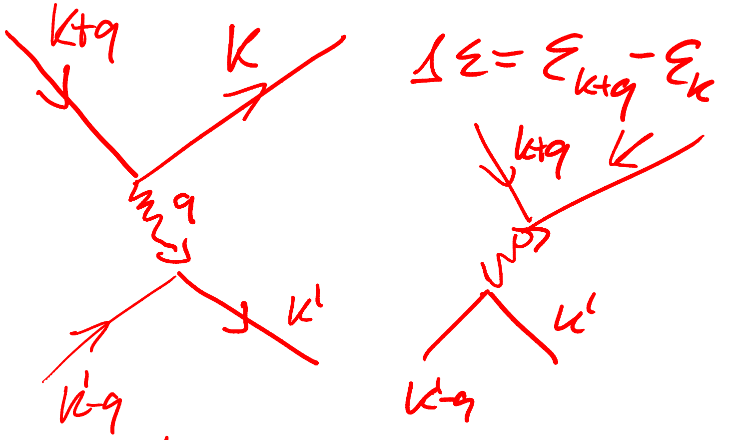
Chapter 4; part 4: BCS Theory

$$H_{eff} = \sum_m{}' \frac{\langle a|H'|m\rangle\langle m|H'|b\rangle}{E_{a/b} - E_m}$$

We had: $$H_{\text{el-ph}} = \int d^3\mathbf{q}\, T(\mathbf{q})\psi^\dagger_{\mathbf{k}}\psi_{\mathbf{k}+\mathbf{q}}(a^\dagger_{\mathbf{q}} + a_{-\mathbf{q}})$$

2nd order perturbation

$$H_{eff} = \int d^3\vec{k}\, d^3\vec{k}'\, d^3\vec{q}\; V\, \psi^+_{\vec{k}'\sigma'}\psi^+_{\vec{k}\sigma}\psi_{\vec{k}+\vec{q}\sigma}\psi_{\vec{k}'-\vec{q}\sigma'}$$



$$V = |T_q|^2(\alpha - \beta)$$

$$\alpha = \frac{1}{\Delta\varepsilon - \hbar\omega_q} \qquad -\beta = \frac{1}{-\Delta\varepsilon - \hbar\omega_q}$$

$$\Rightarrow V = |T_{\vec{q}}|^2 \frac{\hbar\omega_q}{(\Delta\varepsilon)^2 - (\hbar\omega_q)^2}$$

change in e^- energies $\delta\varepsilon = \varepsilon_{\vec{k}+\vec{q}} - \varepsilon_{\vec{k}}$

e^- - photon interaction $T_{\vec{q}}$

two cases: $\Delta\varepsilon^2 > (\hbar\omega_q)^2$

$\rightarrow$ repulsion

$\rightarrow \delta\varepsilon^2 < (\hbar\omega_q)^2$ q large!

$\rightarrow$ attraction

only if $k, k', k+q, k'-q \simeq k_F$

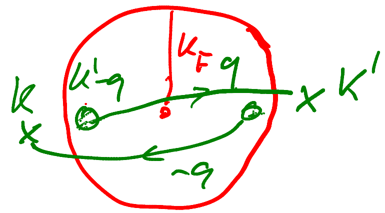
Assumptions
- only "virtual" phonon excitations
- no degeneracy; i.e. $|(\Delta\varepsilon)^2 - (\hbar\omega_q)^2| \gg |T_q|^2$

BCS Hamiltonian : further simplification $\sigma \neq \sigma'$ for symm. band wavefcn. 4.4.2

$$H_{BCS} = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^+_{\vec{k},\sigma} c_{\vec{k},\sigma} + \underline{V} \sum'_{\vec{k},\vec{k}'} c^+_{\vec{k}\uparrow} c^+_{-\vec{k}\downarrow} c_{-\vec{k}'\downarrow} c_{\vec{k}'\uparrow}$$

Further
Assumptions: Sum restricted to small range around k_F

i.e. $|\vec{q}| = |\vec{k}' - \vec{k}| \approx 2k_F$ $\qquad \underline{V<0}$ (attractive)



Keep only terms
$k'' = k' - q$
$-k'' = k + q$
$\Rightarrow k = -k'' - q$
$= -k'$

ignore k, q dependence of V in attractive region

$\longrightarrow$ spontaneous formation of pair excitations $\underline{c^+_{k\uparrow} c^+_{-k\downarrow}}\, |FS\rangle$
instability in this case : cooper pairs
is stable with $\varepsilon < \varepsilon_F$

BCS : calculate density of pair excitations self-consistently

Equivalent approaches:

- variational ansatz $|BCS\rangle = \prod_{\vec{k}} (u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow}) |0\rangle$ Schrieffer
  not particle conserving!
- Mean field theory $\langle c^+_{k\uparrow} c^+_{-k\downarrow} \rangle = \gamma_{\vec{k}} \neq 0$

