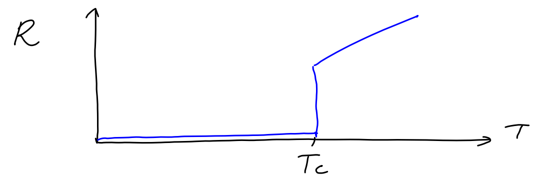
Superconductivity: Elements of BCS theory

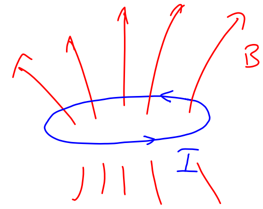
9.11.09 $\boxed{\text{BCS1}}$

Basic properties of superconductors

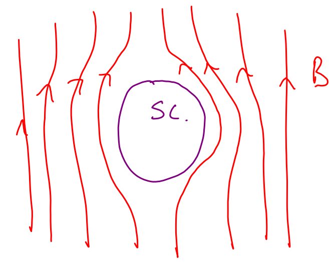
- Perfect conductivity



$\Rightarrow$ 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.

History: $\boxed{\text{BCS2}}$

- 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.

$\boxed{\text{BCS3}}$

Free electron gas (model for normal metals)

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

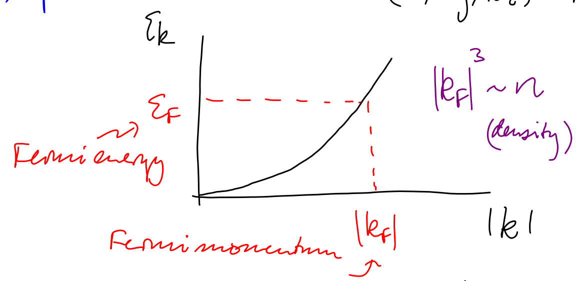
creates electron with momentum k, spin σ

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

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

Properties of H_0: $\varepsilon_k = \frac{k^2}{2m}$

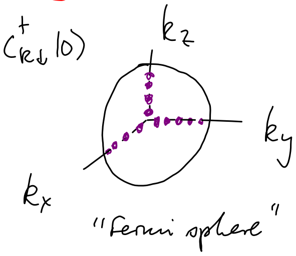
("free" electrons)



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

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

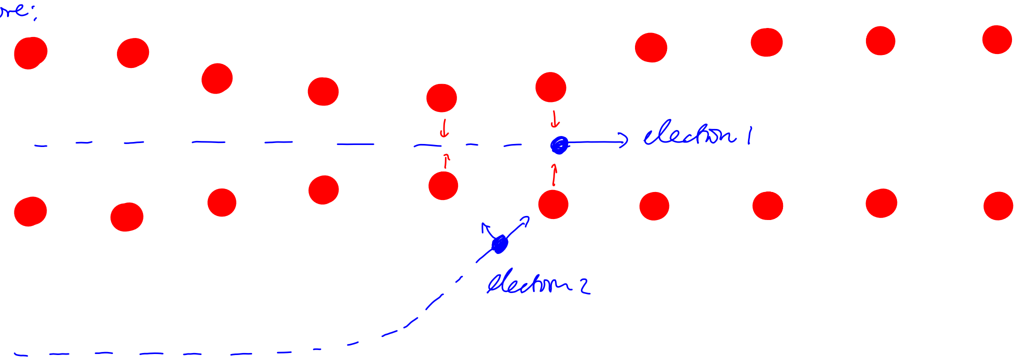
$|k| > |k_F|$: empty: $c_{k\sigma} |F\rangle = 0$



$\boxed{\text{BCS4}}$

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

$\Rightarrow$ "phonon-induced electron-electron interaction"

Herbert Fröhlich, 1950

(PhD student of Arnold Sommerfeld, at LMU!)

"Reduced BCS Hamiltonian"

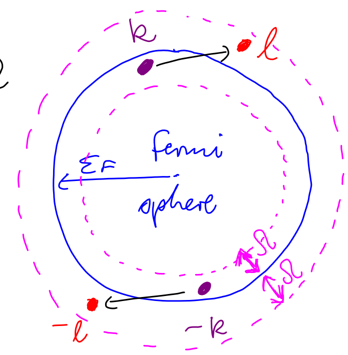
$\boxed{\text{BCS5}}$

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

$$= H_0 + H_1$$

reduced BCS interaction:

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



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"

$\boxed{\text{BCS6}}$

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

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

"bosons", since:

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

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

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

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

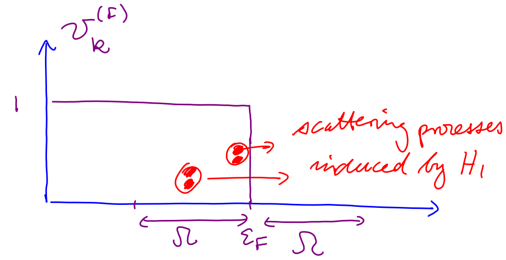
$\Rightarrow$ b's are "bosonic" for $k \neq k'$ (4,5), but "hardcore" for equal k's (2).

Pair scattering for Fermi sea: $\boxed{BCS7}$

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

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

$v_k^{(F)} = \langle F| b_k^\dagger b_k |F\rangle$



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!

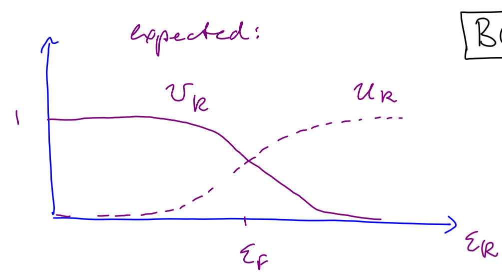
The more pair scattering can occur, the better for lowering ground state energy. Hence, don't fill states strictly up to ε_F, but leave some space for pair scattering!

BCS variational wave function $\boxed{BCS8}$

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. $\Big\} \Longrightarrow |u_k|^2 + |v_k|^2 = 1$ (2)

u_k and v_k are variational parameters, to be chosen such that

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

Normalization: $\boxed{BCS9}$

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

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

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

$|BCS\rangle$ 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 very much simpler.

Justification: Number fluctuations are small in thermodynamic limit: $\boxed{BCS10}$

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

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

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

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

$= \sim$ Volume, since the number of ℓ-states scales with volume (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 $v_\ell = 0$

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

Variational minimization of ground state energy

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$$E_{BCS}(\{v_k\}) = \langle BCS|\hat{H}_{red} - \mu\hat{N}|BCS\rangle \quad (1)$$

μ ↑ Lagrange multiplier, to fix average particle #.

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

analogous to (10.4)

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

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

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

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

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

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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.

$$2|v_k|^2 = 2\cos^2\theta_k = 1 + \cos 2\theta_k \quad (2)$$

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

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

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!!