

SEMICONDUCTOR PHYSICS

UNIT-1

CLASSICAL FREE ELECTRON THEORY :-

In most solids, the two main types of internal energy are (i) the vibrational energy of the atoms about their mean lattice positions and (ii) the kinetic energy of the free electrons.

If an electric field is applied to a solid, the free electrons are accelerated. Their kinetic energy increases. Some of the kinetic energy is lost by collisions with the atom in the lattice. The resulting current is proportional to the average velocity of the free electrons. This velocity is determined by the applied electric field and also the collision frequency.

There are two different velocities associated with the electrons. (i) drift velocity ($v_d = -eE\tau/m$) which is superimposed on a much higher velocity called root mean square velocity (\bar{c}) due to the random motion of the electron which is possible even in the absence of electric field. The random motion which contributes zero current, exists also in the presence of field.

So, if the mass of an electron is m then at absolute temperature T it will possess an average random velocity given by the Kinetic Theory of gases. Thus,

$$\frac{1}{2} m \bar{c}^2 = \frac{3}{2} kT$$

where, $k \rightarrow$ Boltzmann constant.

Suppose an electric field E is applied. Under the influence of the field, the electron acquires a drift velocity. The resulting acceleration of the electron is eE/m where eE is the force acting on the electron. The drift

velocity is much smaller compared to random velocity \bar{c} . further the drift velocity is not retained after a collision with an atom because of the relatively large mass. Hence, just after a collision the drift velocity is zero.

If the mean free path is λ then the time that elapses before the next collision takes place is λ/c . Hence, a drift velocity acquired just before the next collision takes place is

$$u = \text{acceleration} \times \text{time} \\ = \left(\frac{eE}{m} \right) \times \frac{\lambda}{c}$$

Thus, the average drift velocity of the electron is

$$v_d = \frac{u}{2} = \frac{eE}{2m} \times \frac{\lambda}{c}$$

If the number of electrons per unit volume is n , then the no. of electrons crossing unit area for unit time is nothing but current density, j .

Thus,

$$j = ne v_d$$

$$j = ne \left(\frac{eE\lambda}{2mc} \right)$$

$$\therefore \bar{c} = \sqrt{\frac{3KT}{m}} \quad (\text{from eqn. 1})$$

$$\text{Thus, } j = \frac{ne^2 E \lambda}{2m} \sqrt{\frac{m}{3KT}}$$

So, electrical conductivity,

$$\sigma = \frac{j}{E} = \frac{ne^2 \lambda}{\sqrt{12mKT}}$$

$$\rho = \frac{\sqrt{12mKT}}{ne^2 \lambda} \quad \text{--- (2)}$$

Hence, at constant temperature, the electrical conductivity is a constant.

IMPOTENTIALNESS OF CLASSICAL FREE ELECTRON THEORY:-

Some of the drawbacks of classical free electron theory are listed below.

1. classical theory failed to explain the variation of electronic specific heat at low temperatures.
2. The mean free path of electrons in any metal, calculated on the basis of Drude's model (classical theory) was ten times less than the experimentally observed value.
3. classical theory failed to explain the conduction mechanism in semiconductors and insulators.
4. classical model could not explain the origin of Pauli's paramagnetism.

QUANTUM FREE ELECTRON THEORY OF METALS :-

Sommerfeld, with the invention of quantum mechanics, realized that the difficulties with the free electron theory were due to the use of classical Boltzmann statistics and could be resolved by the use of Fermi-Dirac statistics. With this modification, the free electron theory was able to explain those phenomenon which are not explained earlier.

The free electron theory was further modified by taking into account the interaction of free electrons with the residual positive ions in the metals. With this modification it is observed that electrons in metals as well as in non-metals can occupy a discrete set of energy levels which are grouped together into separate energy bands. Thus, the free electrons in metals can have only those energies which lie in one of the allowed energy bands.

FERMI ENERGY AND FERMI DISTRIBUTION FUNCTION :-

Electrons are distributed among the various energy levels in the conduction band at a given temperature. We can not apply Maxwell-Boltzmann distribution to electrons because (i) they obey exclusion principle and (ii) they are indistinguishable particles. The statistical distribution function applicable to quantum particles is the Fermi-Dirac distribution function.

The probability that an electron occupies an energy level E at thermal equilibrium is given by

$$f(E) = \frac{1}{1 + \exp[(E - E_f)/KT]}$$

where E_f is known as Fermi level. The function $f(E)$ is known as Fermi function or Fermi factor.