MFT Ansatz $\hat{A}\hat{B} \approx \langle\hat{A}\rangle\hat{B} + \hat{A}\langle\hat{B}\rangle - \langle\hat{A}\rangle\langle\hat{B}\rangle$ 4.4.3

+ ~~fluctuations~~

"order parameter"

= mean field $\gamma_{\vec{k}} = \langle c^\dagger_{\vec{k}\uparrow} c^\dagger_{-\vec{k}\downarrow}\rangle$ off diagonal

$$H_{BCS} \approx \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} + V \sum'_{\vec{k}\vec{k}'} \left(\gamma_{\vec{k}'} \underline{c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow}} + \gamma^*_{\vec{k}'} \underline{c^\dagger_{\vec{k}\uparrow} c^\dagger_{-\vec{k}\downarrow}} - |\gamma_{\vec{k}}|^2 \right)$$

not particle conserving

Mixing Electrons and holes

$$= \sum_{\vec{k}} \left(c^\dagger_{\vec{k}\uparrow} \; c_{-\vec{k}\downarrow} \right) \begin{pmatrix} \underline{\varepsilon_{\vec{k}}} & \Delta_{\vec{k}} \\ \Delta^*_{\vec{k}} & \underline{-\varepsilon_{\vec{k}}} \end{pmatrix} \begin{pmatrix} c_{\vec{k}\uparrow} \\ c^\dagger_{-k\downarrow} \end{pmatrix} + \text{const}$$

Holes: $c_k \Leftrightarrow c^\dagger_k$ and $\varepsilon_k \to -\varepsilon_k$ (alternative point of view)

where $\underline{\Delta_k = V \sum'_{k'} \gamma_{k'}}$

Solved by

Bogoliubov Transformation

superposition of Electron and hole operators

$$a_k = u_k \underline{c_{\vec{k}\uparrow}} - v_k \underline{c^\dagger_{-k\downarrow}}$$

$$b^\dagger_{-k} = v^*_k c_{k\uparrow} + u^*_k c^\dagger_{-k\downarrow}$$

goal:

Ground state $a_k|GS\rangle = b_k|GS\rangle = 0 \;\; \forall k$

Bogoliubov Transformation

$$\begin{pmatrix} a_k \\ b^+_{-k} \end{pmatrix} = U \begin{pmatrix} \psi_{k\uparrow} \\ \psi^+_{-k\downarrow} \end{pmatrix}$$

U = unitary for Fermions

$$[a_k, a^+_{k'}]_+ = [b_k, b^+_{k'}]_+ = \delta_{kk'}$$

etc

preserves commutation relations

$$U = \begin{pmatrix} u & -v \\ v^* & u \end{pmatrix} \quad \text{with} \quad |u|^2 + |v|^2 = 1$$

for $\Delta_k = 0$ we set $a_k |GS\rangle = 0$

if $u_k = 0$, $v_k = 1$ if $k < k_F$

and $u_k = 1$, $v_k = 0$ if $k > k_F$

then $b_k |GS\rangle = 0$

so Fermi sea is recovered for no interaction.

<u>See exercise!</u> (14,15)

Alternatively for bosons:

$$|u^2| - |v|^2 = 1$$

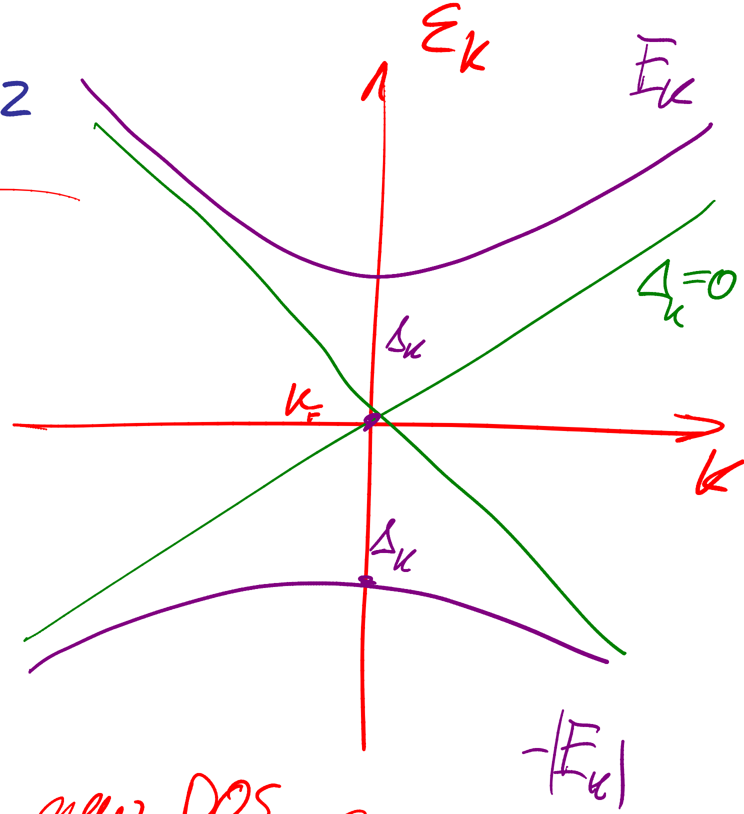
Eigenenergies

$$H_k = \begin{pmatrix} \varepsilon_k & \Delta_k \\ \Delta_k^* & -\varepsilon_k \end{pmatrix}$$

