QUANTUM MECHANICS & QUANTUM COMPUTING

DUAL NATURE OF MATTER:

Light exhibits the phenomena of interference, diffraction, polarization and also photo electric effect and Compton Effect. Interference, diffraction and polarization can be explained by wave nature of light which is based on transfer of energy. The photoelectric effect and Compton Effect are explained by quantum theory. This indicates the particle nature of light which is based on transfer of momentum apart from transfer of energy. So light has dual nature that is wave nature and particle nature.

In 1924 Debroglie proposed that a beam of particles behave as a wave in transferring energy. This is dual nature of matter. He proposed this without any strong experimental support and hence called hypothesis.

Matter Waves: waves associated with the material particle are called mater waves.

Debroglie hypothesis:

The dual nature of light possessing both wave and particle properties was explained by combining plank's expression for energy of a photon $E = h\nu$ with Einstein's mass energy relation $E = mc^2$

$$\therefore \ h\nu = mc^2$$

But we know $\nu = \frac{c}{\lambda}$, we get

$$\frac{hc}{\lambda} = mc^2 \quad \text{or} \quad \lambda = \frac{h}{mc} = \frac{h}{p}$$

The wave length λ is called Debroglie wavelength.

It is defined as the ratio of plank's constant to the momentum of a particle.

$$\therefore \ \lambda = \frac{h}{mv} = \frac{h}{p}$$

Particle does not exhibit the wave nature and particle nature simultaneously.

Debroglie wavelength of electron:

When a potential difference 'V' is applied to the electron it accelerates with velocity 'v' then the work done on the electron is 'eV'. This work done is converted into the kinetic energy of the electron. Thus,

$$eV = \frac{1}{2}mv^2$$

$$2meV = (mv)^2$$

$$mv = \sqrt{2meV}$$

Substitute this value in debroglie wavelength $\lambda = \frac{h}{mv}$.

$$\lambda = \frac{h}{\sqrt{2meV}} = \frac{6.625x10^{-34}}{\sqrt{2x9.1x10^{-31}x1.6x10^{-19}xV}}$$

$$= \frac{12.27}{\sqrt{V}} A^0 \quad \text{or} \quad \frac{1.227}{\sqrt{V}} \text{nm}$$

Properties of matter waves: waves associated with the material particles such as electron, proton, etc., are called matter waves. The wavelength of matter waves is given by $\lambda = \frac{h}{mv}$

1. Greater the mass of the particle, lesser the wavelength
2. Greater the velocity of the particle, lesser the wavelength
3. Wavelength λ is independent of charge of particle.
4. Particle does not exhibit wave nature and particle nature simultaneously
5. Velocity of the matter waves is greater than the velocity of light.

From Debroglie we have $h\nu = mc^2$ or $\nu = \frac{mc^2}{h}$ -------------- (1)

Let v^1 be the velocity of matter waves, we know

$v^1 = \nu\lambda$ or $v^1 = \frac{\nu h}{mv}$ --------- (2)

$$\therefore \; v^1 = \frac{mc^2}{h}\,\frac{h}{mv}$$

$$v^1 = \frac{c^2}{v} > c \qquad \text{(v is velocity of the particle)}$$

But experimentally it is not possible. Because particle does not exceed the velocity of light.

SCHRÖDINGER'S TIME INDEPENDENT WAVE EQUATION:

If particle has wave properties, it is expected that there should be some kind of wave equation which describes the behavior of the particle.

Consider a system of stationary waves associated with a particle. Let x,y,z be the coordinates of the particles and Ψ is the wave displacement for the Debroglie waves at any time 't'. The classical differential equation of a wave motion is given by

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

Where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ and v is the velocity of the wave.

The solution of the equation (1) can be written as,

$$\Psi(x,y,z,t) = \Psi_0(x,y,z)e^{-i\omega t} \text{ ------------(2)}$$

Where $\Psi_0(x,y,z)$ is a function of x,y,z and gives the amplitude at the point considered. Equation (2) can also be expressed as

$$\Psi\,(\overrightarrow{r,t}) = \Psi_0\,(\overrightarrow{x,y,z})\; e^{-i\omega t} \text{ ------------- (3)}$$

Differentiating equation (3) twice, we get

$$\frac{\partial^2\Psi}{\partial t^2} = -\,\omega^2\,\Psi_0(r)\,e^{-i\omega t}$$

$$= -\,\omega^2\,\Psi$$

Substituting this value in equation (1) , we get

$$-\,\omega^2\,\Psi = v^2\;\nabla^2\Psi$$

$$\Rightarrow \nabla^2 \Psi + \frac{\omega^2}{v^2} = 0 \text{ ----------- } (4)$$

But $\omega = 2\pi n = 2\pi \frac{v}{\lambda} \Rightarrow \frac{\varpi}{v} = \frac{2\pi}{\lambda}$

$$\therefore \nabla^2 \Psi + \frac{4\pi^2}{\lambda^2} \Psi = 0 \text{ --------- } (5)$$

Now from the Debroglie relation $\lambda = \frac{h}{mv}$ or $\frac{1}{\lambda^2} = \frac{m^2 v^2}{h^2}$

$$\nabla^2 \Psi + \frac{4\pi^2}{h^2} m^2 v^2 = 0 \text{ --------------- } (6)$$

If 'E' and' V' be the total and potential energies of the particle respectively, then its kinetic energy is given by

$\frac{1}{2} m v^2 = E - V$ or

$m^2 v^2 = 2m (E-V)$ ------------ (7)

From equations (6) and (7), we have

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

$$\nabla^2 \Psi + \frac{8\pi^2 m}{h^2} (E-V) \Psi = 0 \text{ ----------- } (8)$$

Equation (8) is known as Schrödinger's time independent wave equation.

Put $\hbar = \frac{h}{2\pi}$, the above equation can also be expressed as

$$\nabla^2 \Psi + \frac{2m}{\hbar^2} (E - V) \Psi = 0 \text{ ----------- } (9)$$

For free particle V = 0, $\therefore \nabla^2 \Psi + \frac{8\pi^2 m}{h^2} E\Psi = 0$

SCHRÖDINGER'S TIME DEPENDENT WAVE EQUATION :

If particle has wave properties, it is expected that there should be some kind of wave equation which describes the behavior of the particle.

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Where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ and v is the velocity of the wave.

