Band Theory and Electronic Properties of Solids

Phys 674

Physics & Astronomy
King Saud University
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Week No. 01

The Drude Theory of Metals

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Basic Assumptions of the Model

Todays Lecture Outline:

- *Basic Assumptions of the Drude Model for metals*
- *DC ELECTRICAL CONDUCTIVITY OF A METAL*
- *Hall Effect and Magnetoresistance*
- *AC ELECTRICAL CONDUCTIVITY OF A METAL*
- *Thermal Conductivity of Metals*

Basic Assumptions of the Model

Before Drude: #1

① charge was discovered

② Current was " and so as Volt.

③ Faraday law was known (1831)

④ Ohm's law was established (1827)

⑤ light bulb was used (1879)

⑥ AC generator was developed by Tesla (1880)

⑦ electron charge was measured (1897)

Basic Assumptions of the Model

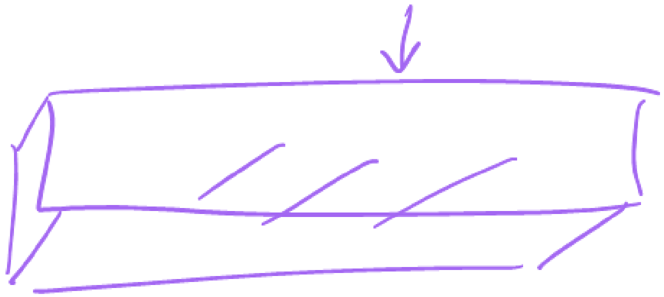
① in 1897 electron was discoverd

② He selected metals

③ Basics of His Theory:

① It depends on same princ. of K.T. of Gas.

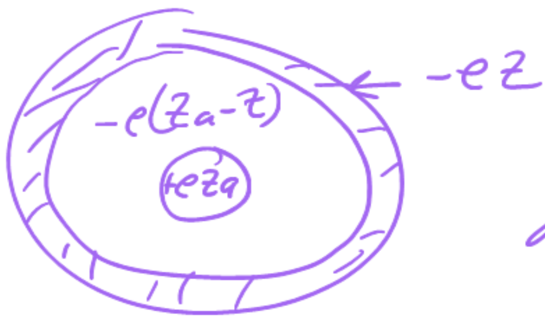
- All atoms are considered as solid sphere
- atoms do not Interact except for collision
- collisions are Instantaneous.
- Neglecting atoms volume.



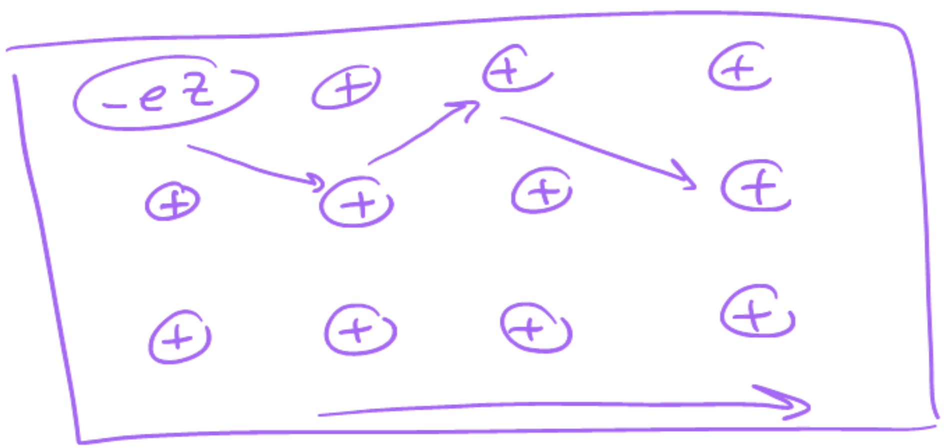
for the electrons:

Basic Assumptions of the Model

① We considered electrons around atom as: core electrons (All electrons In all orbitals except the last "valence" e's)



this is the atom or Independent by its own.



