Lectures on Superconductivity 2023

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Lecture 5
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Normal state: electron-electron interactions and Cooper pair instability

Basic properties of the normal state

Simplest QM model of metal: Sommerfeld model.
N electrons with spin ½ (so 2 spin states ↑, ↓) moving freely in volume $V \equiv L^3$. Apply periodic boundary conditions, then energy eigenstates are

$$\psi_k(\boldsymbol{r}) = \frac{1}{\sqrt{V}} \exp(i\boldsymbol{k}\cdot\boldsymbol{r}) \qquad \text{with } k_x = 2\pi n_x/L \quad \text{(etc.)}$$

and energy

$$\epsilon_k = \hbar^2 k^2/2m$$

so density of states (of both spins) is

$$dn = \frac{2V}{(2\pi)^3} d^3\boldsymbol{k} = \frac{2V}{(2\pi)^3} 4\pi k^2 dk = V \frac{(2m)^{3/2}}{2\pi^2\hbar^3} \epsilon^{1/2} d\epsilon \quad (\equiv V g(\epsilon) d\epsilon)$$

Electrons are fermions, so obey Pauli principle (crucial!)
$\Longrightarrow$ at $T = 0$, electrons occupy lowest-energy N states, that is a sphere in k-space with radius k_F such that

$$\frac{2}{(2\pi)^3} \frac{4\pi}{3} k_F^3 = \mathrm{N}/V \equiv n$$

i.e.

$$k_F = (3\pi^2 n)^{1/3}$$ ← Fermi wave vector, typically $\sim 1\text{Å}^{-1}$

Corresponding energy is

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m}$$ ← Fermi energy, typically $\sim 1 - 10\ eV$ $(\sim 10^4 - 10^5 K)$

For T nonzero, electrons have Fermi distribution

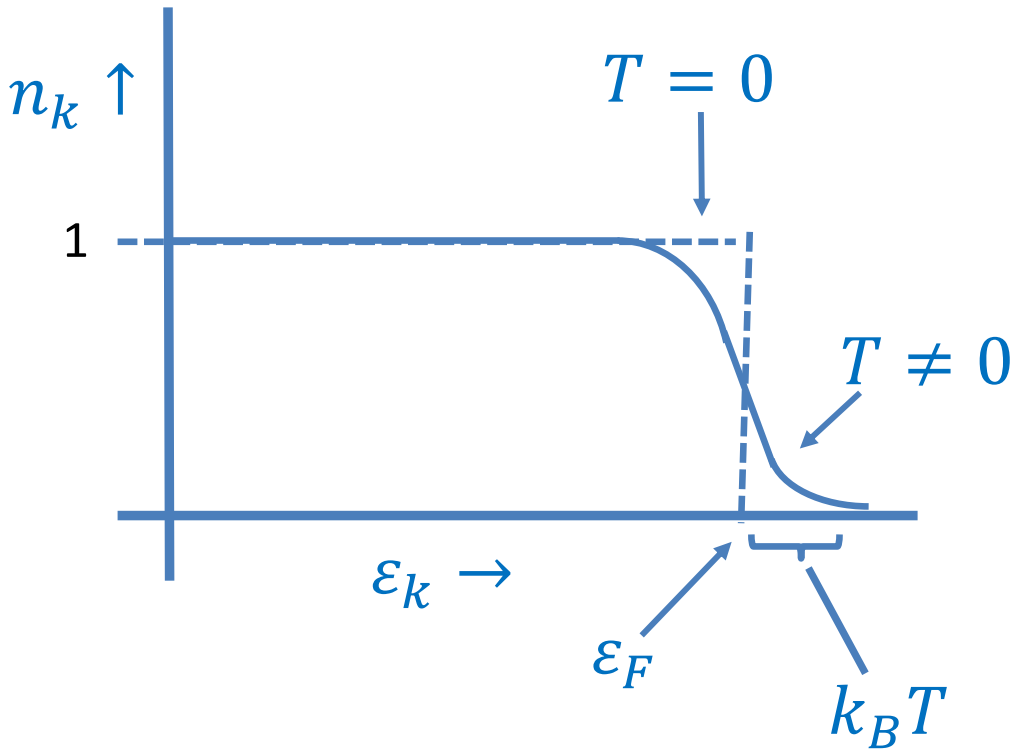
$$n_k = (\exp\beta(\varepsilon_k - \mu) + 1)^{-1}$$

