LECTURE 2B: BCS THEORY OF SUPERCONDUCTIVITY

1. Normal state of a "textbook" metal.

   A. Sommerfeld model

   Free independent electrons obeying Fermi statistics.

   Single-particle states:

$$\Psi_{\underset{\sim}{k}}(\underset{\sim}{r}) = \frac{1}{\sqrt{\Omega}} \exp i\underset{\sim}{k}\cdot\underset{\sim}{r} \qquad \varepsilon_k = \frac{\hbar^2 k^2}{2m}$$

   (Ω ← volume)

   spin component $\sigma = \pm 1/2$

In equilibrium at T, Fermi-Dirac distribution:

$$n(\underset{\sim}{k},\sigma) = \frac{1}{\exp(\varepsilon_k - \mu)/k_B T + 1}$$

(k_F ↙ Fermi wave vector)

at T=0, all states filled for $|k| < k_F$, empty for $|k| > k_F$.

where

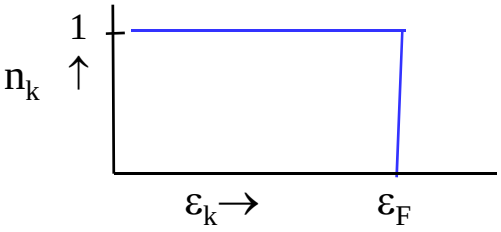
$$k_F \equiv (3\pi^2 n)^{1/3} \qquad (n \equiv N/\Omega)$$

corresponding energy is

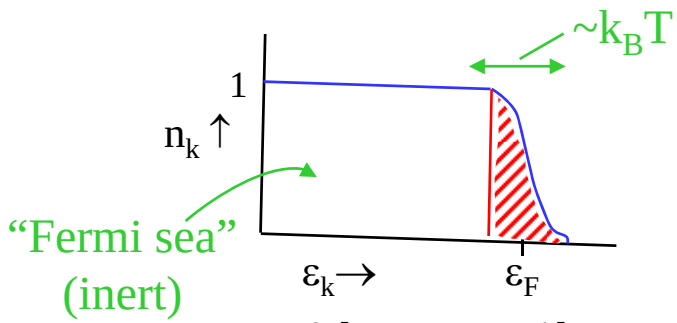
$$\varepsilon_F \equiv \mu(T=0) = \hbar^2 k_F^2 / 2m = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{\Omega}\right)^{1/3}$$ Fermi energy

For typical metal, $\varepsilon_F \sim 10^4 - 10^5 K$ $(\gg T_{melt})$.

At T≠0, μ(T) still ≅ ε_F so distribution modified only in slice of width ~k_B T « ε_F:



$T = 0$



$T \neq 0$ but $\ll \varepsilon_F / k_B$

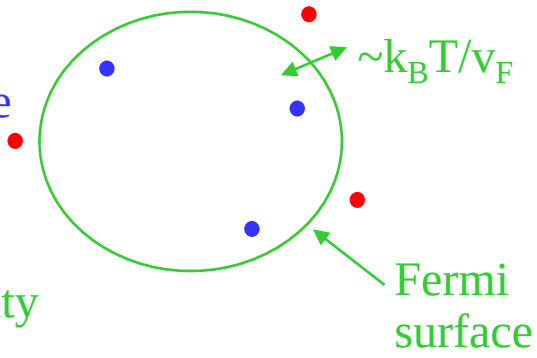
So: all the "action" is in shaded region $|\varepsilon_k - \varepsilon_F| \lesssim k_B T$.

Sommerfeld model (cont.)

Near the surface $|\underset{\sim}{k}| = k_F$ ($\varepsilon_k = \varepsilon_F$) in $\underset{\sim}{k}$-space ("Fermi surface"), we have

$$\varepsilon_k - \varepsilon_F \left(\cong \varepsilon_k - \mu\right) \cong \hbar v_F (|k| - k_F)$$

$(v_F \equiv \hbar k_F / m)$ ← Fermi velocity



and the single-particle density of states (DOS) is given (including a factor of 2 for σ = ↑,↓)* by

$$\frac{dn}{d\varepsilon} = \frac{3n}{2\varepsilon_F} \qquad \text{(Sommerfeld model)}$$

Several basic properties of the system are determined entirely by dn/dε, e.g.

Pauli spin susceptibility $\chi = \mu_B^2 \left(\frac{dn}{d\varepsilon}\right)$

electronic specific heat $c_v = \frac{\pi^2}{3} k_B^2 T \left(\frac{dn}{d\varepsilon}\right)$

Transport in Sommerfeld model:

introduce phenomenological scattering (relaxation) time τ, then dc conductivity given by Drude formula

$$\sigma = ne^2\tau / m$$

However, note that we can equally well write (since $dn/d\varepsilon = 3n/2\varepsilon_F = 3n/(mv_F^2)$)

$$\sigma = \frac{1}{3} v_F^2 \left(\frac{dn}{d\varepsilon}\right) \tau$$

so conductivity (and other transport properties) defined entirely by quantities (v_F, dn/dε) characterizing states close to Fermi surface. (essentially true for all low-energy (low-temperature) properties).