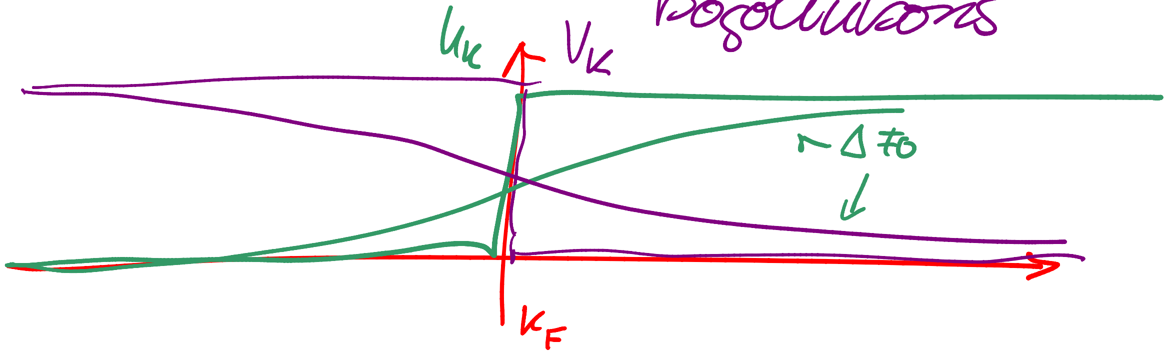
$$E_k = \pm\sqrt{\varepsilon_k^2 + \Delta_k^2}$$

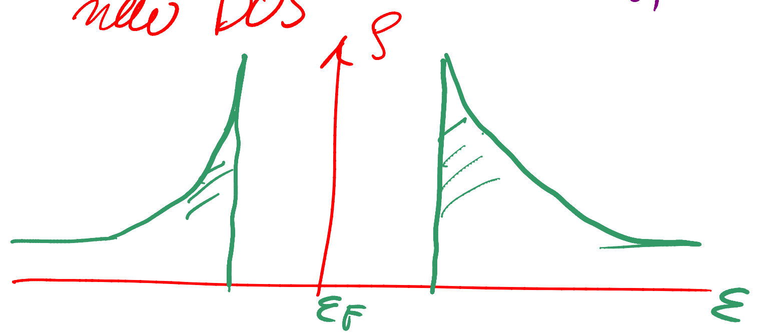
$$u^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_k}{E_k}\right) \qquad v^2 = 1 - u^2$$

$$H = \sum_k |E_{\vec k}| \left(a_{\vec k}^\dagger a_{\vec k} + b_{\vec k}^\dagger b_{\vec k}\right)$$



a_k, b_k are mixtures and are called bogoliubons





Self-consistency: coupling Δ_k is given by expectation value 4.4.6

$a_k|GS\rangle = b_k|GS\rangle = 0$

inverse trafo

$$\gamma_k = \langle c^+_{k\uparrow} c^+_{-k\downarrow} \rangle = \langle (u_k a^+_k + v_k b_{-k})(-v^*_k a_k + u^*_k b^+_{-k}) \rangle$$

$= v_k u^*_k \langle b_{-k} b^+_{-k} \rangle$ anticomm.

$$= v_k u^*_k = \frac{1}{4}\sqrt{1-\frac{\varepsilon_k^2}{E_k^2}} = \frac{1}{4}\frac{\Delta_k}{\sqrt{\varepsilon_k^2+\Delta_k^2}}$$

remember

restricted by approx Debye frequency

$$\Delta_k = \sum_{k'}{}' V \gamma_{k'} = V\int_0^{\hbar\omega_D} d\varepsilon\, g(\varepsilon_F)\, \frac{1}{4}\frac{\Delta}{\sqrt{\varepsilon^2+\Delta^2}} = \Delta\,\frac{V g(\varepsilon_F)}{4}\,\mathrm{arcsinh}\,\frac{\hbar\omega_D}{\Delta}$$

DOS

$$\Rightarrow \Delta = \frac{\hbar\omega_D}{\sinh\left(\frac{4}{V g(\varepsilon_F)}\right)} \approx -2\hbar\omega_D\, e^{+4/g(\varepsilon_F)V}$$

solution for gap

$|V|<0$ and small

Δ exponentially small!

Outcome: new "condensate" state with finite gap (order parameter)

electrons cannot be accelerated, no spin flip possible

to prevent this from happening fields are "energetically" and spontaneously excluded, i.e. ground state expells fields by permanent currents