Condensed Matter Physics

Tries to understand the macroscopic behavior of materials — ie systems with huge (often $\sim 10^{24}$) numbers of interacting particles.

Originally the field was called "solid state physics" and dealt primarily with the electrical properties of solids, ie metals, insulators, semi-conductors.

While condensed matter physics has now grown to include the study of a wider variety of systems, such as liquids, polymers, complex fluids, even biological systems, the focus of this course will remain on the electrical properties of solids.

Even when one knows all the relevant microscopic interactions (for solids these are always the electromagnetic interactions that are the important ones), an exact "first principles" calculation of material properties is usually impossible. The system is just too complex to solve analytically, and or even numerically (except perhaps for some simplest cases).

Example: Suppose we want to compute the properties of a metal from "first principles". We are faced with a problem of $\sim 10^{24}$ atoms consisting of nuclei and electrons, all interacting with long ranged Coulomb forces! Even if we simplify the problem to conduction electrons and "ionic cores" (atomic nuclei + bound inner electrons), the problem remains too complex.

For $N \sim 10^{24}$ ion cores at positions $\vec{R}_\alpha$ with momentum $\vec{P}_\alpha$, and ZN conduction electrons (Z is valence number) at positions $\vec{r}_i$ with momentum $\vec{p}_i$, the Hamiltonian is

$$\mathcal{H} = \sum_\alpha \frac{\vec{P}_\alpha^2}{2M} + \sum_i \frac{\vec{p}_i^2}{2m} \qquad \text{kinetic energy}$$

$$+ \sum_{\alpha,\beta} V_{ion-ion}(\vec{R}_\alpha - \vec{R}_\beta) \qquad \text{ion-ion interaction}$$

$$+ \sum_{i,j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \qquad \text{electron-electron interaction}$$

$$+ \sum_{i,\alpha} V_{e-ion}(\vec{r}_i - \vec{R}_\alpha) \qquad \text{electron-ion interaction}$$

Quantum mechanically, the state of the system is described by the wave function

$$\Psi(\vec{r}_1, s_1, \vec{r}_2, s_2, \cdots , \vec{R}_1, S_1, \vec{R}_2, S_2, \cdots)$$

where s_i and S_α are the spins of electron i and ion α, respectively.

We then need to solve for the eigenstates

$$\mathcal{H}\psi_n = E_n\psi_n \qquad \text{where } \psi \text{ has } \sim 10^{26} \text{ degrees of freedom}$$

To compute properties at finite temperature, we would then take these eigenstates and construct the partition function

$$Z = \sum_n e^{-E_n/k_B T}$$

Clearly this plan of solution is impossible to carry out!

Progress in condensed matter physics is therefore a process of making simplifying assumptions that allow one to do a calculation, then checking the result against experiment to see if there is agreement. When new and unexplained experimental data comes up, the goal is then to see if it can be explained by doing a better calculation within the previous accepted approximations, or whether the new data requires one to relax some approximation and include a previously ignored physical process — then the challenge is in understanding what is the relevant physical process or mechanism that

is responsible for the new effects, and how to make an approximation for this mechanism that will allow one to do a new and better calculation.

Standard approximations to start

1) Assume ions are arranged in fixed positions and cannot move — "static lattice approx"

2) Assume electrons do not interact with each other — "independent electron approx"

3) Assume electrons do not interact with the ions — "free electron approx"

what we are left with after all these approx's is an ideal gas of conduction electrons. We effectively assume that all the e-e or e-ion interactions do is to give instantaneous collisions that serve to keep the electron gas at some fixed temperature T.

Surprisingly, one can explain a lot about metals using this very drastic simple model. We will therefore spend the first part of the course dealing with this free electron model.