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* ↑: In the superconductivity literature it is conventional to use the DOS for (e.g.) ↑ states only, $N(0) \equiv \frac{1}{2}\left(\frac{dn}{d\varepsilon}\right)$

Normal state (cont.)

B. Bloch model

Electrons still independent, but not "free": feel periodic potential of crystal lattice.

Single-particle states now Bloch waves

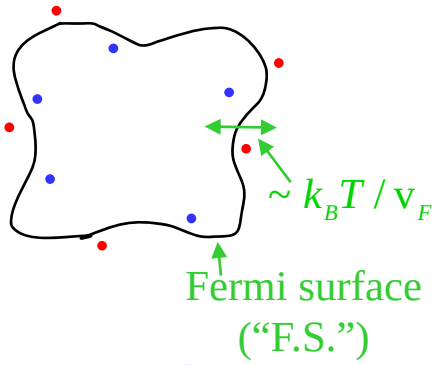
$$\Psi_{kn}(\underset{\sim}{r}) = u_{\underset{\sim}{k}n}(r)\exp i\underset{\sim}{k}\bullet\underset{\sim}{r}$$

band index ↑ ; ↑ has lattice periodicity

Within each band n, energy spectrum is $\varepsilon_n(\underset{\sim}{k})$: in general depends on direction as well as magnitude of $\underset{\sim}{k}$. In most "classic superconductors only one band ("conduction band") is relevant at $T \lesssim T_{melt}$, so drop index n. Thermal equilibrium single-particle distribution is still

$$n(\underset{\sim}{k},\sigma) = \frac{1}{\exp\left(\varepsilon(\underset{\sim}{k}) - \mu\right)/k_B T + 1}$$

so define Fermi surface in $\underset{\sim}{k}$-space as locus of states $\underset{\sim}{k}$ such that $\varepsilon_n(\underset{\sim}{k}) = \mu(0)$ $(\equiv \varepsilon_F)$. In general this is no longer a sphere:



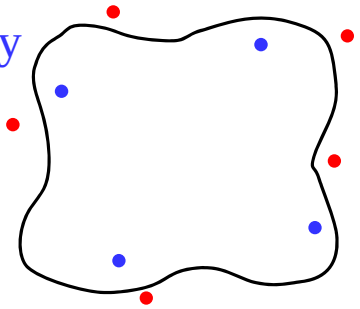
Just as in Sommerfeld case, "elementary" excitations are quasiparticles (•) in states outside Fermi surface and quasiholes (○) inside. We can still define the single-particle DOS (dn/dε) (now depends on the details of spectrum $\varepsilon(\underset{\sim}{k})$) and still have $\chi = \mu_B^2(dn/d\varepsilon)$, $C_v = \frac{\pi^2}{3}k_B^2 T(dn/d\varepsilon)$, but (e.g.) dc conductivity now involves average over F.S.

Most low-energy properties are qualitatively similar in Sommerfeld and Bloch models (! : Hall effect, thermoelectric coefficients . . .). In particular (almost) all low-energy properties are determined by states close to Fermi surface.

Normal state (cont.)

C. Landau-Silin (Fermi-liquid) model

Takes into account (much of) electron-electron interactions both Coulomb and phonon-induced. Low-energy "elementary" excitations are still quasiparticles (•) outside FS and quasiholes (○) inside, but these are now not single electrons (holes) but (e.g.) "electron plus dressing cloud."



Upshot: general picture unchanged, but (a) single-quasiparticle energy spectrum $\varepsilon(\underset{\sim}{k})$ modified, and (b) any macroscopic polarization (e.g. of spin) generates a corresponding molecular field.

Generally, Landau-Silin picture modifies results of Bloch model quantitatively but not qualitatively.

For a qualitative understanding of the superconducting state, it is adequate to start (with BCS) from the simple Sommerfeld picture of the normal state, augmented by a "weak" electron-electron interaction. The "Bloch" and "Landau-Silin" complications change some details of temperature-dependences etc., but rarely affect the properties of the superconducting state qualitatively.

Crucial observation (for "classic" superconductors): always have

$$T_c \ll T_F \left(\equiv \varepsilon_F / k_B\right)$$

Reasonable intuitive hypothesis: only states with $|\varepsilon_k - \mu| \lesssim$ (a few times) T_c involved in formation of superconducting state $\Rightarrow$ mechanism of superconductivity involves only states near Fermi surface.