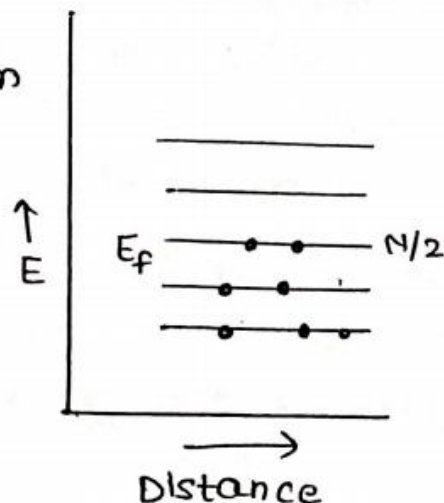
The above equation is known as Fermi-Dirac equation or Fermi-Dirac distribution function.

FERMI LEVEL :- The occupancy of the energy levels by electrons in conductors is described by the Fermi-Dirac distribution function.

$$f(E) = \frac{1}{1 + \exp[(E - E_f)/KT]} \quad \text{--- (1)}$$

FERMI ENERGY :-

Fermi energy represents maximum energy that electrons can have at absolute zero temperature. The top most energy level occupied at absolute zero temp. is called Fermi energy level.



Below fermi energy level, all energy levels are completely occupied and above fermi level, all energy levels are empty.

$$\text{At } 0\text{K}, \quad E_f = \left[\frac{3N}{\pi} \right]^{2/3} \left(\frac{h^2}{8m} \right)$$

at non-zero temp,

$$E_f = E_{f0} \left[1 - \frac{\pi^2}{12} \left(\frac{KT}{E_{f0}} \right)^2 \right]$$

$E_{f0} \rightarrow$ fermi energy at zero kelvin

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FERMI - DIRAC DISTRIBUTION FUNCTION :- fermi-dirac distribution function enables us to find the no. of free electrons per unit volume within energy E to $E+dE$ at temperature T .

The fermi-dirac distribution function is defined as

$$f(E) = \frac{1}{1 + \exp(E - E_f)/KT}$$

$f(E)$ has a value between zero and unity.

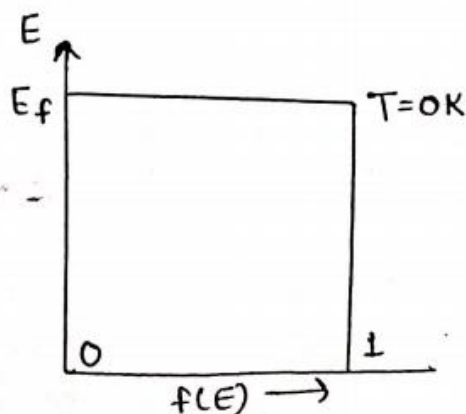
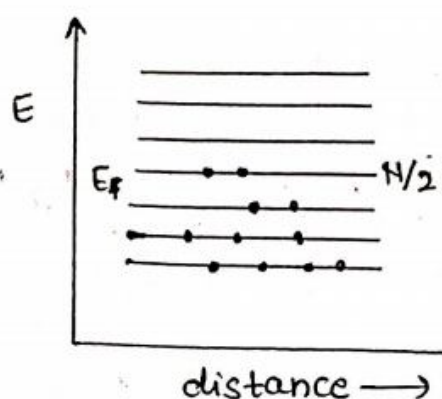
Case 1 :- (a) At $T=0\text{K}$ and $E < E_f$

$$E - E_f = -ve$$

$$\therefore f(E) = \frac{1}{1 + e^{(E - E_f)/KT}} = \frac{1}{1 + e^{(E - E_f)/0}} = \frac{1}{1 + e^{-\infty}} = \frac{1}{1 + 0}$$

$$f(E) = 1 \text{ for } E < E_f$$

$\therefore f(E) = 1$ at $T=0$ (for $E < E_f$), all energy levels below fermi levels are occupied.



(b) When $T=0$ and $E > E_f$

$$\therefore E - E_f = +ve$$

$$\therefore f(E) = \frac{1}{1 + e^{(E-E_f)/0}} = \frac{1}{1 + e^{+\infty}} = \frac{1}{1 + \infty} = \frac{1}{\infty} = 0$$

$$\therefore f(E) = 0, \text{ for } E > E_f$$

\therefore at $T=0$ and $E > E_f$, all energy levels above fermi energy level are vacant.