Basic Assumptions of the Model

For electrons:

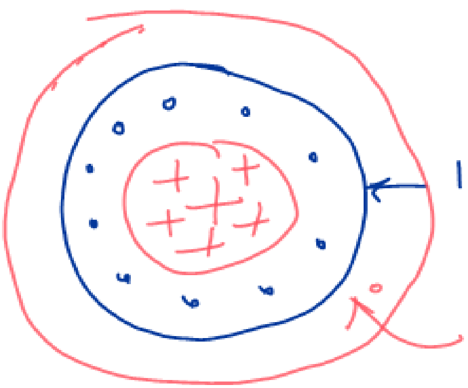
1. Free to move
2. They move in straight lines even after collisions
3. they can collide only with ⊕
4. No interaction with other electron
5. Also no interaction with ions except for coll.
6. After collision: $P = 0$
7. Between the collisions:
   e suffer from 2 forces:
   - $-eE$
   - $-eV \times B$
8. τ = constant.

Basic Assumptions of the Model

example: Na:

Configuration: $1s^2\ 2s^2\ 2p^6\ 3s^1$

10 electrons are core (for $1s^2\ 2s^2\ 2p^6$); $3s^1$ → free electron



10 electrons

1 electron orbits ⇒ Free to move

If there is Electric field E is applied:

⇒ electrons will suffer from collisions

Basic Assumptions of the Model

But overall they will drift as a current

* If momentum of 1 e is $\vec{p}(t)$:

⇒ Newton's 2nd Law : $\frac{d\vec{p}}{dt} = \vec{F}(t)$

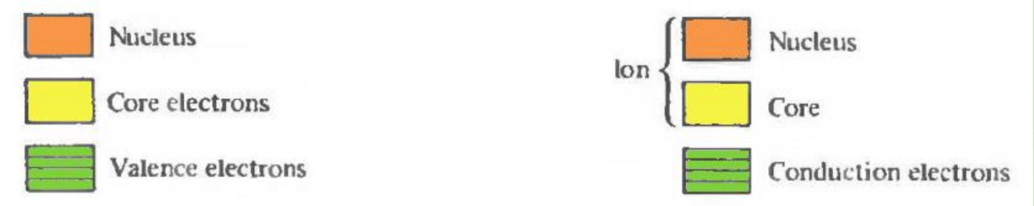
Basic Assumptions of the Model

- Metals are excellent conductors of heat and electricity.
- Indeed. the metallic state has proved to be one of the great fundamental states of matter
- 3 years after Thomson's discovery of electrons (1897); Drude constructed his theory of electrical and thermal conduction by applying the highly successful kinetic theory of gases to a metal, considered as a gas of electrons.
- In its simplest form kinetic theory treats the molecules of a gas as identical solid spheres, which move in straight lines until they collide with one another.
- The time taken up by a single collision is assumed to be negligible, and, except for the forces coming momentarily into play during each collision; no other forces are assumed to act between the particles.

Basic Assumptions of the Model

- This model assumes that electrons can move while nuclei are considered immobile.
- At his time there was no precise notion of the origin of the mobile electrons and the heavier, immobile, positively charged particles. The solution to this problem is one of the fundamental achievements of the modern quantum theory of solids.
- We assume that when atoms of a metallic element are brought together to form a metal; the valence electrons become detached and wander freely through the metal, while the metallic ions remain intact and play the role of the immobile positive particles in Drude's theory.

Fig. 1.1: Schematic picture of an isolated atom (left) and when in a metal the nucleus and ion core retain their configuration in the free atom. But the valence electrons leave the atom to form the electron gas.



Basic Assumptions of the Model

- For single isolated atom:
  - *$+eZ_a$ is the charge of the nucleus (Z_a = atomic no.)*
  - *$-eZ_a$ is the charge of surrounding electrons*
  - *Z of these electrons are weakly bound to the nucleus*
  - *(Z_a-Z) is the no. of tightly bound electrons (core electrons)*
- When these isolated atoms condense to form a metal, the core electrons remain bound to the nucleus to form the metallic ion, but the valence electrons are allowed to wander far away from their parent atoms.
- *These electrons are called: conduction electrons*
- *On average there are: 10^{22} conduction electrons/cm^3*
- These densities are typically a thousand times greater than those of a classical gas at normal temperatures and pressures.

