### **Lecture Notes**

Course/Subject : Applied Physics (R-22)

UNIT : II - Introduction to Quantum Physics and Band Theory of Solids.

## **Introduction to quantum physics:**

### Planck's law (Qualitative)

When a blackbody is heated, it radiates electromagnetic waves of all possible wavelengths. The distribution of total radiated energy among different wavelengths is called spectral distribution of energy.

In 1900, Max Planck introduced the idea of quantum nature of radiation and derived the equation for spectral distribution which was found to be valid for all wavelengths of black body radiation.

Max planck developed quantum theory of radiation based on the following assumptions

- a) A black body contains simple harmonic oscillators of atomic dimensions and all possible frequencies. Such oscillators are called Planck oscillators.
- b) The energy of these Planck oscillators is quantized and is equal to nhv, where v is the frequency of oscillation, h is the Planck's constant and n is the interger.
- c) A Planck oscillator of frequency v can radiate or absorb energy in terms of hv.

By considering Maxwell Boltzmann distribution law to the Planck oscillators, Max Planck derived the following relation for spectral distribution of black body radiation

$$E_{\lambda}d\lambda = \frac{8\pi ch}{\lambda^5} \frac{1}{e^{\frac{hc}{\lambda KT}} - 1} d\lambda$$

This relation was found to be valid for all wavelengths of black body radiation spectrum.

### Wave particle duality and de-Broglie hypothesis:

Light or radiation has dual nature i.e., particle nature (Compton effect and photo electric effect) and wave nature (interference and diffraction). This idea of dual nature of radiation was extended to material particle by the scientist de-Broglie in 1924 and put forward the hypothesis.

#### de-Broglie hypothesis:

Any moving particle has got a wave associated with it. Such waves are named as **matter** waves or de-Broglie matter waves.

### **Expression for the wavelength of matter wave:**

de-Broglie derived the expression for the wavelength of matter wave based on the quantum nature of radiation and using Einstein's mass-energy relation.

According to quantum theory of radiation, radiation is composed of photons and the energy of a photon is given by E = hv -----(1)

where v is the frequency of radiation.

Considering photon as particle, let 'm' be the mass of the photon, then according to Einstein's mass-energy relation,

$$E = mc^2 - (2)$$

Equating equations 1 and 2

$$hv = mc^2$$

but 
$$v = \frac{c}{\lambda}$$

therefore  $\frac{hc}{\lambda} = mc^2$ 

$$\lambda = \frac{h}{mc}$$

Extending the theory to material particle of mass 'm' moving with velocity 'v', the wavelength of associated matter wave is,  $\lambda = \frac{h}{mv}$ 

#### **Characteristics of Matter waves:**

Since wavelength of matter wave is  $\lambda = \frac{h}{mv}$ ,

- 1. Lighter the particle, greater is the wavelength associated with it.
- 2. Lesser the velocity of the particle, longer the wavelength associated with it.
- 3. For v = 0,  $\lambda = \infty$ . This means that only with moving particle, matter waves is associated.
- 4. Whether the particle is charged or not, matter waves is associated with it.
- 5. It can be proved that matter waves travel faster than light.

We know that  $E = mc^2$  and E = hv,

$$hv = mc^2$$

$$v = \frac{mc^2}{h}$$

The wavelength of matter wave is  $\lambda = \frac{h}{mv}$ 

Therefore the velocity of matter wave (say v<sub>m</sub>) is

$$v_m = \lambda v = \frac{h}{mv} \frac{mc^2}{h} = \frac{c^2}{v}$$

As the particle velocity 'v' cannot exceed velocity of light,  $v_m$  is greater than the velocity of light.

- 6. No single phenomena exhibit both particle nature and wave nature simultaneously.
- 7. The wave nature of matter introduces an uncertainty in the finding the position and momentum of the particle when both are determined simultaneously.

## SCHRÖDINGER'S TIME INDEPENDENT WAVE EQUATION:

Schrödinger, in 1926, developed wave equation for the matter wave associated with moving particles. One of its forms can be derived by simply incorporating the deBroglie wavelength expression into the classical wave eqn.

Let us consider a particle of mass 'm' moving with velocity 'v' is associated with a group of matter waves. Let  $\psi(x,t)$  be the displacement of the matter wave and x,y,z be the coordinates of the particle.

The classical wave equation in space is given by

$$\frac{\partial^2 \Psi}{\partial t^2} = V^2 \left( \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) - - - - - - - (1)$$

or 
$$\frac{\partial^2 \Psi}{\partial t^2} = V^2 \nabla^2 \Psi - - - - - - - (2)$$

where 
$$\nabla = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$
 is called the Laplacian operator.