Digression: What do the eigenfunctions and eigenvalues of $\hat{\rho}_2$ look like in the original Sommerfeld model at T=0 (free Fermi gas without interactions)?

A natural choice: 1 in plane-wave state $\underset{\sim}{k}$, spin state σ, 2 in plane-wave state $\underset{\sim}{k}'$, spin state σ', e.g.

$$\chi(r_1\sigma_1 r_2\sigma_2) = \Omega^{-1}\exp i\underset{\sim}{k}\cdot\underset{\sim}{r},\ \exp i\underset{\sim}{k}'\cdot\underset{\sim}{r}_2\uparrow_1\downarrow_2 \begin{cases}\text{occupied if } |\underset{\sim}{k}|,\ |\underset{\sim}{k}'|<k_F\\ \text{unoccupied otherwise}\end{cases}$$

but this is not correctly antisymmetrized, so correct form is

$$\chi^{(i)}_{\text{singlet}} = \tfrac{1}{\sqrt{2}}\cdot\tfrac{1}{\Omega}(\exp i\underset{\sim}{K}\cdot R)(\cos \underset{\sim}{q}\cdot\rho)\cdot\tfrac{1}{\sqrt{2}}(\uparrow_1\downarrow_2-\downarrow_1\uparrow_2)$$

relative

COM

$$\chi^{(i)}_{\text{triplet}} = \tfrac{1}{\sqrt{2}}\tfrac{1}{\Omega}(\exp i\underset{\sim}{K}\bullet R)(\sin \underset{\sim}{q}\cdot\rho)\cdot\begin{cases}\uparrow_1\uparrow_2\\ \tfrac{1}{\sqrt{2}}(\uparrow_1\downarrow_2+\downarrow_1\uparrow_2)\\ \downarrow_1\downarrow_2\end{cases}$$

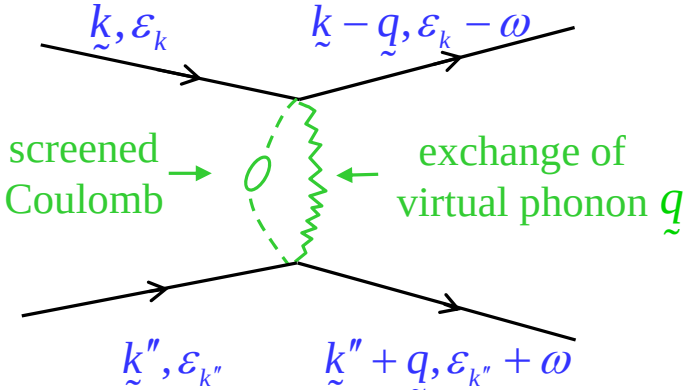
in each case, $n_i = 1$ if $|\underset{\sim}{K}+\underset{\sim}{q}/2|, |\underset{\sim}{K}-\underset{\sim}{q}/2| < k_F$

$n_i = 0$ otherwise.

hence a total of ~N^2 eigenvalues = 1, all others zero.

Electron-electron interaction:

Bardeen-Pines interaction:
screened Coulomb + exchange of virtual phonons.



Exact form:

$$V_{BP}(q,\omega) = \frac{(dn/d\varepsilon)^{-1}}{1+q^2/q_{TF}^2}\ \frac{\omega^2}{\omega^2-\omega_{ph}^2(q)}$$

$(\varepsilon^2\frac{dn}{d\varepsilon}/\varepsilon_0)^{1/2}$ — freq. of phonon with wave vector $\underset{\sim}{q}$

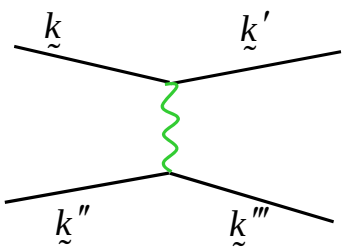
note attractive for $\omega < \omega_{ph}(\underset{\sim}{q})$. (~ ω_D, Debye frequency)

BCS replace by model interaction

$$V(r) = -V_0\delta(\underset{\sim}{r})$$

with restriction

$$|\varepsilon_k-\mu|, |\varepsilon_{k'}-\mu|,\ldots < \omega_D$$



THE COOPER PROBLEM

2 electrons interacting with one another while excluded from the Fermi sea, in spin singlet state with COM momentum K=0.