(c) When $T=0$ and $E = E_f$

$$\therefore E - E_f = 0$$

$$\therefore f(E) = \frac{1}{1 + e^{0/0}} = \text{Indeterminate}$$

This implies that the occupancy of fermi level at 0K, ranges from zero to one.

Case II (a) when $T > 0$ and $E < E_f$:-

The quantity $E - E_f$ will be negative and the quantity $e^{(E-E_f)/KT}$ is greater than 0 but less than 1.

$$\therefore f(E) = \frac{1}{1 + e^{(E-E_f)/KT}}$$

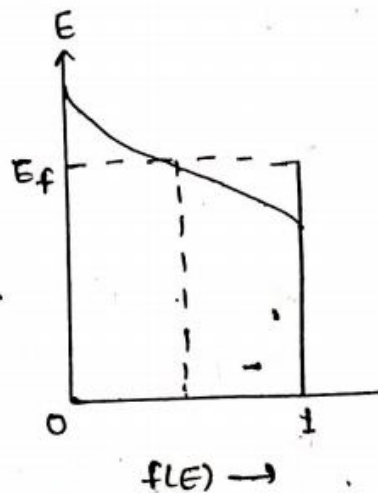
is less than 1 but greater than $\frac{1}{2}$.

(b) when $T > 0$ and $E > E_f$:- for $E > E_f$, the quantity $E - E_f$ will be positive and the quantity $e^{(E-E_f)/KT}$ is greater than 1.
 $\therefore f(E)$ is greater than 0 but less than $\frac{1}{2}$.

(c) when $T > 0$ and $E = E_f$:-

when $E = E_f$, it means an electron is at fermi level at $T > 0$.
Then the quantity $e^{E-E_f/KT}$ will be equal to 1.

$$f(E) = \frac{1}{1 + e^{E-E_f/KT}} = \frac{1}{1 + 1} = \frac{1}{2}$$



DENSITY OF ENERGY STATES:-

The density of states is defined as the number of energy states available per unit volume of a metal in the energy range between E and $E+dE$, where dE is an infinitesimally small energy interval. It is denoted by $g(E)$. The product $g(E)dE$ gives the no. of states per unit volume between the energy levels E and $E+dE$.

To estimate the total no. of electrons in a metallic conductor, it is essential to know about the no. of energy levels available and the probability of electrons available in each electronic energy level. Thus, if $g(E)dE$ represents the no. of quantum energy levels available in the energy range E and $E+dE$ and Fermi-Dirac function $f(E)$ gives the probability of electrons occupying an energy level E , then the no. of electrons per unit volume having energies between E and $E+dE$ is given by

$$N(E)d(E) = g(E)d(E) \times f(E) \quad \text{--- (1)}$$

Derivation to find $g(E)dE$:- The energy of a particle in a three dimensional potential well is given by

$$E = \frac{h^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2) \quad \text{--- (2)}$$

Let us consider,

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

Therefore, equ. (2) becomes

$$E = \frac{h^2}{8ma^2} n^2 \quad \text{--- (3)}$$

Equation $n_x^2 + n_y^2 + n_z^2 = n^2$ represents a sphere. Each value of n_x, n_y, n_z denotes a distribution of points in a sphere. Therefore, to know the actual no. of states in a sphere with all possible energies, a sphere with radius n is constructed. Thus, each point in

In this sphere represents an energy state. A unit volume of this sphere consists of one energy state since all the values of n_x , n_y and n_z are restricted to positive values, only one octant of the sphere is available.

To obtain an expression for the number of energy levels between E and $E+dE$, let us consider two spherical surfaces with radii n and $n+dn$ in the n -space as shown in figure. Consider the following two known principles of further study.

- (i) Only in one octant all the integers n_x , n_y and n_z and hence we have to consider only $\frac{1}{8}$ th volume of the sphere with n -as radius.
- (*) two electrons of opposite spin can occupy each state
- (2) Each state can accommodate two electrons. So the effective no. of states will be double

$$\left(\frac{1}{8}\right) \times 2 \times \frac{4\pi}{3} [(n+dn)^3 - n^3]$$

$$= \frac{2}{8} \left(\frac{4}{3}\right) \pi [n^3 + dn^3 + 3n^2 dn + 3dn^2 \cdot n - n^3]$$

since dn is smaller, the higher orders of dn are neglected,

so, this is approximately equal to

$$= \frac{2}{8} \left(\frac{4}{3}\right) \pi (3n^2 dn)$$

$$= \frac{\pi n^2 dn}{2} \quad (4)$$

Thus, density of energy state is

$$g(n)dn = \frac{\pi n^2 dn}{2}$$

using equ. (3) and remembering that n is a function of E , one can write the density