Drude Model (~1900)

Classical ideal gas of free electrons
to describe behavior of conduction electrons in a metal

what's a metal? Atoms of atomic number Z_a with valence Z. From each atom, Z electrons "detach" from the ionic core and are free to wander through the material. These are the conduction electrons (so each ion remains with $Z_a - Z$ bound core electrons)

N_a is number of atoms

$N = ZN_a$ is number of conduction electrons

conduction electron density in volume V

$$m = \frac{N}{V} = 0.6022 \times 10^{24} \frac{Z \rho}{A}$$

↑ Avogadro's number

ρ = mass density of metal (g/cm^3)

A = atomic mass of atom $(g/mole)$

Another measure of electron density is

r_s = radius of sphere whose volume is the volume per conduction electron

$$\frac{4}{3}\pi r_s^3 = \frac{V}{N} = \frac{1}{m} \implies r_s = \left(\frac{3}{4\pi m}\right)^{1/3}$$

Convenient to give r_s in units of the Bohr radius $a_0 = 0.529 \times 10^{-8}$ cm

Some metals

Element	Z	$n \ (\times 10^{22}/cm^3)$	r_s/a_0
Li	1	4.7	1.72
Na	1	2.65	2.08
K	1	1.40	2.57
Rb	1	1.15	2.75
Cs	1	0.91	2.98
Cu	1	8.47	1.41
Ag	1	5.86	1.60
Au	1	5.90	1.59
Be	2	24.7	0.99
Mg	2	8.61	1.41
Ca	2	4.61	1.73
Sr	2	3.55	1.89
Ba	2	3.15	1.96

generally $r_s/a_0 \sim 2-3$

Drude model

Conduction electron obeys equation of motion:

$$\frac{d\vec{p}}{dt} = \vec{f}_{ex}(t) + \vec{f}_{coll}(t)$$

$\vec{f}_{ex}$ is external applied force, typically from applied electric and magnetic fields.

$\vec{f}_{coll}$ is force due to "collisions" — imagined to be collisions between the electron and either the ions or other electrons (both these turn out to be wrong)

Assume collisions are <u>instantaneous</u> — ie time for a collision is $\ll$ time between collisions (somehow long range coulomb forces are being replaced by short ranged "collisions"!)

Between collisions, electron moves like a free particle acted on by force $\vec{f}_{ex}$.

Collisions are instantaneous events that change electron velocity randomly — serve to keep electron gas in thermal equilibrium

Collision occur at rate $1/\tau$

τ = "relaxation time"

Average equation of motion over all electrons

$$\langle \vec{p} \rangle = \frac{1}{N} \sum_i \vec{p}_i$$

$$\frac{d \langle \vec{p} \rangle}{dt} = \vec{f}_{ext}(t) + \langle \vec{f}_{coll} \rangle$$

What is $\langle \vec{f}_{coll} \rangle$?

Electron enters collision with momentum $\vec{p}_{initial}$.
Electron exits collision with momentum $\vec{p}_{final}$
Change in momentum is $\vec{p}_{final} - \vec{p}_{initial}$
Rate of collisions $\frac{1}{\tau}$

So: $\langle \vec{f}_{coll} \rangle = \dfrac{\langle \vec{p}_{final} - \vec{p}_{initial} \rangle}{\tau}$

Now by assumption, the electron exists a collision
with random momentum chosen from the
equilibrium distribution. $\Rightarrow \langle \vec{p}_{final} \rangle = 0$
 (since equilib distrib depends only on $|\vec{p}|$)

$$\langle \vec{f}_{coll} \rangle = - \frac{\langle \vec{p}_{initial} \rangle}{\tau}$$

But $\langle \vec{p}_{initial} \rangle = \langle \vec{p} \rangle$ average momentum

So finally $\langle \vec{f}_{coll} \rangle = - \dfrac{\langle \vec{p} \rangle}{\tau}$ and

$$\boxed{\frac{d \langle \vec{p} \rangle}{dt} = \vec{f}_{ex}(t) - \frac{\langle \vec{p} \rangle}{\tau}}$$

Hence forth we drop the brackets $\langle\rangle$, and $\vec{p}$ will be used to denote the <u>average</u> momentum of the electrons