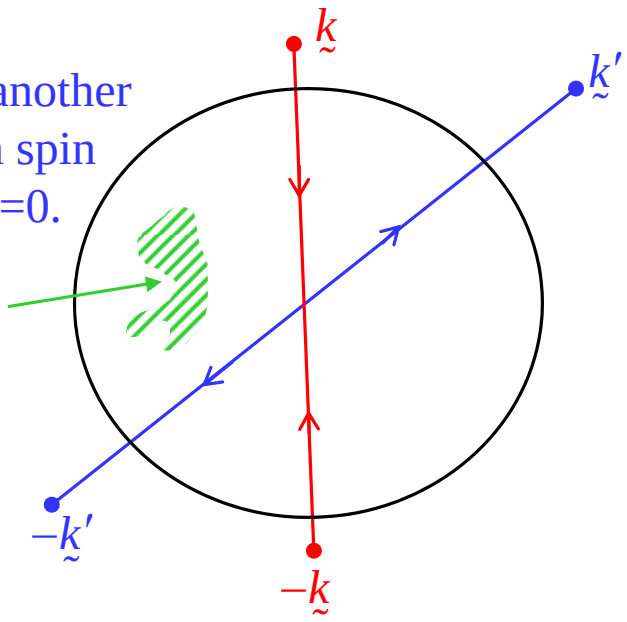
So orbital wave function is

$$\psi_{orb}(\underset{\sim}{r}_1, \underset{\sim}{r}_2) = \psi_{orb}(\underset{\sim}{r}_1 - \underset{\sim}{r}_2)$$

$$\equiv \sum_k e^{i\underset{\sim}{k}\cdot(\underset{\sim}{r}_1 - \underset{\sim}{r}_2)} \psi_k$$

$$\psi_k = \psi_{-k}, \sum_k |\psi_k|^2 = 1$$

antisymmetrization normalization



Define $\varepsilon_k \equiv \frac{\hbar^2 k^2}{2m} - \varepsilon_F$ and measure energy from $2\varepsilon_F$ (min. energy of 2 free particles excluded from Fermi sea)

Then Schrödinger equation is in Fourier-transformed form

$$2\varepsilon_k \psi_k + \sum_{k'} V_{kk'} \psi_{k'} = E\psi_k$$

or

$$\psi_k = -\frac{1}{2\varepsilon_k - E} \sum_{k'} V_{kk'} \psi_{k'}$$

For BCS form of potential $V_{kk'} = \begin{cases} -V_0, \text{ if } |\varepsilon_k|, |\varepsilon_{k'}| < \varepsilon \\ 0, \text{ otherwise} \end{cases}$

take Ψ_k independent of $\hat{k}$, i.e. $\psi_k \equiv C(\varepsilon)$:

$$C(\varepsilon) = \frac{V_c}{2\varepsilon - E} \int_c^{\varepsilon_c} d\varepsilon' \, \rho(\varepsilon') C(\varepsilon')$$

single-spin DOS

approximate $\rho(\varepsilon')$ by N(0);then can take C=const.and integrate over ε:

$$1 = N(0)V_0 \int_0^{\varepsilon_c} \frac{d\varepsilon}{2\varepsilon - E} \cong \frac{N(0)V_0}{2} ln\left(\frac{2\varepsilon_c}{|\varepsilon|}\right) (|E| \ll \varepsilon_c)$$

$$\Rightarrow E \cong -2\varepsilon_c \exp -2/N(0)V_0$$

$\Rightarrow \exists$ bound state for arbitrarily small attraction.

BCS Ansatz

In real life, most natural to minimize not $\hat{H}$ but $\hat{H}-\mu\hat{N}$ so most natural to measure single-particle energies ε_k from μ.

Thus from now on

$$\varepsilon_k \equiv \frac{\hbar^2 k^2}{2m} - \mu$$

So kinetic energy (KE) is (with $-\mu\hat{N}$ subtracted)

$$\hat{T} \equiv \sum_{k\sigma} \varepsilon_k \hat{n}_{k\sigma}$$

For the moment, keep potential energy general:

$$V \equiv \frac{1}{2}\sum_{ij} V(\hat{\underset{\sim}{r}}_i - \hat{\underset{\sim}{r}}_j)$$

Problem: Minimize expectation value of $\hat{H}-\mu\hat{N} \equiv \hat{T}+\hat{V}$.

Generalized BCS state:

$$\Psi_N(t) = \mathbb{N}\cdot\mathcal{A}\cdot\varphi(\underset{\sim}{r}_1\underset{\sim}{r}_2\sigma_1\sigma_2 : t)\varphi(\underset{\sim}{r}_3\underset{\sim}{r}_4\sigma_3\sigma_4 : t)\ldots\varphi(\underset{\sim}{r}_{N-1}\underset{\sim}{r}_N\sigma_{N-1}\sigma_N : t)$$

"BEC"

normalization antisymmetrizer

i.e. a sort of "BEC of di-electronic molecules."

