

PH8252 PHYSICS FOR INFORMATION SCIENCE

UNIT- I

ELECTRICAL PROPERTIES OF MATERIALS

Part B

1. (a) Starting with the classical free electron theory of metals obtain an expression for electrical and Thermal conductivity and hence prove Wiedemann – Franz law. (OR)

(b) State and prove Wiedemann - Franz law. Why does the Lorentz number determined experimentally does not agree with the value calculated from the classical formula? (OR)

(c) Obtain Weideman-Franz law using the expressions of electrical and thermal conductivity and Find expression for Lorentz number. (OR)

(d) Deduce mathematical expressions for electrical conductivity and thermal conductivity of a Conducting material and hence obtain Wiedemann – Franz law. (OR)

(e) (i) Give the postulates of free electron theory.

(ii) Derive the mathematical expressions for electrical and thermal conductivity for a free electron and deduce Wiedemann – Franz law.

Classical Free Electron Theory:

Postulates:

(1) A Solid metal is composed of atoms and the atoms have large number of free electrons.

(2) The valence electrons of atoms are free to move about the whole volume of the metals like the molecules of a perfect gas in a container.

(3) In the absence of an electric field, the free electrons move in random directions and collide with other free electrons and positive ion core. All the collisions are elastic. i.e., there is no loss of energy.

(4) When an electric field is applied, the free electrons are accelerated in the direction opposite to the direction of applied electric field.

(5) Since the electrons are assumed to be a perfect gas, they obey the laws of kinetic theory of gases.

(6) The velocity and energy distribution of the electrons are governed by classical Maxwell distribution function.

Expression for Electrical Conductivity:

Definition:

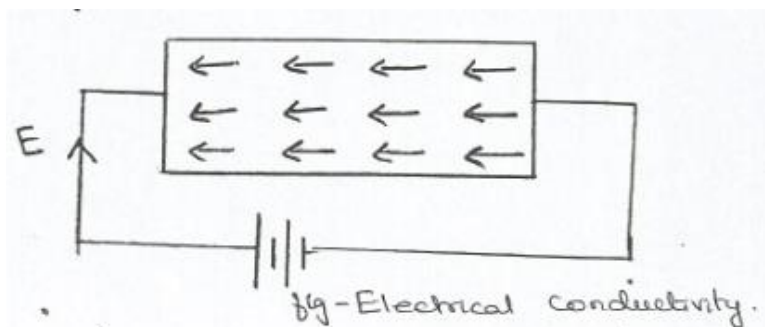
Electrical conductivity is defined as the quantity of charge flowing across unit area of cross – section of the material per unit time under unit potential gradient.

Derivation:

In the absence of external electric field, the free electrons in a metal experience random motion in all possible directions.

When an electric field of strength E is applied, the free electrons experience a force F is given by

$F = eE$, where e is the charge of the electron. Due to this force, the free electrons will acquire an acceleration 'a'.



From Newton's second law of motion, the force on the electron

$$F = ma$$

Equating both the forces, $ma = eE$

$$\text{Therefore, } a = \frac{eE}{m} \text{ ----- (1)}$$

Due to the applied field, the electron accelerated continuously.

The average velocity acquired by the free electron in a particular direction due to the applied electric field is called drift velocity (V_d).

If τ_c is the collision time, then

$$a = \frac{V_d}{\tau_c}$$

$$V_d = a\tau_c$$

Substituting the value of 'a' from eqn (1) we get,

$$V_d = \frac{eE\tau_c}{m} \text{ ----- (2)}$$

Current density (J) is defined as the charge crossing unit area per unit time.

If 'n' is the number of conduction electrons per unit volume, then the current density is given by

$$J = neV_d$$

$$= ne \frac{eEC}{m}$$

$$J = \frac{ne^2C}{m} E$$

$$\frac{J}{E} = \frac{ne^2}{m} C \text{ ----- (3)}$$

According to ohm's law, current density (J) is expressed as

$$J \propto E$$

$$J = \sigma E$$

$$\frac{J}{E} = \sigma \text{ ----- (4)}$$

Comparing eqn (3) and (4), we have

$$\sigma = \frac{ne^2}{m} C \text{ ----- (5)} \quad \left\{ \text{Where } \sigma' \text{ is the electrical conductivity.} \right.$$

This is the expression for electrical conductivity.

Electrical conductivity in terms of mobility:

$$\text{Mobility of the electron, } \mu = \frac{V_d}{E}$$

$$\mu = \frac{eCE}{mE}$$

$$\mu = \frac{eC}{m}$$

$$C = \frac{\mu m}{e}$$

Substitute the value of C in eqn (5) we get

$$\sigma = \frac{ne^2}{m} \times \frac{\mu}{e} m$$

$$\sigma = ne\mu \text{ ----- (6)}$$

This is the expression for the electrical conductivity in terms of number of electrons and mobility.

Variation of electrical conductivity with temperature:

Based on kinetic theory, the kinetic energy of electron is related to the temperature by

$$\frac{1}{2}me^2 = \frac{3}{2}KT \quad \{\text{Where K is Boltzmann's constant.}\}$$

Therefore

$$V^2 = \frac{3KT}{m}$$

$$V = \sqrt{\frac{3KT}{m}} \quad \text{----- (7)}$$

The average distance travelled between two successive collisions is called the mean free path (λ)

$$\text{i.e, } \lambda = VC$$

$$\tau = \frac{\lambda}{V}$$

Substituting eqn (7) we get

$$\tau = \lambda \sqrt{\frac{m}{3KT}}$$

Substituting the value of τ in eqn (5), we get

$$\sigma = \frac{ne^2}{m} \lambda \sqrt{\frac{m}{3KT}}$$

$$\sigma = \frac{ne^2}{\sqrt{3KTm}} \lambda$$

Hence as temperature increases, conductivity decreases.