The general solution of the above equation is

$$\Psi = \Psi_0 \sin(\omega t) = \Psi_0 \sin(2\pi v t) - (3)$$

Where  $\Psi_0$  is the amplitude.

Differentiating  $\Psi$  w.r.to t,

$$\frac{\partial \Psi}{\partial t} = 2\pi \nu \Psi_0 \cos(2\pi\nu t)$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -4\pi^2 \nu^2 \Psi_0 \sin(2\pi\nu t) = -4\pi^2 \nu^2 \Psi - - - - - - - - (4)$$

Substituting 4 in 2, we get

$$-4\pi^{2}\nu^{2}\Psi = V^{2}\nabla^{2}\Psi - - - - - - - - (4)$$

But  $V = v\lambda$  or  $v=V/\lambda$ ,

Equation 4 becomes,  $-4\pi^2 \frac{V^2}{\lambda^2} \Psi = V^2 \nabla^2 \Psi$ 

Implies 
$$\nabla^2 \Psi + \frac{4\pi^2}{\lambda^2} \Psi = 0$$

Substituting  $\lambda = \frac{h}{mV}$ , we get

$$\nabla^2 \Psi + \frac{4\pi^2 (m^2 V^2)}{h^2} \Psi = 0 - - - - - 5$$

and total energy(E)=K.E.(K)+P.E.(U)

$$(\frac{1}{2})mV^2=(E-U)$$
, implies  $m^2V^2=2m(E-U)$ .

Substituting in equation 5,

$$\nabla^{2}\Psi + \frac{4\pi^{2}\{2m(E-U)\}}{h^{2}}\Psi = 0$$

$$\nabla^{2}\Psi + \frac{\{2m(E-U)\}}{h^{2}}\Psi = 0 - - - - - - 6$$

This is the Schrödinger Time Independent Wave Equation.

### **Physical Significance of Wave Function:**

Max Born in 1926 gave a satisfactory interpretation of the wave function  $\Psi$  associated with a moving particle. He postulated that the square of the magnitude of the wave function  $|\Psi|^2$  (or

 $\Psi \Psi^*, \Psi^*$  is complex conjugate of  $\Psi$ ), evaluated at a particular point represents the probability of finding the particle at the point.

 $|\Psi|^2$  is called the probability density and  $\Psi$  is the probability amplitude. Thus the probability of the particle within an element volume dv is  $|\Psi|^2$ dv. Since the particle is certainly somewhere, the integral at

 $|\Psi|^2$  dt over all space must be unity i.e.

$$\iiint \mid \Psi \mid^2 dv = 1$$

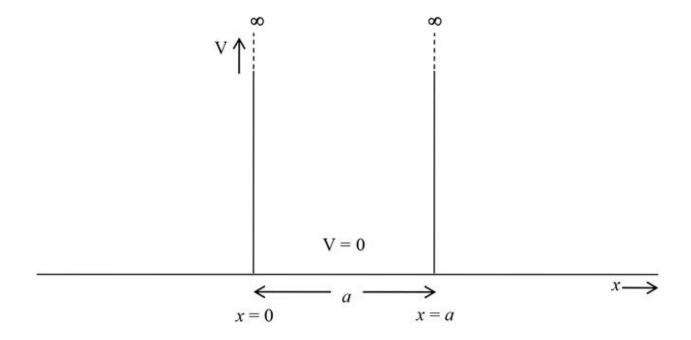
In one dimension, say along x axis

$$\int |\Psi|^2 \, \mathrm{d} x = 1$$

A wave function that obeys the above equations is said to be normalized.

### PARTICLE IN ONE DIMENSIONAL POTENTIAL BOX:

Consider a particle of mass 'm' moving along the x-axis between x=0 and x=a inside a onedimensional box of infinite height and width



### Fig. Particle in a potential well of infinite height.

Assume that the particle is freely moving inside the box. The motion of the particle is restricted by the walls of the box. The particle is bouncing back and forth between the walls of the box at x = 0 and x = a. For a freely moving particle at the bottom of the potential well, the potential energy is very low. Since the potential energy is very low, moving particle energy is assumed to be zero between x = 0 and x = a.

The potential energy of the particle outside the walls is infinite due to the infinite P.E outside the potential well.