Basic Assumptions of the Model

The basic assumptions of the Drude model are:

- ❑ Between collisions the interaction of a given electron, both with the others and with the ions, is neglected and thus the electron will move in a straight line (no external fields applied).
- ❑ In the presence of externally applied fields each electron is taken to move as determined by ***Newton's laws of motion*** in the presence of those external fields, but neglecting the additional complicated fields produced by the other electrons and ions.
- ❑ The neglect of electron-electron interactions between collisions is known as the ***independent electron approximation***.
- ❑ The corresponding neglect of electron-ion interactions is known as the ***free electron approximation***
- ❑ the free electron approximation must be abandoned if one is to arrive at even a qualitative understanding of metallic behavior.

Basic Assumptions of the Model

The basic assumptions of the Drude model are:

- Collisions in the Drude model, as in kinetic theory, are instantaneous events that abruptly alter the velocity of an electron. Drude attributed them to the electrons bouncing off the impenetrable ion cores
- We shall assume that an electron experiences a collision with a probability per unit time $1/\tau$. We mean by this that the probability of an electron undergoing a collision in any infinitesimal time interval of length dt is just dt/τ.
- τ: Relaxation time OR Collision time OR the mean free time
- the collision time τ is taken to be independent of an electron's position and velocity
- Electrons are assumed to achieve thermal equilibrium with their surroundings only through collisions

DC ELECTRICAL CONDUCTIVITY OF A METAL

DC electrical Conductivity

like above : $\frac{dP}{dt} = F \Rightarrow P = Ft$ . . . (1)

let $t = \tau$ (collision relaxation time)

$\therefore \quad \vec{P} = F\tau$ - - - - - (2)

$\because \quad \vec{F} = q\bar{E}$. - . . - - - (3)

$\Rightarrow \quad \vec{P} = q\vec{E}\tau$ - - - - - (4)

Current density $\vec{J} = q \cdot n \cdot v$

$= \frac{nqP}{m}$ - - - (5)

DC ELECTRICAL CONDUCTIVITY OF A METAL

(4) in (5) for P:

$$\therefore \vec{J} = \frac{nq}{m} \cdot qE\tau = \frac{nq^2\tau}{m} \cdot \vec{E} \quad \text{--- (6)}$$

Ohm's Law: $\vec{J} = \sigma \vec{E}$ --- (7)

by Comparison: $\sigma = \frac{nq^2\tau}{m}$ --- (8)

Where σ: conductivity.

$\therefore \sigma \propto n$: No. of electrons

$\propto q^2$: charge of $e = -1.6 \times 10^{-19}$ C

$\propto \frac{1}{m}$: mass " e

DC ELECTRICAL CONDUCTIVITY OF A METAL

and $\sigma \propto \tau$

But τ depends on:

1. density
2. Temp.
3. purity of conductor

Testing Drude model using Hall eff.

if $R_H = -\frac{1}{ne} \Rightarrow n = -\frac{1}{R_H \cdot e}$

this density of electrons is observed using Hall exp. let $n \equiv n^o$

note that in:
monovalent D.M. is sccessfull.
- but in Divalent and Trivalent
$\Rightarrow$ D.M. Fails.
why?
It Ignores effects such as: Fermi surface and electron Correlations

Valency	Element	n $(10^{22}/\text{cm}^3)$	n^o/n
1	Li	4.70	0.8
	Na	2.65	1.2
	K	1.40	1.1
	Rb	1.15	1.0
1	Cu	8.47	1.5
	Ag	5.86	1.3
	Au	5.90	1.5
2	Be	24.7	-0.2
	Mg	8.61	-0.4
3	Al	18.1	-0.3
	In	11.5	-0.3