DC electric conductivity

Ohms Law: $\underline{V = IR}$

voltage↑ current↑ → resistance

$V = EL$, E is electric field, L is length
$I = jA$, $\vec{j}$ is current density, A is crosssection area

$\Rightarrow E = j\dfrac{AR}{L} = j\rho$

where $R = \dfrac{L\rho}{A}$, ρ is the <u>resistivity</u>

$j = \left(\dfrac{1}{\rho}\right)E = \sigma E$, σ is the conductivity

Expect ρ, σ to be independent of system volume

Compute σ within Drude model:

$\vec{f}_{ex} = -e\vec{E}$ $-e$ is electron charge
                    $\vec{E}$ is uniform dc electric field

$\dfrac{d\vec{p}}{dt} = \vec{f}_{ex} - \dfrac{\vec{p}}{e} = -e\vec{E} - \dfrac{\vec{p}}{e}$

for steady state d.c. behavior, average momentum is constant in time, so $d\vec{p}/dt = 0$

$$\Rightarrow \quad \vec{p} = -e\vec{E}\tau$$

Current density $\vec{j} = -ne\vec{v}$

$\vec{v} = \frac{\vec{p}}{m}$ is average electron velocity

n is electron density

$$\vec{j} = -ne\frac{\vec{p}}{m} = -\frac{ne}{m}(-e\vec{E}\tau) = \frac{ne^2\tau}{m}\vec{E}$$

$$\Rightarrow \quad \boxed{\sigma = \frac{ne^2\tau}{m}}$$

Since the collisions are just treated phenomelogically in the Drude model, rather than coming from a more microscopic theory that would allow one to compute τ, the above is really just a way to determine Drude's relaxation time τ from experimental measurement of conductivity σ.

Typical resistivities ρ at room temperature are

$$\rho \sim 10 \,\mu\Omega\text{-cm} \quad (\text{micro ohm cm})$$

gives $\tau \sim 10^{-14} - 10^{-15}$ sec

Is this a reasonable value for τ?

mean free path = average distance between collisions

$$\ell = v_0 \tau$$

$$\quad \overset{\uparrow}{\text{average electron speed}}$$

For a classical ideal gas of electrons

$$\langle \tfrac{1}{2} m v_0^2 \rangle = \tfrac{3}{2} k_B T$$

gives

$\quad v_0 \sim 10^7$ cm/sec   at room temperature

using $\tau \sim 10^{-14}$ to 10^{-15} sec   at room temp

gives $\quad \ell \sim 1$ to 10 Å

Above value of ℓ is comparable to inter ionic spacings, it seems that Drude model is consistent with idea that collisions are due to electrons colliding with ions.

But: at lower $T \sim 77°K$, v_0 is smaller since $v_0 \sim \sqrt{T}$, but ρ is measured to be smaller too!

at $T \sim 77°K$, $\rho \sim 1$ $\mu\Omega$-cm $\Rightarrow$ $\tau \sim 10^{-13}$ to 10^{-14} sec

$\quad v_0 \sim .5 \times 10^7$ cm/sec $\Rightarrow \ell \sim 5$ to 50 Å

When we consider the more correct quantum mechanical treatment of the electron gas, we will find that actually $v_0 \sim 10^8$ cm/sec and is roughly independent of temperature, thus giving $\ell \sim 100$ to 1000 Å at low $T \sim 77°K$. This is too big to be explained by a simple picture of colliding with static ions!

In quantum picture, ~~we will~~ where electron is viewed like a wave, we will see that a periodic array of static ions does not, in fact, scatter the electron at all! Collisions are therefore not with the ions, but rather occur when an ion is displaced from its periodic array position due to thermal vibrations. These thermal vibrations of the ions are "phonons". Electric resistivity is thus due (except at very low temp) due to "electron-phonon" scattering.

O O O
O O ← ion displaced from its perfect periodic position
O O O   causes scattering of electron wave.