The particle cannot escape from the box

i.e. 
$$V = 0$$
 for  $0 < x < a$ 

$$V = \infty$$
 for  $0 > x > a$ 

Since the particle cannot be present outside the box, its wave function is zero

ie 
$$|\psi|^2 = 0$$
 for  $0 > x > a$ 

$$|\psi|^2 = 0$$
 for  $x = a \& x = 0$ 

The Schrödinger time independent wave equation in one – dimension

$$\frac{d^2\Psi}{dx^2} + \frac{\{2m(E-U)\}}{\hbar^2}\Psi = 0 - - - - 1$$

Between the walls, the potential experienced by the particle is zero, i.e., U=0

Therefore equation 1 becomes

$$\frac{d^2\Psi}{dx^2} + \frac{2mE}{\hbar^2}\Psi = 0 - - - - 2$$

Let 
$$\frac{2mE}{h^2} = K^2$$
 -----3

Eqn.(2) becomes 
$$\frac{d^2\Psi}{dx^2} + \frac{2mE}{\hbar^2}\Psi = 0 - - - - 4$$

Eqn. (3) is similar to eq. of harmonic motion and the general solution of above eqn. is written as

$$\Psi(x) = A \sin kx + B \cos kx - (5)$$

where A, B and k are unknown quantities.

To find A and B, we apply the boundary conditions,

- a) When x = 0,  $\Psi(x) = 0$ . Substituting in equation 5, we get 0 = 0 + B, implies B = 0 and equation 4 becomes  $\Psi(x) = A \sin kx$ -----(6)
- b) When x = a,  $\Psi(x) = 0$  implies Asin Ka=0. Since A $\neq$ 0, SinKa=0 This is possible when Ka = n  $\Pi$  or  $k = n \Pi/a$ -----(7)

Substituting the value of k in eqn. (3)

$$\frac{2mE}{\hbar^2} = \left[\frac{n\pi}{a}\right]^2$$

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

The wave eqn. can be written as

$$\Psi(x) = A\sin\left(\frac{n\pi}{a}\right)x - (9)$$

To find the value of A, we apply the normalization condition. As the electron is definitely present between the two walls, the probability that the particle is found inside the box is unity.

$$\int_0^a |\Psi(x)|^2 dx = 1$$

$$\int_0^a \left| A \sin \left( \frac{n\pi}{a} \right) x \right|^2 dx = 1$$

$$A^{2} \int_{0}^{a} \sin^{2}\left(\frac{n\pi x}{a}\right) dx = 1$$

$$A^{2} \int_{0}^{a} \frac{1}{2} \left[1 - \cos\left\{\frac{2n\pi x}{a}\right\}\right] dx = 1$$
Or 
$$\frac{A^{2}}{2} \left[x - \frac{a}{2\pi n} \sin\frac{2\pi nx}{a}\right]_{0}^{a} = 1$$

implies 
$$\frac{A^2L^{\infty}}{2} = 1 \text{ or } A = \sqrt{\frac{2}{a}}$$

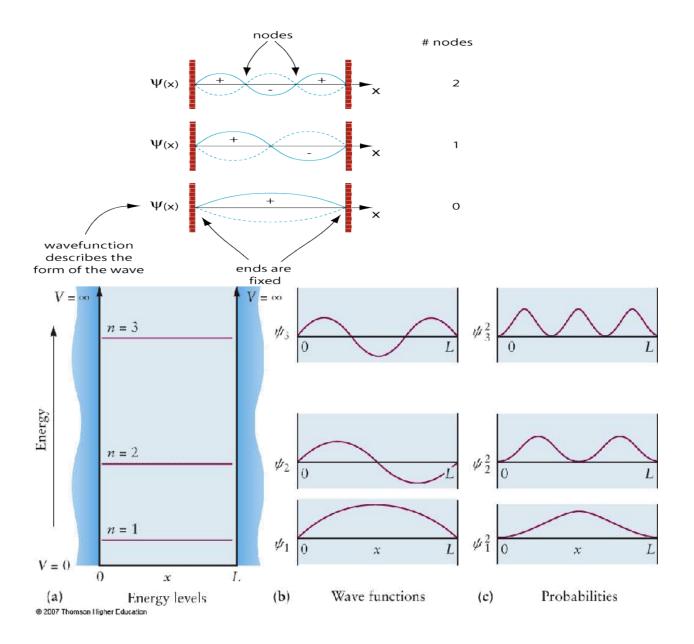
The normalized wave functions and corresponding energies En, are called eigen functions and eigen values.

Substituting the value of A in equation 9, we get

$$\Psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}\right) x - - - - - 10$$

Eqn. (8) represents an energy level for each value of n and the corresponding wave function is given in eqn. (10). Therefore the particle in the box can have discrete values of energies which are quantized.