The solution of the equation (1) can be written as,

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Where $\Psi_0(x,y,z)$ is a function of x,y,z and gives the amplitude at the point considered. Equation (2) can also be expressed as

$$\Psi\,(\overrightarrow{r,t}) = \Psi_0\,(\overrightarrow{x,y,z})\ e^{-i\omega t} \text{ ------------- (3)}$$

Differentiating the above equation, we get

$$\Psi = \Psi_0\, e^{-i\omega t}\ (-i\omega)$$

$$\frac{\partial\Psi}{\partial t} = (-i2\pi\nu)\Psi = (-i2\pi\frac{E}{h})\Psi = \left(-i\frac{E}{\hbar}\right)\Psi \quad \text{or}$$

$$-\frac{\hbar}{i}\frac{\partial\Psi}{\partial t} = E\Psi$$

$$i\hbar\frac{\partial\Psi}{\partial t} = E\Psi \text{ ----------- (4)}$$

From the Schrödinger's time independent wave equation,

$$\nabla^2\Psi + \frac{2m}{\hbar^2}(E - V)\Psi = 0$$

$$\nabla^2\Psi = -\frac{2m}{\hbar^2}(E - V)\,\Psi$$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\,\Psi = E\Psi \text{ -------- } (5)$$

Substituting the value of EΨ from equ.(4) into equ.(5), we get

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\,\Psi = i\hbar\frac{\partial\Psi}{\partial t} \text{ ---------- } (6)$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi = i\hbar\frac{\partial\Psi}{\partial t} \quad \text{or}$$

$H\Psi = E\Psi$ where $H = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)$ is called Hamiltonian which gives the total energy of the particle.

Equation (6) is called Schroedinger's time dependent equation which is applicable to nonrelativistic particles.

PHYSICAL SIGNIFICANCE OF THE WAVE FUNCTION 'Ψ':

Max Born in 1926 gave a satisfactory explanation for the wave function 'Ψ' associated with a moving particle.

Born postulated that the square of the magnitude of the wave function $|\Psi^2|$ or $(\Psi\Psi^* \; if \; \Psi \; is complex)$ represents the probability of finding the particle in the given region.

$|\Psi^2|$ is called probability density and Ψ is probability amplitude. Thus the probability of the particle within an element volume dxdydz (or) dV is $|\Psi^2|$dxdydz.

Since the particle is certainly somewhere in the given region, the integral of $|\Psi^2|$dxdydz over all the space must be unity. i.e,

$$\iiint_{-\infty}^{+\infty} |\Psi^2| \; dxdydz = 1$$

A wave function that obeys the above equation is called ***normalized.*** Every acceptable wave function must be normalizable and should fulfill the following conditions:

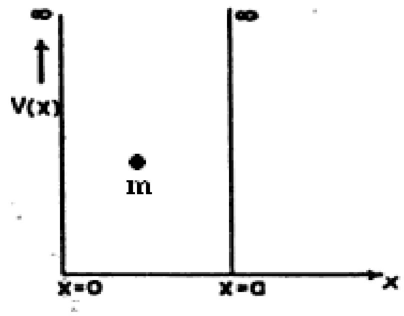
1. It must be finite every where

2. It must be single valued

3. It must be continuous and have a continuous first derivative every where

PARTICLE IN ONE DIMENSIONAL POTENTIAL BOX:

When a motion of a particle is confined to a limited region such that the particle moves back and forth in the region, the particle is said to be in bound state.



Consider a particle of mass 'm' bouncing back and forth between the rigid walls of a one dimensional box.

Suppose that a particle does not lose energy when it collides with walls, so that its total energy remains constant. This box can be represented by a potential well or box of width 'a'.

The potential energy 'V'of the particle is infinitely high beyond the walls, while inside the box 'V' is uniform.

This potential well can mathematically describe as:

$V(x) = \infty$ for $x < 0$ and $x > a$

$= 0$ for $0 < x < a$

The uniform potential of the particle inside the box is taken as zero for simplicity.

From Schrodinger's wave time independent wave equation, we have

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\Psi = 0 \qquad \text{or} \qquad (\because V = 0 \text{ inside the box})$$

$$\frac{d^2\Psi}{dx^2} + k^2\Psi = 0 \text{ ------------ (1)}$$

Where $k^2 = \frac{8\pi^2 m}{h^2} E$ ---------- (2)

The solution of the above equation is of the form

$\Psi(x) = A \sin kx + B \cos kx$ ----------- (3)

Where A and B are arbitrary constants can be obtained by applying the boundary conditions of the problem.

(i) $\Psi(x) = 0$ at $x = 0$

(ii) $\Psi(x) = 0$ at $x = a$

From the first boundary condition, $0 = 0 + B \Rightarrow B = 0$.

Hence $\Psi(x) = A \sin kx$ ---------- (4)

From the second boundary condition, $0 = A \sin ka$ ($\because$ already we got B=0)

If $A \sin ka = 0$, either $A = 0$ or $\sin ka = 0$.

$A = 0$ is not applicable. So $\sin ka = 0$, $ka = n\pi$ or $k = \frac{n\pi}{a}$

$$K^2 = \frac{n^2\pi^2}{a^2} \text{ ---------- (5)}$$

$\therefore$ The solution can be written as $\Psi(x) = A \sin \frac{n\pi x}{a}$ -------- (6)

From equations (2) and (5) $\frac{8\pi^2 m}{h^2} E = \frac{n^2\pi^2}{a^2}$ or

$$\boxed{E_n = \frac{n^2 h^2}{8a^2 m}} \text{ ----------- (7)} \quad n = 1, 2, 3 \ldots$$

It is clear that inside the potential box, the particle can have discrete energy levels. That is the energy of the particle is quantized.

Determination of constant 'A' (by using normalization condition):

The wave function of the motion of the particle is

$$\Psi_n = A \sin \frac{n\pi x}{a} \quad \text{for } 0 < x < a$$

$$= 0 \quad \text{for } x < 0, x > 0$$

The probability of finding the particle in the box at some where is unity.

$$\therefore \int_0^a |\Psi(x)|^2 dx = 1 \quad \text{or}$$

$$\int_0^a A^2 \sin^2 \frac{n\pi x}{a} dx = 1 \quad \text{or}$$

$$A^2 \int_0^a \sin^2 \frac{n\pi x}{a} dx = 1 \quad \text{or}$$

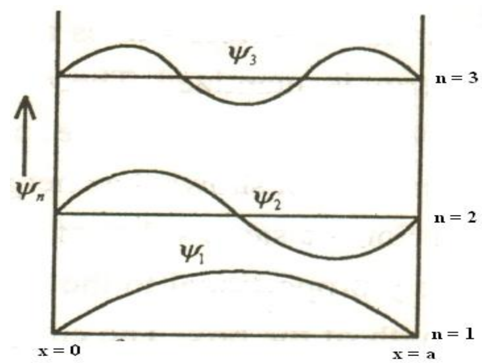
$$A^2 \int_0^a \frac{1}{2}\left[1 - \cos\frac{2n\pi x}{a}\right] dx = 1 \quad \text{or}$$

$$\frac{A^2}{2}\left[x - \sin\frac{2n\pi x}{a}\frac{a}{2n\pi}\right]_0^a = 1 \quad \text{or}$$

$$\frac{A^2 a}{2} = 1 \quad \text{or} \quad [\because \sin n\pi = 0 \text{ for all n}]$$

$$A = \sqrt{\frac{2}{a}}$$

$$\Psi(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} \text{ ------------- (8)}$$



Equation (8) gives the wave function of the particle enclosed in infinitely deep potential well.

The wave functions for the first three values of 'n' are shown in figure.

OPERATORS IN QUANTUM MECHANICS:

Total Energy Operator: From Hamiltonian equation, H = $\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)$ which gives total energy of the particle.

