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Ashcroft & Mermin

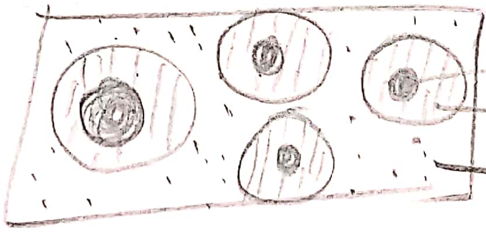
Drude Theory of Metals:

Metals :– Excellent conductors of heat & electricity, ductile & malleable, has luster. Why these properties?

Drude's is the first theory (1900).
→ inspired by kinetic theory of gases & applied to electrons.

Assumptions:

Atom with Z_a atomic number gives out Z electrons to the e^- gas. Atoms becomes ions with +ve charge of $Z_a - Z$.



What is the density of the e^- gas?

$$\#\text{ of } e^- \text{ per unit volume} = \frac{\text{mass of metal}}{\text{volume}} \times \frac{\text{no. of atoms}}{\text{mass of metal}} \times \frac{\text{no. of } e^-\text{s}}{\text{atom}}$$

$$= \text{density } \rho_m \times \frac{6.023 \times 10^{23}}{\text{atomic mass in grams}} \times Z$$

12 gms of Carbon has 6.023×10^{23} carbon atoms
1 mole.

$$n = 6.023 \times 10^{23} \cdot \frac{Z \rho_m}{A}$$

A → atomic mass in grams

Thus, volume occupied by a single electron $= \frac{1}{n}$ & its radius is given by

$$\frac{1}{n} = \frac{4\pi r_s^3}{3}$$

& the radius of the sphere within which only a single e^- is present is

$$r_s = \left(\frac{3}{4\pi n}\right)^{1/3}.$$

Compare the radius r_s of an electron volume in metals with a_0, the radius of Hydrogen atom in ground state $a_0 = \frac{\hbar^2}{me^2}$. $\frac{r_s}{a_0}$, a dimensionless number then gives an idea about how "spread out" the e^-s are in the metal. $a_0 = 0.5$ Å, and $\frac{r_s}{a_0}$ of metals are usually 2 to 3 ($\approx 1.0 - 1.5$ Å) but can also be between 3 & 6 for Alkali metals.

This density is much larger than that of the density of gases analyzed using kinetic theory.

Assumptions of Drude model:

(1) Interaction of e^-s with other e^-s neglected → Independent e^- approximation
very difficult to reinstate

Interaction of e^-s with ions neglected - free e^- approximation.
relatively easy to correct this.

② Collisions between $\bar{e}$'s neglected. Collisions between $\bar{e}$'s & ions accounted for → which changes the velocity of $\bar{e}$'s abruptly. Between two collisions $\bar{e}$'s travel freely.

③ Average time between collisions assumed to be $\underline{\tau}$ (relaxation time). Thus the probability for collision between t & $t+dt$ is dt/τ. τ is assumed to be independent of $\bar{e}$'s position & velocity.

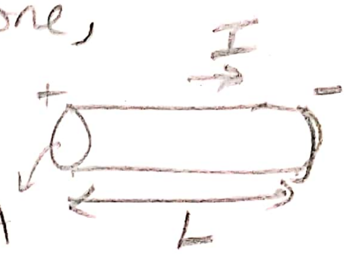
④ How heating a metal affects the electron? The velocity of an $\bar{e}$ right after a collision is determined by the temperature at the place where the collision happened. Thus, heats gets to the ions & from ions, get passed onto $\bar{e}$'s.

With the above assumptions, let us begin to calculate conductivity of a metal. The goal of the derivation is to calculate an observable, macroscopic property from non-observable microscopic properties. Then this relation can be inverted to calculate the non-observable quantities by measuring observable quantities.

DC conductivity of a Metal :-

Ohm's law : $V = IR$ → depends on dimension of the conductor. (Extrinsic)

To convert the law into intrinsic one, remember that



current density $j = \frac{I}{A}$.