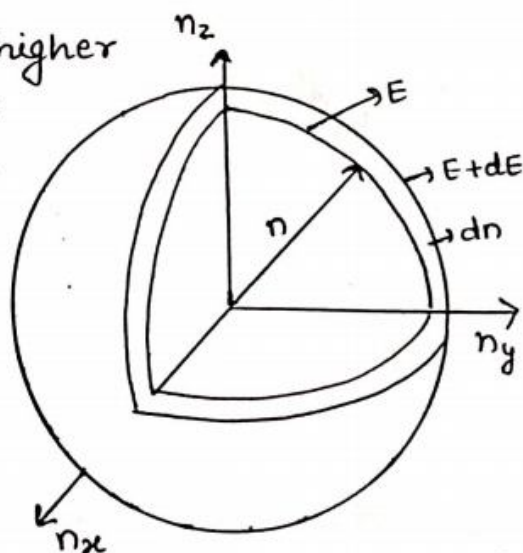


fig: positive octant of n -space

of energy states having energy values lying between E and $E + dE$ as

$$g(E)dE = \frac{\pi n^2 dn}{V} \quad \text{--- (5)}$$

from eqn. (3), we have

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

$$\text{and } 2n dn = \frac{8ma^2 E}{h^2} dE$$

$$dn = \left(\frac{1}{2n}\right) \left(\frac{8ma^2}{h^2}\right) dE \quad \text{--- (6)}$$

Substituting the value of n and dn from eqn. (3) and (6) and simplifying, we get through the following steps:

$$g(E)dE = \frac{1}{V} \left(\frac{\pi n}{V}\right) \left[\frac{8ma^2 E}{h^2}\right]^{1/2} \times \left(\frac{1}{2n}\right) \left(\frac{8ma^2}{h^2}\right) dE$$

$$g(E)dE = \frac{\pi}{2V} \left[\frac{8m}{h^2}\right]^{3/2} E^{1/2} dE \quad \text{--- (7)}$$

With $a^3 = V$, Equation (7) is for $V=1$

If $N(E)dE$ is the no. of electrons per unit volume in the metal with energy values between E and $E+dE$, then the product of $g(E)dE$ and the probability function will give $N(E)dE$.

$$N(E)dE = g(E)dE \{F(E)\}$$

at 0°K,
$$F(E) = \frac{1}{1 + \exp[(E - E_f)/kT]} = 1$$

Thus,

$$\boxed{\int N(E)dE = \int g(E)dE = \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{3/2} \int_0^{E_f} E^{1/2} dE} \quad \text{--- (8)}$$

KRONIG - PENNEY MODEL :-

The Kronig - Penney model is a simplified model for an electron in a one dimensional periodic potential. It explains the behaviour of an electron in a periodic potential. Kronig and Penney suggested a simplified model potential consisting of an infinite row of rectangular potential wells separated by barriers of width b , with space periodicity ' a ' which is the periodicity of the lattice. Each well represents an approximation to the potential produced by one ion.

So, In the region $0 < x < a$, the potential energy is equal to zero and in the region $-b < x < 0$, the potential energy is V_0 i.e

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < a \\ V_0 & \text{for } -b < x < 0 \end{cases} \quad (1)$$

The possible states that the electron can occupy in such a square well potential can be determined by 1D Schrodinger equation.

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)]\psi = 0 \quad (2)$$

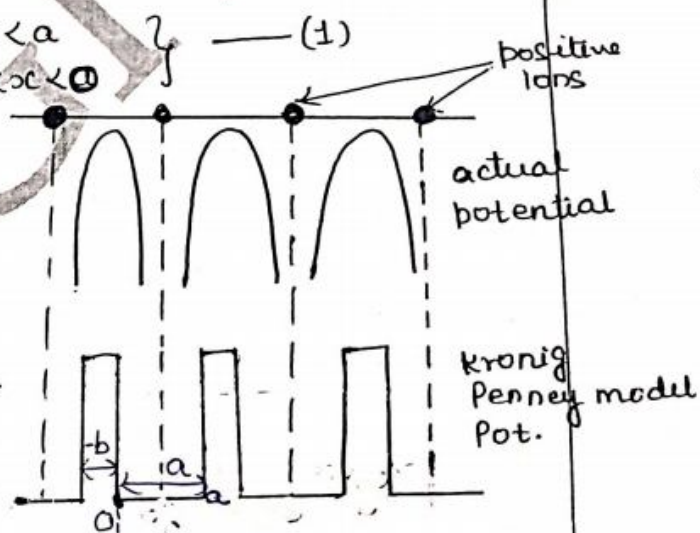
Here, m is the mass of electron. Equ. (2) for the two regions I and II takes the form