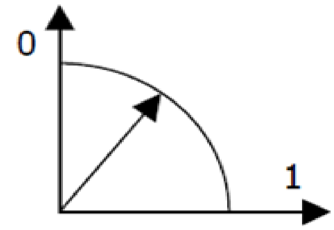
Kinetic Energy operator: Kinetic energy = $\frac{1}{2}mv^2 = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$ $(\because$ p=mv)

Velocity operator (v): $\frac{p^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2 = (mv)^2 = -\hbar^2\nabla^2$ or $v = -\frac{i\hbar}{m}\nabla$

Momentum operator: p = -$i\hbar\nabla$

QUBITS-CLASSICAL BITS:

In classical computers, data is stored in the form of a digital bit. Digital bits have only one value: true or false, on or off, one or zero;



The silicon chip processes one calculation at a time, sequentially, and information is processed in one direction only. Quantum computing, on the other hand, uses atoms in place of traditional processors. Each bit of information carried in quantum computers is called a 'qubit', which can represent 0, 1, and any value in between at the same time. In a graphical sense, a vector pointing in a direction intermediate between those representing 0 and 1 represents the in-between position known as superposition.

The linear combination of $|0\rangle$ and $|1\rangle$ (ket 0 and ket 1) can be written as

$$|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

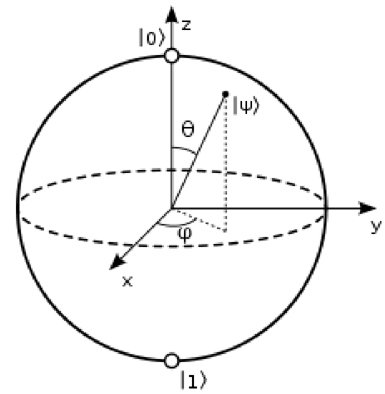
Where α and β are complex numbers, $\alpha = \cos\frac{\theta}{2}$; $\beta = e^{i\phi}\sin\frac{\theta}{2}$

α and β are constrained by the equation $|\alpha|^2 + |\beta|^2 = 1$

Physical representation of qubits:

Qubit	0	1
Photon: Linear polarization	Vertical $\downarrow$	Horizontal $\leftrightarrow$
Photon: Circular polarization	Left	Right
Electron: Spin	$+\frac{1}{2}\downarrow$	$-\frac{1}{2}\uparrow$
Atom: Energy levels	Ground state	Excited state

BLOCH SPHERE:



Bloch sphere is a sphere of unit radius and the state of a qubit is geometrically represented by a vector in this sphere as shown in figure.

A qubit can be in 0 or 1 or superposition of both states. These states are represented by $|0\rangle$ and $|1\rangle$.

The qubit obey the laws of quantum mechanics and is represented by $|\Psi\rangle$.

A classical bit could be only at the "North pole" or "south pole" of the sphere where the values $|0\rangle$ and $|1\rangle$ respectively. The rest of the surface of the sphere is inaccessible to the classical bit, but qubit state can be represented by any point on the sphere surface.

$|\Psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$ --------- (1)

As shown in the figure 'θ' is angle between the state vector $|\Psi\rangle$ and z-axis, ϕ is the projection of $|\Psi\rangle$

<u>Case i:</u> For ϕ =0 and θ = 0;

$|\Psi\rangle = \cos\frac{0}{2}.|0\rangle + (\cos 0 + i\sin 0)\sin 0 . |1\rangle$ (from equ.(1))

$|\Psi\rangle = 0$ ∴ The state corresponding to $|0\rangle$ is along z-axis.

<u>Caseii</u>: For ϕ =0 and θ = 180; $|\Psi\rangle$=.0 + 1. $|1\rangle$ = $|1\rangle$

The state $|\Psi\rangle$ corresponds to $|1\rangle$ is along –ve z-axis

→ If we consider $\boxed{\theta = 90^0}$, then the vector is in xy plane.

i) For $\phi = 90^0$, $|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$ is superposition state along +ve y-axis

ii) For $\phi = -90^0$, $|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$ is superposition state along -ve y-axis

iii) For $\phi = 0^0$, $|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ is superposition state along +ve x-axis

iv) For $\phi = 180^0$, $|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ is superposition state along -ve x-axis

ADVANTAGES OF QUBITS:

Quantum Computation: Increase in Computing Power

Using quantum parallelism, a quantum computer can calculate or factor any huge number that is currently difficult on a classical computer. For example, factoring a number with 400 digits will take the existing fastest supercomputers billions of years to accomplish. A quantum computer can obtain the answer within a year. Therefore, quantum computers capable of performing difficult mathematical calculations that are impossible using semiconductor computers.

Quantum Cryptography: Advances in Security

Quantum cryptography allows two parties to exchange public keys in a private channel and thus secure privacy in quantum communication. The quantum mechanics will not allow any eavesdropper to obtain the private key. Two legitimate parties will reveal a random subset of the key bits and check the error rate to test for eavesdropping. In so doing, even though eavesdropping will not be prevented, any attempt, regardless how subtle and complicated, to break into the communication channel will be detected.

Teleportation

Teleportation is the capabilities to make an object or a person disintegrate in one place while a perfect replica (duplicate) appears in another. According to the uncertainty principle, the duplicating process will disturb or destroy the original objects; the more an object is duplicated, the more it is destroyed.

Artificial Intelligence:

The theories of quantum computation suggest that every physical object, even the universe, is in some sense. Computers should be able to model every physical process. Ultimately this suggests that computers will be capable of simulating conscious rational thought. And a quantum computer will be the key to achieving true artificial intelligence

HEISENBERG UNCERTAINTY PRINCIPLE:

According to Heisenberg it is impossible to determine the exact position and momentum of a moving particle.

If Δx denotes the error (uncertainty) in the measurement of the position of the particle along x-axis and Δp represents the error in the measurement of momentum, then

$$\Delta x . \Delta p = h \text{ ------------ (1)}$$

Where h is plank's constant. The above equation represents the uncertainty involved in the measurement of both the position and momentum of the particle.

In more optimized form the above equation can be written as

$$(\Delta x.\ \Delta p) \geq \frac{\hbar}{2} \text{ or } \frac{h}{4\pi} \text{ ------------ (2)}$$

If the time during which a system occupies a certain state is not greater than Δt, then the energy of the state cannot be known to within ΔE, where:

$$(\Delta E)\ (\Delta t) \geq \frac{\hbar}{2} \text{ ----------- (3)}$$

P.Srinivasa Rao

Free Electron theory of metals

Classical free electron theory:

Merits:

1. This theory verifies ohm's law.

2. This theory explains electrical conductivity and thermal conductivities of metals.

3. This theory explains optical properties of metals such as optical absorption, reflection and opaque nature of metals etc.