$1/k_BT$

chemical potential. $\approx \varepsilon_F$

Crucial point: at least for "classical" metals, at all T below melting, $kT \ll \varepsilon_F$

$\Longrightarrow$ properties of metals overwhelmingly determined by states near Fermi energy



density of states

Particularly important quantity: DOS (of both spins) per unit energy per unit volume for states near Fermi surface,

$$(dn/d\epsilon) \equiv g(\varepsilon_F) = \frac{(2m)^{3/2}}{2\pi^2\hbar^3}\epsilon_F^{1/2} = 3n/2\varepsilon_F$$

In terms of this,

electronic specific heat $C_V = \frac{\pi^2}{3}k_B^2 T\frac{dn}{d\epsilon}$ (so $\sim k_B T/\varepsilon_F$ times classical value ${}^3/_2\, nk_B$)

Pauli spin susceptibility $\chi_p = \mu_B^2\frac{dn}{d\epsilon}$ ($\sim k_B T/\varepsilon_F$ times classical value $n\mu_B^2/k_B T$)

($\times\ \mu_0$ in S1)

To discuss transport properties in Sommerfeld model, introduce phenomenological scattering time

$\tau \equiv \ell/v_F$ ← $\equiv \hbar k_F/m \equiv$ "Fermi velocity" (typically $\sim 3\text{x}10^6 m/sec \sim 0.01c$)

mean free path

then $\sigma = \frac{e^2}{3}\left(\frac{dn}{d\epsilon}\right)\text{v}_F^2\tau = \frac{ne^2\tau}{m}$

dc conductivity

FS properties

for a good metal (e.g. Cu) at RT, $\rho \equiv \sigma^{-1} \sim$ a few hundred μohm*cm

room temperature

Some important corrections to Sommerfeld model:

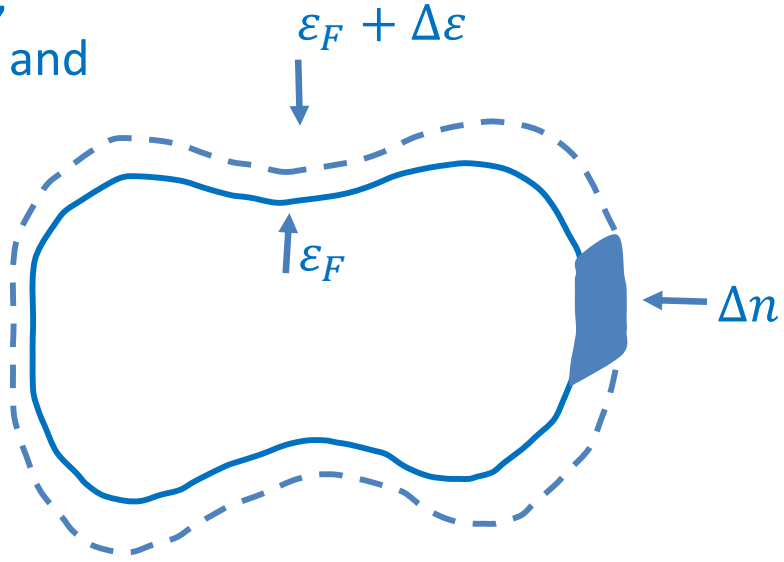
1. Crystal periodicity ⟹ Bloch Model:

   Electrons still non-interacting, but move in periodic potential of $ions$; main consequences:

   (a) band structure ⇒ not all crystalline solids metallic (but at least those with odd number of electrons/unit cell should be)

   (b) within single band, $\varepsilon(\boldsymbol{k}) \neq \hbar^2 k^2/2m$

⇒ locus of ε_F in general not spherical. However, can still define DOS at Fermi energy, $dn/d\epsilon$, and formula for C_V and χ_p in terms of it unchanged



2. Effect of (mostly short-range repulsive) interactions ⇒ Landau-Silin model: low lying excitations now "quasiparticles" (≈ electron plus screening charge) with effective mass m^*, interact via Weiss-type molecular fields.

Neither Bloch nor Landau-Silin modifications change basic structure of BCS theory, so shall assume simple Sommerfeld model plus weak attraction (see below).

How to generate effective attraction between electrons in a metal?

