$\Rightarrow \boxed{E_{BCS} \overset{(11.3)}{=} \sum_l \xi_k (1 + \cos 2\theta_l) + \frac{1}{4}\sum_{ll'} V_{ll'} \sin 2\theta_l \sin 2\theta_{l'} \underbrace{e^{i(\phi_l - \phi_{l'})}}_{\equiv 1}} \tag{4}$$

To avoid that sum over different phase factors averages to zero, choose

$\phi_l = \phi$ = independent of l $\Rightarrow$ "all pairs have same phase" !!

(e.g. $\phi = 0$)

important!!

$$\boxed{\text{BCS 13}}$$

Minimize: $\partial_{\theta_k} E_{BCS} = 0$ (1)

since both sums $\sum_k$ and $\sum_{k'}$ make equal contributions

$$\xi_k(-2)\sin 2\theta_k + \frac{2\cdot 2}{4}\sum V_{lk} \sin 2\theta_l \cos 2\theta_k \overset{(12.4)}{=} 0 \tag{2}$$

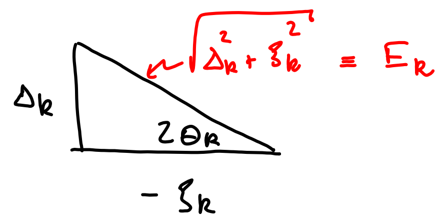
$\frac{(2)}{\cos 2k}$:

$$\tan 2\theta_k = \frac{1}{\xi_k}\underbrace{\sum_l V_{lk} \overbrace{\tfrac{1}{2}\sin 2\theta_l}^{(12.3):\ u_l v_l^*}}_{\equiv -\Delta_k} = -\frac{\Delta_k}{\xi_k} \tag{3}$$

where $\Delta_k \equiv -\sum_l V_{lk}\, u_l v_l$ (4)

Graphical representation of

$\tan 2\theta_k \overset{(3)}{=} -\frac{\Delta_k}{\xi_k}$:



(5)

$$\boxed{\text{BCS 14}}$$

(13.5) implies: $2u_l v_l \overset{(12.3)}{=} \sin 2\theta_l \overset{(13.5)}{=} \frac{\Delta_l}{E_l}$ (1)

and for later use: $v_l^2 - u_l^2 \overset{(12.1)}{=} \cos^2\theta_l - \sin^2\theta_l = \cos 2\theta_l \overset{(14.1)}{=} -\frac{\xi_l}{E_l}$ (2)

[The choice of sign in (2) ensures $\left.\begin{array}{l} u_l \to 1 \\ v_l \to 0 \end{array}\right\}$ for $\xi_l \to \infty$ as expected from page $\boxed{\text{BCS 8}}$ (3)

(14.1) into (13.4):

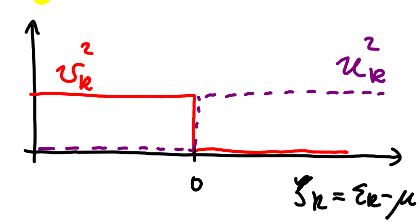
$$\boxed{\Delta_k = -\sum_l V_{kl}\frac{\Delta_l}{2E_l}}$$

"Gap equation" (4)

Trivial solution:

$\Delta_k = 0 \ \forall k$, $\Rightarrow E_k \overset{(13.5)}{=} |\xi_k|$

$v_k^2 - u_k^2 \overset{(14.2)}{=} -\frac{\xi_k}{|\xi_k|} = -\mathrm{sgn}(\xi_k)$

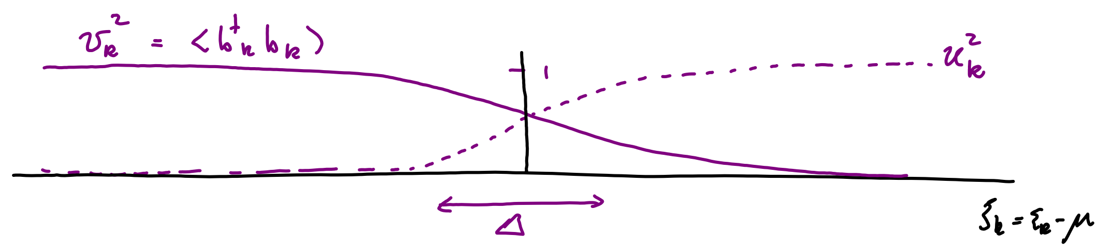


$\Rightarrow v_k = \theta(-\xi_k)$, $u_k = \theta(\xi_k)$ $\Rightarrow$ FREE FERMI SEA.