Failures of classical free electron theory:

1. The phenomena such as photo electric effect, Compton Effect and black body radiation could not be explained by classical free electro theory.
2. According to classical theory the value of specific heat of metals is given by 4.5R (R =Universal gas constant) where as the experimental value is nearly 3R(Dulang Petit law)
3. Electrical conductivity of semiconductor or insulator could not be explained by using this model.
4. According to classical free electron model $\frac{K}{\sigma T}$ is constant.(Wide mann-franz law) as this not constant at low temperatures.
5. Ferromagnetism could not be explained by this theory
6. According to classical free electron theory,
   Resistivity

$$\rho = \frac{m}{ne^2\tau_c} = \frac{m}{ne^2}\sqrt{\frac{3KT}{m}}\frac{1}{\lambda} = \frac{\sqrt{3KTm}}{ne^2\lambda}$$

$$\rho = \sqrt{T}$$

But according to experiments $\rho \alpha T$

QUANTUM FREE ELECTRON THEORY:

Somerfield applied quantum mechanics to explain conductivity phenomenon in metals. He has improved the Drude- Lorentz theory by quantizing the free electron energy and retaining the classical concept of force motion of electrons at random.

ASSUMPTIONS

1. The electrons are free to move with in the metal like gaseous molecules. They are confined to the metal due to surface potential.

2. The velocities of electrons obey Fermi-Dirac distribution because electrons are spin – half particles.

3. The electrons would go into different energy levels and obey Pauli's exclusion principle.

4. The motion of the electron is associated with a wave called matter wave, according to the deBroglie hypothesis.

5. The electrons can not have all energies but will have discrete energies according to the equation $E_{n=} \frac{n^2h^2}{8ma^2}$ where a is the dimension of the metals.

Derive an expression for electrical conductivity by using quantum free electron theory

According to Quantum theory

$$p = mv = \hbar K \text{ -----(1)}$$

Where $\hbar = \frac{h}{2\pi}$, $K = \frac{2\pi}{\lambda}$

Differentiating equation (1) w.r.t to t

$$a = \frac{dv}{dt} = \frac{\hbar}{m}\frac{dK}{dt}$$

At equilibrium the lorentz force $F = -eE$ acting on the electron is equal and opposite to the product of mass and acceleration of the electron

i.e.

$$eE = ma$$

$$\Rightarrow m\frac{\hbar}{m}\frac{dK}{dt} = eE$$

$$\Rightarrow dK = \frac{eE}{\hbar}dt \text{ ---(2)}$$

Integrating (2) between the limits 0 and t

$$\int_0^t dK = \int_0^t \frac{eE}{\hbar}dt$$

$$K(t) - K(0) = \frac{eE}{\hbar}t$$

$\Delta K = \frac{eE}{\hbar}t_c$ where t_c =men collision time.

But $J = ne\Delta v$ and $\Delta v = \hbar\frac{\Delta K}{m}$

$$\Delta v = \hbar\frac{\Delta K}{m} = \frac{\hbar}{m}\frac{eE}{\hbar}t = \frac{eEt}{m}$$

$$\therefore J = \frac{ne^2Et}{m^*}$$

From microscopic form of Ohm's law

$$J = \sigma E$$

$\therefore \sigma = \frac{ne^2t}{m^*}$ This is the expression for the electrical conductivity.

FERMI DIRAC DISTRIBUTION:

In quantum theory different electrons occupy different energy levels at O`K. Electrons obey Pauli's exclusion principle. As the electrons receive energy they are excited to higher levels which are unoccupied at O K. The occupation of electrons obeys Fermi-Dirac distribution law. The particles that obey Fermi-Dirac distribution law are called Fermions.

The Fermi-Dirac distribution function at a temperature T is given by

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

Where E_f =Fermi energy, $f(E)$=the probability that a state of energy (E) is filled.

(I) At T=O K for $E>E_f$ $E=\frac{n^2h^2}{8ma^2}$

$$f(E)=\frac{1}{e^{\infty}+1}=1$$

This means that all the energy state below E_f are filled.

For $E>E_f$

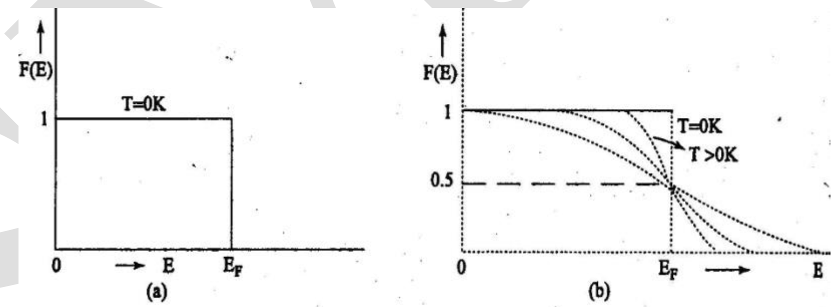
$f(E)=\frac{1}{e^{\infty}+1}=0$ Means that all the energy levels above E_f are empty.

From this we define Fermi level as it is the level at 0K below which all the levels are filled and above which all the levels are empty or it is the highest occupied state at 0K

(2) At T>0 and $E=E_f$

$$f(E)=\frac{1}{1+1}=\frac{1}{2}$$

Fermi level is the state at which the probability of electron occupation is ½ at any temperature.



FERMI ENERGY:

The no. of available electrons per unit volume in metal is given by

$$n = \int_0^{E_F} F(E)\, Z(E)\, dE \quad \text{----------} \ (1)$$

where F(E) is probability of occupation of electrons in energy level with energy E

Z(E) is available energy states per unit volume

$$\therefore \ n = \int_0^{E_F} \frac{1}{1+\exp\left(\frac{E-E_F}{K_B T}\right)} \frac{\pi}{2}\left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}} \ dE$$

In metal at T = 0k, E<E_F, F(E) = 1

$$\therefore \ n = \int_0^{E_F} \frac{\pi}{2}\left(\frac{8m}{h^2}\right) E^{\frac{1}{2}} dE$$

$$= \frac{\pi}{2}\left(\frac{8m}{h^2}\right) E^{\frac{1}{2}} \int_0^{E_F} E^{\frac{1}{2}} \ dE$$

$$= \frac{\pi}{2}\left(\frac{8m}{h^2}\right) E^{\frac{1}{2}} \left(\frac{E^{\frac{3}{2}}}{\frac{3}{2}}\right)_0^{E_F}$$

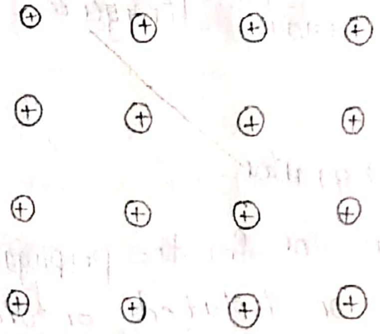
$$= \frac{\pi}{3}\left(\frac{8m}{h^2}\right) E^{\frac{1}{2}} \ E_F^{\frac{3}{2}}$$