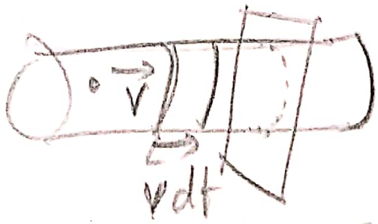
Electric field $E = \frac{V}{L}$

and resistivity ρ is given through the relation $R = \frac{\rho . L}{A}$.

Thus $E . \cancel{L} = (j . A)\left(\frac{\rho \cancel{L}}{A}\right) \Rightarrow E = \rho j$.

Since E & j are vectors, we write

$$\vec{E} = \rho \vec{j}$$



Calculation of current from microscopic quantities:

In a time dt, $\bar{e}$s traveling with an average velocity $\vec{v}$ will travel a distance $L = \vec{v}\,dt$.

So in a time dt, the number of electrons crossing an area A is

the number of electrons per unit volume
× Area A × Length L

$= n \cdot A \cdot \vec{v}\, dt$

And the charges flowing across area A is $-e \times \#$ of $\bar{e}$ (charge)
in a time dt $= -ne\vec{v} A dt$

Thus, current, defined as charges flowing across the wire in unit time is $I = ne\vec{V}A$.

$$\therefore \quad j = \frac{I}{A} = -ne\vec{v}$$

j: macroscopic quantity

n: number density of $\bar{e}$'s

e: charge of $\bar{e}$

$\vec{v}$: average velocity of $\bar{e}$

n, e, $\vec{v}$: microscopic quantities

When there is no electric field, the average velocity of $\bar{e}$'s is zero, because $\bar{e}$'s can move in all possible directions, thereby canceling the currents produced. Thus $\langle \vec{v} \rangle = 0$.

[This is why we wrote $E = \rho j$ as a vector equation].

Thus, when $E = 0$, $j = 0$.

When we apply a voltage 'V' across the wire, the $\bar{e}$'s feel an electric field locally, where

$$E = \frac{V}{L}.$$

Say an $\bar{e}$ emerges from a collision at $t=0$ with a velocity $\vec{v}_0$ and feels the presence of an electric field $\vec{E}$. After a time 't', its velocity is $\vec{v}_0 + a.t = \vec{v}_0 + \frac{F}{m}.t$.

a ↓ acceleration

But $\vec{F} = -e\vec{E}$ in an electric field.

Therefore, $\vec{v} = \vec{v}_0 + \left(\frac{-eE}{m}\right).t$

The average velocity of an $\bar{e}$ after a collision at time t is, then,

$$\langle \vec{v} \rangle = \langle \vec{v}_0 \rangle + \left\langle \frac{-eEt}{m} \right\rangle$$

Since we have assumed that $\vec{v}_0$, the velocity right after collision is directionless, $\langle \vec{v}_0 \rangle = 0$. And $\langle t \rangle = \tau$, the relaxation time.

$$\therefore \langle \vec{v} \rangle = \frac{-eE\tau}{m}$$

and $\vec{j} = -ne\vec{v} \Rightarrow \boxed{\vec{j} = \frac{ne^2\tau}{m}.E}$

Thus, <u>Conductivity</u> of a metal, with electron density 'n', is

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

Since we have found a way to calculate the number density n $\left(= 6.023 \times 10^{23} \cdot \frac{Z \rho_m}{A}\right)$, and know m & e, and can also measure the macroscopic quantity σ (conductivity or $1/\sigma = \rho$) we can evaluate the relaxation time as

$$\tau = \frac{m}{\rho n e^2}.$$

If we plug in the numbers, we find that

$$\tau \approx 10^{-14} \text{ to } 10^{-15} \text{ seconds.}$$

That is the time taken by e^-s on flight between collisions.

How to verify this?

If we know the average velocity of e^-s, we can calculate the distance traveled between collisions and see if that is a reasonable number. How to calculate average velocity of e^-s in the absence of $\vec{E}$? We can guess that the velocity has to do with temperature.

Drude, from kinetic theory of gases, used equipartition theorem, that every degree of freedom gets $\frac{1}{2} k_B T$ to calculate $\langle v \rangle$.

WRONG!