Expression for Thermal Conductivity

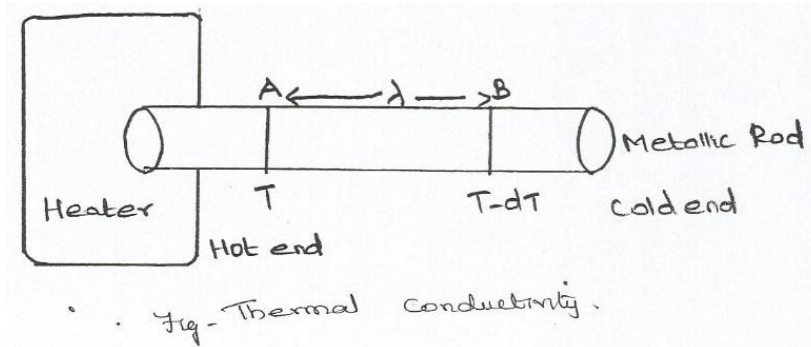
Definition:

Thermal conductivity is defined as the amount of heat flowing across unit area of cross section of the material per unit time under unit temperature gradient.

$$\text{i.e. } K = \frac{Q}{\frac{dT}{dx}}$$

Derivation:

Consider a uniform metallic rod containing free electrons. One end of the rod is heated using a heater. Let A and B be the two cross sections of temperatures T and (T-dT) separated by a distance of mean free path (λ)



Let heat flow from hot end to cold end. The electrons lose its kinetic energy due to collision at A and gains at B.

At A, the average kinetic energy = $\frac{3}{2}KT$

At B, the average kinetic energy = $\frac{3}{2}K(T-dT)$

Excess Kinetic energy carried out by the electrons from A to B = $\frac{3}{2}KT - \frac{3}{2}K(T-dT)$

$$= \frac{3}{2}KT - \frac{3}{2}KT + \frac{3}{2}KdT$$

$$= \frac{3}{2}KdT.$$

Let the free electron density be 'n' and velocity of electron be 'v'. Let us assume that there is an equal probability for the electrons to move in all '6' directions.

Hence, the number of electrons crossing per unit area per unit time from A to B = $\frac{1}{6}nv$

Excess of energy carried from A to B for unit area in unit time = $\frac{1}{6}NV \times \frac{3}{2}KdT$

$$= \frac{1}{4}nvKdT$$

Similarly, the deficiency of energy carried from B to A for unit area in unit time = $-\frac{1}{4}nvKdT$

Hence, the net energy transferred from A to B for unit area in unit time

$$Q = \frac{1}{4}nvKdT - \left[-\frac{1}{4}nvKdT \right]$$

$$Q = \frac{1}{2}nvKdT \text{ ----- (2)}$$

From eqn(1) $Q = K \frac{dT}{dx} = K \frac{dT}{\lambda} \text{ -----(3)}$

Comparing eqn (2) and (3) we get

$$K = \frac{1}{2}nvK\lambda$$

We know, $\lambda = V\tau$

Therefore $K = \frac{1}{2}nvKV\tau$

$$K = \frac{1}{2}nv^2K\tau \text{ ----- (4)}$$

This is the classical expression for Thermal conductivity.

WIEDEMANN – FRANZ LAW

Statement:

The ratio of thermal conductivity to the electrical conductivity of a metal is directly proportional to the absolute temperature of the metal.

i.e. $\frac{K}{\sigma} \propto T$

Where $K \rightarrow$ Thermal conductivity

$\sigma \rightarrow$ Electrical conductivity

$T \rightarrow$ Absolute Temperature.

From classical theory,

$$K = \frac{1}{2}nv^2K\tau \quad \text{and} \quad \sigma = \frac{ne^2C}{m}$$

$$\begin{aligned} \frac{K}{\sigma} &= \frac{\frac{1}{2}nv^2K\tau}{\frac{ne^2C}{m}} \\ &= \frac{1}{2} \frac{mv^2K}{e^2} \end{aligned}$$

We know that the kinetic energy of an electron,

$$\begin{aligned} \frac{1}{2}mv^2 &= \frac{3}{2}KT \\ \frac{K}{\sigma} &= \frac{3}{2}KT \times \frac{K}{e^2} = \frac{3T}{2} \left(\frac{K}{e}\right)^2 \\ \frac{K}{\sigma} &= \frac{3T}{2} \left(\frac{K}{e}\right)^2 T \\ \frac{K}{\sigma} &= LT, \quad \text{where } \frac{3}{2} \left(\frac{K}{e}\right)^2 \end{aligned}$$

Hence $\frac{K}{\sigma} \propto T$

This dependence of $\frac{K}{\sigma}$ on absolute temperature is Wiedemann – Franz law.

LORENTZ NUMBER

According to Wiedemann – Franz law,

$$\frac{K}{\sigma} = LT \quad (\text{or}) \quad \frac{K}{\sigma T} = L$$

“The ratio of thermal conductivity to the product of electrical conductivity and absolute temperature of a metal is a constant. The constant L is known as Lorentz number”. Whose value is $2.44 \times 10^{-8} \text{ watt ohm K}^{-2}$ at 293K.

$$L = \frac{3}{2} \left(\frac{K}{e} \right)^2$$

2. (a) Starting with the Fermi distribution function, obtain an expression for Fermi energy of an electron in a metal at $T=0\text{K}$ and hence an expression for the average energy of an electron. (OR)

(b) Write an expression for the Fermi energy distribution function and discuss the behaviour with change in temperature. Plot $f_{ed}(E)$ versus E for $T = 0\text{K}$ and $T > 0\text{K}$. (OR)

(c) Define Fermi energy. Obtain an expression for average energy of an electron at $T = 0\text{K}$.

