

Electron Transport ← Electricity and heat are carried by free electrons in metals.

(1) Phase velocity and group velocity Wave is represented in general

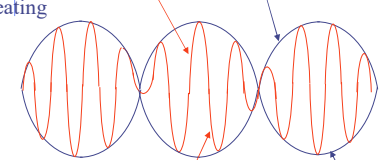
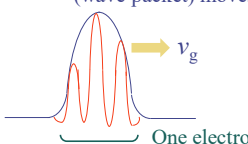
$$U = U_0 e^{i(kx - \omega t)}$$

Convolution of two slightly different waves with $\omega \pm \Delta\omega$ and $k \pm \Delta k$ is,

$$U = U_0 [e^{i[(k+\Delta k)x - (\omega+\Delta\omega)t]} + e^{i[(k-\Delta k)x - (\omega-\Delta\omega)t]}]$$

$$= U_0 e^{i(kx - \omega t)} [e^{i(\Delta k \cdot x - \Delta\omega \cdot t)} + e^{-i(\Delta k \cdot x - \Delta\omega \cdot t)}]$$

$$= 2U_0 e^{i(kx - \omega t)} \cos(x\Delta k - t\Delta\omega)$$

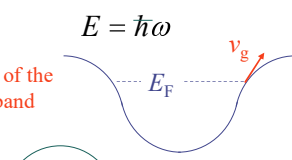
Beating  A lump of wave (wave packet) moves by v_g . 

Velocity of the original wave (Phase velocity) $v = \frac{\Delta x}{\Delta t} = \left[\begin{matrix} \\ \end{matrix} \right]$ Velocity of the envelop (Group velocity) $v_g = \left[\begin{matrix} \\ \end{matrix} \right]$

One electron

(2) From energy band $E(k)$

$$v_g = \frac{\partial \omega}{\partial k} = \frac{1}{\hbar} \frac{\partial E(k)}{\partial k}$$

Tangent of the energy band 

For 3D

$$\vec{v}_g = \frac{1}{\hbar} \left(\frac{\partial E(k)}{\partial k_x}, \frac{\partial E(k)}{\partial k_y}, \frac{\partial E(k)}{\partial k_z} \right)$$

Differentiated by t

$$\frac{\partial v_g}{\partial t} = \frac{1}{\hbar} \frac{\partial^2 E(k)}{\partial k^2} \frac{\partial k}{\partial t}$$

External field ε during δt gives rise to work $\delta E = -e\varepsilon v_g \delta t$

But $\delta E = \left(\frac{\partial E}{\partial k} \right) \delta k = \hbar v_g \delta k$ leads to $-e\varepsilon v_g \delta t = \hbar v_g \delta k$ giving $\hbar \frac{\partial k}{\partial t} = \left[\begin{matrix} \\ \end{matrix} \right]$

Thus $\frac{\partial v_g}{\partial t} = \frac{1}{\hbar^2} \frac{\partial^2 E(k)}{\partial k^2} (-e\varepsilon)$ Alternatively, differentiate $p = \hbar k$

$ma = F$ → 加速度 $\frac{\partial p}{\partial t} = \hbar \frac{\partial k}{\partial t} = F = -e\varepsilon$ 力

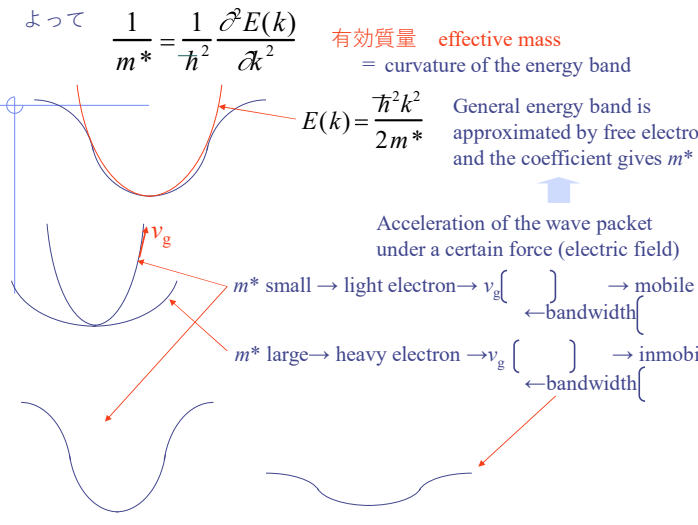
よって $\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 E(k)}{\partial k^2}$ 有効質量 effective mass = curvature of the energy band

$E(k) = \frac{\hbar^2 k^2}{2m^*}$ General energy band is approximated by free electron and the coefficient gives m^*

Acceleration of the wave packet under a certain force (electric field)

m^* small → light electron → $v_g \left[\begin{matrix} \\ \end{matrix} \right] \rightarrow$ mobile ← bandwidth $\left[\begin{matrix} \\ \end{matrix} \right]$

m^* large → heavy electron → $v_g \left[\begin{matrix} \\ \end{matrix} \right] \rightarrow$ immobile ← bandwidth $\left[\begin{matrix} \\ \end{matrix} \right]$