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0 \quad (\text{for } 0 < x < a) \quad (3)$$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} [E - V_0] \psi = 0 \quad (\text{for } -b < x < 0) \quad (4)$$

Now let $\alpha^2 = \frac{2mE}{\hbar^2}$

and $\beta^2 = \frac{2m}{\hbar^2} [V_0 - E]$ (here we assume $E < V_0$)



The equ. (3) and (4) become

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0 \quad (\text{for } 0 < x < a) \quad \text{--- (5)}$$

$$\text{and } \frac{d^2\psi}{dx^2} - \beta^2\psi = 0 \quad (\text{for } -b < x < 0) \quad \text{--- (6)}$$

Since $\psi(x)$ is the periodic function, it can be expressed as $\psi(x) = e^{(ikx)} \phi(x)$

If ϕ_1 and ϕ_2 are the values of $\phi(x)$ in the two regions I and II, then equ. (5) and (6) take the form

$$\frac{d^2\phi_1}{dx^2} + 2ik \frac{d\phi_1}{dx} + (\alpha^2 - k^2)\phi_1 = 0 \quad \text{--- (7)}$$

$$\text{and } \frac{d^2\phi_2}{dx^2} + 2ik \frac{d\phi_2}{dx} + (\beta^2 - k^2)\phi_2 = 0 \quad \text{--- (8)}$$

The general solutions of equ. (7) and (8) are

$$\phi_1 = A e^{i(\alpha-k)x} + B e^{-i(\alpha+k)x} \quad \text{--- (9)}$$

$$\phi_2 = C e^{(B-ik)x} + D e^{-(B+ik)x} \quad \text{--- (10)}$$

Here A, B, C and D are constant to be determined by the following conditions.

$$(\phi_1)_{x=0} = (\phi_2)_{x=0}; \quad \left(\frac{d\phi_1}{dx}\right)_{x=0} = \left(\frac{d\phi_2}{dx}\right)_{x=0}$$

$$\text{and } (\phi_1)_{x=a} = (\phi_2)_{x=-b}; \quad \left(\frac{d\phi_1}{dx}\right)_{x=-a} = \left(\frac{d\phi_2}{dx}\right)_{x=-b}$$

Applying these conditions in equ. (9) and (10), solving we get,

$$\boxed{\gamma \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka} \quad \text{--- (11)}$$

$$\text{where, } \gamma = \frac{mV_0 ab}{\hbar^2} \quad \text{--- (12)}$$

Case I. When $\gamma \rightarrow \infty$ then equ. (12) has a solution

only if

$$\sin \alpha a = 0$$

$$\text{or } \sin \alpha a = \sin n\pi \quad (\text{where } n \text{ is an integer})$$

$$\alpha a = n\pi$$

$$\text{or } \alpha^2 a^2 = n^2 \pi^2$$

$$\text{or } \frac{2mE}{\hbar^2} a^2 = n^2 \pi^2 \quad \left(\text{Since } \alpha^2 = \frac{2mE}{\hbar^2} \right)$$

$$\text{or } \boxed{E = E_n (\text{say}) = \frac{n^2 \pi^2 \hbar^2}{2ma^2}} \quad \text{--- (13)}$$

equ. (13) represents the energy levels of a particle in one dimensional box of atomic dimension.

Case II:- When $\gamma \rightarrow 0$, the equ. (11) reduces to

$$\cos \alpha a = \cos ka$$

$$\alpha a = ka$$

$$\alpha^2 = k^2$$

$$\frac{2mE}{\hbar^2} = k^2$$

$$\boxed{E = \frac{\hbar^2 k^2}{2m}} \quad \text{--- (14)}$$

$$\text{or } \boxed{E = \frac{\hbar^2 k^2}{8\pi^2 m}} \quad \text{--- (15)}$$

$$\text{or } E = \frac{1}{2m} \left(\frac{2\pi}{\lambda} \right)^2 \left(\frac{\hbar^2}{4\pi^2} \right) = \frac{\hbar^2}{2m} \left(\frac{1}{\lambda} \right)^2$$

according to de-Broglie relation $\lambda^2 = \left(\frac{h}{mv} \right)^2$

$$\text{Hence, } E = \frac{\hbar^2}{2m} \cdot \left(\frac{m^2 v^2}{h^2} \right) = \frac{1}{2} m v^2$$

which is appropriate to the completely free particle. This shows that the allowed energy states of electrons are continuous.