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Even though we know that, because of quantum mechanics, this evaluation would be wrong, we proceed: For $\bar{e}$'s, the average kinetic energy, with 3 degrees of freedom, is

$$\frac{1}{2} m \langle v \rangle^2 = \frac{3}{2} k_B T.$$

From this Drude calculated the mean free path $\lambda = \langle v \rangle \tau$ to be about 1 to 10 Å. This is the same distance as interatomic spacing. Everything works out! Electrons collide with ions in the lattice and the time taken between collisions and the mean free path turns out to be of the correct magnitude.

$\Rightarrow$ In reality, the mean free paths of $\bar{e}$'s in metals can go upto 1000 Å's or more. Drude was wrong because he did not use QM.

Because τ, calculated using Drude's model, is unreliable, we will look for quantities (macroscopic) that are independent of τ: Conductivity in the presence of magnetic field $\rightarrow$ Hall effect.

To derive conductivity of metals in the presence of magnetic field, we should first write the equation of motion of an electron:

How does the momentum of electron vary in the presence of electric / magnetic fields?

*Learn how to derive differential equation describing a process.

Given $\vec{p}(t)$, the momentum of e^- at time t, what will its momentum be at $t+dt$, $\vec{p}(t+dt)$?

Remember that the probability of collision of e^- with ions in the interval t & $t+dt$ is dt/τ.
So the probability for no collision is $1-dt/\tau$.
In the period τ without collision, the e^- acquires an additional momentum $\boxed{f(t)\,dt + O(dt)^2}$ from external fields. i.e., $\vec{p}(t) \to \vec{p}(t) + \vec{f}(t)dt$

Thus, the momentum at time $t+dt$ is

$$\vec{p}(t+dt) = \text{probability of no collision} \times \text{momentum at } t+dt$$
$$+ \left(\text{probability of collision} \times \text{momentum after collision at } t+dt\right)$$

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$$\bar{p}(t+dt) = \left(1 - \frac{dt}{\tau}\right)\left[\bar{p}(t) + \bar{f}(t)\,dt + \mathcal{O}(dt)^2\right]$$

$$+ \frac{dt}{\tau}\left[\text{momentum after collision at } t+dt\right]$$

↳ this is $\mathcal{O}(dt)$ because after collision, velocity is randomized.

upto first order in dt [ignoring $\mathcal{O}(dt^2)$],

$$\bar{p}(t+dt) = \bar{p}(t) + \bar{f}(t)\,dt - \frac{p(t)\cdot dt}{\tau} + \mathcal{O}(dt^2)$$

$$\frac{\bar{p}(t+dt) - \bar{p}(t)}{dt} = \frac{-\vec{p}(t)}{\tau} + \vec{f}(t)$$

Taking the limit $dt \to 0$, we get

$$\boxed{\frac{d\vec{p}(t)}{dt} = \frac{-\vec{p}(t)}{\tau} + \vec{f}(t)}$$

If there is no external Electric or magnetic field, $\bar{f}(t) = 0$ and the solution for the above diff. eqn is

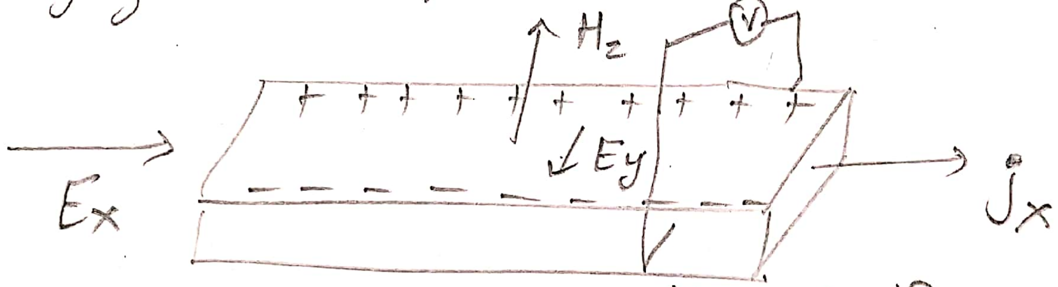
$$\boxed{\vec{p}(t) = \vec{p}_0\, e^{-t/\tau}}$$

which implies that the average momentum along any given direction is zero after relaxation time.