The normalized wave functions  $\Psi 1$ ,  $\Psi 2$ ,  $\Psi 3$  given by eqn (10) are plotted.



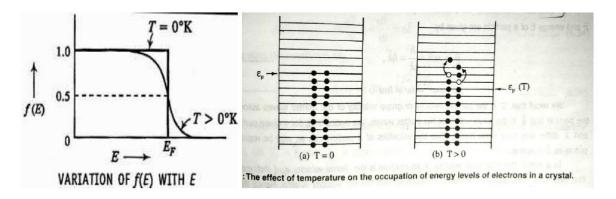
Note: Distance between the walls is taken as "a" or "L"

## Fermi Dirac Distribution:-

A metal piece contains very large number of electrons. Each electron possesses quantized energy states and obeys Pauli's exclusion principle. Hence they satisfy Fermi-Dirac statistics. The probability F(E) of an electron occupying energy level  $E_i$  is given by

$$F(E_i) = \frac{1}{\exp(\frac{E_i - E_f}{kT}) + 1}$$

Where  $F(E_i)$  is called Fermi function which is defined as the probability of electron occupation in the given energy state ( $E_i$ ) at thermal equilibrium.  $E_f$  is Fermi energy,  $E_i$  is energy of  $i^{th}$  state and k is Boltzmann constant.



The plot of F(E) Vs E is as shown in fig.

**Conclusions:** At **T=OK**, the Fermi Dirac distribution of electrons can be understood mathematically from the following two cases.

Case -1: If E>E<sub>F</sub>, 
$$e^{\frac{(E_i-E_F)}{kT}}$$
 =  $\infty$ 

Therefore,  $F(E_i)=1/\infty$  then  $F(E_i)=0$ . It indicates that energy levels above Fermi level are empty.

Case -2: If  $E < E_F$ ,  $e^{\frac{(E_i - E_F)}{kT}} = 0$  then  $F(E_i) = 1$ . It indicates that energy levels below Fermi levels are full of electrons. The Fermi level is a boundary energy level which separates the filled energy state and empty states at 0k. The energy of the highest filled state at 0k is called Fermi Energy  $E_F$  and the energy level is known as Fermi Level.

Case-3: At T>OK, if  $E_i=E_F$  then  $F(E_i)=1/2$ . i.e 50%. Therefore Fermi level is the energy level for which the probability of filled states is 50% at any temperature.

2. When **T>0**,  $F(E_F)<1$  for  $E_i<E_F$ 

$$F(E_i)>0$$
 for  $E_i>E_F$ 

$$F(E_i) = \frac{1}{2}$$
 for  $E_i = E_F$ 

As temperature increases more and more electrons jump to the levels above EF leaving vacancies as shown in the fig.

- 3. The electrons in the levels above EF and vacancies in the levels below EF are responsible for conduction in semiconductors.
- 4. If the temperature is raised further, the resistance of the metals increases due to decrease of mobility.
- 5. At **T>0K**, the Fermi energy level decreases.

### **Introduction to electron theory**

The electron theory aims to explain the structure and bulk properties of solids through their electronic structure. The theory has been developed in three main stages.

### The classical free electron theory

The classical free electron theory was introduced by P. Drude in 1900 and developed by Lorentz in 1909. According to this theory, the metals containing the free electrons and obey the laws of classical mechanics.

#### The quantum free electron theory

Somerfield developed this theory in 1928. According to this theory the free electrons obey quantum laws and are called fermions. According to this theory, the free electrons moving inside a solid experience a constant potential field.

### The zone theory

Bloch stated this theory in 1928. According to this theory, the free electrons moving inside a solid or metal, experiences a periodic potential field due to the positive ion core in the lattice.

### **CLASSICAL FREE ELECTRON THEORY:**

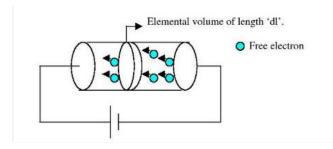
The classical free electron theory is based on the following postulates or assumptions

1. The valence electrons of atoms are free to move about the whole volume of the metal, like the molecules of a perfect gas in a container.

- 2. The free electrons move in random direction and collide with either positive ions fixed to the lattice and the collisions are elastic in nature i.e., there is no loss of energy.
- 3. The electron velocities in a metal obey classical Maxwell-Boltzmann distribution of velocities and the RMS velocity of these electrons is given by  $\bar{C} = \sqrt{\frac{3KT}{M}}$ .
- 4. Mutual repulsion between electrons is ignored and hence potential energy is taken as zero. Therefore the total energy of the electron is equal to its kinetic energy.
- 5. As the potential experienced by the free electrons inside the metal is zero and at the walls, infinite, the electrons are confined inside the metal specimen.