Nontrivial solution has $\Delta_k \neq 0$ (to be determined below). $\boxed{BCS15}$

find u_k, v_k:
$$v_k^2 + u_k^2 \overset{(8.2)}{=} 1 \qquad (1)$$
$$v_k^2 - u_k^2 \overset{(14.2)}{=} -\frac{\xi_k}{E_k} \qquad (2)$$

$\frac{1}{2}[(1) \pm (2)]$:
$$\left.\begin{array}{l} v_k^2 \\ u_k^2 \end{array}\right\} = \frac{1}{2}\left(1 \mp \frac{\xi_k}{E_k}\right) = \frac{1}{2}\left(1 \mp \frac{\xi_k}{\sqrt{\Delta^2 + \xi_k^2}}\right)$$



Pair correlations "reshuffle" electrons from below to above the Fermi level.
This costs kinetic energy but gains potential energy!

To evaluate non-trivial solution with $\Delta_k \neq 0$, use BCS model: $\boxed{BCS15}$

$$V_{kk} \overset{(5.2)}{=} \begin{cases} -V_0 \,(<0) & \text{for } |\xi_k| < \Omega \\ 0 & \text{otherwise} \end{cases} \qquad (1)$$

$$\Rightarrow \quad \Delta_k \overset{(14.4)}{=} \begin{cases} \Delta & \text{for } |\xi_k| < \Omega \\ 0 & \text{otherwise} \end{cases} \qquad (2)$$

$\xi = \varepsilon - \mu$

with
$$1 \overset{(14.4)}{=} V_0 \sum_{|\xi_k| < \Omega} \frac{1}{2E_k} \qquad (3)$$

Now: $\left(\delta k = \frac{2\pi}{L}\right)$

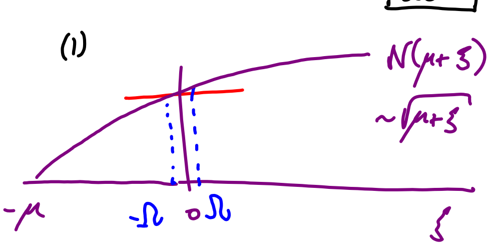
$$\sum_k = \frac{1}{(\delta k)^3}\int d^3k = \frac{L^3}{(2\pi)^3}\int_0^\infty dk\, k^2 \cdot 4\pi = \int_0^\infty d\varepsilon_k\, \mathcal{N}(\varepsilon_k) = \int_{-\mu}^\infty d\xi\, \mathcal{N}(\mu+\xi) \qquad (4)$$

where $\varepsilon_k = \frac{k^2}{2m} \Rightarrow \frac{d\varepsilon_k}{dk} = \frac{k}{m} \Rightarrow \sqrt{2m\varepsilon_k}\, d\varepsilon_k = dk\, \frac{k}{m}\cdot k \qquad (5)$

$$\Rightarrow \quad \frac{L^3}{4\pi^2}\, dk\, k^2 = \frac{L^3}{4\pi^2}\sqrt{2m^3\varepsilon_k}\, d\varepsilon_k \equiv \mathcal{N}(\varepsilon_k)\, d\varepsilon_k = \mathcal{N}(\mu+\xi)\, d\xi \qquad (6)$$