Solu:

The probability $F(E)$ of an electron occupying a given energy level at absolute temperature is called Fermi – Dirac distribution function. It gives the probability of filling the electron within the Fermi energy level.

$$\text{It is given by } F(E) = \frac{1}{1 + e^{(E - E_F)/KT}}$$

Where $F(E) \rightarrow$ Fermi function.

$E \rightarrow$ Energy of the level whose occupancy is considered.

$E_F \rightarrow$ Fermi energy of the system.

$K \rightarrow$ Boltzmann constant.

$T \rightarrow$ Absolute temperature.

Effect of temperature on Fermi function

1. At $T = 0\text{K}$:

(a) For $E < E_F$ $(E - E_F)$ is negative

$$\begin{aligned} F(E) &= \frac{1}{1 + e^{(E - E_F)/KT}} = \frac{1}{1 + e^{-E_F/0}} \\ &= \frac{1}{1 + e^{-\infty}} = \frac{1}{1} = 1 \end{aligned}$$

$$F(E) = 1$$

i.e, 100% chance for the electron to occupy the energy levels below Fermi energy. Energy levels below E_F are filled at $T = 0K$.

(b) For $E > E_F$, $(E - E_F)$ is positive

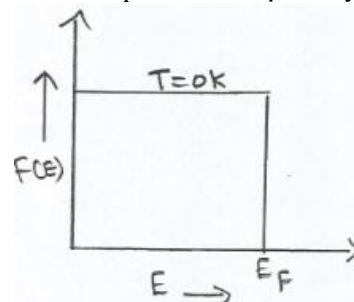
$$F(E) = \frac{1}{1 + e^{(E - E_F)/KT}} = \frac{1}{1 + e^{E/0}}$$

$$= \frac{1}{1 + e^{\infty}} = \frac{1}{1 + \infty} = \frac{1}{\infty}$$

$$F(E) = 0$$

i.e, 0% chance for the electrons to occupy the energy level above Fermi energy. All the energy levels above E_F are empty at $T = 0K$.

This means that at $T = 0K$, all quantum states with energy below E_F are completely occupied and those above E_F are unoccupied as shown in below fig.



(2) At $T > 0K$ and $E = E_F$

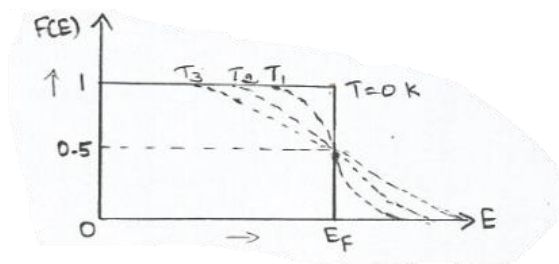
$$F(E) = \frac{1}{1 + e^0}$$

$$= \frac{1}{1 + 1} = \frac{1}{2}$$

$$F(E) = 0.5$$

i.e, 50% chance for the electron to occupy the Fermi energy level, with increase in temperature, Fermi function varies with 'E'.

$$T_3 > T_2 > T_1 > 0K$$



3. At $T \rightarrow \infty$, $KT \gg E_F$

Electron lose their quantum mechanical behaviour. The Fermi distribution function reduces to classical Boltzmann distribution function.

3. (a) Derive an expression for density of states and hence deduce the expression for Fermi energy at Zero kelvin. (OR)

(b) Explain the meaning of 'density of states'. Derive an expression for the number of allowed States for unit volume of a solid. (OR)

(c) Obtain an expression for density of states (OR)

(d) What is density states? Derive an expression for the density of states.

Definition:

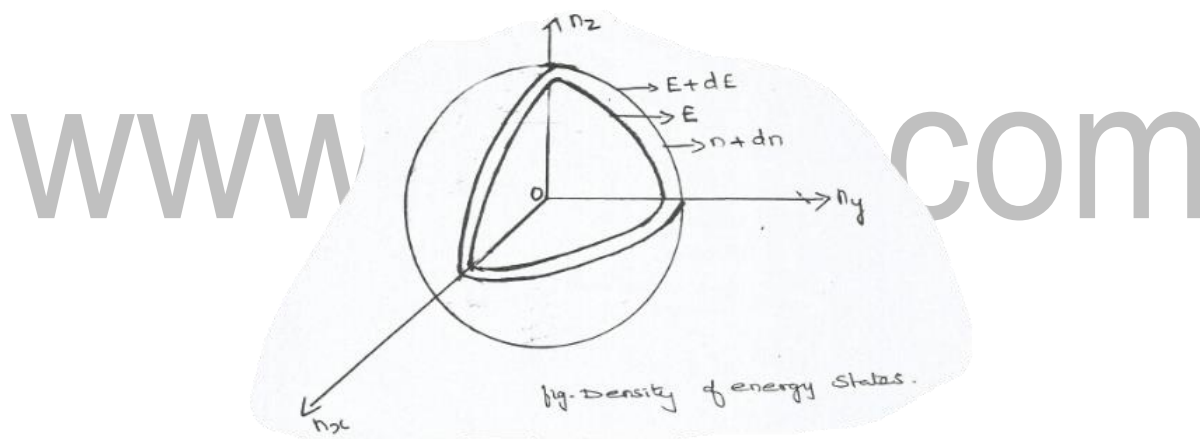
Density of energy state is defined as the number of energy states $N(E) dE$ per unit volume of the material in an energy interval E and $E+dE$. It is denoted by $Z(E)dE$.

$$Z(E)dE = \frac{N(E)dE}{V}$$

It is used to calculate the number of charge carriers per unit volume of any solid.