### **Drift velocity**

If no electric field is applied on a conductor, the free electrons move in random directions, just as gas molecules move randomly in a gas container. They collide with each other and also with the positive ions. Since the motion is completely random, average velocity in any direction is zero. If a constant electric field is established inside a conductor, the electrons experience a force F = -eE due to which they move in the direction opposite to direction of the field. As a result, in addition to the random velocity, the electrons gain an additional velocity due to the applied electric field. This velocity is called **drift velocity** " $V_d$ ".



### **Merits of Classical Free Electron theory:**

- ➤ It verifies Ohm's law
- > It explains the electrical and thermal conductivities of metals
- ➤ It derives Wiedmann-Franz law: i.e. the ratio of thermal conductivity to electrical

conductivity of a metal is directly proportional to absolute temperature.

 $K/\sigma \propto T$ 

or

 $K/\sigma T = L$ , where L is a constant called Lorentz number.

> It explains optical properties of metals

### **Drawbacks of Classical free electron theory**

Classical free electron theory has the following drawbacks

- The phenomena such as photoelectric effect, Compton Effect and spectral distribution of blackbody radiation could not be explained by classical free electron theory
- According to this theory,  $K/\sigma T = L$ , a constant (Wiedmann-Franz law) for all temperatures. But this is not true at low temperatures.
- > The theoretically predicted value of specific heat of a metal does not agree with the experimentally obtained value.
- ➤ Electrical conductivity of semiconductors and insulators couldn't be explained by this theory
- This theory fails to explain ferromagnetism and superconductivity.

## **Kronig – Penny Model:-**

According to Kronig-penny theory the electrons move in a periodic potential produced by the positive ion cores. The potential energy of the electron varies periodically with the periodicity of positive ion core and potential energy of electron is zero at the positive ion sites (near the nucleus of the positive ion) and maximum between the two ions. The two positive ions are separated by the interatomic distance 'a' as shown in fig.

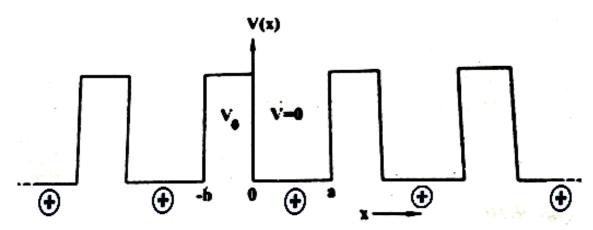


Fig. One dimensional Periodic potentials in a crystal

From the fig.:

The variation of P.E of electron,  

$$V(x) = \{ 0, \text{ for Region-I}, 0 < x < a \}$$
  
 $\{ V_0, \text{ for Region-II}, -b < x < 0 \}$ 

Here we have two regions.

The 1-dimensional Schroedinger Time Independent wave equation is,

$$\begin{split} &\frac{d^2\Psi}{dx^2} + \frac{2m}{\mathfrak{h}^2} \, ( \ E-V(x)) \Psi = 0 \\ &\text{Since, } V(x) = 0, \qquad \frac{d^2\Psi}{dx^2} + \frac{2m}{\mathfrak{h}^2} \, E \Psi = 0 \\ &\text{Consider,} \qquad \frac{2m}{\mathfrak{h}^2} \, E = \alpha^2 \\ &\text{Then, } \frac{d^2\Psi}{dx^2} + \alpha^2 \, \Psi = 0 \quad ------(1) \end{split}$$

The 1-dimensional Schroedinger Time Independent wave equation is,

$$\begin{split} &\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} \, ( \ E\text{-V}(x)) \Psi = 0 \\ &\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} \, ( \ E\text{-V}_0) \Psi = 0 \quad \text{[ since V(x) =V_0 ]} \\ &\frac{d^2\Psi}{dx^2} - \frac{2m}{\hbar^2} \, (V_0\text{- E}) \Psi = 0 \quad \text{[since V}_0\text{>> E ]} \end{split}$$

Consider, 
$$\frac{2m}{\mathfrak{h}^2}$$
 (V<sub>0</sub>- E) =  $\beta^2$   
Then,  $\frac{d^2\Psi}{dx^2}$  -  $\beta^2\Psi$  = 0 -----(2)

The solutions of equations (1) & (2) can be obtained by using Bloch theorem

i.e., 
$$\Psi_K(x) = e^{\pm iKx} U_K(x)$$
....(3)

and 
$$U_K(x) = U_K(x+a)$$

Differentiating equation(3) w. r.to. 'x' twice and substituting in eqns (1)&(2) and applying boundary conditions and solving,

we get the solution,

$$\frac{P}{\alpha a} \sin \alpha a + \cos \alpha a = \cos Ka \qquad ....(4)$$

It is also called as Kronig - Penny equation.