Hence: **BCS17**

$$1 \overset{(15.3)}{=} V_0 \frac{1}{2} \int_{-\mu}^{\infty} d\xi \, \mathcal{N}(\mu+\xi) \frac{\Theta(\Omega - |\xi|)}{\sqrt{\Delta^2 + \xi^2}} \qquad (1)$$



$$\simeq V_0 \cancel{\tfrac{1}{2}} \int_{\overset{0}{\cancel{-\Omega}}}^{\Omega} d\xi \, \mathcal{N}(\mu) \frac{1}{\sqrt{\Delta^2 + \xi^2}} \qquad (2)$$

assume: $\Delta \ll \Omega \ll \mu$

$$\frac{1}{V_0 \mathcal{N}(\mu)} = \sinh^{-1} \underbrace{\frac{\sqrt{\Delta^2 + \Omega^2}}{\Delta}}_{\simeq \Omega} \qquad (3)$$

$$\left[\sinh \frac{1}{x} = \frac{1}{2}\left(e^{\frac{1}{x}} - e^{-\frac{1}{x}}\right) \simeq \frac{1}{2} e^{\frac{1}{x}} \text{ for } x \ll 1 \right]$$

$$\Delta = \Omega \left[\sinh\left(\frac{1}{V_0 \mathcal{N}(\mu)}\right)\right]^{-1} = 2\Omega \, e^{-\frac{1}{V_0 \mathcal{N}(\mu)}} \qquad (4)$$

(since typically, $V_0 \mathcal{N}(\mu) \lesssim 0.3$, approx OK with error of $\lesssim 1\%$)

We get a non-perturbative result for Δ!!

Condensation energy: **BCS18**

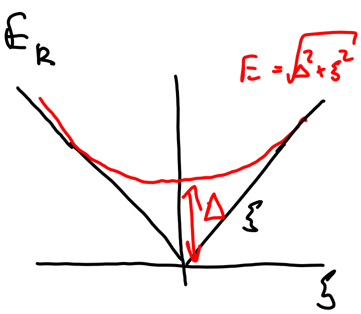
$$\Delta E_{BCS} \overset{(12.4)}{=} \langle BCS | \hat{H} - \mu \hat{N} | BCS \rangle - \langle F | \hat{H} - \mu \hat{N} | F \rangle \qquad (1)$$

$$= \left[\sum_k \left(\xi_k - \frac{\xi_k^2}{E_k} \right) - \frac{\Delta^2}{V_0} \right] - \sum_{|\varepsilon_k| < \varepsilon_F} 2\xi_k$$

Exercise:

$$= -\frac{1}{2} \Delta^2 \mathcal{N}(\mu) \sim \text{Volume}$$, hence extensive gain!

Excited states: $\left.\begin{matrix} c^\dagger_{k\sigma} |BCS\rangle \\ c_{k\sigma} |BCS\rangle \end{matrix}\right\}$ both have energy E_k

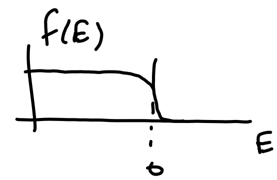


BCS19

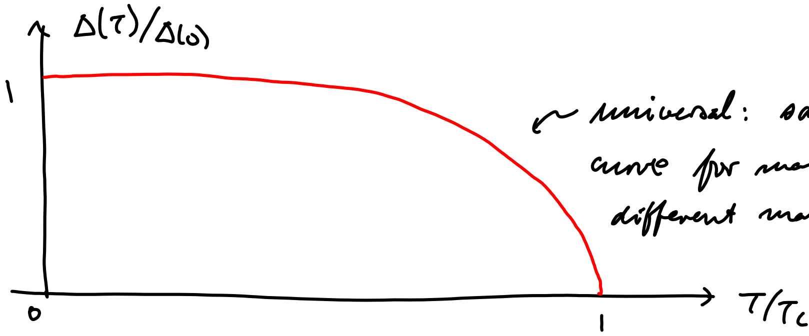
Finite temperature gap equation:
(obtained by minimizing free energy $H - TS$):

$$1 = -\sum_{\ell} V_{k\ell} \frac{\Delta_\ell}{2E_\ell}\left(1 - 2f(E_\ell)\right) \qquad (1)$$

where $f(E_\ell) = \dfrac{1}{e^{\beta E_\ell}+1}$ = Fermi function $\qquad$ (2)



Solution:
(can be shown)



← universal: same curve for many different materials!