DC ELECTRICAL CONDUCTIVITY OF A METAL

- Based on Ohm's Law: $V = IR$ (1.1)
- The Drude model provides an estimate of the resistance *R*
- Or using resistivity: $\mathbf{E} = \rho\mathbf{j}$ (1.2)
- $\mathbf{j} = I/A$ and thus: $R = \rho L/A$
- $\mathbf{j} = -ne\mathbf{v}_{avg}$ (1.3)
- where *n = no.* electrons per unit volume
- $\mathbf{v}_{avg}$ is defined as:

$$v_{avg} = -\frac{e\boldsymbol{E}\tau}{m}$$

$$\therefore \mathbf{j} = \left(\frac{ne^2\tau}{m}\right)\mathbf{E} \qquad (1.4)$$

$$\because \mathbf{j} = \sigma\boldsymbol{E}$$

$$\therefore \sigma = \frac{ne^2\tau}{m} \qquad (1.5)$$

- This establishes the linear dependence of **j** on **E**

DC ELECTRICAL CONDUCTIVITY OF A METAL

- Hence, the relaxation time is:

$$\tau = \frac{m}{\rho n e^2} \qquad (1.6)$$

- At any time *t,* the average electronic velocity **v** is just **p**(t)/m, where **p** is the total momentum per electron. Hence the current density is:

$$\mathbf{j} = \frac{ne\boldsymbol{p}}{m} \qquad (1.7)$$

DC ELECTRICAL CONDUCTIVITY OF A METAL

ELECTRICAL RESISTIVITIES OF SELECTED ELEMENTS[a]

ELEMENT	77 K	273 K	373 K	$\frac{(\rho/T)_{373\ K}}{(\rho/T)_{273\ K}}$
Li	1.04	8.55	12.4	1.06
Na	0.8	4.2	Melted	
K	1.38	6.1	Melted	
Rb	2.2	11.0	Melted	
Cs	4.5	18.8	Melted	
Cu	0.2	1.56	2.24	1.05
Ag	0.3	1.51	2.13	1.03
Au	0.5	2.04	2.84	1.02
Be		2.8	5.3	1.39
Mg	0.62	3.9	5.6	1.05
Ca		3.43	5.0	1.07
Sr	7	23		
Ba	17	60		
Nb	3.0	15.2	19.2	0.92
Fe	0.66	8.9	14.7	1.21
Zn	1.1	5.5	7.8	1.04
Cd	1.6	6.8		
Hg	5.8	Melted	Melted	
Al	0.3	2.45	3.55	1.06
Ga	2.75	13.6	Melted	
In	1.8	8.0	12.1	1.11
Tl	3.7	15	22.8	1.11
Sn	2.1	10.6	15.8	1.09
Pb	4.7	19.0	27.0	1.04
Bi	35	107	156	1.07
Sb	8	39	59	1.11

DRUDE RELAXATION TIMES IN UNITS OF 10^{-14} SECOND[a]

ELEMENT	77 K	273 K	373 K
Li	7.3	0.88	0.61
Na	17	3.2	
K	18	4.1	
Rb	14	2.8	
Cs	8.6	2.1	
Cu	21	2.7	1.9
Ag	20	4.0	2.8
Au	12	3.0	2.1
Be		0.51	0.27
Mg	6.7	1.1	0.74
Ca		2.2	1.5
Sr	1.4	0.44	
Ba	0.66	0.19	
Nb	2.1	0.42	0.33
Fe	3.2	0.24	0.14
Zn	2.4	0.49	0.34
Cd	2.4	0.56	
Hg	0.71		
Al	6.5	0.80	0.55
Ga	0.84	0.17	
In	1.7	0.38	0.25
Tl	0.91	0.22	0.15
Sn	1.1	0.23	0.15
Pb	0.57	0.14	0.099
Bi	0.072	0.023	0.016
Sb	0.27	0.055	0.036

Example 1

The resistivity of Cu is 1.7×10^{-8} Ωm at 300 K and the electron density is 8.5×10^{28} m^{-3}.