In second-quantization notation:

$$\Psi_N(t) = \left\{\sum_{\alpha\beta}\int\int d\underset{\sim}{r}\, d\underset{\sim}{r}'\, \varphi(\underset{\sim}{r}\underset{\sim}{r}'\alpha\beta : t)\psi_\alpha^\dagger(\underset{\sim}{r})\psi_\beta^\dagger(\underset{\sim}{r}')\right\}^{N/2} |vac\rangle$$

Our task: Find (t-independent) form of $\varphi(rr' : \alpha\beta)$ which minimizes $\langle\hat{T}+\hat{V}\rangle$.

For case of interest (superconducting metal) assume

(a) COM at rest
(b) singlet pairing

$$\Rightarrow \varphi(\underset{\sim}{r}_1\underset{\sim}{r}_2\sigma_1\sigma_2) = \frac{1}{\sqrt{2}}(\uparrow_1\downarrow_2 - \downarrow_1\uparrow_2)\times\varphi(\underset{\sim}{r}_1 - \underset{\sim}{r}_2)$$

Then:

$$\Psi_N = \mathbb{N}''\left(\sum_{\underset{\sim}{k}} c_k a^+_{\underset{\sim}{k}\uparrow} a^+_{-\underset{\sim}{k}\downarrow}\right)^{N/2} |vac\rangle \qquad c_k \equiv \Omega^{-1/2}\int \exp i\underset{\sim}{k}\cdot\underset{\sim}{\rho}\,\varphi(\underset{\sim}{\rho})d\underset{\sim}{\rho}$$

If we set $2\sum_k \frac{|c_k|^2}{1+|c_k|^2} = N$, then $\mathbb{N}'' = 1$. So …

BCS Ansatz for Groundstate (in "particle-conserving" form):

$$\Psi_N = \left(\sum_k c_k a^+_{k\uparrow} a^+_{-k\downarrow}\right)^{N/2} |vac\rangle$$

with normalization

$$2\sum_k \frac{|c_k|^2}{1+|c_k|^2} = N$$

Alternative (conventional, particle-nonconserving) form of Ψ_N

$$\Psi_N = \prod_k (u_k + v_k a_{k\uparrow}^{\ +} a^+_{-k\downarrow})\,|vac\rangle$$

with $|u_k|^2 + |v_k|^2 = 1$, $\quad v_k / u_k = c_k \quad \left(\Rightarrow |v_k|^2 = \frac{|c_k|^2}{1+|c_k|^2}\right)$

Some properties of the BCS groundstate (most easily proved using conventional (particle-nonconserving) form):

1. $\langle n_{k\sigma}\rangle \equiv \langle a^+_{k\sigma} a_{k\sigma}\rangle = \frac{|c_k|^2}{1+|c_k|^2} \qquad \left(\equiv |v_k|^2\right)$

2. $\langle a^+_{k\uparrow} a^+_{-k\downarrow} a^+_{-k'\downarrow} a^+_{k'\uparrow}\rangle = F_k^* F_{k'}$, where

$$F_k \equiv \frac{c_k}{|+|c_k|^2} \qquad (\equiv u_k^* v_k)$$

3. The 2-particle density matrix has, besides $0(N^2)$ eigenvalues of $0(1)$, a single eigenvalue $\sim 0(N)$, with associated eigenfunction (up to normalization)

$$\chi_0(\underset{\sim}{r}_1\sigma_1 \underset{\sim}{r}_2\sigma_2) = \frac{1}{\sqrt{2}}(\uparrow_1\downarrow_2 - \downarrow_2\uparrow_2) \times F(\underset{\sim}{r})$$

$\underset{\sim}{r}_1 - \underset{\sim}{r}_2$

$$F(\underset{\sim}{r}) \equiv \sum_k F_{\underset{\sim}{k}} \exp i\underset{\sim}{k}\cdot\underset{\sim}{r}$$

i.e. COM momentum zero and relative wave function $F(\underset{\sim}{r})$. The associated eigenvalue is

$$N_0 = \sum_k |F_k|^2 \sim 0(N)$$

Thus, $F(\underset{\sim}{r})$ is the closest analog of the relative w.f. $\Psi(\underset{\sim}{r})$ in the 2-particle problem, and is often called the "wave function of the Cooper pairs."