BCS20

BCS-mean field

$$H_{red} = \sum_{k\sigma} \xi_k c^\dagger_{k\sigma} c_{k\sigma} - V_0 \sum_k{}' c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \sum_\ell{}' c_{-\ell\downarrow} c_{\ell\uparrow} \qquad (1)$$

$\varepsilon_k, \varepsilon_\ell$ within Ω of ε_F

mean field approximation:

$$\Big[\overset{1}{\langle c^\dagger c^\dagger\rangle} + \overbrace{c^\dagger c^\dagger - \langle c^\dagger c^\dagger\rangle}^{2}\Big]\Big[\overset{3}{\langle cc\rangle} + \overbrace{cc - \langle cc\rangle}^{4}\Big] \qquad (2)$$

$$\overset{1\cdot 2}{=} \langle c^\dagger c^\dagger\rangle\langle cc\rangle + \overset{1\cdot 4}{\langle c^\dagger c^\dagger\rangle(cc - \langle cc\rangle)} + \overset{2\cdot 3}{(c^\dagger c^\dagger - \langle c^\dagger c^\dagger\rangle)\langle cc\rangle} + \underbrace{3\cdot 4}_{\text{neglect}} \qquad (3)$$

$$\simeq \langle c^\dagger c^\dagger\rangle cc + c^\dagger c^\dagger\langle cc\rangle - \langle c^\dagger c^\dagger\rangle\langle cc\rangle \qquad (4)$$

$$H^{MF}_{red} = \sum_{k\sigma} \xi_k : c^\dagger_{k\sigma} c_{k\sigma} : + \underbrace{(-V_0)\sum_k{}'\langle c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\rangle}_{\equiv \Delta^*} \sum_\ell{}' c_{-\ell\downarrow} c_{\ell\uparrow} + \sum_k{}' c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \underbrace{(-V_0)\sum_\ell{}'\langle c_{-\ell\downarrow} c_{\ell\uparrow}\rangle}_{\equiv \Delta} - \frac{1}{V_0}|\Delta|^2 \qquad (5)$$

$$= \sum_{k\sigma} \xi_k : c^\dagger_{k\sigma} c_{k\sigma} : + \sum_k{}' \left(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow}\Delta + \Delta^* c_{-k\downarrow} c_{k\uparrow}\right) - \frac{1}{V_0}|\Delta|^2 \qquad (6)$$

BCS21

$$H^{red}_{MF} = \sum_k H_k^{MF} - \frac{|\Delta|^2}{V_0} \quad \leftarrow \text{ignore these constants henceforth} \tag{1}$$

$$H_k^{MF} = \xi_k c^\dagger_{k\uparrow} c_{k\uparrow} - \xi_{-k} c_{-k\downarrow} c^\dagger_{-k\downarrow} - \left(c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \Delta + \Delta^* c_{-k\downarrow} c_{k\uparrow}\right) \tag{2}$$

$$= \begin{pmatrix} c^\dagger_{k\uparrow} & c_{-k\downarrow} \end{pmatrix} \underbrace{\begin{pmatrix} \xi_k & \Delta \\ \Delta^* & -\xi_{-k} \end{pmatrix}}_{h_{\alpha\alpha'}} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\uparrow} \end{pmatrix} = \sum_\sigma E_\sigma \hat{\gamma}^\dagger_{k\sigma} \hat{\gamma}_{k\sigma} \tag{3}$$

$$= \sum_{\alpha\alpha'} c^\dagger_\alpha(k)\, h_{\alpha\alpha'}(k)\, c_\alpha(k)$$

with $c_\alpha(k) \equiv \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \equiv \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix}$, $\quad c^\dagger_\alpha(k) = (c_1^\dagger, c_2^\dagger) = (c^\dagger_{k\uparrow}, c_{-k\downarrow})$ (4)