3

Effective mass of 1D tight-binding band

$$E(k) = \alpha + 2\beta \cos ka$$

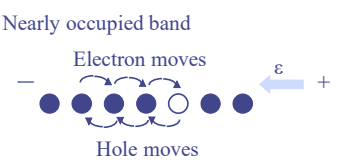
$$\frac{\partial^2 E}{\partial k^2} = \left[\begin{matrix} \\ \end{matrix} \right]$$

$$m^* = -\frac{\hbar^2}{2\beta a^2 \cos ka}$$

$m^* < 0$ for upper half of the band: hole

The wave packet is accelerated in the opposite direction as like a positively charged particle.

Nearly occupied band

Electron moves  Hole moves

$$E(k) = \frac{\hbar^2 k^2}{2m^*} = -\frac{\hbar^2 k^2}{2|m^*|} < 0$$

The upper, the more stable like a balloon.

Hole : $m^* < 0, E < 0$, a particle with positive charge

4

(3) Electric conduction

Equation of motion under electric field ϵ (classical mechanics!)

$$m \frac{dv}{dt} + \frac{m}{\tau} v = -e \epsilon$$

加速度 摩擦力 電場による力

1) Remove the force, so $\epsilon=0$ leads to

$$\frac{dv}{dt} = \left[\quad \right] \Rightarrow v = \left[\quad \right] \quad \tau : \text{relaxation time}$$

Electron is scattered to $v=0$ within time τ .

2) Steady state at $\epsilon \neq 0$ leads to $\frac{dv}{dt} = 0$

$$v = \left[\quad \right] \text{ so the current density is } j = -nev = \left[\quad \right] \text{ and}$$

conductivity is $\sigma = \frac{j}{\epsilon} = \left[\quad \right]$

or using mobility $\mu = \frac{e\tau}{m}$ to afford $\sigma = \left[\quad \right]$

5

Resistivity $\rho = \frac{1}{\sigma} \propto \frac{1}{\tau}$ Only τ is temperature dependent

In reality $\frac{1}{\tau} = \frac{1}{\tau_{ph}} + \frac{1}{\tau_i}$

Phonon scattering $\frac{1}{\tau_{ph}} = C_v \cdot T \rightarrow$ at high T above room T $\frac{1}{\tau_{ph}} \propto T$

Impurity scattering (independent of temperature)

Lattice specific heat : const. at high T (Dulong-Petit's rule)

at low T $\frac{1}{\tau_{ph}} \rightarrow 0$ thus $\rho \propto \frac{1}{\tau_i} = \text{const.}$

at high T (>100 K) $\rho \propto \frac{1}{\tau_{ph}} \propto T$

$C_v \rightarrow T^3$ and becomes slightly steeper around 50K.

Constant resistivity from impurity scattering (残留抵抗 residual resistance)

Resistivity of metals decreases at low temperatures, and becomes constant at very low temperatures.

6

(4) Hall effect

x//: apply current j_x ,
z//: apply magnetic field B
y//: measure the generated voltage E_y .

Electrons in electric and magnetic fields feel

$$\vec{F} = e(\vec{v} \times \vec{B} + \vec{E})$$

Lorentz force force of electric field

No current //y leads to

$$F_y = ev_x B - eE_y = 0 \Rightarrow E_y = \left[\quad \right]$$

Put this in $j_x = -nev_x$ and $E_y = \left[\quad \right] j_x B$

R_H : Hall coefficient cf. hole

Hall coefficient $R_H > 0$ hole
 $R_H < 0$ electron

$R_H \rightarrow$ carrier concentration n gives \rightarrow Hall $\left[\quad \right] \mu = \frac{e\tau}{m}$
 $\sigma = ne\mu$

7

(5) Thermal conductivity (of metals is due to free electrons)

Thermal conductivity carried by free electrons
in analogy with thermal conductivity carried by phonons (lattice vibration)

$\kappa = \frac{1}{3} C_v v_F l_F$ mean free path (at E_F)
1/3 for x, y, z directions electron heat capacity velocity (at E_F) $l_F = v_F \tau$

$$\kappa = \frac{1}{3} \frac{\pi^2}{3} D(E_F) k_B^2 T \cdot v_F \cdot v_F \tau$$

$$= \frac{\pi^2 N k_B^2 T \tau}{3m} \quad D(E_F) = \frac{3N}{2E_F} = \frac{3N}{mv_F^2}$$

$$\frac{\kappa}{\sigma} = \frac{\frac{\pi^2 N k_B^2 T \tau}{3m}}{\frac{Ne^2 \tau}{m}} = \left[\quad \right] T$$