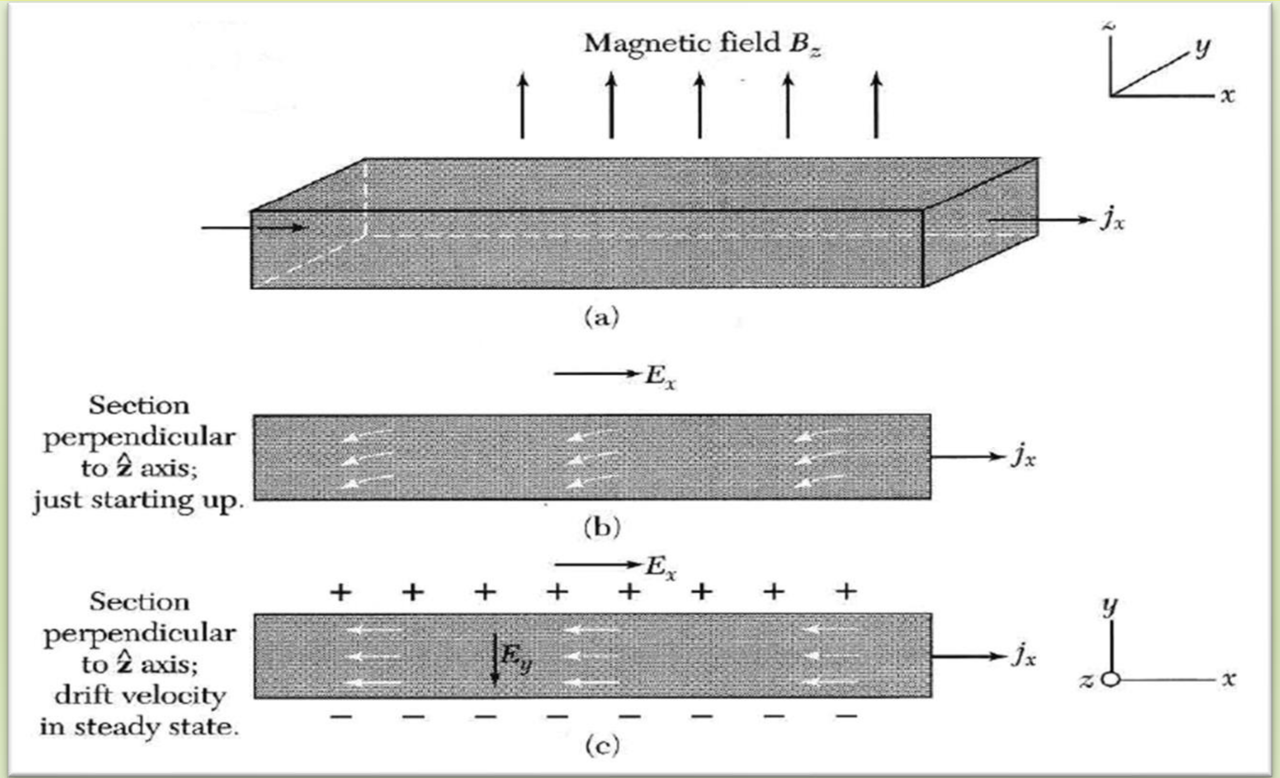
(a) Calculate the relaxation time of electrons in Cu at 300 K .

(b) Calculate the mean free path of the electrons using Drude approximation

$$\tau = \frac{m_e}{\rho n e^2} = \frac{9.1\times10^{-31}}{1.7\times10^{-8}.\,8.5\times10^{28}(1.6\times10^{-19})^2} = 2.38\times10^{-14}\ s$$

Hall Effect and Magnetoresistance

- Hall assumed that if the current of electricity in a fixed conductor is itself attracted by a magnet, the current should be drawn to one side of the wire, and therefore the resistance experienced should be increased but without experimental results.