Goal: diagonalize to get $\quad H_k^{MF} = \sum_\alpha E_\alpha(k)\, \gamma^\dagger_\alpha(k)\, \gamma_\alpha(k)$ (5)

BCS22

Diagonalize: Let $(V_\alpha)^{\bar\alpha}$ be eigenvectors of h with eigenvalues $E_{\bar\alpha}$,

$$h_{\alpha\alpha'} (V_{\alpha'})^{\bar\alpha} = E_{\bar\alpha} (V_\alpha)^{\bar\alpha} , \tag{1}$$

orthogonal: $\quad \sum_\alpha (V_\alpha)^{\bar\alpha} (V^*_\alpha)^{\bar\alpha'} = \delta_{\bar\alpha\bar\alpha'}$ (2)

Then the matrix $\quad W_{\alpha\bar\alpha} \equiv (V_\alpha)^{\bar\alpha}$ (3)

with inverse $\quad (W^{-1})_{\bar\alpha\alpha} = (V^*_\alpha)^{\bar\alpha} = W^*_{\alpha\bar\alpha} \overset{(3)}{=} (W^\dagger)_{\bar\alpha\alpha}$ (4)

(so that $(W^{-1}W)_{\bar\alpha\bar\alpha'} = \delta_{\bar\alpha\bar\alpha'}$)

diagonalizes h: $\quad W^{-1}_{\bar\alpha'\alpha}\, h_{\alpha\alpha'}\, W_{\alpha\bar\alpha} \overset{(1)}{=} E_{\bar\alpha}\, \delta_{\bar\alpha\bar\alpha'}$ (5)

Shorthand: $\quad W^{-1} h W = E\, \mathbb{1}$ (6)

BCS23

$$H_k^{mf} = \sum_{\alpha\alpha'} c^\dagger_\alpha(k)\, h_{\alpha\alpha'}(k)\, c_{\alpha'}(k) \qquad (1)$$

$$= c^\dagger h\, c = \underbrace{c^\dagger W}_{\gamma^\dagger} E \underbrace{W^\dagger c}_{\gamma} = \gamma^\dagger E \gamma \qquad (2)$$

$$= \sum_\alpha E_\alpha \gamma^\dagger_\alpha(k)\, \gamma_\alpha(k) \qquad \text{(has desired form 21.5)} \qquad (3)$$

with $\gamma_\alpha(k) = \sum_{\alpha'} W^\dagger_{\alpha\alpha'} c_{\alpha'}$, $\gamma^\dagger_\alpha(k) = \sum_{\alpha'} c^\dagger_{\alpha'}(k) W_{\alpha'\alpha}$ (4)

Now, diagonalize: $h = \begin{bmatrix} \xi_k & |\Delta| e^{i\phi} \\ |\Delta| e^{-i\phi} & -\xi_{-k} \end{bmatrix}$ (5)

$\xi_{-k} \leftarrow \xi_k$

eigenvalues: (6)

$$\left.\begin{matrix} E_1(k) \\ E_2(k) \end{matrix}\right\} = \pm \underbrace{\sqrt{|\Delta|^2 + \xi_k^2}}_{E_k}$$

eigenvectors: (7)

$$V^{\alpha=1}(k) = \begin{pmatrix} u_k \\ v_k e^{-i\phi} \end{pmatrix}, \qquad V^{\alpha=2}(k) = \begin{pmatrix} -v_k e^{i\phi} \\ u_k \end{pmatrix}$$

coefficients: (8)