$E_F = \frac{1}{2} m v_F^2$

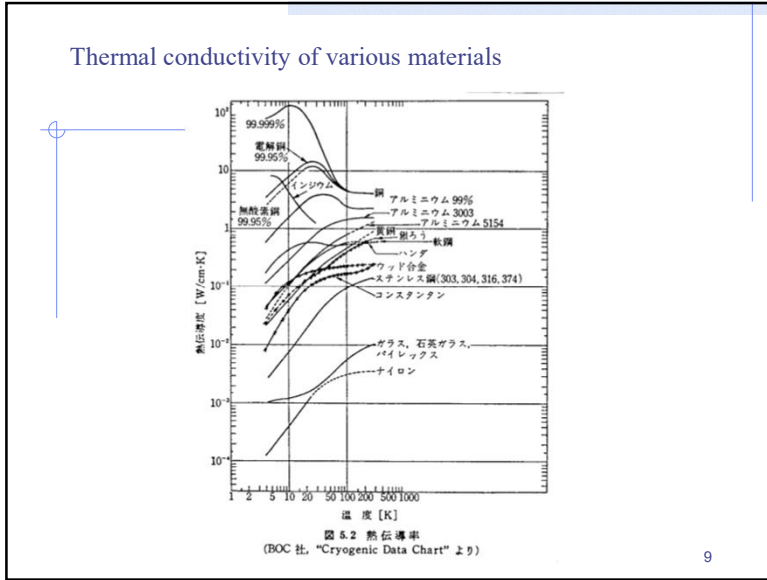
High T $\sigma \propto 1/T$ $\kappa \propto 1/T$

Intermediate $\sigma \propto 1/T^2$ $\kappa \propto 1/T^2$

Low T $\sigma = \text{const.}$ $\kappa \propto 1/T$

$\frac{\kappa}{\sigma T} = L$ Lorenz number = const. (Wiedeman-Franz law)

8



(6) Cyclotron oscillation

Electron moves circularly under magnetic field.

Equation of motion under electric and magnetic fields

$$\frac{d\vec{p}}{dt} = m \frac{d\vec{v}}{dt} = e\vec{v} \times \vec{B}$$

Lorentz force

For magnetic field $B//z$

$$\frac{dv_x}{dt} = -\frac{eB}{m} v_y = -\omega_c v_y \quad \frac{dv_y}{dt} = \omega_c v_x \quad \omega_c = \frac{eB}{m}$$

Electron moves circularly in the xy plane

Reciprocal space

Real space

Fermi surface

90° behind the reciprocal space

Thus

$$\begin{cases} v_x = v_0 \cos \omega_c t \\ v_y = v_0 \sin \omega_c t \end{cases}$$

$$\begin{cases} x = -\frac{v_0}{\omega_c} \sin \omega_c t \\ y = \frac{v_0}{\omega_c} \cos \omega_c t \end{cases}$$

where

$$|r| = \frac{v_0}{\omega_c} = \frac{m}{eB} v_0 = \frac{|p|}{eB}$$

and

$$\frac{dE(k)}{dt} = \frac{dE}{d\vec{p}} \frac{d\vec{p}}{dt} = \vec{v} \cdot (e\vec{v} \times \vec{B}) = 0$$

Exterior product of \vec{v} and \vec{B} is $\perp \vec{v}$. Its inner product is 0.

Electron moves on a constant energy surface (= Fermi surface).

Absorbs the microwave with $\omega_c = \frac{eB}{m}$

Cyclotron resonance

$\hbar\omega_c = \text{const.}$

Microwave absorption

Experimental estimation of m^*

Cross section of $H \perp$ surface and the Fermi surface

(7) Quantum Oscillation

Circular motion is quantized just like a hydrogen atom.

(circle) = (wavelength) \times (integer) Bohr's quantization condition

$$2\pi r = n\lambda = n \frac{h}{p} \Rightarrow r \cdot p = n\hbar$$

Using $|r| = \frac{|p|}{eB}$ for circular motion $\frac{p}{eB} \cdot p = n\hbar$

Kinetic energy

$$E = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2)$$

$$= \frac{\hbar^2}{2m} 2 \frac{eB}{\hbar} n + \frac{\hbar^2}{2m} k_z^2$$

$$= \left[\quad \right] n + \frac{\hbar^2}{2m} k_z^2$$

$S_k = \pi(k_x^2 + k_y^2)$ using the area of this circle

$$S_k = \frac{2\pi eB}{\hbar} n$$

S_k is quantized as integer times of $\frac{2\pi eB}{\hbar}$

this area

The area has the same interval.

$n=3$
 $n=2$
 $n=1$

$n=1$ circle = λ $E = \hbar\omega_c$
 $n=2$ circle = 2λ $E = 2\hbar\omega_c$
 $n=3$ circle = 3λ $E = 3\hbar\omega_c$

$\hbar\omega_c = \frac{\hbar e B}{m}$

Orbit is restricted to these circles (also circle in the real space).