Derivation:

Let us consider two energy values E and $E+dE$. The number of energy states between E and $E+dE$ can be found by finding the number of energy states between the shells of radius n and $n+dn$, from the origin.



The number of energy states within a sphere of radius 'n' $= \frac{4}{3}\pi n^3$.

Since the quantum numbers (n_x, n_y, n_z) can have only positive integer values, only one octant of the sphere is considered.

i.e., $\frac{1}{8}$ th of the spherical volume.

Therefore the number of available energy states within one octant of the sphere of radius 'n'.

$$= \frac{1}{8} \left[\frac{4}{3}\pi n^3 \right]$$

Similarly, the number of available energy states within one octant of the sphere of radius $n+dn$

$$= \frac{1}{8} \left[\frac{4}{3} \pi (n + dn)^3 \right]$$

∴ The number of available energy states between the shells of radius n and $n+dn$ is

$$N(E) dE = \frac{1}{8} \frac{4}{3} \pi [(n + dn)^3 - n^3]$$

$$= \frac{\pi}{6} (n^3 + d n^3 + 3ndn^2 + 3n^2 dn - n^3)$$

$$= \frac{\pi}{6} \times 3n^2 dn$$

[Neglecting higher power of dn as it is very small]

$$= \frac{\pi}{2} n^2 dn$$

$$\therefore N(E)dE = \frac{\pi}{2} n \times ndn. \text{----- (1)}$$

We know the energy of an electron in a cubical metal piece of sides 'a' is given by

$$E = \frac{n^2 h^2}{8ma^2}$$

$$\Rightarrow n^2 = \frac{8ma^2 E}{h^2}$$

$$\text{Or } n = \left(\frac{8ma^2 E}{h^2} \right)^{1/2} \text{----- (2)}$$

Differentiating n^2 term, we get

$$2ndn = \frac{8ma^2}{h^2} dE$$

$$\therefore ndn = \frac{8ma^2}{2h^2} dE \text{----- (3)}$$

Substituting eqn (2) and eqn (3) in eqn (1), we get

$$\textcircled{1} \Rightarrow N(E)dE = \frac{\pi}{2} n \times \pi dn$$

$$= \frac{\pi}{2} \left(\frac{8ma^2 E}{h^2} \right)^{1/2} \frac{8ma^2}{2h^2} dE$$

$$= \frac{\pi}{2} \times \frac{1}{2} \left(\frac{8ma^2}{h^2} \right)^{3/2} E^{1/2} dE$$

$$N(E)dE = \frac{\pi}{4} \left(\frac{8ma^2}{h^2} \right)^{3/2} E^{1/2} dE$$

According to Pauli's exclusion principle, only two electrons of opposite spin can occupy each state.

$$\therefore N(E)dE = 2 \times \frac{\pi}{4} \left(\frac{8ma^2}{h^2} \right)^{3/2} E^{1/2} dE$$

$$N(E)dE = \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{3/2} a^3 E^{1/2} dE$$

Density of states is given as number of energy states per unit volume.

$$\begin{aligned} Z(E) dE &= \frac{N(E)dE}{V} \\ &= \frac{\frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{3/2} a^3 E^{1/2} dE}{a^3} \\ &= \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{3/2} E^{1/2} dE \end{aligned}$$

$$Z(E)dE = \frac{4\pi}{h^3} (2m)^{3/2} E^{1/2} dE$$

This is the expression for density of energy states.

$$\begin{aligned} (8m)^{3/2} &= (8m)^1 (8m)^{1/2} \\ &= 4 \times 2m (4 \times 2m)^{1/2} \\ &= 4 \times (2m)^1 (2^2 \times 2m)^{1/2} \\ &= 4 \times 2 \times (2m)^1 (2m)^{1/2} \\ &= 8 (2m)^{3/2} \end{aligned}$$

Carrier concentration in metals:

The carrier concentration is the number of electrons per unit volume in a given energy range of interval.

$$\text{i.e. } n_c = \int Z(E) F(E) dE.$$

Energy band

$$= \int \frac{4\pi}{h^3} (2m)^{3/2} E^{1/2} \frac{1}{1+e^{(E-E_F)/KT}} dE$$

Energy band

$$= \frac{4\pi}{h^3} (2m)^{3/2} \int E^{1/2} \frac{1}{1+e^{(E-E_F)/KT}} dE$$

Energy band

This is the expression for density of charge carriers or carrier concentration at any temperature.

When $T = 0K$, $F(E) = 1$ Since, $(E < E_F)$

$$\begin{aligned} n_c &= \int_0^{E_F} \frac{4\pi}{h^3} (2m)^{3/2} E^{1/2} dE \\ &= \frac{4\pi}{h^3} (2m)^{3/2} \int_0^{E_F} E^{1/2} dE \end{aligned}$$

$$\begin{aligned}
&= \frac{4\pi}{h^3} (2m)^{3/2} \left(\frac{E_F^{3/2}}{\frac{3}{2}} \right) \\
&= \frac{2}{3} \times \frac{4\pi}{h^3} (2m)^{3/2} E_F^{3/2} \\
&= \frac{8\pi}{3h^3} (2m)^{3/2} E_F^{3/2} \\
&= \frac{8\pi}{3} \left(\frac{2m}{h^2} \right)^{3/2} E_F^{3/2}.
\end{aligned}$$

Expression for Fermi energy:

The general expression for the number of electrons lying in the energy interval dE is

$$n_c = \int Z(E) F(E) dE.$$

Energy band

When $T = 0K$, $F(E) = 1$ ($\because E < E_F$)

$$\begin{aligned}
\therefore n_c &= \int_0^{E_F} \frac{4\pi}{h^3} (2m)^{3/2} E^{1/2} dE \\
&= \frac{4\pi}{h^3} (2m)^{3/2} \int_0^{E_F} E^{1/2} dE \\
&= \frac{4\pi}{h^3} (2m)^{3/2} \left(\frac{E_F^{3/2}}{3/2} \right) \\
&= \frac{2}{3} \times \frac{4\pi}{h^3} (2m)^{3/2} E_F^{3/2} \\
&= \frac{8\pi}{3h^3} (2m)^{3/2} E_F^{3/2} \\
&= \frac{8\pi}{3} \left(\frac{2m}{h^2} \right)^{3/2} E_F^{3/2}
\end{aligned}$$

$$E_F^{3/2} = \frac{3n_c}{8\pi} \left(\frac{h^2}{2m} \right)^{3/2}$$

$$\therefore E_F = \left(\frac{3n_c}{8\pi} \right)^{2/3} \frac{h^2}{2m}$$

This is the expression for the Fermi energy of electron in solids at absolute zero.

4. (a) Derive the energy value of a particle in a three dimensional box. (OR)

(b) Derive Schrodinger equation for a particle in three dimensional box. Determine the Eigen values and Eigen functions for the same (OR)

(c) Obtain the Eigen values and Eigen functions of an electron enclosed in a 3-dimensional potential box (OR)

(d) Derive the energy value of a particle in a three dimensional box (OR)

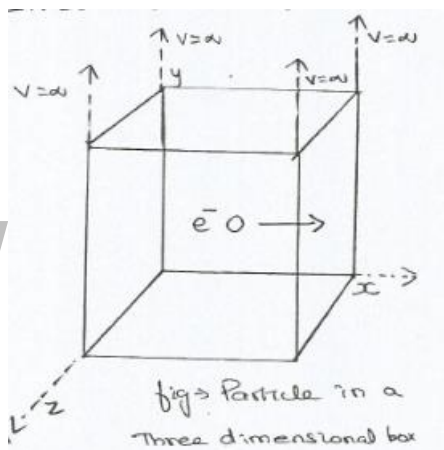
(e) Derive an expression for the density of single particle states as a function of energy For a free electron gas in three dimension?

Let us consider a particle enclosed in a three dimensional potential box of length a, b and c along X, Y and Z axis respectively.

In three dimensional potential box, the particle can move in any direction in space. Hence it has three quantum numbers n_x , n_y and n_z corresponding to the three coordinate axes X, Y and Z.

The energy of the particle = $E_x + E_y + E_z$. We know, for one dimensional potential box of width 'a'.

$$E_n = \frac{n^2 h^2}{8ma^2}$$



Then for three dimensional potential box of length a,b,c can be written as,

$$E_{n_x n_y n_z} = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8mb^2} + \frac{n_z^2 h^2}{8mc^2}$$

For a cubical box, $a = b = c$

$$\therefore E_{n_x n_y n_z} = \frac{h^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2) \text{ ----- (1)}$$

The corresponding normalized wave function of an electron in a cubical box can be written as

$$\Psi_{n_x n_y n_z} = \sqrt{\frac{2}{a}} \sqrt{\frac{2}{a}} \sqrt{\frac{2}{a}} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a}$$

$$\Psi_{n_x n_y n_z} = \sqrt{\frac{8}{a^3}} \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a} \text{ ----- (2)}$$

From equation (1) and (2) we can understand that several combinations of the three quantum numbers lead to different Eigen values and Eigen functions.

Degenerate State:

If a state has quantum numbers.

$$n_x = 1, n_y = 1 \text{ and } n_z = 2$$

$$\text{then } n_x^2 + n_y^2 + n_z^2 = 1+1+4 = 6$$

Similarly for $n_x = 1, n_y = 2, n_z = 1$ combination and $n_x = 2, n_y = 1, n_z = 1$.

$$n_x^2 + n_y^2 + n_z^2 = 6$$

$$\therefore E_{112} = E_{121} = E_{211} = \frac{6h^2}{8ma^2}$$

The corresponding wave functions are written as

$$\Psi_{112} = \sqrt{\frac{8}{a^3}} \sin \frac{\pi x}{a} \sin \frac{\pi y}{a} \sin \frac{2\pi z}{a}$$

$$\Psi_{121} = \sqrt{\frac{8}{a^3}} \sin \frac{\pi x}{a} \sin \frac{2\pi y}{a} \sin \frac{\pi z}{a}$$

$$\Psi_{211} = \sqrt{\frac{8}{a^3}} \sin \frac{2\pi x}{a} \sin \frac{\pi y}{a} \sin \frac{\pi z}{a}$$

For several combinations of quantum numbers, if we have same energy Eigen value but different Eigen functions, then such a state is called degenerate state.

$$\text{Example: } E_{112} = E_{121} = E_{211}$$

$$\Psi_{112} \neq \Psi_{121} \neq \Psi_{211}$$

Non-degenerate state:

For certain combination of quantum numbers if there is only one wave functions corresponding to a particular energy, then such states are called non-degenerate states.

Example: For $n_x = 2, n_y = 2$ and $n_z = 2$

$$\text{We have } E_{222} = \frac{12h^2}{8ma^2} \text{ and}$$

$$\Psi_{222} = \sqrt{\frac{8}{a^3}} \sin \frac{2\pi x}{a} \sin \frac{2\pi y}{a} \sin \frac{2\pi z}{a}.$$

5.(a) Derive an expression for the effective mass of an electron moving in energy bands of a solid show that it varies with the wave vector. (OR)

(b) Write a note on the effective mass of electron and the concept of hole.
(OR)

(c) (i) Explain effective mass of an electron and deduce an expression for the effective mass

(ii) Explain the concept of hole (OR)

(d) Explain the origin of band gap when an electron is moving in a periodic potential. Also explain the effective mass of electron in a periodic potential.