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

BCS24

Details:

$$\begin{pmatrix} \xi & |\Delta| e^{i\phi} \\ |\Delta| e^{-i\phi} & -\xi \end{pmatrix}\begin{pmatrix} s \\ c \end{pmatrix} = E \begin{pmatrix} s \\ c \end{pmatrix} \qquad |s|^2 + |c|^2 = 1 \qquad (1)$$

$$\xi s + |\Delta| e^{i\phi} c = E s \quad \Rightarrow \quad c = \frac{(E-\xi)}{|\Delta|} s\, e^{-i\phi} \qquad (2)$$

$$|\Delta| e^{-i\phi} s - \xi c = E c \quad \Rightarrow \quad s = \frac{(E+\xi)}{|\Delta|} c\, e^{i\phi} \qquad (3)$$

consistency requires: (3) into (2):

$$\frac{E^2 - \xi^2}{|\Delta|^2} = 1 \quad \Rightarrow \quad E_\pm = \pm \underbrace{\sqrt{|\Delta|^2 + \xi^2}}_{E_k} \qquad (4)$$

solve for c: $|c|^2 |\Delta|^2 \overset{|(2)|^2}{=} (E-\xi)^2 |s|^2 = (E-\xi)^2(1 - |c|^2)$ (5)

$$\Rightarrow |c|^2(|\Delta|^2 + (E-\xi)^2) = (E-\xi)^2 \qquad (6)$$

$$|c|^2 \overset{(6')}{=} \frac{E-\xi}{2E} = \frac{1}{2}\left(1 - \frac{\xi}{E}\right) \qquad (7)$$

$$\Rightarrow |s|^2 = \frac{1}{2}\left(1 + \frac{\xi}{E}\right) \qquad (8)$$

$$\left[\begin{aligned} &|\Delta|^2 + (E-\xi)^2 \\ &= E^2 - 2E\xi + \xi^2 + \Delta^2 \\ &= 2E^2 - 2E\xi \\ &\to 2E(E-\xi) \qquad (6') \end{aligned}\right]$$

BCS25

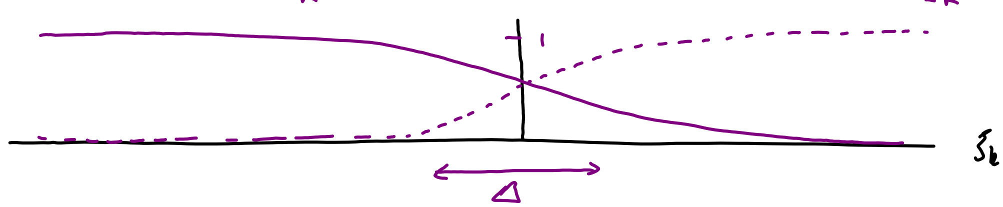
First eigenvalue: $E_1(k) = +E_k$

$$V_1(k) = \begin{pmatrix} s_1 \\ c_1 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}}\left(1 + \frac{\xi_k}{E_k}\right)^{1/2} \\ \frac{1}{\sqrt{2}}\left(1 - \frac{\xi_k}{E_k}\right)^{1/2} e^{-i\phi} \end{pmatrix} \equiv \begin{pmatrix} u \\ v e^{-i\phi} \end{pmatrix}$$

Second eigenvalue: $E_2(k) = -E_k$

$$V_2(k) = \begin{pmatrix} s_2 \\ c_2 \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}}\left(1 - \frac{\xi_k}{E_k}\right)^{1/2} e^{i\phi} \\ \frac{1}{\sqrt{2}}\left(1 + \frac{\xi_k}{E_k}\right)^{1/2} \end{pmatrix} \equiv \begin{pmatrix} -v e^{i\phi} \\ u \end{pmatrix}$$

$v_k \equiv \frac{1}{\sqrt{2}}\left(1 + \frac{\xi_k}{E_k}\right)^{1/2}$ $\qquad$ $u_k \equiv \frac{1}{\sqrt{2}}\left(1 - \frac{\xi_k}{E_k}\right)^{1/2}$



BCS25

New eigenmodes: $\gamma_\alpha(k) = \sum_{\alpha'} W^\dagger_{\alpha\alpha'} c_{\alpha'} = \sum_{\alpha} \left(V^*_{\alpha'}\right)^\alpha c_{\alpha'}$ (1)

$$\begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^\dagger_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} \gamma_1(k) \\ \gamma_2(k) \end{pmatrix} = \begin{pmatrix} u_k & v_k e^{i\phi} \\ -v_k^{-i\phi} & u_k \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} \quad \text{(2)}$$