In three dimension
 $B \uparrow$
 $n=1, 2, 3$
Landau tube: cylindrical slices of the Fermi surface

Fermi surface

z direction motion
 $\frac{\hbar^2}{2m} k_z^2$ remains \rightarrow Spiral in the real space

E
 E_F
 $B=0$ $D(E)$

E
 $5\hbar\omega_c$
 $4\hbar\omega_c$
 $3\hbar\omega_c$
 $2\hbar\omega_c$
 $\hbar\omega_c$
 $B \neq 0$ $D(E)$

Interval of the Landau levels is 0 at $B = 0$, and increases with increasing B .

1D energy band for z has density of states, $D(E) \propto E^{-1/2}$ with a peak at $E = 0$.

13

Changing B \rightarrow large B

E
 E_F
 $D(E)$

E
 E_F
 $D(E)$

Occupied upper most Landau level
 = Most outer orbit
 = Equator of the Fermi surface
 = (In general) extremal cross section

When this crosses E_F by changing B , $D(E_F)$ makes peaks

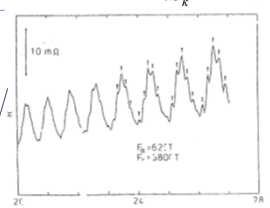
The periodicity is $S_k = \frac{2\pi e}{\hbar} B_n n = \frac{2\pi e}{\hbar} B_{n+1} (n+1)$

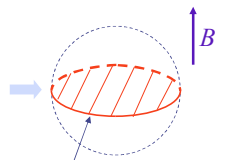
Erasing n from this to give

$$\frac{1}{B_{n+1}} - \frac{1}{B_n} = \Delta\left(\frac{1}{B}\right) = \left[\right]_{14}$$

14

Many properties of metals oscillate when B is scanned at low T .
 The periodicity is $\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar S_k}$





This area

Electrical Resistivity
 Magnetic Susceptibility
 Specific Heat

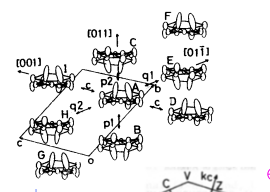
Shubnikov-de Haas oscillation
 de Haas-van Alphen oscillation
 Fermiology to investigate Fermi surface

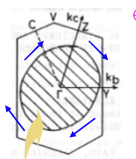
D. Shoenberg, *Magnetic Oscillations in Metals*, Cambridge (1984).
 J. Wosnitzer, *Fermi Surfaces of Low-Dimensional Organic Metals and Superconductors*, Springer (1996).
 M. V. Kartsovnik, *Chem. Rev.* **104**, 5737 (2004).

15

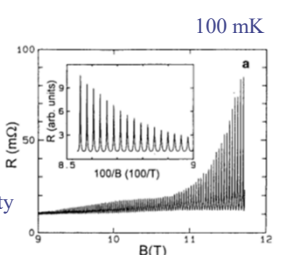
Shubnikov- de Haas Oscillation in β -(BEDT-TTF)₂I₃

Oscillation of electrons rotating around the Fermi surface is observed at low T (< 1 K) and under strong magnetic field (> 10 T).





⊕ Magnetic Field
 1 electron per unit cell
 Hatched Area
 Periodicity
 $\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar S_k}$