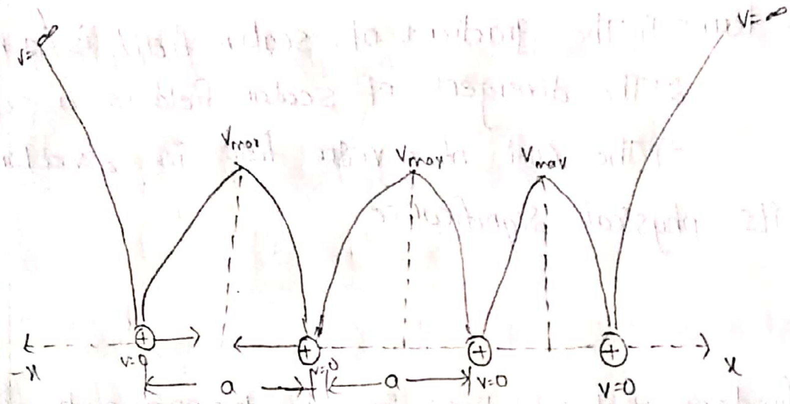
Or $E_F^{3/2} = \frac{3n}{\pi}\left(\frac{8m}{h^2}\right)^{-\frac{3}{2}}$

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

* 6.1 Band theory of solids *

Bloch theorem:- → General solution modulating with period function





→ According to block the potential varying with the periodicity 'a'

i.e., the potential is minimum at the +vely charge nuclei as

$\boxed{V_x = 0}$

→ And in between the two positively charged nuclei the potential v is maximum

i.e $\boxed{V_x = V_{max}}$

→ According to Bloch the potential $v(x)$ is varies as $v(x+a)$

i.e; $\boxed{v(x) = v(x+a)}$

Where a is the periodicity

→ Generally, the motion of the Electron in the metal can be represented by a fundamental wave equ

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

∴ The general solution of the above shrowdinger wave equation will be taken as

$$\boxed{\psi(x) = e^{\pm ikx}}$$

→ But, according to Bloch $V(x) = V(x+a)$ then, the shroowdinger wave equation can be written as

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

then, the general solution of above equation can be taken as

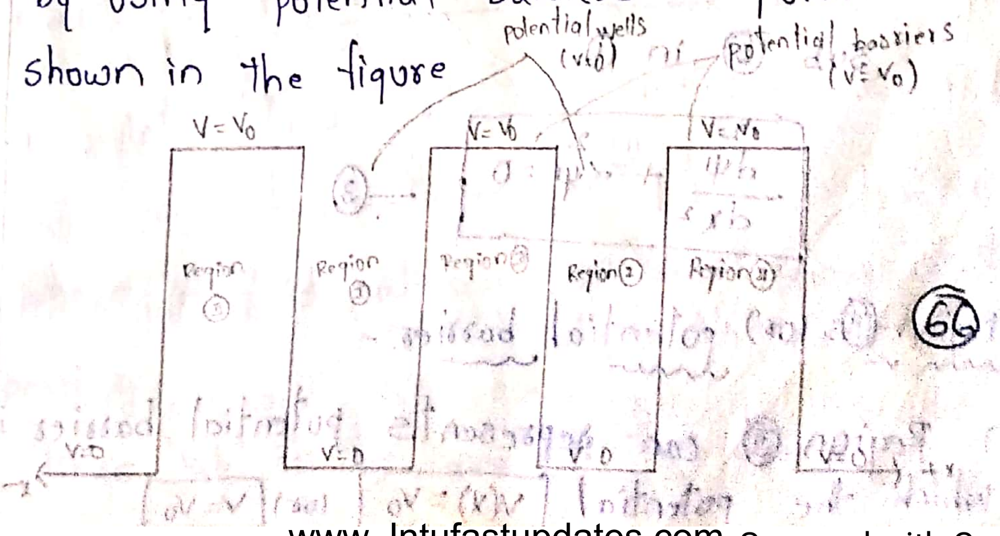
$$\boxed{\psi(x) = U_k(x)\, e^{\pm ikx}}$$

where, $U_k(x)$ → periodic function.

i.e., Bloch states that the plane wave solutions of the wave equations are modulating with the periodic functions.

Kronig-penney Model (or) The periodic motion of electron in atomic lattice

The periodic motion of electron in atomic lattice was explained by the scientist kronig & penney by using potential barriers and potential wells as shown in the figure



→ In the figure, the region Ⓘ can represents potential wells in which the potential $V=0$.

→ In the figure, the region Ⓘⓘ can represents potential barrier, the potential 'v' is maximum.

→ let the maximum potential will be taken as 'V_0'

$$\therefore \boxed{V(x) = V_0}$$

Region Ⓘ (or) potential well :-

→ Region Ⓘ can represents potential well in which the potential $V=0$.

→ Let us consider a particle which is present in potential well than the shroudinger wave equation can be written as

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

In potential $V=0$

$$\therefore \boxed{\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0} \quad \text{—} ①$$

$0 < x < a$

→ let $\boxed{\alpha^2 = \frac{2mE}{\hbar^2}}$ — ②

sub ② in ①

$$\boxed{\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0} \quad \text{—} ③$$

Region Ⓘⓘ (or) potential barrier:-

→ Region Ⓘⓘ can represents potential barrier in which the potential $V(x) = V_0$ (or) $V = V_0$

→ let us consider a particle which is present in potential barrier, than the shroudinger wave Equation can be written as

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_p)\psi = 0 \quad \text{—④}$$

In potential barrier $V = V_0$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi = 0 \quad \text{—⑤}$$

→ let $\beta^2 = \frac{2m}{\hbar^2}(E-V_0)$ —⑥

sub ⑥ in ⑤

$$\frac{d^2\psi}{dx^2} + \beta^2\psi = 0 \quad \text{—⑦}$$

→ According to bloch the general solution of the above differential equation can be taken as

$$\psi = e^{\pm ik} U_k(x) \quad \text{—⑧}$$

Now differentiate above equation twice w.r.t 'x' and those values substitute in equ. ③ & ④ then finally we will get the condition as

$$\frac{mV_0ab}{\hbar^2}\frac{\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka \quad \text{—⑨}$$