Determination of the optimum form of the pair wave function $F(\underset{\sim}{r})$ (or equivalently of its Fourier transform $F_{\underset{\sim}{k}}$) :

We need to minimize $\left\langle \hat{T} \right\rangle + \left\langle \hat{V} \right\rangle$. In terms of F_k,

$\left\langle \hat{T} \right\rangle = (const.+) \sum_k |\varepsilon_k| \left(1 - \sqrt{1 - 4|F_k|^2}\right)$ (*note* = 0 for $F_k = 0$)

Evaluation of $\left\langle \hat{V} \right\rangle$: For the BCS-ansatz form of Ψ, only 3 types of term contribute:

(1) Hartree: $\left\langle \hat{V} \right\rangle_H = \frac{1}{2} V(0) N^2 = const.$(ind. of F_k) $\Rightarrow$ ignore

(2) Fock: $\left\langle \hat{V} \right\rangle_F = \frac{1}{2} \sum_{k\sigma} V(\underset{\sim}{k} - \underset{\sim}{k}') \left\langle n_{\underset{\sim}{k}\sigma} \right\rangle \left\langle n_{\underset{\sim}{k}'\sigma} \right\rangle$.

In the most general case this is not ignorable. However, we will see that $\langle n_{k\sigma} \rangle$ differs from its N-state value appreciably only for $|\varepsilon_k| \lesssim k_\varepsilon T_c$, so if scale of variation of $V(\underset{\sim}{k} - \underset{\sim}{k}')$ is $\gg k_0 T_c / V_F$ the Fock term is approximately unaffected by the onset of pairing $\Rightarrow$ can ignore.

(3) Pairing:

$$\langle V \rangle_{pair} = \sum_{kk'} V_{kk'} \left\langle a^+_{k\uparrow} a^+_{-k\downarrow} a_{-k'\downarrow} a_{k'\uparrow} \right\rangle = \sum_{kk'} V_{kk'} F_k F^*_{k'}$$

Thus:

$$\left\langle \hat{H} - \mu \hat{N} \right\rangle \{F_k\} = \sum_k |\varepsilon_k| \left(1 - \sqrt{1 - 4|F_k|^2}\right) + \sum_{kk'} V_{kk'} F_k F^*_{k'}$$

note in limit of 2-particle problem ($\mu \to 0$, $F_k \to 0$) this just reduces to

$$\left\langle \hat{H} - \mu \hat{N} \right\rangle \{F_k\} = \sum_k \frac{\hbar^2 k^2}{2 m_r} |F_k|^2 + \sum_{kk'} V_{kk'} F_k F^*_{k'}$$

i.e. 2-particle energy with $\Psi_k \to F_k$. So, correction to Cooper problem ($F_k \to 0$ but μ still = $\varepsilon_F \neq 0$) is nonlinear term of the form

$$\sum_k |\varepsilon_k| |F_k|^4 + 0(F_k^\varepsilon)$$

whose effect is to limit magnitude of F_k.

BCS Gap Equation:

$$\left\langle \hat{H} - \mu \hat{N} \right\rangle = \sum_k \varepsilon_k \left(1 - \sqrt{1 - 4 |F_k|^2} \right) + \sum_{kk'} V_{kk'} F_k F_{k'}^*$$

Vary with respect to F_k^* :

$$\frac{2 |\varepsilon_k| F_k}{\sqrt{1 - 4 |F_k|^2}} + \sum_{k'} V_{kk'} F_{k'} = 0 \qquad (*)$$

This is just the BCS gap equation in disguise! To see this, introduce

$$E_k \equiv \frac{|\varepsilon_k|}{\sqrt{1 - 4 |F_k|^2}}, \quad \Delta_k \equiv \frac{F_k}{|F_k|} \left(E_k^2 - \varepsilon_k^2 \right)^{1/2} \qquad \left(\text{so } F_k = \frac{\Delta_k}{2E_k} \right)$$

then (*) is written

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

standard form of BCS gap equation.

For BCS model potential

$$V_{kk'} \equiv \begin{cases} -V_0, & |\varepsilon_k|, |\varepsilon_{k'}| < \varepsilon_c (\sim \omega_D) \\ 0, & \text{otherwise} \end{cases}$$

$\Delta_k = \text{const.} \equiv \Delta$. The overall phase of Δ is physically meaningless, so set Δ real. Then for $\Delta \ll \varepsilon_c$ the self-consistent solution is

$$\Delta = 2\varepsilon_c \exp -1/N(0)V_0$$

DOS for 1 spin $\left(\equiv \frac{1}{2} \frac{dn}{d\varepsilon} \right)$

Note that the usual case $N(0)V_0 \ll 1$,

$$\Delta \ll \varepsilon_c \sim \omega_D \ll \varepsilon_F$$

so approximation of taking into account only states close to the Fermi surface is well justified.

Digression: Why does BCS model potential give such quantitatively good results? (e.g. for T-dependence of various properties)

Answer: Provided range of variation of "true" potential is $\gg T_c$, can always carry out renormalization and obtain BCS model form, with only unknown V(0) fixed (for given ε_c) by experimental value of Δ (or T_c).