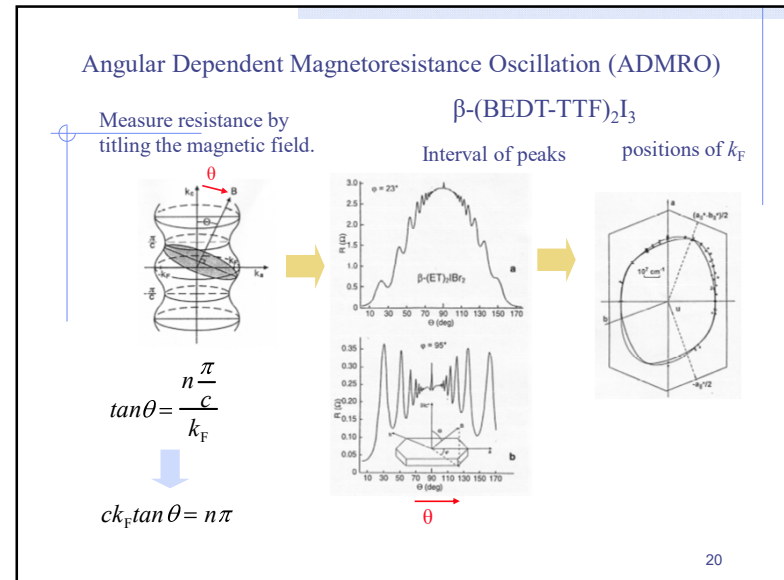
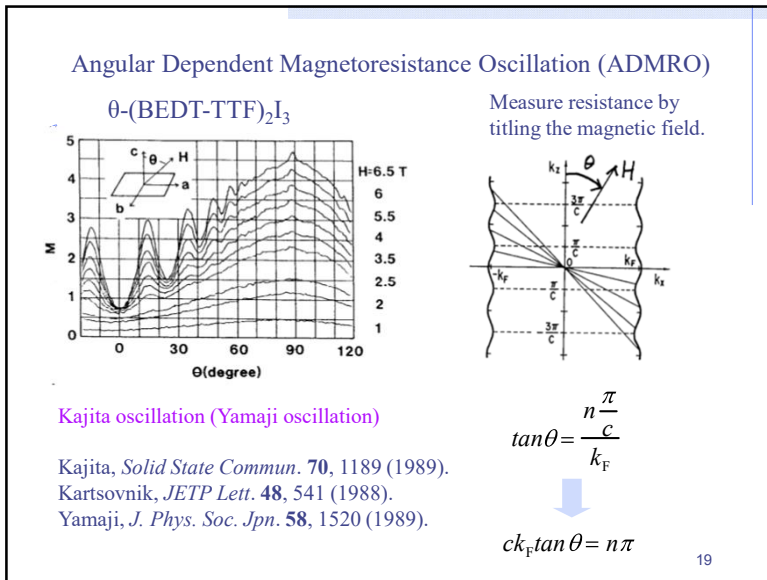
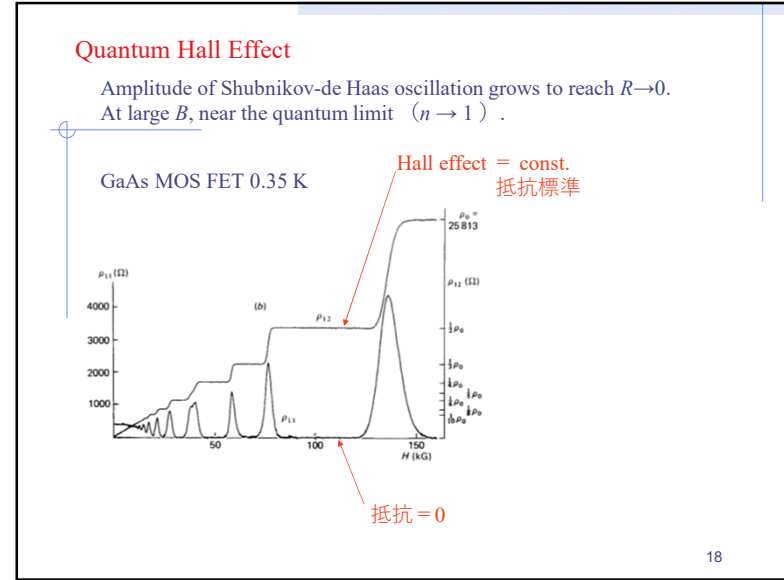
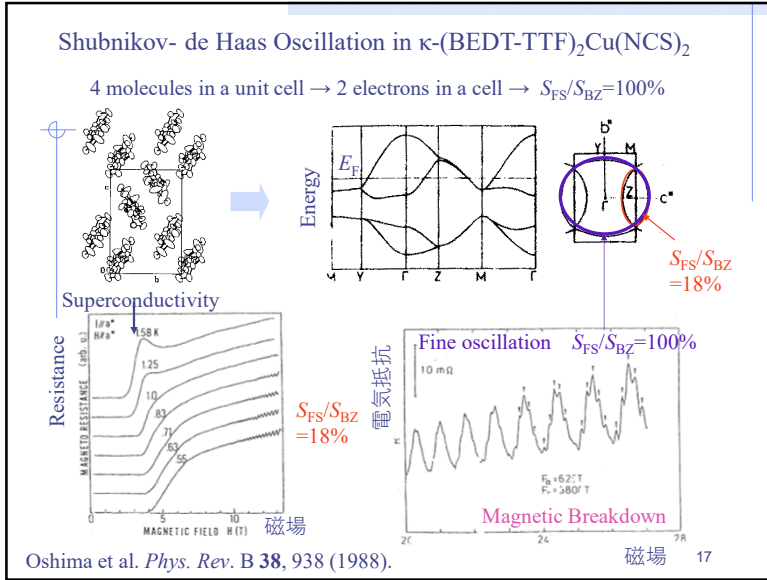
Resistance R (mΩ)

Magnetic Field B (T)

Fermi surface is 50% of the 1st Brillouin zone.

Kang, et al. *Phys. Rev. Lett.* **62**, 2559 (1989).

16



Conventional ADMRO due to the Fermi surface of Cu

Open orbit (red arrow) and **Close orbit** (blue arrow) are shown in the Fermi surface diagrams. The magnetoresistance graph shows Resistance vs. Magnetic Field with a saturation point and $\Delta\rho = B^2$. The Fermi surface map shows directions $[110]$, $[111]$, $[001]$, and $111[110]$.