let $P = \frac{mV_0ab}{\hbar^2}$ —⑩

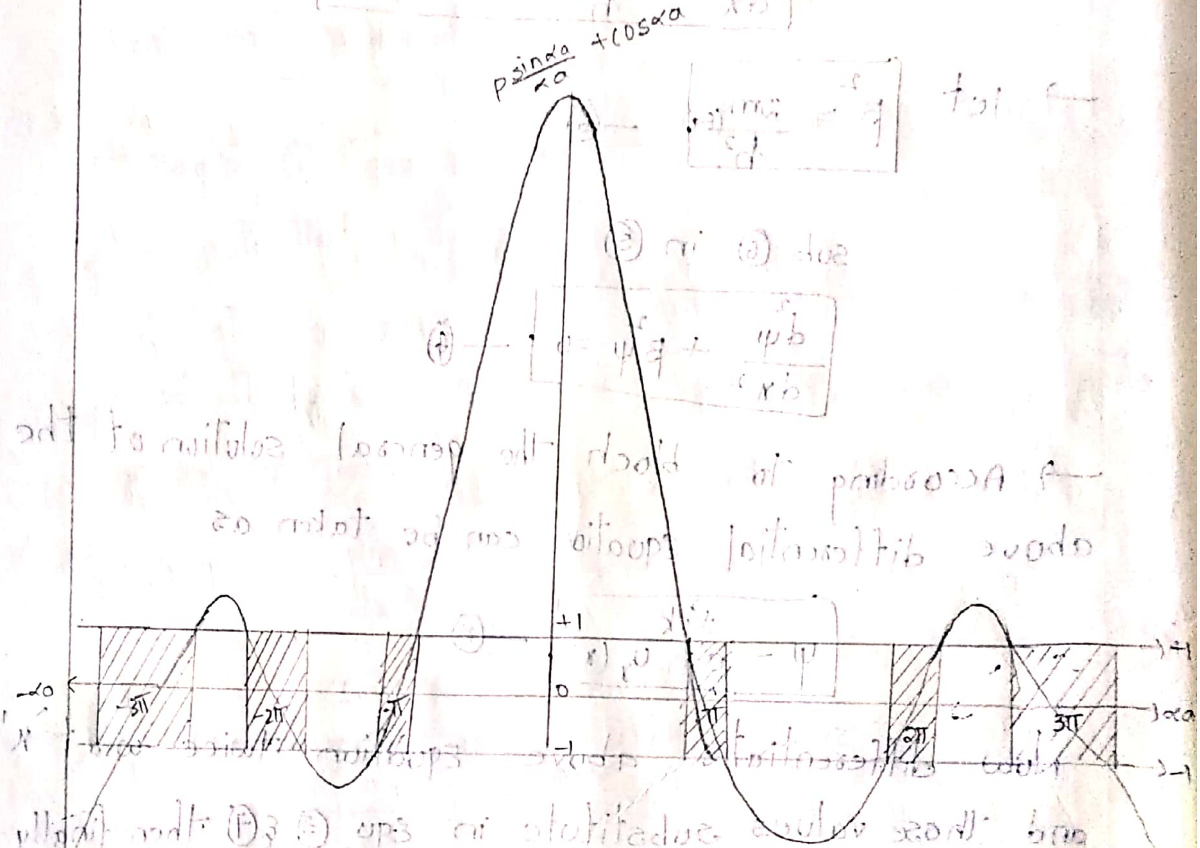
where 'P' is called scattering power of the barrier.

Here 'V_0b' is the area of the barrier.

Now sub ⑩ in ⑨

$$\boxed{P\frac{\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka} \quad —⑪$$

→ Now plot a graph between $P\frac{\sin\alpha}{\alpha a} + \cos\alpha a$ to αa for a particular value $P = \frac{3\pi}{2}$ then the graph is as shown in the figure.



→ from the above graph we conclude the following points.

1. The allowed bands of 'αa' are shown by shaded regions which are seperated by forbidden bands.

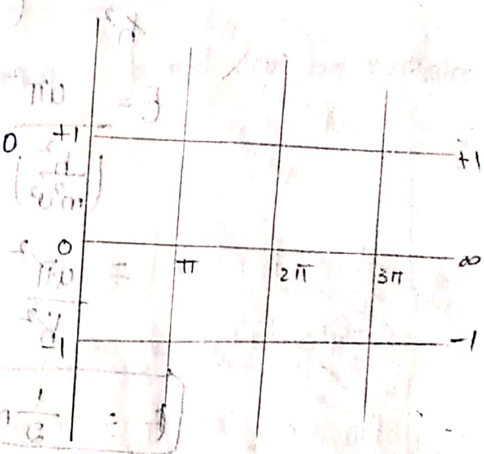
i.e., $\left[\alpha^2 = \frac{2mE}{\hbar^2}\right]$.

2. If the value 'αa' increases then the width of the allowed band increases then the forbidden band decreases.

3. If the scattering power of the barrier 'p' increases then the width of the forbidden band increases then the allowed band decreases.

$$\because \left[P = \frac{m V_0 a b}{\hbar^2} \right]$$

4. If the scattering power of the barrier $P \to \infty$ then the allowed band reduces and these will be appear as single lines as shown in the figure.



i.e., $\sin \alpha a = 0$

But we know that $\sin n\pi = 0$

$$\alpha a = n\pi$$

$$\alpha = \frac{n\pi}{a}$$

$$\alpha^2 = \frac{n^2\pi^2}{a^2}$$

where $\alpha^2 = \frac{2mE}{\hbar^2}$

$$\therefore \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

$$E = \frac{n^2\pi^2}{a^2} \times \frac{\hbar^2}{2m}$$

$$= \frac{n^2\pi^2}{2ma^2} \times \frac{h^2}{4\pi^2}$$

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

$n = 1, 2, 3, \ldots$

5. If the scattering power of the barrier $P \to 0$ then the forbidden band will disapper and the particle will be free in b/w ±1 as shown in the figure.

from Equ (11) $\boxed{P=0}$

Then, $\cos \alpha a = \cos ka$

$$\alpha a = ka$$

$$\alpha = \frac{ka}{a}$$

$$\alpha = k$$

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

$$\frac{2mE}{\hbar^2} = \left(\frac{2\pi}{\lambda}\right)^2$$

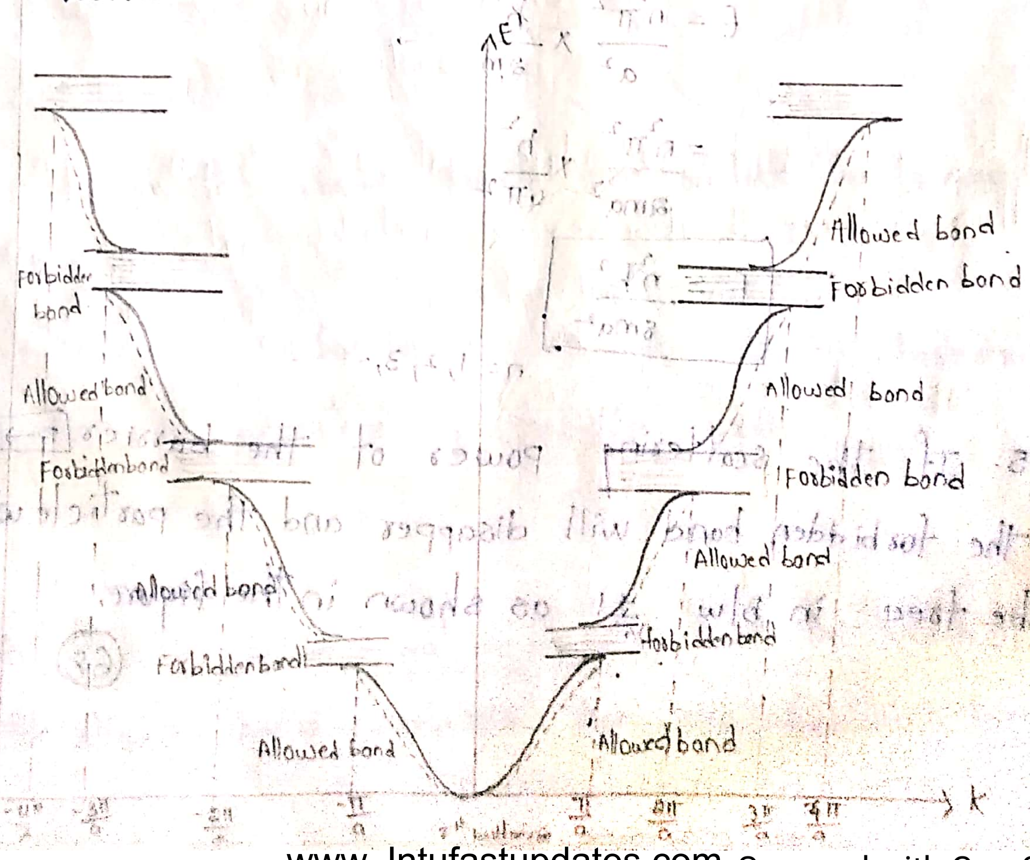
$$E = \frac{4\pi^2}{\left(\frac{h^2}{m^2v^2}\right)} \times \frac{\hbar^2}{2m}$$