Hall Effect and Magnetoresistance

❑ Motion of electrons in magnetic and electric fields:

$$F = m\frac{d\mathbf{v}}{dt} = \hbar\frac{d\mathbf{k}}{dt} = -e\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right) \qquad (1.8)$$

If no magnetic field applied:

$$\rightarrow \hbar\frac{d\mathbf{k}}{dt} = -e\,\mathbf{E} = \mathbf{F} \qquad (1.9)$$

Integrating both sides and rearranging terms

$$\delta\mathbf{k} = -\frac{e}{\hbar}\mathbf{E}t$$

$$\rightarrow \hbar\frac{\delta\mathbf{k}}{t} = -e\mathbf{E} = \mathbf{F}$$

Adding the friction effect (proportional to $1/\tau$)

$$\hbar\left(\frac{d}{dt} + \frac{1}{\tau}\right)\delta\mathbf{k} = \mathbf{F} \qquad (1.10)$$

Hall Effect and Magnetoresistance

- Equation (1.10) has two terms:

$\hbar \frac{d}{dt} \delta \boldsymbol{k}$ (acceleration term)

and: $\hbar \frac{\delta \boldsymbol{k}}{\tau}$ (force of friction term).

Magnetic field adds:

$$\mathbf{F} = -e\left(\frac{1}{c}\mathbf{v}\times\mathbf{B}\right) \quad (1.11)$$

- Please note that the *c* is added only if using the CGS system of units.
- The force shown in eq. (1.8) is the total force on the electron and is called: *Lorentz force*

Hall Effect and Magnetoresistance

- Using $m\boldsymbol{v} = \hbar\delta\boldsymbol{k}$: then use B at z direction, (1.8) leads to:

$$m\left(\frac{d}{dt}+\frac{1}{\tau}\right)\mathbf{v} = -e\left(\mathbf{E}+\frac{1}{c}\mathbf{v}\times\mathbf{B}\right) \qquad (1.12)$$

$$m\left(\frac{d}{dt}+\frac{1}{\tau}\right)v_x = -e\left(E_x+\frac{B}{c}v_y\right) \qquad (1.13)$$

$$m\left(\frac{d}{dt}+\frac{1}{\tau}\right)v_y = -e\left(E_y-\frac{B}{c}v_x\right) \qquad (1.14)$$

$$m\left(\frac{d}{dt}+\frac{1}{\tau}\right)v_z = -eE_z \qquad (1.15)$$

$$\bar{v}\times\bar{B} = \begin{vmatrix} i & j & k \\ v_x & v_y & v_z \\ B_x & B_y & B_z \end{vmatrix}$$

note : $B_y = B_x = 0$, $B = B_z$

$$\therefore \bar{v}\times\bar{B} = i\,(v_y B_z - 0) = i\, v_y B$$
$$- j\,(v_x B_z - 0) = j\, v_x B$$
$$+ k\,(0-0)$$

Hall Effect and Magnetoresistance

- At equilibrium, derivative → 0

$$v_x = -\frac{e\tau}{m}E_x - \omega_c \tau v_y \qquad (1.16)$$

$$v_y = -\frac{e\tau}{m}E_y + \omega_c \tau v_x \qquad (1.17)$$

$$v_z = -\frac{e\tau}{m}E_z \qquad (1.18)$$

- In Hall experiment, a new voltage builds up across the conductor due to the build-up of charges:

$$\left.\begin{aligned} &\because v_y = -\frac{e\tau}{m}E_y + \omega_c \tau v_x \\ &\therefore \frac{e\tau}{m}E_y = \omega_c \tau v_x - v_y \\ &v_y = 0, \ \therefore \frac{e\tau}{m}E_y = \omega_c \tau v_x \end{aligned}\right\} \qquad (1.19)$$

Hall Effect and Magnetoresistance

$$\because v_x = -\frac{e\tau}{m}E_x - \omega_c \tau v_y = -\frac{e\tau}{m}E_x$$

$$\therefore \frac{e\tau}{m}E_y = \omega_c \tau \left(-\frac{e\tau}{m}E_x \right)$$

$$\therefore E_y = \omega_c \tau \left(-E_x \right)$$

$$\therefore E_y = -\omega_c \tau E_x$$

$$\therefore E_y = -\frac{eB\tau}{mc}E_x \qquad (1.20)$$

In SI System :

$$\left.\begin{aligned} E_y &= -\frac{eB\tau}{m}E_x \\ R_H &= \frac{E_y}{J_x B} \end{aligned}\right\} \qquad (1.21)$$