Allowed Energy zones:-

Equ. (11) provides the allowed solutions to the Schrodinger equation. As the relation involves trigonometric functions, only certain values of α are possible. The right hand side of equ. (11) is cosine function and can take values only

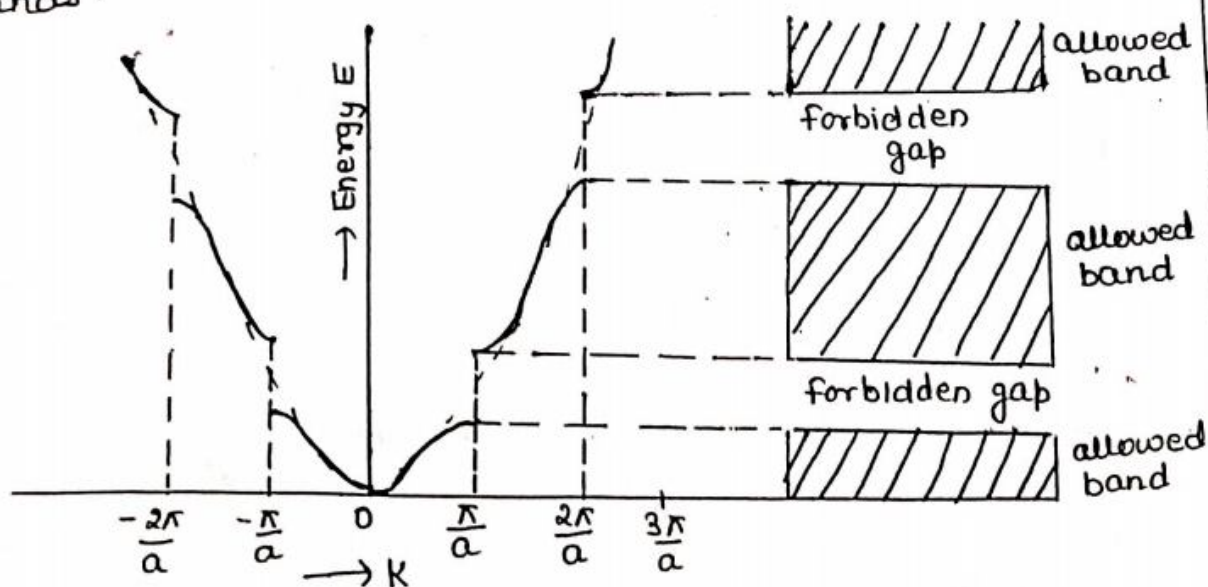
between -1 and $+1$. Therefore, the left side of the equ. is restricted to vary between those two limits. Hence, only certain values of α are allowed. It means that energy E is restricted to lie within certain ranges.

This concept is best understood by drawing the plot of energy E as a function of the wave number K . which is known as $E-K$ diagram. The plot is shown in figure. The parabolic relation between E and K obtained in case of free electron is interrupted at certain values of K , as shown by the broken curve.

fig. shows discontinuities in E . The discontinuities occur at $Ka = \pm n\pi$ i.e. at

$$K = \pm \frac{\pi}{a}, \pm \frac{2\pi}{a}, \pm \frac{3\pi}{a}, \dots \quad (16)$$

The energy spectrum of the electron consists of alternate regions of allowed energy (continuous) and forbidden energy. These regions are usually referred as the allowed and forbidden energy bands.



Electron energy E versus wave no. K plot for a solid.

Concept of Brillouin zone:-

In $E-K$ diagram, the energy gaps appear as regions for which there are no real values of K . (Imaginary values are possible but they lie in the forbidden region). The other inference is that beyond few discontinuities in the $(E-K)$ curve, the electron energy becomes very large and we are not usually concerned with them. The regions between the energy discontinuities are called Brillouin zones labeled 1st Brillouin zone, 2nd Brillouin zone, etc.