$$= \frac{4\pi^2}{h^2} \times \frac{m^2v^2}{2m} \times \frac{h^2}{4\pi^2}$$

$$\boxed{E = \frac{1}{2}mv^2}$$

The above equation represents K.E of free particle.

E-K diagram (or) Brillion zones:



→ Brillon showed that the allowed regions and forbidden regions is in the form of zones which are called brillion zone

→ These are shown on the graph between E and k

→ According to him the first Brillion zone is $\frac{-\pi}{a} \to \frac{\pi}{a}$

The II^{nd} Brillion zone is $\left\{\frac{-2\pi}{a} \to \frac{-\pi}{a}\right\}$ and $\left\{\frac{\pi}{a} \to \frac{2\pi}{a}\right\}$

The III^{rd} Brillion zone is $\left\{\frac{-3\pi}{a} \to \frac{-2\pi}{a}\right\}$ and $\left\{\frac{2\pi}{a} \to \frac{3\pi}{a}\right\}$

origin of formation of Energy bands :-

The origin of formation of energy band can be explained by using of example.

Ex:- carbon

(Z = 6)

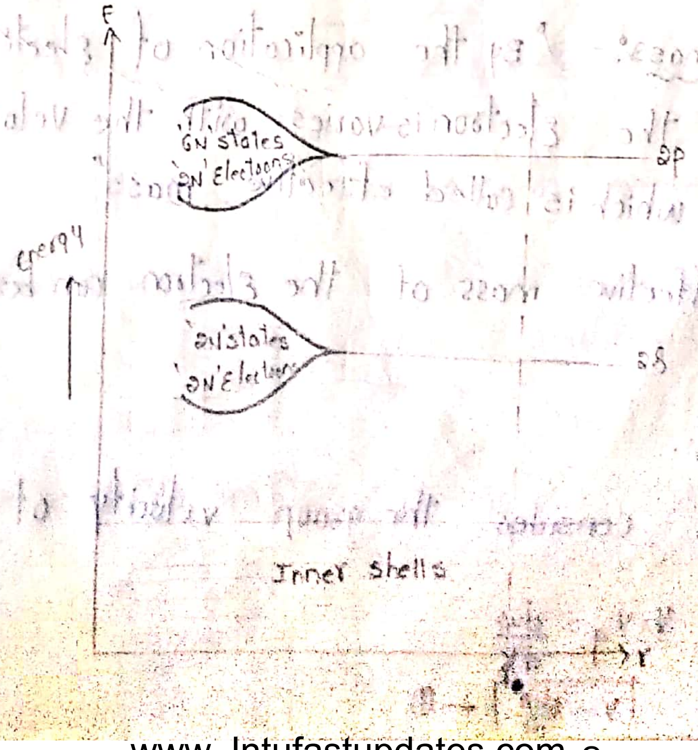
Electronic configuration $1s^2 2s^2 2p^2$

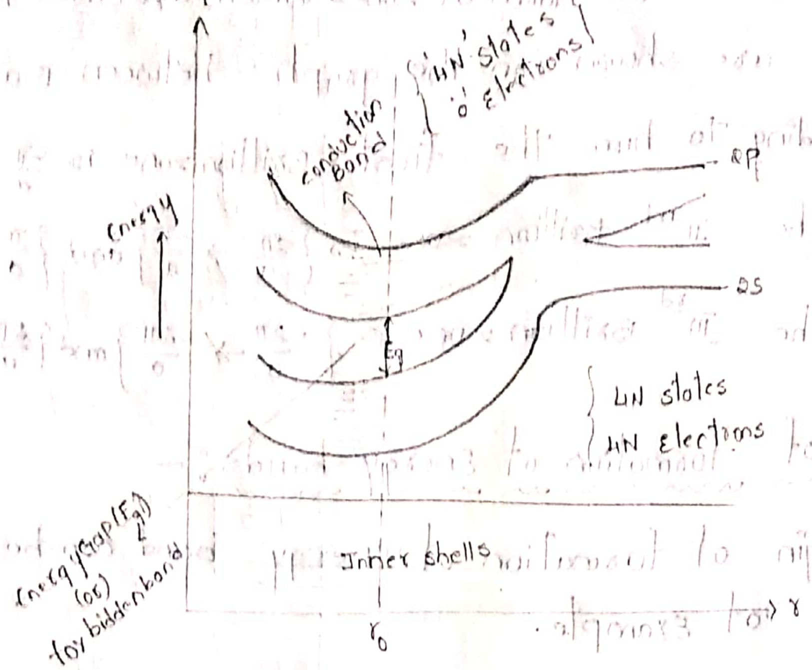
i.e., the outermost orbit electrons in carbon is '4'.

The valency of carbon is '4'.

→ The orbital representation diagram of carbon is as shown in the figure.

If suppose 'N' be the no. of atoms in the carbon element then the orbital representation is as shown in the figure.





* Imp **classification of materials into conductors, semi-conductors & insulators :-**

Based on the energy gap between the conduction band and valency band the solids are classified into three types.

They are:

1. conductors.
2. semi-conductors.
3. Insulators.

effective mass:- "By the application of electric field the mass of the electron is varies with the velocity of the electron which is called effective mass."