Where the cyclotron frequency is:

$$\omega_c = \frac{eB}{mc}$$

Hall Effect and Magnetoresistance

- R_H is called: Hall coefficient:

$$\therefore j_x = \frac{ne^2\tau}{m} E_x$$

$$\therefore R_H = \frac{-\frac{eB\tau}{m} E_x}{\frac{ne^2\tau}{m} E_x B}$$

$$\therefore R_H = -\frac{1}{ne} \qquad (SI) \qquad (1.22)$$

- This is a very striking result, for it asserts that the Hall coefficient depends on no parameters of the metal except the density of carriers

Hall Effect and Magnetoresistance

- Since we have already calculated *n* assuming that the atomic valence electrons become the metallic conduction electrons, a measurement of the Hall constant provides a direct test of the validity of this assumption.
- In trying to extract the electron density *n* from measured Hall coefficients one is faced with the problem that, contrary to the prediction of (1.22), they generally do depend on magnetic field
- Furthermore, they depend on temperature and on the care with which the sample has been prepared
- This result is somewhat unexpected, since the relaxation time τ, which can depend strongly on temperature and the condition of the sample, does not appear in (1.22).
- However, at very low temperature, the measured Hall constants do appear to approach a limiting value.

Hall Effect and Magnetoresistance

Some Hall coefficients at high and moderate fields are listed in the table . Note the occurrence of cases in which R_H is actually positive, apparently corresponding to carriers with a ***positive*** charge. A striking example of observed field dependence totally unexplained by Drude theory is shown in the Figure on the next slide

HALL COEFFICIENTS OF SELECTED ELEMENTS IN MODERATE TO HIGH FIELDS[a]

METAL	VALENCE	$-1/R_H nec$
Li	1	0.8
Na	1	1.2
K	1	1.1
Rb	1	1.0
Cs	1	0.9
Cu	1	1.5
Ag	1	1.3
Au	1	1.5
Be	2	−0.2
Mg	2	−0.4
In	3	−0.3
Al	3	−0.3

[a] These are roughly the limiting values assumed by R_H as the field becomes very large (of order 10^4 G), and the temperature very low, in carefully prepared specimens. The data are quoted in the form n_0/n, where n_0 is the density for which the Drude form (1.21) agrees with the measured R_H: $n_0 = -1/R_H ec$. Evidently the alkali metals obey the Drude result reasonably well, the noble metals (Cu, Ag, Au) less well, and the remaining entries, not at all.

According to D.M.:

$$R_H = \frac{-1}{n_0 e} \quad --- (1)$$

n here is only conduction electrons

for electron-based; R_H must be -tive

However; we have R_H (+tive)

this is Because D.M. fails to Include holes

from table:

Alkali metals: Li, Na, K, Rb and Cs : Valency = +1

$$(1) \Rightarrow \frac{-1}{R_H n e c} = \frac{n_0 e}{n e} = \frac{n_0}{n}$$

in this case:

all these metals $\rightarrow \sim 1$ $(n_0 \approx n)$

$\Rightarrow$ sucsess of D.M.

* in Noble metals: Cu, Ag and Au (Also Valency = 1)

$\frac{n_c}{n} > 1 \Rightarrow$ D.M. is not in full agreement with exp.

* Be + Mg (Valency = 2)

$\frac{n_c}{n}$ is -tive (D.M. fails)

it fails in sign and magnetude

why?

Diavalent metals often have multiple Conduction Bands

$\Rightarrow$ more Complex Charge Carrier dynamics

- tive sign is due to holes + the above.

Hall Effect and Magnetoresistance

In Al: Trivalen (+3)

same as in Diavalent.

Resuls:

1. D.M. failed to Include Band structure
2. " " " " multiple charge Type
3. " " " " Fermi surface

Hall Effect and Magnetoresistance

- The Drude result confirms Hall's observation that the resistance does not depend on field, for when $j_y = 0$ (as is the case in the steady state when the Hall field has been established), the expected result for the conductivity in zero magnetic field.