Where, P = Scattering power of the potential barrier

$$P = \frac{maV0\omega}{\hbar^2}$$
;  $V_0\omega = Barrier strength$ .

## Kronig - Penny Graph :-

The left hand side of equation (4) is plotted as a function of ' $\alpha$ a' for the value of P=  $6\pi$  as shown in fig. Coska imposes a limitation on the values of the left side function .i.e. from +1to -1.

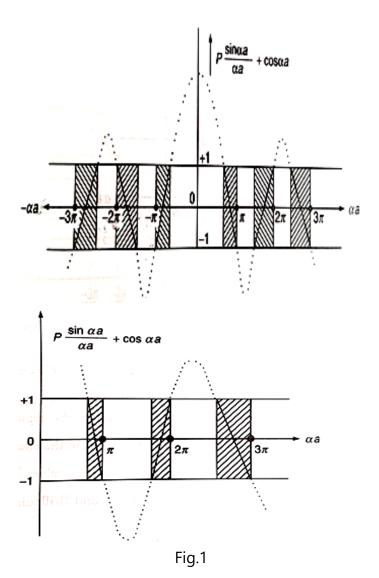
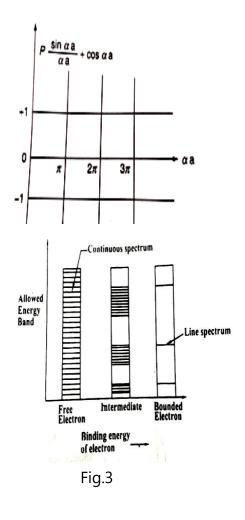


Fig.2



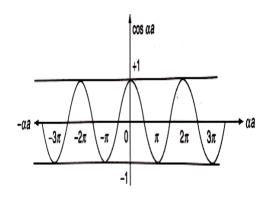


Fig.4 Fig.5

### **Conclusions-**

- (i). The energy spectrum has a number of allowed energy and forbidden energy bonds, as shown in fig. 1.
- (ii). As the value of '  $\alpha a$  ' increases the width of the allowed ENERGY band increases and width of the forbidden band decreases as shown in fig. 2.
- (iii). As  $P \rightarrow \infty$ , the allowed energy band becomes infinitely narrow and the energy spectrum is a line spectrum as shown in fig. 3.
- (iv) As scattering power (P) increases, the strength of potential barrier increases and the width of the allowed energy band decreases.
- (v) When  $P \rightarrow 0$  then electrons move freely over the lattice without energy potential. Hence all the energies are allowed to the electrons and produce the continuous spectrum as shown in fig. 4
- (vi) Thus by varying P from 0 to  $\infty$ , we get the energy spectra of all energies as shown in fig. 5.

## **Brilliouin Zones (or) E-K Diagram:-**

Brillouin zones are the boundaries that are marked by the values of waves vector K, in which the electrons can have allowed energy values. These represent the allowed values of K of the electrons in 1D, 2D & 3D.

We have, the energy of the electron in a constant potential box is,

$$E = \frac{n^2h^2}{8ma^2}....(1), Where a = length of the box.$$

But, K = 
$$\frac{n\pi}{a}$$
 »  $\boxed{K^2}$  =  $\frac{n^2\pi^2}{a^2}$   $\frac{n^2}{a^2}$  =  $\frac{K^2}{\pi^2}$ .....(2)

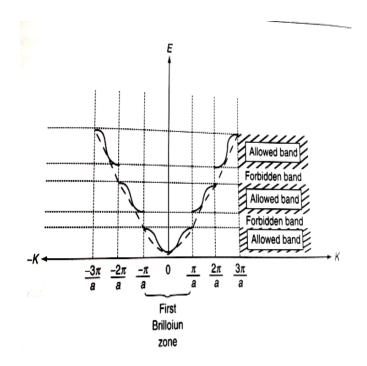
Substitute eqn. (2) in (1), we get

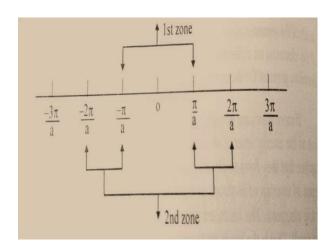
: 
$$E = \frac{K^2h^2}{8m\pi^2}$$
; i.e.,  $E \alpha K^2$ ...It represents Parabolic equation.