At first sight, have only interaction with static lattice (accounted for in Bloch picture) and Coulomb interaction,

$$\sum_{ij} e^2/4\pi\epsilon_0|\boldsymbol{r}_i - \boldsymbol{r}_j| \ ,$$

which is purely repulsive. However:

(a) Effective Coulomb interaction is screened. To get qualitative feeling, consider response of electrons to charged impurity (ions form constant $+ve$ background.)

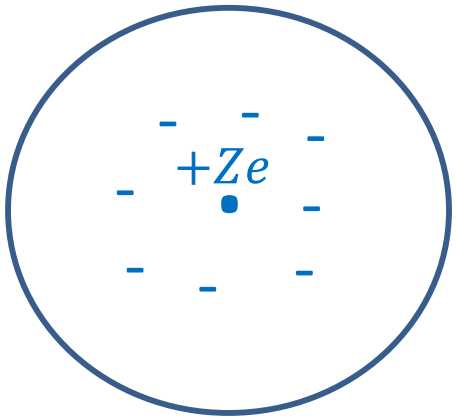
Quantitatively: effective potential at $\boldsymbol{r}$ is

$$V_{eff}(r) = V_{ext}(r) + V_{ind}(r)$$

$+Z\,e^2/r$

due to induced electron cloud

total charge enclosed ≈ 0



$$\nabla^2 V_{ind}(r) = -\rho_{ind}\,(r)/\epsilon_0$$

induced charge density

$$\rho_{ind}(r) = -\chi_0 V_{eff}(r)$$

response induced in non-interacting gas (actually $\sim dn/d\epsilon$)

Taking Fourier transforms and solving gives

$$V_{eff}(q) = \frac{Z\kappa_0}{1 + q^2/q_{TF}^2}$$

$(dn/d\epsilon)^{-1}$

Thomas-Fermi wave vector, $\equiv (e^2/\epsilon_0\kappa_0)^{1/2}$ $\sim 1 - 2\text{Å}^{-1}$

i.e.

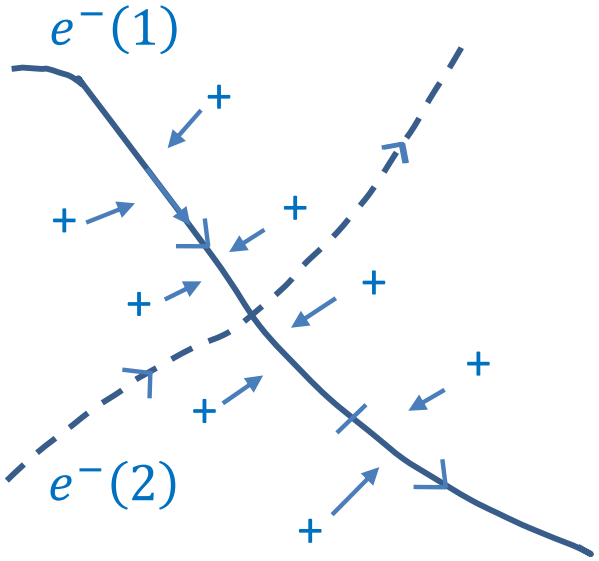
$$V_{eff}(r) \approx \frac{Ze^2}{r}\exp - q_{FT}r$$

Intuitively, same should hold for effective interaction of two electrons…

however, interaction is still repulsive…

How to generate attraction….? (cont.)

2. Effect of ionic motion (phonons): $+ve$ ions attracted to path of $e^-(1)$; but sluggish + slow to relax → after passage of $e^-(1) + ve$ charge remains, can attract $e^-(2)$. Thus,



$e^-(2)$ attracted to past position of $e^-(1)$!
(note: works even if solid not crystalline!)

Illustrative analogy:
2 particles 1, 2 coupled with strength g to SHO of mass m and natural frequency ω_0. Results in time-dependent effective interaction $V_{eff}^{12}(t)$ whose Fourier transform is

simple harmonic oscillator

$$V_{eff}^{12}(\omega) = \frac{g^2}{m}\frac{1}{\omega^2 - \omega_0^2}$$

attraction for $\omega < \omega_0$

Putting considerations 1 and 2 together (and with lots of algebra!) we find that a plausible form of effective interaction of 2 electrons in metal is

Frequency of phonon with wave vector q

$$V_{eff}(q,\omega) = \frac{\kappa_0}{1 + q^2/q_{TF}^2}\left\{1 + \frac{\omega_{ph}^2(q)}{\omega^2 - \omega_{ph}^2(q)}\right\}$$

Bardeen-Pines interaction
Attractive for $\omega < \omega_{ph}(q)$

: If this were exactly right, all metals should be superconductors!