Figure 1.4
The quantity $n_0/n = -1/R_H nec$, for aluminum, as a function of $\omega_c\tau$. The free electron density n is based on a nominal chemical valence of 3. The high field value suggests only one carrier per primitive cell, with a positive charge. (From R. Lück, *Phys. Stat. Sol.* **18**, 49 (1966).)

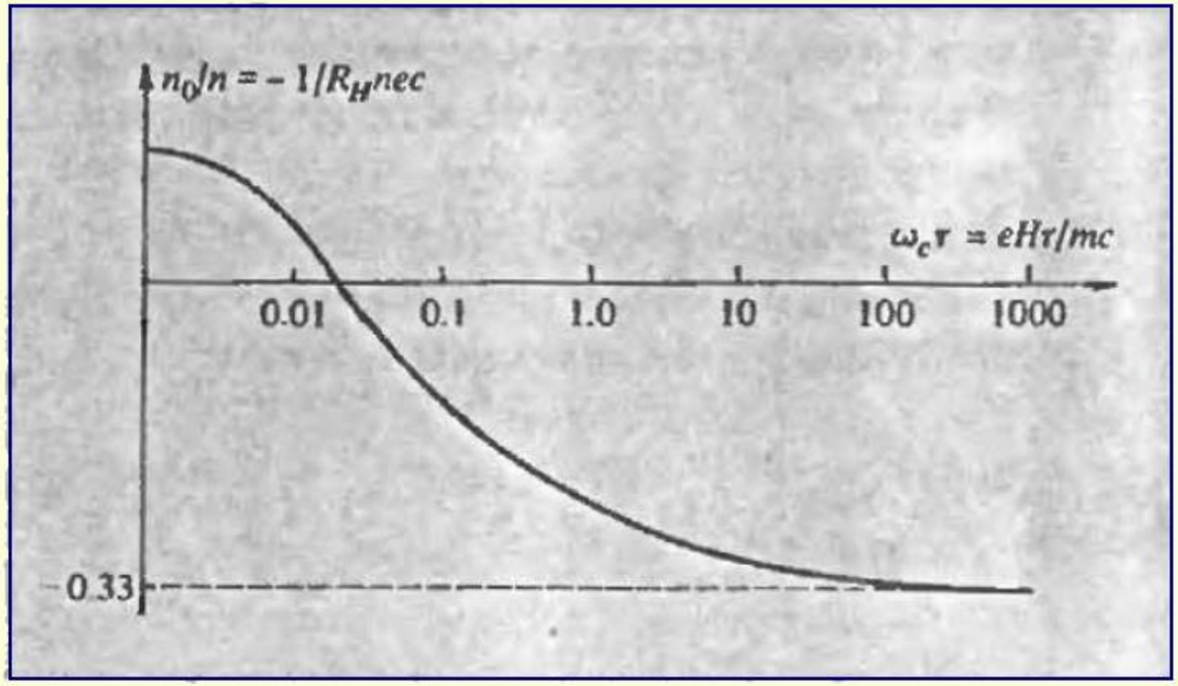


Figure Compares exp. Result with D.M. for $\frac{n_0}{n}$ vs. $\omega_c \tau$ for Al.

D.M. expects that $\frac{n_0}{n} = -0.33$ for all $\omega_c \tau$ valu

→ D.M. fail

ii D.M. did not predict good Result for Al because Al conduction depends on more complex interactions such as Band struct. effect and holes participation.

Q: Why D.M. agree at high $\omega_c \tau$ values?

$\omega_c \tau$ gets large if:

① τ is large ② ω_c is high

In these 2 cases $\frac{n_c}{n} \to 1$

∴ D.M. is not approporiate for Law

wcτ to Intermediate values.

in Conclusion:

Hall effect was very Important

to expose the limitations of D.M.

this was one of the Driving forces towards

more work that end up with quantum

based results: Fermi surface, Band structure

and Band Theory of solids ## ##

Hall Effect and Magnetoresistance

- However, more careful experiments on a variety of metals have revealed that there is a magnetic field dependence to the resistance, which can be quite dramatic in some cases.
- Here again the quantum theory of solids is needed to explain why the Drude result applies in some metals and to account for some truly extraordinary deviations from it in others.

Thanks