Magnetoresistance does not saturate at the angles when the orbit is closed.

21

Optical Properties of Metals (Plasmon)

When light is irradiated, how the ac electric field enters.

$$D(\omega) = \epsilon_0 E(\omega) + P \quad D(\omega) = \epsilon \epsilon_0 E(\omega)$$

These lead to $\epsilon(\omega) = \frac{D(\omega)}{\epsilon_0 E(\omega)} = 1 + \frac{P(\omega)}{\epsilon_0 E(\omega)}$

Eq. of motion vibrated by the electric field E : $m \frac{d^2 x}{dt^2} = -eE$

$E, x \propto e^{i\omega t}$ leads to $-m\omega^2 x = -eE \rightarrow x = \left[\right]$

$P = -nex = \left[\right]$ **Plasma frequency**

Put this in the above eq. to $\epsilon(\omega) = \left[\right] = 1 - \frac{\omega_p^2}{\omega^2}$

Maxwell eq. $\mu_0 \frac{\partial^2 D}{\partial^2} = \nabla^2 E$ with $E \propto e^{i(Kr - \omega t)}$ to give

$$\mu_0 \epsilon_0 \epsilon(\omega)^2 = K^2 \rightarrow \omega^2 - \omega_p^2 = c^2 K^2$$

22

$\omega^2 - \omega_p^2 = c^2 K^2$ $\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$

$\omega < \omega_p \rightarrow K$ imaginary

Diminish as $E \propto e^{-Kr}$ in metals
Light cannot enter, and is reflected: metallic luster.
 ω_p : near ultraviolet in ordinary metals near infrared in organics

$\omega > \omega_p \rightarrow K$ real
 $E \propto e^{-iKr}$ Metals are transparent to UV.

$\omega = \omega_p \rightarrow D=0 \rightarrow E = -\frac{1}{\epsilon_0} P = \frac{nex}{\epsilon_0}$

$$m \frac{d^2 x}{dt^2} = -\frac{ne^2}{\epsilon_0} x \rightarrow \frac{d^2 x}{dt^2} + \omega_p^2 x = 0$$

Characteristic oscillation of electron ω_p : plasma oscill.....

longitudinal rarefaction wave

23

Thermoelectric power: temperature difference \rightarrow voltage cf. Thermocouple

$\Delta V = S(T_2 - T_1)$

Thermopower or Seebeck coefficient 熱電率 $1 \mu\text{V/K} \sim 1 \text{mV/K}$

Waste heat \rightarrow Several 100 K \rightarrow Generator

$S > 0$ hole
 $S < 0$ Electron
Charge polarity determinator instead of Hall effect

$S \propto T$ metal
 $S \propto 1/T$ semiconductor

DOS gradient \rightarrow Different electron numbers above E_F \rightarrow voltage

24

Magnetism

Molecular orbital of transition metal compounds

Ligand orbital: bonding
Transition metal d-orbitals: antibonding
s, p levels are further antibonding
All valence electron enters in the d levels

Splitting of the d levels (Coordination Splitting)
For octahedral

Two e_g orbitals directed to the ligands are lifted, and more antibonding.

Three t_{2g} orbitals have nodes in the direction of the ligands, and are nonbonding.

$\Delta = 1 \sim 2 \text{ eV}$

Absorb visible light
→ Transition metal compounds are colored.

Ligand Field Theory or Crystal Field Theory
Molecular Field Theory of
Transition Metal Compounds

25

For octahedral

high spin

$S = 1/2, 1, 3/2, 2, 5/2, 2, 3/2, 1, 1/2, 0$

$\text{Ti}^{3+}, \text{Ti}^{2+}, \text{Cr}^{3+}, \text{Cr}^{2+}, \text{Fe}^{3+}, \text{Fe}^{2+}, \text{Co}^{2+}, \text{Ni}^{2+}, \text{Cu}^{2+}, \text{Zn}^{2+}$

$\text{V}^{4+}, \text{V}^{3+}, \text{Mn}^{4+}, \text{Mn}^{3+}, \text{Mn}^{2+}, \text{Co}^{3+}, \text{Ni}^{3+}, \text{Cu}^+$

$\text{Ti}^0, \text{V}^0, \text{Cr}^0, \text{Mn}^0, \text{Fe}^0, \text{Co}^0, \text{Ni}^0$

$4, 5, 6, 7, 8, 9, 10$

For $d = 4 \sim 7$, when crystal field $>$ Hund rule, low spin state achieved

Transition from high spin to low spin by changing T
Spin crossover

Low spin d^6 is nonmagnetic

$S = 1, 1/2, 0, 1/2$

χT vs T graph showing a peak at 176 K for $[\text{Fe}^{\text{II}}(\text{phen})_2(\text{NCS})_2]$ between low spin and high spin states.