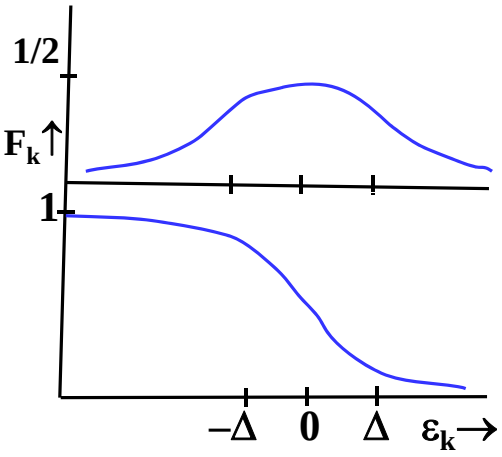
Behavior of Fk and ⟨nk⟩ in BCS groundstate:

$$F_k = \Delta_k / 2E_k \sim \Delta / |\varepsilon_k| \quad \text{for } |\varepsilon_k| \gg \Delta$$

$$\langle n_k \rangle = \frac{1}{2}\left(1 - \frac{\varepsilon_k}{E_k}\right)$$

$$\sim 0\left(\Delta/\varepsilon_k\right)^2 \quad \text{for } \varepsilon_k \gg \Delta$$

$$\sim 1 - 0\left(\Delta/\varepsilon_k\right)^2 \text{ for } \varepsilon_k \ll -\Delta$$

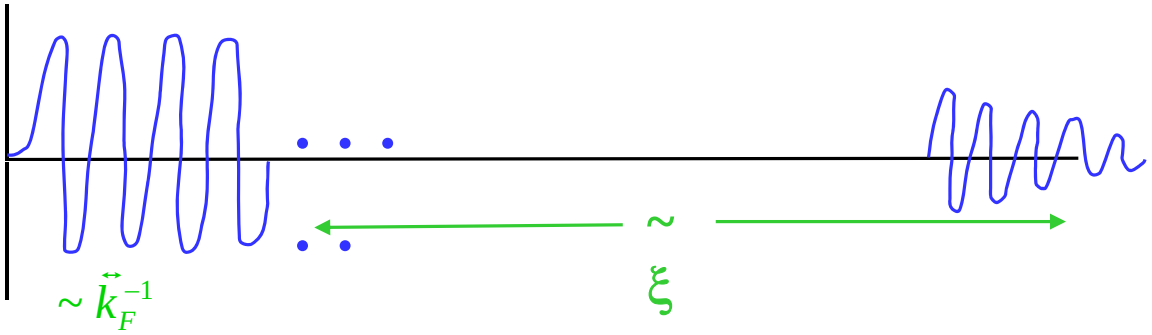


Form of "pair wave function":

$$F(r) = \sum_k F_k e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}}$$

$$= \sum_k \frac{\Delta}{2\varepsilon_k} e^{i\underset{\sim}{k}\cdot\underset{\sim}{r}} \cong \Delta N(0)\frac{\sin k_F r}{k_F r}\exp -r/\xi$$

$$\xi \sim \hbar v_F / \Delta \quad \leftarrow \text{ typically } \sim 10^3 - 10^4 \text{ Å}$$



The "number of Cooper pairs" is the eigenvalue N_0 of $\hat{\rho}_2$. This is given by the normalization of $F(\underset{\sim}{r})$, i.e.

$$N_0 = \Omega \int d\underset{\sim}{r}\,|F(\underset{\sim}{r})|^2 = \Omega \sum_{\underset{\sim}{k}} |F_k|^2 = \frac{\pi}{4}\Delta N(0)\Omega$$

or since $N(0) \sim n/\varepsilon_F$, $\sim 10^{-3} - 10^{-4}$

$$N_0 \sim N(\Delta/\varepsilon_F)$$

so "condensate fraction" N_0/N is very small!

DEFINITION OF AN ORDER PARAMETER IN BCS THEORY

The most natural definition of an order parameter would probably be

$$\Psi = F(0) = \sum_k F_k$$

However, it is actually more convenient to use the fact that for a constant (i.e. k-independent) (possibly nonequilibrium) value Δ of Δ_k there is a simple relation between Δ and Ψ:

$$\Psi = \sum_k \frac{\Delta}{(\varepsilon_k^2 + |\Delta|^2)^{1/2}} = \Delta N(0) \ln 2\varepsilon_c / |\Delta|.$$

So it is equally possible to treat Δ as the order parameter. Then

$$\left.\begin{aligned} \langle T \rangle &= \sum_k \varepsilon_k \left(1 - \frac{\varepsilon_k}{E_k}\right) = N(0)\Delta^2 \left(\ell n\left(\frac{2E_c}{\Delta}\right) - \frac{1}{2}\right) \\ \langle V \rangle &= -V_0 \Psi^2 = -V_0 N^2(0)\Delta^2 \ell n^2\left(\frac{2E_c}{\Delta}\right) \end{aligned}\right\} \Delta \ll E_c$$