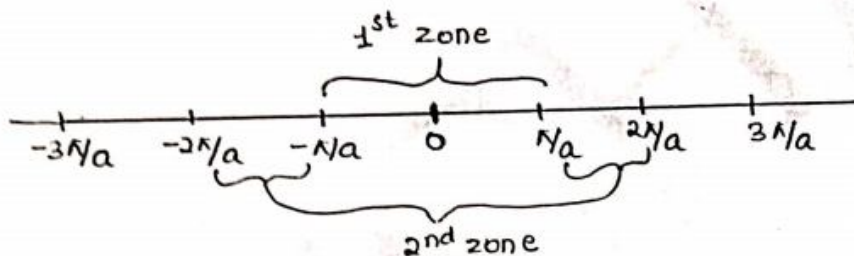


fig: Brillouin zones

Brillouin zones in two dimension:-

In general, the condition for any discontinuity is

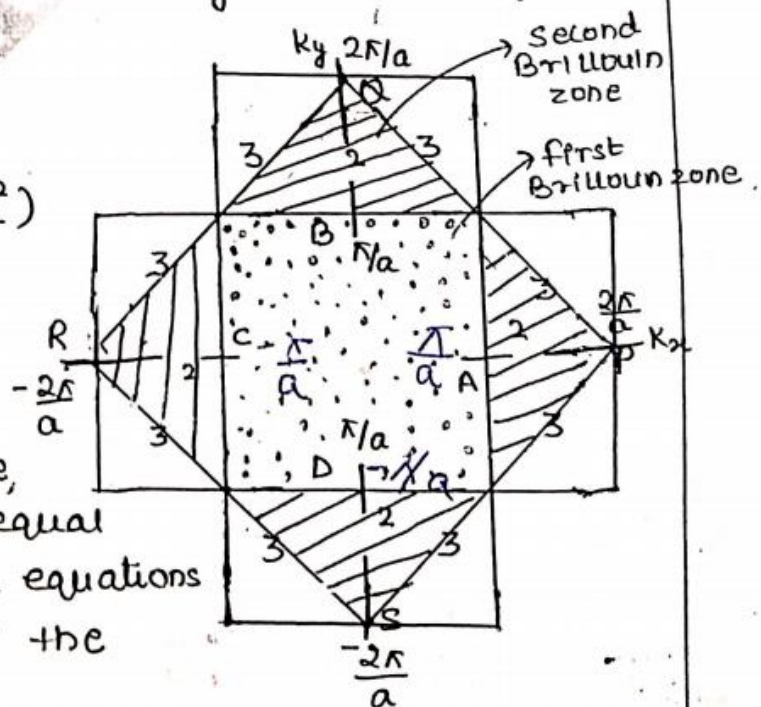
$$K = \pm \frac{n\pi}{a}$$

for 2D case,

$$K_x n_1 + K_y n_2 = \frac{\pi}{a} (n_1^2 + n_2^2)$$

where, n_1 and n_2 are integers referring to each of the axis.

To sketch the first zone, n_1 and n_2 are made equal in turn to ± 1 or 0. The equations giving the borders of the first zone are



$$n_1 = \pm 1, n_2 = 0 \text{ giving } K_x = \pm \frac{\pi}{a}$$

$$n_1 = 0, n_2 = \pm 1 \text{ giving } K_y = \pm \frac{\pi}{a}$$

It is a square passing through the points A, B, C and D gives the first Brillouin zone. The second Brillouin zone should pass through the point P, Q, R and S.

To get the sketch of the second zone, we must use the next set of integers above those for the first zone.

$$n_1 = +1, n_2 = +1 \text{ giving } K_x + K_y = \frac{2\pi}{a}$$

$$n_1 = -1, n_2 = +1 \text{ giving } -K_x + K_y = \frac{2\pi}{a}$$

$$n_1 = +1, n_2 = -1 \text{ giving } K_x - K_y = \frac{2\pi}{a}$$

$$n_1 = -1, n_2 = -1 \text{ giving } -K_x - K_y = \frac{2\pi}{a}$$

EFFECTIVE MASS OF ELECTRON:-

An electron in a crystal interacts with the crystal lattice. Therefore, its behaviour towards external forces is different from that of a free electron.

The deviation of the electron behaviour in the crystal lattice from the free electron behaviour can be taken into account simply by considering the electron to have an "effective mass m^* " rather than its free space, mass m .

The effective mass m^* depends on the nature of the crystal lattice and varies with the direction of motion of the electron in the lattice. m^* may be much larger or much smaller than m and it may even be negative.