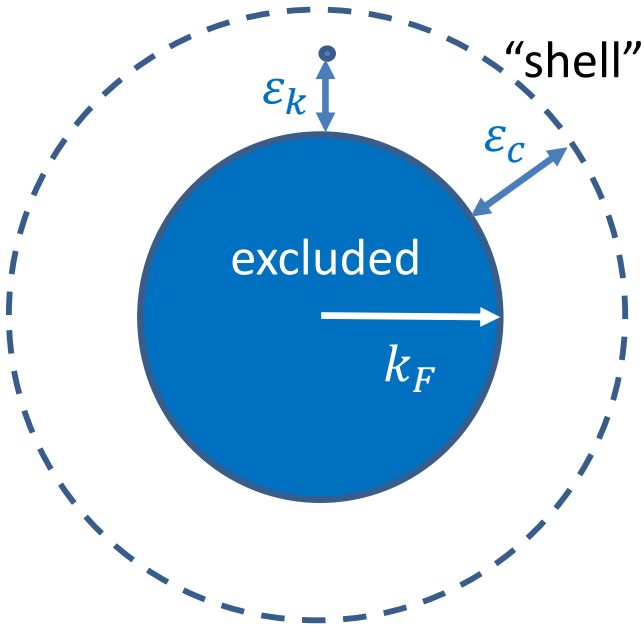
⇒ need more precise calculation taking into account details of band structure, etc.*

But, at end of day, plausible that for at least some metals the "static" $(\omega \to 0)$ interaction can be attractive….

*Some predictions spectacular, e.g. of superconductivity in metallic hydrides with $T_c \sim {}^2/_3$ of RT.

The Cooper problem

2 electrons in singlet spin state, interacting via contact potential $V_0\delta(r)$ (V_0 either sign), but excluded from the Fermi sea (and also from high-energy states with $\varepsilon > \varepsilon_F + \varepsilon_c$). Suppose COM is at rest, then orbital wave function is



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

$$= \sum_{k\ in\ shell} c_k \exp i\boldsymbol{k}\cdot(\boldsymbol{r}_1 - \boldsymbol{r}_2) \quad \text{with} \quad c_k = c_{-k} \quad \sum_k |c_k|^2 = 1$$

↑ $\equiv \boldsymbol{r}$, relative coordinate

↑ Pauli

↑ normalization

It is convenient to measure the kinetic energy $\langle\hat{T}\rangle$ from the value it would have if both electrons were exactly on the Fermi surface ($k = k_F$). Thus,

$$\langle\hat{T}\rangle = \sum_{k\ in\ shell} 2\varepsilon_k |c_k|^2 \qquad \varepsilon_k \equiv \frac{\hbar^2 k^2}{2m} - \varepsilon_F$$

$$(so\ 0 < \varepsilon_k < \varepsilon_c)$$

The potential energy is

$$\langle \hat{V} \rangle = \int \mathrm{V}(\boldsymbol{r})|\psi(\boldsymbol{r})|^2 d\boldsymbol{r} = V_0|\psi(0)|^2 = V_0 \sum_{\leftarrow kk' \text{ in shell}} c_k^* c_{k'}$$

Hence, minimizing $\langle T \rangle + \langle \mathrm{V} \rangle$ subject to the normalization condition and measuring the energy E from $2\varepsilon_F$, we find the $TISE$ ← time-independent Schrödinger equation

$$(2\varepsilon_k - E)c_k = -\mathrm{V}_0 \sum_{k'} c_{k'}$$

or rearranging and replacing

$$c_k \to c(\varepsilon), \sum_{k'} \to \frac{1}{2}\int g(\varepsilon')c(\varepsilon')d\varepsilon' ,$$

(note no spin sum!)

$$c(\varepsilon) = \frac{-\mathrm{V}_o}{2\varepsilon - E}\int_0^{\varepsilon_c} \frac{d\varepsilon'}{2}\big(g(\varepsilon')\big)c(\varepsilon') \qquad (*)$$

Note that so far, the case of 2 electrons interacting in free space is a special case, with ε_F set $= 0$. In that case (in 3D) the DOS $g(\varepsilon') \propto \varepsilon'^{1/2}$, and for small enough V_o equation (*) has no bound-state $(\varepsilon < 0)$ solution, giving the known result:

> in (3D) free space, an arbitrarily weak attractive potential does not give a bound state.