26

For tetrahedral : upside down. always high spin

$S = 1/2, 1, 3/2, 2, 5/2, 2, 3/2, 1, 1/2$

Order of Δ : spectroscopic series
 $\text{I} < \text{Br} < \text{Cl} < \text{F} < \text{OH} < \text{H}_2\text{O}$
 $< \text{NCS}^- \sim \text{NH}_3 < \text{en} < \text{phen} < \text{CN}^-$

strong $\text{C} < \text{N} < \text{O} < \text{F}$
weak I

For example, FeCl_4^- is Fe^{3+} so d^5 for Fe^0 minus 3 leads to d^5 , so $S = 5/2$

27

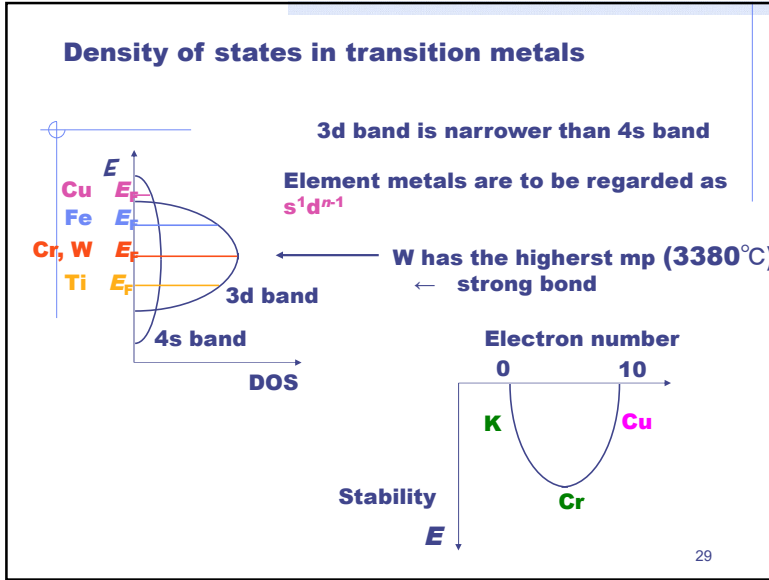
周期表

s-ブロック d-ブロック p-ブロック

ランタノイド

アクチノイド

28



Magnetic Susceptibility

Application of H to materials gives rise to magnetization M . B in the material is $B = \mu_0(H + M)$

$\chi = M / H$ Magnetic Susceptibility

- $\chi < 0$ $B < \mu_0 H$ Diamagnetism: Materials without spins
- $\chi > 0$ $B > \mu_0 H$ Paramagnetism: Materials with unpaired spins

Diamagnetism of Atoms

Materials with unpaired spins → Atomic orbital motion

charge cyclotron frequency ω_c

(Mag. Moment) = $I \times$ (Circular Area)

$$\mu = -\frac{Ze^2 B}{4m} \langle x^2 + y^2 \rangle = -\frac{Ze^2 B}{6m} \langle r^2 \rangle$$

leads to $\frac{2}{3} \langle r^2 \rangle$

$$\chi = \frac{N\mu}{B} = -\frac{NZe^2}{6m} \langle r^2 \rangle$$
 Diamagnetism inherent in the atoms $\chi < 0$

Sum of atomic diamagnetism gives the Pascal diamagnetism.

Page number: 30

Dielectrics in a capacitor

Capacitors: $Q = CV$ $q = \epsilon E$ $E = V/d$
 $C = \epsilon S/d$ $Q = qS$

$\epsilon_0 = 0.088 \text{ pF/cm}$

Insert dielectrics with keeping q

Actual field: $E = E_0 - 4\pi P$
 Original electric field: $\epsilon_0 E = D - P$
 $q' = q - \sigma$

$D = E + 4\pi P$ cgs $D = \epsilon_0 E + P$ MKS
 $D = \epsilon E$ dielectric const. $D = \epsilon_0 \epsilon_r E$

E decreases 1/ε of D e.g. Si (ε = 11.9) → 1/11.9 water → 1/80

Insert dielectrics with keeping $V \rightarrow C$ is $\times \epsilon$

In particular, $\sigma = q$ perfect polarization → $E = 0$ and $\epsilon = \infty$
 → Metal ($E = 0$ in a metal)

Always $P > 0 \rightarrow \epsilon > 1$

Page number: 31

Curie Paramagnetism

Magnetic moment from unpaired electrons $\mu = \gamma \hbar S = -g\mu_B S$

Zeemann splitting due to the magnetic field H
 $E = -g\mu_B H S = -\mu H$

Split to two for $S = 1/2$. In thermal equilibrium:

$$\frac{N_{\uparrow}}{N} = \frac{e^{\mu H / k_B T}}{e^{\mu H / k_B T} + e^{-\mu H / k_B T}} \quad \frac{N_{\downarrow}}{N} = \frac{e^{-\mu H / k_B T}}{e^{\mu H / k_B T} + e^{-\mu H / k_B T}}$$

lead to $M = \mu_B (N_{\uparrow} - N_{\downarrow}) = N \mu_B \tanh \frac{\mu H}{k_B T} \approx N \mu \left(\frac{\mu H}{k_B T} \right) \ll 1$ so

$$\chi = \frac{M}{H} = \frac{N \mu^2}{k_B T} = \frac{C}{T}$$
 Curie constant
 Except for $S=1/2$ $C = \frac{NS(S+1)g^2 \mu_B^2}{3k_B}$

χ is inversely proportional to T . only comes from S .