Definition:

The mass acquired by an electron when it is accelerated in a periodic potential is called effective mass of an electron. It is denoted by m^* .

Explanation:

When an electron is accelerated by an electric or magnetic field in a periodic potential, the mass of the electron is not a constant, it varies with respect to the field applied. This varying mass is called effective mass (m^*).

Derivation:

Consider an electron of charge e and mass m acted on by an electric field E .

The acceleration $a = \frac{eE}{m}$ is not a constant in the periodic lattice of the crystal. Its variation is caused by the variation of electron's mass when it moves in the crystal lattice.

$$\therefore a = \frac{eE}{m^*}$$

The electrical force on the electron $F = m^*a$ ----- (1)

Considering the free electron as a wave packet, the group velocity V_g corresponding to the particle's velocity can be written as

$$V_g = \frac{d\omega}{dk} \text{----- (2)}$$

Where $\omega \rightarrow$ angular frequency of the electron.

$K \rightarrow$ wave vector

We know, $\omega = 2\pi\gamma$

$$E = h\gamma \Rightarrow \gamma = \frac{E}{h}$$

$$\therefore \omega = \frac{2\pi E}{h} = \frac{E}{h}$$

Substituting in eqn (2) we get

$$V_g = \frac{d\omega}{dk} = \frac{1}{h} \frac{dE}{dk}$$

$$\begin{aligned} \text{Now acceleration } a &= \frac{dV_g}{dt} = \frac{1}{h} \frac{d^2E}{dt dk} \\ &= \frac{1}{h} \frac{d^2E}{d^2K} \frac{dk}{dt} \text{ ----- (3)} \end{aligned}$$

$$\begin{aligned} \text{We know momentum } p &= \frac{h}{\lambda} = \frac{h}{2\pi} \frac{2\pi}{\lambda} \\ &= \frac{1}{h} K \quad \text{Where } K = \frac{2\pi}{\lambda} \end{aligned}$$

$$\text{Now } \frac{dp}{dt} = h \frac{dk}{dt}$$

$$\text{The force acting on the electron } F = \frac{dp}{dt}$$

$$\therefore F = \frac{1}{h} \frac{dk}{dt}$$

$$\text{or } \frac{F}{h} = \frac{dk}{dt}$$

Substituting this in eqn (3), we get

$$\begin{aligned} a &= \frac{1}{h} \frac{d^2E}{dK^2} \frac{F}{h} \\ &= F \frac{1}{h^2} \frac{d^2E}{dK^2} \\ \therefore F &= \frac{h^2}{d^2E/dk^2} a \text{ -----(4)} \end{aligned}$$

Comparing eqn(1) and (4), we get

$$m^* = \frac{h^2}{d^2E/dk^2}$$

Hence the effective mass of an electron in a periodic potential depends on $\frac{d^2E}{dk^2}$.

Special Cases:

Case (1): If $\frac{d^2E}{dk^2}$ is positive, then m^* is also positive.

Case (2): If $\frac{d^2E}{dk^2}$ is negative, then m^* is also negative.

Case (3): If $\frac{d^2E}{dk^2}$ is zero, then m^* becomes infinity.

Case (4): If $\frac{d^2E}{dk^2}$ is more, then the electrons behave as light particle

Case (5): If $\frac{d^2E}{dk^2}$ is small, then the electrons behaves as heavy particles.

Concept of hole (or) Negative effective mass:

* The effective mass plays an important role in the conduction process in semiconductors and insulators since they have filled valence band.

* The effective mass is found to be negative near the zone edges of almost filled valence bands i.e., the electrons in these regions are accelerated in a direction opposite to the direction of the applied force. This is called the negative mass behaviour of electrons.

* The electron with the negative effective mass is called hole.

* The holes are not real particles like electron or positrons, but it is only a way of looking at the negative effective mass behaviour of electrons near the zone edge.

* The motion of negative effective mass of electron is looked upon as the motion of positive holes or positive vacant sites in a nearly filled band.

* Thus, the hole is a vacant state in the valence band of a semiconductor or insulator. When an electric field is applied, it behaves as a particle having positive electron mass and the same positive charge as the numerical value of the electron's charge.

6. (a) Explain the band theory of solids in detail and classify solids into conductors, semi-Conductors and insulators with neat diagram(OR)

(b) Explain how band theory is used to classify solids.(OR)

(c) How does the band theory of solids lead to the classification of solids into conductors, Semiconductors and insulators?

Energy Bands in Solids:

Consider a solid metal which contains N number of atoms packed closely together. Each atom in the metal has discrete set of electron energy levels. i.e., 1s, 2s, 2p, 3s,.....

The energies of electrons within any one isolated atom obey the following conditions.

* Electrons occupy the specified electronic energy levels of each atom. They cannot occupy the space between the levels.

* Electrons fill the lowest energy level first.

* According to Pauli's exclusion principle, only two electrons of opposite spin can occupy an energy level.