(cf. coordinate-space discussion in lecture 3)

Now the crunch: for the Cooper problem, $g(\varepsilon)$ needs to be given its value at the Fermi energy, *i.e.* the constant value $(dn/d\varepsilon)$ (note in free space this would be the case in 2D). Thus, taking this out of the integral.

$$\mathrm{c}(\epsilon) = \frac{-\frac{1}{2}\left(\frac{dn}{d\epsilon}\right)\mathrm{V}_0}{2\epsilon - E}\int_0^{\epsilon_c} d\epsilon' c(\epsilon')$$

or integrating both sides over ϵ and cancelling the factor $\int_0^{\epsilon_c} c(\epsilon')d\epsilon'$,

$$1 = -\frac{1}{2}\left(\frac{dn}{d\varepsilon}\right)V_0\int_0^{\varepsilon_c}\frac{d\varepsilon}{2\varepsilon - E}$$

We seek a solution with $E < 0$. For V_0 positive (repulsion) no such solution exists. But for V_0 negative (attraction)

$$1 = \frac{1}{2}\left(\frac{dn}{d\epsilon}\right)|\mathrm{V}_0|\ell n\left(\frac{2\varepsilon_c}{-E} + 1\right) \Rightarrow E = -2\varepsilon_c\left(\exp\left(4/\left[\frac{dn}{d\epsilon}|\mathrm{V}_0|\right]\right) - 1\right)^{-1}$$

or in the limit $|\mathrm{V}_0| \to 0$,

$$E = -2\varepsilon_c \exp -4/\left[\left(\frac{dn}{d\epsilon}\right)|\mathrm{V}_0|\right]$$

Thus, state is "bound" in sense that $E < 0$. Is it also "bound" in the sense that $\psi(r) \to 0$ for $r \to \infty$? Yes!

$$\psi(r) = (\text{const.})\frac{1}{r}\frac{\partial}{\eth r}\int_{k_F}^{k(\varepsilon_c)} \frac{\cos kr}{2\varepsilon_k + |E|}\, dk \sim (\cos/\sin k_F r) \times f(r)$$

where $f(r) \sim 1/r$ at small r , $\sim 1/r^2$ at large r (so ψ normalizable). Crossover occurs at distance $r \sim \xi_c$, where

$$\xi_c \sim \hbar v_F/|E| \sim (\hbar v_F/\varepsilon_c)\exp +4/\left(\frac{dn}{d\varepsilon}|V_0|\right)$$

so "effective radius" of pair $\to \infty$ for $|V_0| \to 0$.

What do we expect at nonzero T? Crudely speaking, if we replace in $\int c(\epsilon)d\epsilon$ the lower limit 0 by a value $\sim |E|_{T=0}$, solution disappears. But effect of nonzero T is to "blur" sharp cutoff at $\epsilon = 0$ by amount $\sim k_B T$. Hence expect solution disappears for $T \sim T_c$ where

$$T_c \sim |E|/k_B \sim (\varepsilon_c/k_B)\exp -4/\left[\left(\frac{dn}{d\varepsilon}\right)|V_0|\right].$$

Summary of lecture 5:

A minimal model for superconductivity is the free-electron (Sommerfeld) model plus a weak attractive electron-electron interaction. The overall interaction can be attractive because

(a) the "bare" Coulomb repulsion is strongly screened, and

(b) virtual polarization of the ionic lattice (exchange of virtual phonons) can give rise to an interaction which is attractive at low frequencies.

In the presence of a weak attractive contact interaction $-|V_0|\delta(r)$, a pair of electrons excluded from the Fermi sea form a bound state with energy $\mathrm{E}\sim -2\varepsilon_c exp-4/[(dn/d\epsilon)|V_0|]$ and radius $\sim\hbar v_F/|E|$. At nonzero T the bound state disappears around $T_c\sim|E|/k_B$.