Random spins / Aligned under magnetic field / More aligned at low T .

Page number: 32

Magnetic Order

Ferromagnetism : all parallel
The whole material is a magnet.

$J > 0$
 $S_i // S_j$ is stable

Antiferromagnetism :
alternately opposite directions

$J < 0$
Antiparallel S_i and S_j

Spin Hamiltonian

$$\hat{H} = -\sum_{i,j} 2J_{ij} \bar{S}_i \bar{S}_j - g\mu_B H \sum_i \bar{S}_i$$
 Interaction Zeemann splitting

S_i is a vector like (S_x, S_y, S_z) : (Heisenberg model).
When spin is always directed in one direction (z) due to the large magnetic anisotropy coming from the crystal field, we only consider S_z . (Ising model)

When $S_i = 1/2, S_j = 1/2$, (Interaction) = $-J/2$
When $S_i = 1/2, S_j = -1/2$, (Interaction) = $J/2$ } Energy difference J

Note: (Interaction) is defined as $-\sum_{i,j} J_{ij} \bar{S}_i \bar{S}_j$ in old literatures.
 J is twice larger. 33

Molecular Field (Mean Field) Approximation

Focusing on S_i , and use average sum for \sum_j

$$\hat{H} = \sum_i S_i (-\sum_j 2J_{ij} S_j - g\mu_B H) = -g\mu_B (H_{\text{eff}} + H) \sum_i S_i$$

$$H_{\text{eff}} = \frac{1}{g\mu_B} \sum_j 2J_{ij} \langle S_j \rangle$$

Interaction with S_j is replaced by a field (effective or internal field)(有效或内部磁場) generated on S_i .

S_j changes every moment, but S_j is approximated by the average $\langle S_j \rangle$
(分子場近似 or 平均場近似 Molecular Field or Mean Field Approximation)

Statistical distribution similar to the Curie paramagnetism gives

$$M = \frac{N\mu^2 H}{k_B T} \xrightarrow{H \rightarrow H_{\text{eff}} + H} M = \chi_0 (H_{\text{eff}} + H)$$

where $M = Ng\mu_B \langle S \rangle$ leads to $\sum_j 2J_{ij} \langle S_j \rangle$ } 分子磁場係數

$$H_{\text{eff}} = \frac{1}{N(g\mu_B)^2} M = aM$$

Put this in the above eq. to give

$$M = \chi_0 (aM + H)$$

$$M \left[\frac{1}{1 - \chi_0 a} \right] = \chi_0 H \rightarrow \chi = \frac{M}{H} = \frac{\chi_0}{1 - \chi_0 a} = \frac{C}{T - \theta}$$

Curie-Weiss則 34

$$\theta = \frac{1}{k_B} \sum_j 2J_{ij} = \frac{2zJ}{k_B}$$

← Coordination number z for nearest neighbor J 's

Weiss温度

$J > 0 \rightarrow \theta > 0$ Ferromagnetism

Curie温度 T_c

$T \rightarrow T_c: \chi \rightarrow \infty$
 $T < T_c: M \neq 0$ for $H=0$
Spontaneous Magnetism \rightarrow Magnet
 T_c Fe 1043 K Ni 627 K

Magnetization of Ferromagnet
Hysteresis

Usual ferromagnet has randomly oriented magnetic domains (磁区), but magnetic field aligns the spin orientation to make a bulk magnet.

35

Magnetic Susceptibility of Metal Electrons (Pauli paramagnetism)

$\downarrow \uparrow$ is more stable than \uparrow under magnetic field.

$$E_{\uparrow} = \frac{\hbar^2 k^2}{2m} - \mu H$$

$$E_{\downarrow} = \frac{\hbar^2 k^2}{2m} + \mu H$$

Magnetization is

$$M = \mu(N_{\uparrow} - N_{\downarrow})$$

$$= \mu \frac{1}{2} D(E) \times 2\mu H$$

Susceptibility $\chi = \frac{M}{H} = \mu^2 D(E_F)$

Pauli paramagnetism is $\chi > 0$ and T independent.

電子比熱係數 $\gamma = \frac{\pi^2}{3} D(E_F) k_B^2$ leads to $\frac{\chi}{\gamma} = \left[\dots \right] = \text{const.}$ Wilson比

Ratio of χ and γ does not change depending on m^* .