This is because the e's collide with ions within a time τ and randomize their velocities. So the average is zero. The long-time evolution of $\vec{p}(t)$ is determined by $\vec{f}(t)$.

Quantification of Hall effect :-

In 1879, Hall tried to measure the increase in resistance when a current-carrying wire is placed in a magnetic field.



As the e's move through the metal, the magnetic field $\perp$ to their velocity direction will push them to the sides of the conductor. [right hand rule]. When they are against the side walls, they cannot move further & will create a transverse voltage, measured across the side walls. The force on the e's depend, through Lorentz force

$$\vec{F} = -e\vec{v} \times \vec{H},$$

on both the current and on the magnetic field.

The transverse electric field E_y opposes this Lorentz force and balances it out.
Thus E_y would be proportional to the current I and magnetic field H. The proportionality constant, called Hall coefficient, is

$$\boxed{R_H = \frac{E_y}{j_x \cdot H_z}}$$

This can be used to determine the sign of the charge carriers. If the current is made of e^-s, then they will be pushed to one side & if it is made of positive charges (holes) they will also be pushed to the same side, because for the same current direction, the +ve charges flow along the direction & -ve charges flow opposite to the current direction. Then, the sign of E_y will be different, depending upon the sign of the charge carriers.

Let us calculate R_H using Drude's model.

Using our equation for e^-s under forces,

$$\boxed{\frac{d\vec{p}}{dt} = \frac{-\vec{p}}{\tau} + \vec{f}(t)}$$

where $\vec{f}(t)$ here is $-e\vec{E} + \frac{\vec{p}}{mc} \times \vec{H}$,

cgs units.

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we get $\frac{d\vec{p}}{dt} = \frac{-\vec{p}}{\tau} - e\left(E + \frac{\vec{p}}{mc} \times \vec{H}\right)$

In steady state, the current, & hence $\vec{p}$ is independent of time. $\therefore \frac{dp}{dt} = 0$.

Thus,

$$-\frac{p_x}{\tau} - e\left(E_x + \frac{H_z p_y}{mc}\right) = 0$$

and

$$-\frac{p_y}{\tau} - e\left(E_y - \frac{H_z p_x}{mc}\right) = 0$$

say $\omega_c = \frac{eH_z}{mc}$

then

$$p_x + \omega_c \cdot \tau \cdot p_y = -eE_x \cdot \tau$$

& $$p_y - \omega_c \tau p_x = -eE_y \cdot \tau$$

Converting the $\bar{e}$ momentum $\vec{p}$ to current density $\vec{j}$ by multiplying the above eqns with $\frac{-ne}{m}$,

$$-ne\underbrace{\frac{p_x}{m}}_{v_x} + \omega_c \cdot \tau \cdot \left(-ne\underbrace{\frac{p_y}{m}}_{v_y}\right) = \left(\frac{ne^2\tau}{m}\right) \cdot E_x$$

$$= j_x + \omega_c \tau \cdot j_y = \sigma_0 \cdot E_x$$

where $\sigma_0 = \frac{ne^2\tau}{m}$ is the conductivity we derived a while ago.

& $$j_y - \omega_c \tau j_x = \sigma_0 E_y$$

In the above equations, $j_y = 0$.
There is no transverse current.

$$\therefore \quad -\omega_c \tau j_x = \sigma_0 E_y$$

$$\text{or} \quad E_y = \left(\frac{-\omega_c \tau}{\sigma_0}\right) j_x$$

Substituting for $\omega_c = \frac{eH_z}{mc}$ & $\sigma_0 = \frac{ne^2\tau}{m}$,

$$E_y = \left[\frac{-1}{nec}\right] j_x H_z .$$

Since we have defined earlier the Hall coefficient as

$$R_H = \frac{E_y}{j_x H_z},$$

we see that $\boxed{R_H = -\frac{1}{nec}}$.

n = electron density (or hole) & e = electronic charge.
c = velocity of light.

<u>R_H just depends on the charge carrier density!!!</u>

No dependence on τ (which was wrong anyway).

This result is valid even today, in the limit of low temperatures, high magnetic fields and very pure samples. → can be used to measure charge density.