Bogoljubov-Valatin transformation

$$\boxed{\begin{aligned} \gamma^\dagger_{k\uparrow} &= u_k c^\dagger_{k\uparrow} + v_k e^{-i\phi} c_{-k\downarrow} & (QP)_\uparrow &= \bullet\!\uparrow + \circ\!\downarrow \\ \gamma^\dagger_{-k\downarrow} &= -v_k e^{-i\phi} c_{k\uparrow} + u_k c^\dagger_{-k\downarrow} & (QP)_\downarrow &= \circ\!\uparrow + \bullet\!\downarrow \end{aligned}} \quad \text{(3)}$$

$$H^{MF}_k = E_1(k)\,\gamma_1^\dagger(k)\,\gamma_1(k) + E_2(k)\,\gamma_2^\dagger(k)\,\gamma_2(k) \quad \text{(4)}$$

$$= E_k \gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} + (-E_k)\,\gamma_{-k\downarrow}\gamma^\dagger_{-k\downarrow} \quad \text{(5)}$$

$$\boxed{H^{MF} = \sum_k E_k \left(\gamma^\dagger_{k\uparrow}\gamma_{k\uparrow} + \gamma^\dagger_{k\downarrow}\gamma_{k\downarrow}\right) + \text{const.}} \quad \text{(6)}$$

↑ spin ↑ and ↓ quasiparticles are degenerate

Inverse transformation of (25.2): (BCS 27)

$$\begin{pmatrix} c_{k\uparrow} \\ c^{+}_{-k\downarrow} \end{pmatrix} \overset{(21.6)}{=} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \overset{(1)}{=} \begin{pmatrix} u & -v e^{i\phi} \\ v e^{-i\phi} & u \end{pmatrix} \begin{pmatrix} \gamma_{k\uparrow} \\ \gamma^{+}_{-k\downarrow} \end{pmatrix} \quad (1)$$

$$c_{k\uparrow} = u_k \gamma_{k\uparrow} - v_k e^{i\phi} \gamma^{+}_{-k\downarrow} \quad (2)$$

$$c_{-k\downarrow} = v_k e^{i\phi} \gamma^{+}_{k\uparrow} + u_k \gamma_{-k\downarrow} \quad (3)$$

Can easily be checked:

$$\{\gamma_{k\sigma}, \gamma^{+}_{k'\sigma'}\} = \delta_{kk'} \delta_{\sigma\sigma'}, \quad \{\gamma_{k\sigma}, \gamma_{k'\sigma'}\} = 0, \quad \{\gamma^{+}_{k\sigma}, \gamma^{+}_{k'\sigma'}\} = 0$$

$\Rightarrow$ Quasi-particles are also fermionic, just as original electrons.

BCS ground state is defined by $\gamma_{k\sigma} |BCS\rangle = 0$

Self-consistency condition:

$$\Delta = (-V_0) \sum_k{}' \langle c_{-k\downarrow} c_{k\uparrow} \rangle$$

$$= -V_0 \sum_k \langle BCS | (v_k e^{+i\phi} \gamma^{+}_{k\uparrow} + u_k \gamma_{-k\downarrow}) (u_k \gamma_{k\uparrow} - v_k e^{i\phi} \gamma^{+}_{-k\downarrow}) |BCS\rangle$$

only non-zero contribution!

$$= V_0 \sum_k u_k v_k e^{i\phi}$$

$$= V_0 \sum_k \frac{\Delta}{2E_k} e^{i\phi}$$

$$uv = \tfrac{1}{2}\left(1 + \tfrac{\xi}{E}\right)^{1/2}\left(1 - \tfrac{\xi}{E}\right)^{1/2} = \tfrac{1}{2}\left(\frac{E^2 - \xi^2}{E^2}\right)^{1/2} = \tfrac{1}{2}\frac{\Delta}{E}$$

$$\boxed{1 = V_0 \sum_k \frac{1}{2E_k}}$$ gap equation.