Let us consider an electron moving along the x-axis in a crystal lattice to which an external electric field E has been applied. The external force acting on the electron is eE . Suppose that the electron gains velocity v over a distance ' dx ' in time ' dt '. The resulting change in its energy is given by

$$dE = eE dx = eE v dt \quad (\because v = dx/dt)$$

We know that the velocity v of a particle is the same as the group velocity v_g of the de-Broglie waves associated with the particle ($v = v_g$)

Thus,
$$dE = eE v_g dt$$

Now, we have

$$E = h\nu = \frac{h}{2\pi} \omega \quad (\because \nu = \frac{\omega}{2\pi})$$

Differentiating it, we have

$$dE = \frac{h}{2\pi} d\omega = \frac{h}{2\pi} \frac{d\omega}{dk} dk \quad \text{---(2)}$$

But $\frac{d\omega}{dk} = v_g$

$$\therefore dE = \frac{h}{2\pi} v_g dk$$

Comparing it with equ. (1), we get

$$eE dt = \frac{h}{2\pi} dk$$

$$\frac{dk}{dt} = \frac{2\pi}{h} eE \quad \text{---(3)}$$

The group velocity v_g can be written in terms of energy E as

$$v_g = \frac{d\omega}{dk} = \frac{2\pi}{h} \frac{dE}{dk} \quad (\text{by equ. 2})$$

Differentiating w.r. to time we get

$$\frac{dv_g}{dt} = \frac{2\pi}{h} \frac{d^2 E}{dt \cdot dk} = \frac{2\pi}{h} \frac{d^2 E}{dk^2} \cdot \frac{dk}{dt}$$

$$\text{or } \frac{d v_g}{dt} = \frac{4\pi^2}{h^2} \frac{d^2 E}{d k^2} eE \quad (\text{by eqn. 3})$$

Employing $v_g = v$ again, this can be written as

$$\frac{d v}{dt} = \left(\frac{4\pi^2}{h^2} \frac{d^2 E}{d k^2} \right) eE \quad \text{--- (4)}$$

This equation connects the force eE on the electron with the acceleration dv/dt through the proportionality factor $\frac{4\pi^2}{h^2} \frac{d^2 E}{d k^2}$. It is same as Newton's second law,

so, if we set

$$\frac{1}{m^*} = \frac{4\pi^2}{h^2} \frac{d^2 E}{d k^2}$$

$$\text{or } m^* = \frac{h^2}{4\pi^2 d^2 E / d k^2}$$

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

This is the expression for the effective mass of electron.

Significance of effective mass of electron:-

Effective mass of electron has a special importance because the result of free electron theory can be applied in band theory of solids by replacing the rest mass ' m ' of electron by effective mass m^* of electron. The effective mass is used in transport calculations, such as transport of electrons under the influence of fields or carrier gradients in different semiconductors. It is also used to calculate the density of states.

Concept of phonons: (Quantisation of Lattice vibrations :-

The energy of a Lattice vibration is quantised. The quantum of energy is called a "phonon". Thus, elastic waves in crystals are made up of phonons. Thermal vibrations in crystals are thermally - excited phonons.

Phonons have zero spin (like photons). Hence, they obey Bose-Einstein statistics.

The energy of each mode of vibration in an elastic wave of frequency ν is

$$E = (n + \frac{1}{2}) h\nu = (n + \frac{1}{2}) (\frac{h}{2\pi}) \omega,$$

where n is the no. of phonons in the mode, $(\frac{h}{2\pi})\omega$ is the quantum of elastic energy i.e. energy of phonon and $\frac{1}{2}(\frac{h}{2\pi})\omega$ is the zero-point energy of the mode.

The quantisation of lattice vibration energy has an important consequence when a lattice vibration is involved in an interaction. Since the energy of a mode of vibration has to be $(n + \frac{1}{2})(\frac{h}{2\pi})\omega$ with n any positive integer and since to a first order approximation, the energy changes only to adjacent allowed values, we must have

$$\Delta E = \pm (\frac{h}{2\pi})\omega$$

and correspondingly

$$\Delta n = \pm 1$$

This means that the energy - change corresponds to a gain or loss of a single phonon at a time.

Experimental Evidence for phonon:-

- (1) The lattice contribution to the heat capacity of solids approaches zero as the temperature

approaches zero. This can be explained only if the lattice vibrations are quantised.

- ii) X-rays and neutrons are scattered inelastically by crystals. The change of energy and momentum in this process corresponds to the creation or absorption of one or more phonons. By measuring the energy and momentum of the scattered X-rays or neutrons, we can determine the properties of phonons.