These expressions are valid for arbitrary Δ. Minimization of $\langle H - \mu N \rangle \langle T \rangle + \langle V \rangle$ leads back to the BCS expression for the equilibrium value Δ_0 of Δ:

$$\Delta_0 = 2\varepsilon_c \exp -1/N(0)V_0$$

and substitution of this into $\langle T \rangle$ and $\langle V \rangle$ leads to

$$\langle H - \mu N \rangle = N(0)\Delta^2 \left\{ \ell n\left(\frac{\Delta}{\Delta_0}\right) - \frac{1}{2} \right\} \qquad \left(+0\left(\frac{1}{\ell n \varepsilon_c / \Delta}\right)\right)$$

Note that the leading dependence on ε_c has fallen out. This expression has (of course!) a minimum at $\Delta = \Delta_0$, with a value (the "condensation energy" relative to the N state) of

$$E_{case} = -\tfrac{1}{2} N(0)\Delta_0^2$$

and a second derivative

$$\frac{\partial^2 E_{case}}{\partial \Delta^2} = +2N(0)$$

which stabilizes the equilibrium value similarly to a Ψ^4 term. (Note: Near T_c, $F(\Delta) = -\alpha(T)|\Delta|^2 + \tfrac{1}{2}\beta(T)|\Delta|^4$, so analogy to Bose case is more exact.)

ELEMENTARY EXCITATIONS FROM THE BCS GROUNDSTATE

Recall that in the particle-nonconserving formulation the groundstate can be written

$$\Psi_N = \prod_k (u_k + \mathrm{v}_k a^+_{k\uparrow} a^+_{-k\downarrow}) \,|\, \mathrm{vac}\rangle$$

i.e. the occupation state of the pair of plane-wave states $\downarrow \underset{\sim}{k} \uparrow, -\underset{\sim}{k} \downarrow\rangle$ (4D Hilbert space!) is

$$\Psi_{GI} = u_k \,|00\rangle + v_k \,|11\rangle \qquad (\text{“ground pair”})$$

The 4D Hilbert space is spanned by $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. So we can construct two types of excited state in this space

$$\Psi_{BP} = |01\rangle, |10\rangle \qquad (\text{“broken pair”})$$

$$\Psi_{EP} = u^*_k \,|00\rangle - u^*_k \,|11\rangle \qquad (\text{“excited pair” orthogonal to } \Psi_{EP})$$

The energy of the GP state is

$$E_{GP} = |\,\varepsilon_k\,| \left(1 - \sqrt{1 - 4\,|\,F_k\,|^2}\right) + 2F_k \sum_{k'} V_{kk'} F^*_{k'} \quad \left(F_k = \tfrac{\Delta_k}{2E_k}\right)$$

The BP states have $F_k = 0$ *i.e.* $\langle V \rangle = 0$, and $\langle T \rangle = \varepsilon_k$, so $E_{BP} = |\,\varepsilon_k\,|$ while the EP states have $\mathrm{F_k} \to -\mathrm{F_k}$ in the potential term, and their KE is given by $(|\,v_k\,|^2 \to |\,u_k\,|^2)$ $|\,\varepsilon_k\,| \left(1 + \sqrt{1 - 4\,|\,F_k\,|^2}\right)$. Hence

$E_{BP} - E_{GP} = \Re_k$, $E_{EP} - E_{GP} = 2\Re_k$, where

$$\Re_k \equiv |\,\varepsilon_k\,| \sqrt{1 - 4\,|\,F_k\,|^2} + 2F_k \sum_{k'} V_{kk'} F^*_{k'}$$

$$= |\,\varepsilon_k\,| \sqrt{1 - 4\,|\,F_k\,|^2} + \frac{|\Delta_k|^2}{E_k} = \varepsilon_k \left(1 - \frac{\Delta^2}{E_k^2}\right)^{1/2} + \frac{|\Delta_k|^2}{E_k}$$

$$= \frac{\varepsilon_k^2}{E_k} + \frac{|\Delta_k|^2}{E_k} \equiv E_k$$

$\Rightarrow$

EXCITATION ENERGY OF BP STATES IS Ek, OF EP 2Ek

$\Rightarrow$ in BCS model (Δ_k = const. $\equiv \Delta$), minimum excitation energy of system is $|\Delta|$ (hence, Δ is “energy gap”)

$\Rightarrow$ at low T, no. of excitations ~N exp $-\Delta/k_B$ T.

for e.g. N~10^{27}, Δ ~ 20 K, T ~ 5 mK, this is «1!