## **Graph:-**

A graph is drawn between the total energy (E) and the wave vector k, for various values of k.

i.e, 
$$K = \frac{n\pi}{a}$$
;  $n = \pm 1, \pm 2, \pm 3,...$ 





 $1^{st}$  Brillouin Zone (1BZ):-  $-\frac{\pi}{a}$  to  $\frac{\pi}{a}$   $2^{nd}$  Brillouin Zone (2BZ):-  $-\frac{\pi}{a}$  to  $\frac{-2\pi}{a}$  and  $\frac{\pi}{a}$  to  $\frac{2\pi}{a}$  Similarly  $3^{rd}$ ,  $4^{th}$  Brillouin Zones can be obtained. Brillouin Zones are separated by forbidden gap.

### **Effective mass of the electron:**

When an electron in a period potential is accelerated by an electric field (or) magnetic

field, then the mass of the electron is called effective mass (m\*).

Let an electron of charge 'e' and mass 'm' moving inside a crystal lattice of electric field (E).

## According to Newton's law

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

$$v_g = \frac{d\omega}{dk} = \frac{d(2\Pi\nu)}{dk} = 2\Pi \frac{d\nu}{dk} = {2\Pi \choose h} \frac{d(h\nu)}{dk} = \frac{1}{h} \frac{dE}{dk} - \dots (2)$$

where, the energy E = hu and  $\hbar = \frac{h}{20}$ 

Acceleration a = 
$$\frac{dv_g}{dt} = \frac{d(\frac{1dE}{hdk})}{dt} = \frac{1}{h} \frac{d^2E}{dk.dt} = \frac{1}{h} \left(\frac{d^2E}{dk.dk}\right) \left(\frac{dk}{dt}\right) = \frac{1}{h} \left(\frac{d^2E}{dk^2}\right) \left(\frac{dk}{dt}\right)$$
 (3)

Since 
$$\hbar k = p$$
  

$$\hbar (dk/dt) = (dp/dt)$$

$$\hbar (dk/dt) = F$$

$$(dk/dt) = F/\hbar$$

Equation (3) become

$$\therefore a = \frac{1}{h^2} \left( \frac{d^2 E}{dk^2} \right) F$$

Substitute 'a' value in equation (1)

$$m*=[\frac{\hbar^2}{(\frac{d^2E}{dk^2})}]$$
-----(4)

This equation indicates that the effective mass is determined by  $\frac{d^2E}{dk^2}$ .

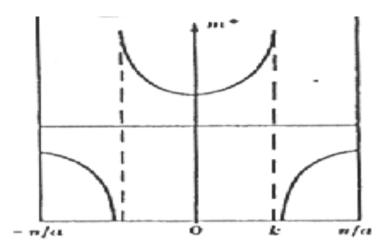
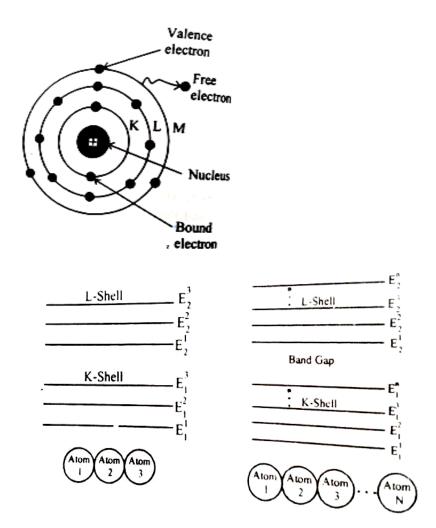


Fig. Effective mass as a function of k

# Origin of Energy band formation in Solids:-

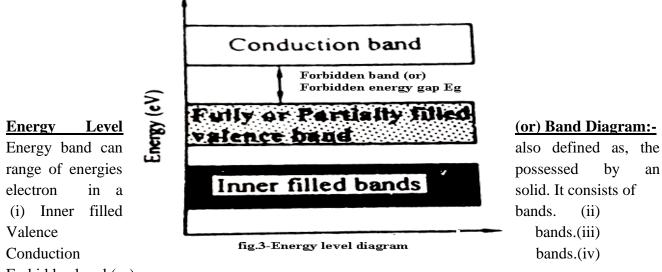
Band theory of solids explains, the formation of energy bands and determines whether a solid is a conductor, insulator or a semi conductor.