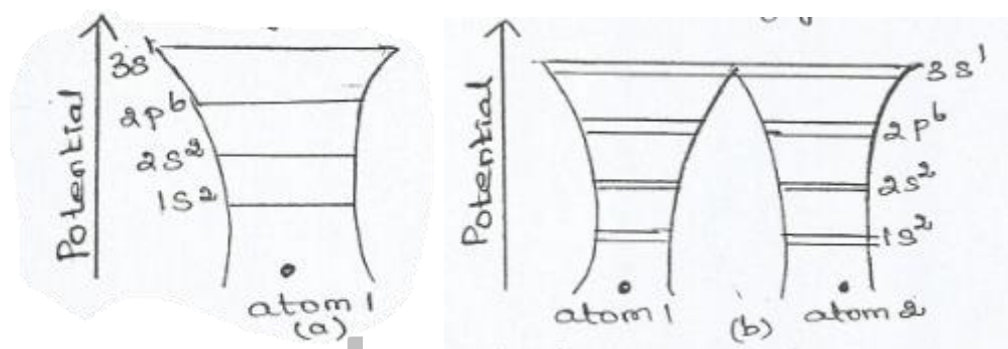
Imagine the N atoms in a solid to be isolated from one another, they would have completely coinciding schemes of energy levels.

When two atoms are brought close together to interact, each of the allowed electron energy levels within the atoms splits into two distinct but closely spaced

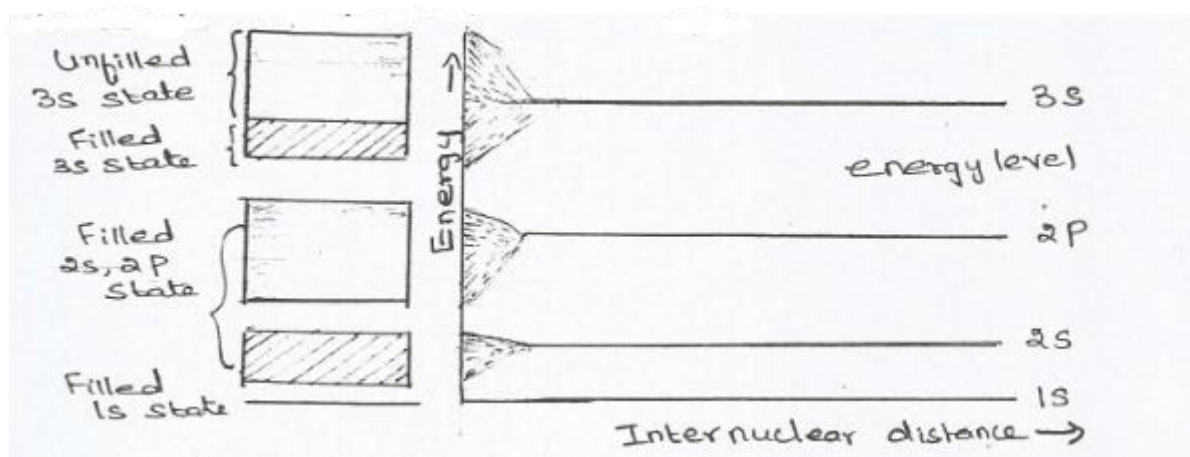
energy levels as the atoms combine to form the two-atom system. When more and more atoms are packed closely together, each set of split energy levels contains more and more levels spread over the same energy range allowed at that particular radius from the nuclei.

So, in a crystalline solid, the energy levels within each set become so closely spaced in energy that they form a continuous energy band.

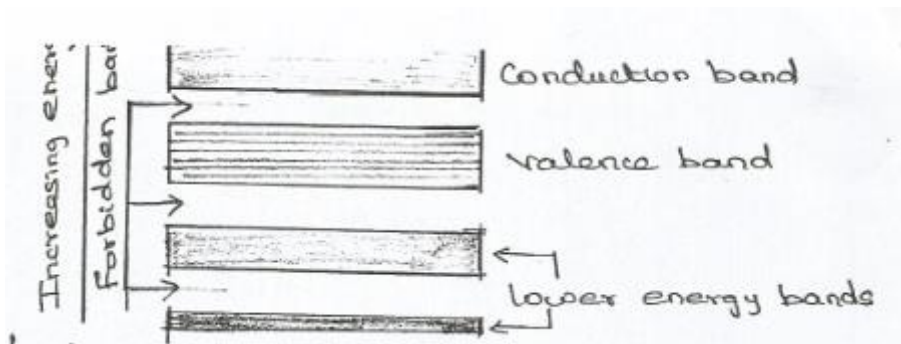
For example, consider a sodium metal which has 11 electrons with electronic configuration $1s^2 2s^2 2p^6 3s^1$. The energy spectrum of a single atom is shown in fig (a) and when two sodium atoms are assembled to form a sodium molecule the energy spectrum becomes as fig (b)



It is found that for a sodium molecule each atomic levels are split into two atoms are assembled to form a solid, then we have N number of very closely spaced sub levels so called energy band.



In solids, the bands of permissible energy levels are called the allowed bands. These may either be filled with electrons or empty. The energy bands between these allowed bands are called forbidden bands or energy gap. These bands correspond to the gaps between electron energy levels within the isolated atoms.



The highest energy band that is occupied by electrons is the valence band. The valence band consists of group of states containing the outermost electrons or valence electrons of an atom.

Above the valence band, there exists the band of next higher permitted energies called conduction band. It is separated from the valence band by a gap. The conduction band corresponds to the first excited states and it is normally the lowest unfilled energy band. The electrons can move freely and they are generally called as conduction electrons.

Classification of Metals, semiconductors and Insulators:

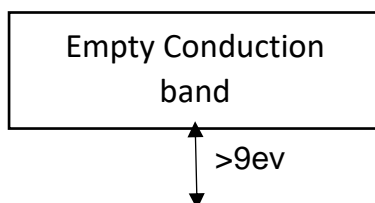
Based on band theory, solid-state materials can be classified into three groups.

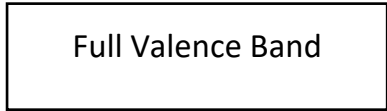
- (i) Insulators
- (ii) Semiconductors and
- (iii) Conductors

(i) Insulators:

Insulators are materials in which valence electrons are tightly bonded to their parent atoms, thus requiring very large electric field to remove them from the attraction of the nuclei

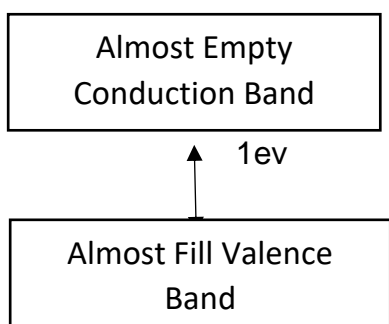
- * At OK, the valence band is completely filled and conduction band is empty.
- * The forbidden gap is very large – The energy gap exceeds $\sim 9\text{eV}$.
- * Insulators have very high electrical resistance and do not conduct electric current.
- * When large amount of energy is applied the electrons cannot Jump from valence band to conduction band.





(ii) Semiconductor:

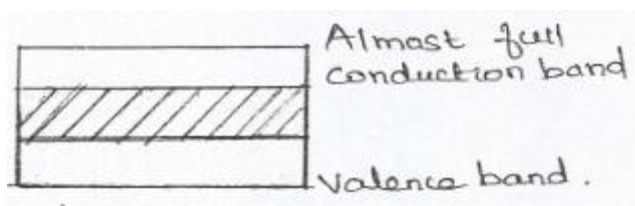
Material whose electrical properties lie in between insulators and good conductors are known as semiconductor material. (Example Ge, Si). In terms of energy band, semiconductors are materials which have almost an empty conduction band and almost filled valence band with a very narrow energy gap separating the two.



- * There is a small energy gap of the order of 1ev
- * Semiconductors at OK behave like insulators.
- * The electrons require a small energy to jump from valence band to conduction band. This energy may be in the form of heat or light.
- * Even at room temperature the thermal energy is sufficient to transfer electrons from valence band to conduction band.
- * In semiconductors the resistance decrease with increase in temperature.
- * Semiconductors have electrical resistance between those of conductors and insulators.

(iii) Conductors (or) Metals:

Conductors are materials which has plenty of free electrons for conduction. In conductors the valence band is only partially filled and overlap occurs between valence band and conduction band.



- * Electrons are free to move in both the valence and conduction bands.

- * There is no forbidden band gap.
- * Large number of free electrons are available.
- * Conductors have low electrical resistance.
- * Conduction is due to flow of electrons.

7. (a) Discuss the behaviour of an electron in a periodic potential and Explain tight binding approximation with suitable diagrams.(OR)

(b) Explain briefly about electron in periodic potential and describe tight binding approximation.

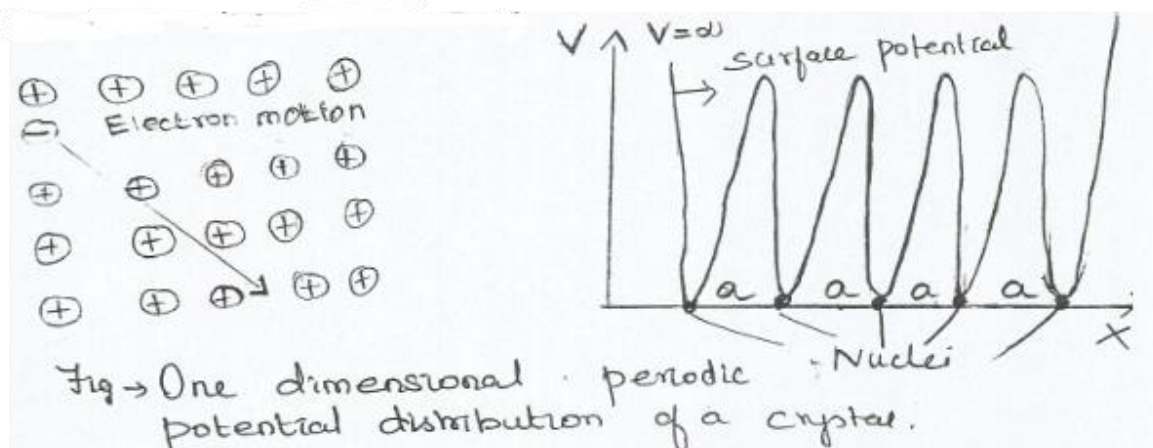
Electron in periodic potential:

Definition:

When an electron moves through a solid, its Potential energy varies periodically with the periodicity equal to period of interatomic distance. This is called periodic potential.

Explanation:

In a metal piece, the positive are arranged in a regular and proper order in a lattice. Hence a periodic potential exists in a metal. Also the potential is minimum near the centre of positive ions and is maximum between the centres of ions.



Therefore, the potential energy of the electron nearby the centre of positive ions is maximum and will not be able to move freely. But the electrons which are above these potential peaks are free to move inside the metal and hence they are termed as free electrons.

Tight Binding Approximation

In solids, there exist ionic cores which are tightly bounded to the lattice location, while the electrons are free to move throughout the solid. This is called free electron approximation.

Tight binding approximation is exactly an opposite approach when compared to free electron approximation. In tight binding approximation, the atoms are free while the electrons are tightly bounded to the atom.

The following are the points of approximation in this binding.

- * The potential energy of the electron accounts for the total energy.
- * The width of forbidden bands is large as compared to the allowed bands.
- * The lattice constant is so large that the wave functions of adjacent atoms do not overlap.
- * The interaction between neighbouring atoms is relatively weak.
- * The wave functions and allowed energy levels of the crystal as a whole are closely related to the wave functions and energy levels of isolated atoms.