# **Energy Bands:-**



When two atoms of equal energy levels are brought closer together, the original energy levels  $E_1\&\ E_2$  splits each into two energy levels. i.e., the K- shell energy  $E_1$  splits into  $E_1{}^1\&\ E_1{}^2$ , similarly the L-shell energy  $E_2$  splits into  $E_2{}^1\&\ E_2{}^2$ 

When 3-atoms are brought closer together, the original energy levels  $E_1\& E_2$  splits into 3 energy levels as  $E_1^1$ ,  $E_1^2$ ,  $E_1^3\& E_2^1$ ,  $E_2^2$ ,  $E_2^3$  respectively. Therefore, if 'N' no. of atoms of equal levels are brought closer to form a solid, then forms a closely spaced continuous energy levels, called as <u>energy bands</u>.



Forbidden band (or) energy gap.

(i) Inner filled bands:- During the formation of energy bands the inner filled energy levels forms a energy band called as inner filled bands. It is completely filled with electrons.

### (ii) Valence bands:-

The electrons in the outermost orbits of atoms forms a energy band, called as valence band. It is completely filled (or) partially filled with electrons, based on the type of materials.

#### (iii) Conduction band:-

If the electrons come out from valence band for conduction, then they forms a energy band, called as Conduction band. It is partially filled (or) empty band.

### (iv) Forbidden band:-

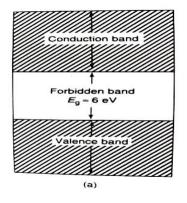
Energy bands are separated by small regions which do not allow any energy levels. Such regions between the energy bands are called as forbidden energy gap or forbidden bands.

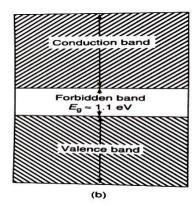
### **Classification of Solids:-**

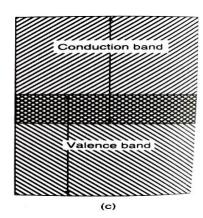
Based on band theory, arrangement of electrons and forbidden energy gap, the solid materials are classified into 3 types.

They are,

- 1. Conductors
- 2. Insulators,
- 3. Semi conductors







## 1) Conductors:-

Solid materials which conduct electric current when potential difference is applied across them, are known as Conductors.

In conductors, the forbidden energy gap is zero (Eg = 0) i.e., both valence band & conduction band overlap with each other as shown in Fig.1.

In conduction band plenty of free electrons are available. These electrons move freely from valence band to conduction band & constitute electrical current. Ex:- Cu, Al,Fe,....etc.

### 2) Insulators:-

Solid materials which don't conduct electric current are known as insulators.

In insulators, the forbidden energy gap is very high (Eg> 3 eV). Due to this electrons cannot jump from valence bond to conduction band. In insulators, the valence electrons are bound tightly to their parent atom.

At 0k, the valence bond is completely filled & energy gap between C.B & V.B is of the order of 10ev. The resistivity of insulator is of the order of  $10^7 \,\Omega$ -m. Ex:- Glass, wood, plastic

### 3) Semi conductors:-

Solid materials, whose electrical conductivity lies between conductors & insulators are called as semi conductors. Conductivity of semi conductors is in the order of  $10^4$  to  $10^{-4}$  mho m<sup>-1</sup>.

In semi conductors, the forbidden energy gap is very small (Eg= 1.1ev or Eg < 3 eV). Ex:-Ge, Si.

For Ge, forbidden energy gap (Eg) = 0.72 eV and Si, Eg = 1.1 eV At T = 0 k, semi conductor becomes an insulator.

# \*\*\*Distinguish between Conductors, Semiconductors and Insulators:-

Conductors	Semiconductors	Insulators
1.valence band and conduction	1. valence band and conduction	1. valence band and conduction
bands overlap with each other	bands do not overlap with each	bands do not overlap with each
	other	other
2.Forbidden Energy gap is zero	2. energy gap is very small	2. energy gap is very high
i.e., Eg = 0	i.e., Eg= 1.1ev or Eg < 3 eV	i.e., Eg> 3 eV).
3. Conductivity is vey high	3. Conductivity is medium	3. Conductivity is very less or zero
4. Resistivity is very less	4. Resistivity is medium	4. Resistivity is very high
5.They have +ve temperature	5. They have -ve temperature	5. They have -ve temperature
Coefficient of resistance	Coefficient of resistance	Coefficient of resistance
6. Charge carriers are electrons	6. Charge carriers are electrons and holes	6. No Charge carriers
7. Ex:- Cu, Al,Fe,etc.	7. Ex:-Ge, Si.	7. Ex:- Glass, wood, plastic