→ The effective mass of the electron can be represented as 'm^*'

Derivation:-

→ let us consider the group velocity of the particle

$$V = v_g = \frac{d\omega}{dK}$$

$$\boxed{V = \frac{d\omega}{dk}} \quad \text{--- (1)}$$

where,

$\omega \longrightarrow$ angular frequency

$$\boxed{\omega = 2\pi\nu}$$

from ① ⇒ $V = \frac{d(2\pi\nu)}{dk}$ —②

$E = h\nu \Rightarrow \boxed{\nu = \frac{E}{h}}$

from ②

$$V = \frac{d}{dk}\left(\frac{2\pi}{h}\right)E$$

$$\boxed{v = \frac{1}{\hbar}\frac{dE}{dk}} \quad —③$$

Now differentiate above equation w.r.t 't'

$$\frac{dv}{dt} = \frac{d}{dt}\left[\frac{1}{\hbar}\frac{dE}{dk}\right]$$

$$a = \frac{1}{\hbar}\left[\frac{d^2E}{dk\,dt}\right]$$

$$a = \frac{1}{\hbar}\frac{d^2E}{dk\,dt}\left[\frac{dk}{dk}\right]$$

$$a = \frac{1}{\hbar}\frac{d^2E}{dk^2}\cdot\left(\frac{dk}{dt}\right) \quad —④$$

We know that $\boxed{P = \hbar k}$ —⑤

Now differentiating above equation w.r.t to 't'

$$\boxed{\frac{dP}{dt} = \hbar\frac{dk}{dt}} \quad —⑥$$

We know that, the rate of change of momentum is called force.

$$\boxed{\frac{dP}{dt} = F} \quad —⑦$$

sub ⑦ in ⑥

$$F = \hbar\frac{dk}{dt}$$

$$\boxed{\frac{dk}{dt} = \frac{F}{\hbar}} \quad —⑧$$

sub ⑧ in ④

$$a = \frac{1}{\hbar}\left[\frac{d^2E}{dk^2}\right]\frac{F}{\hbar}$$

$$a = \frac{F}{\hbar^2}\left(\frac{d^2E}{dk^2}\right) \quad —⑨$$

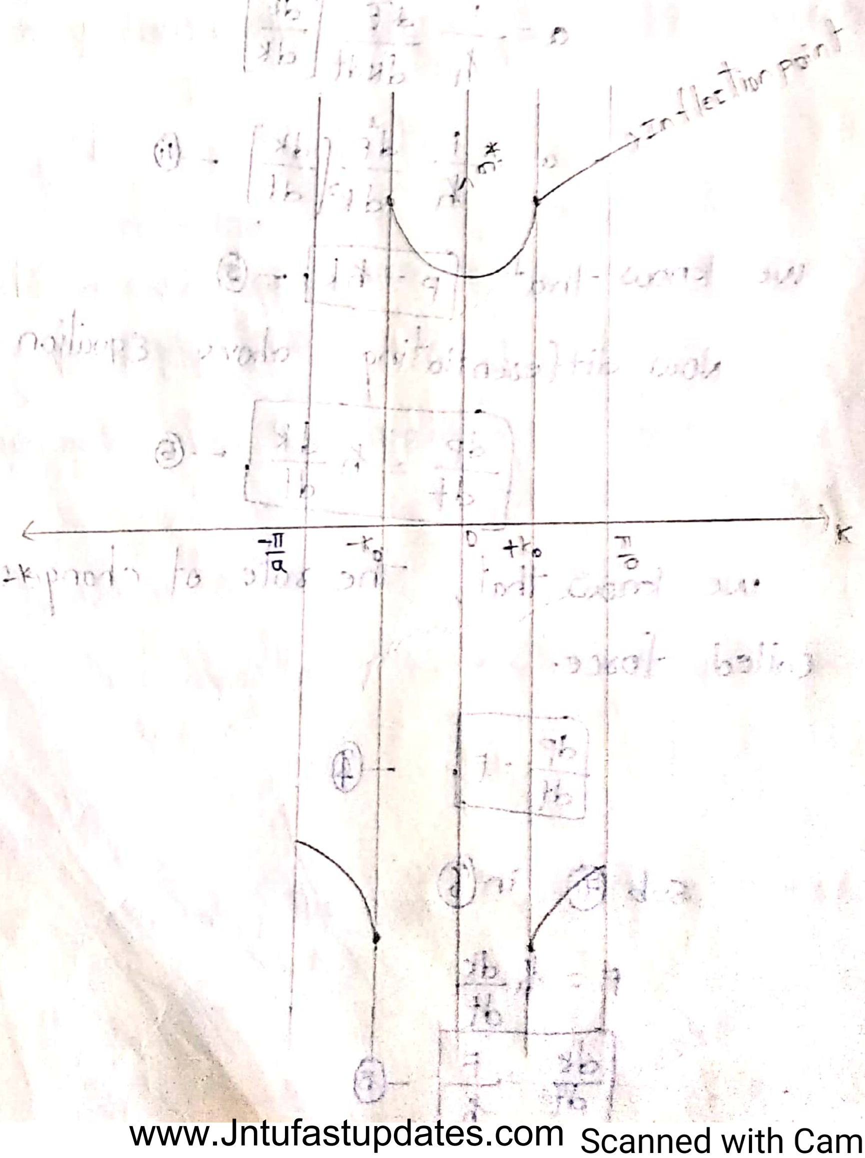
$$\boxed{F = m^* a} \quad —⑩$$

sub ⑩ in equ ⑨

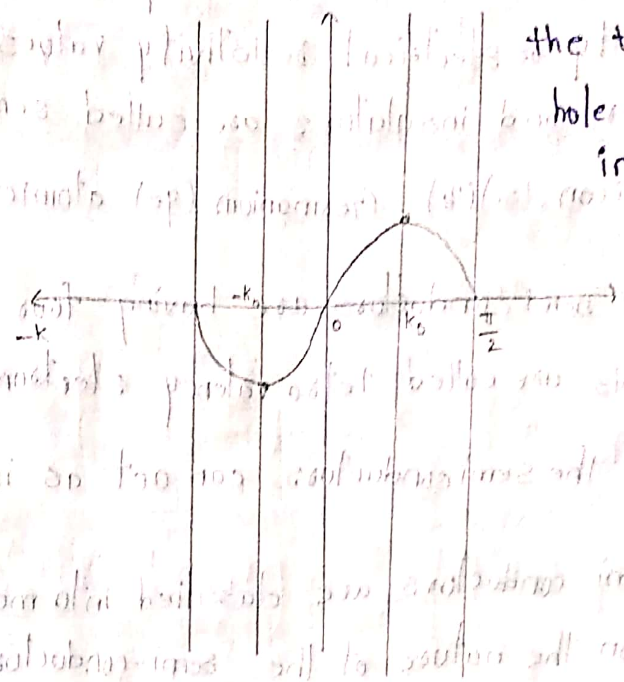
$$a = \frac{m^* a}{\hbar^2}\left[\frac{d^2E}{dk^2}\right]$$

$$\boxed{m^* = \frac{\hbar^2}{\left[\frac{d^2E}{dk^2}\right]}}$$

∴ The above Equation represents the effective mass of the electrons



→ The point at which the -vely charged Electron can behaves as the +vely charged hole is called inflection point.



Questions :-

1. State & derive effective mass of Electron and Explain the concept of hole?

2. Explain the origin of formation of energy bands in solids?

3. Differentiate (or) classify the materials into conductors, semi-conductors and insulators?

4. Explain the kronig - penney model (or) Explain the periodic motion of electron in atomic lattice?

5. State & Explain the block theorm?

→ The mass of the Electron is a function of velocity. By the application of electric field the mass of the Electron is also increasing with velocity 'v' upto a point 'k_0'. (71)

→ Beyond the point 'k_0' the velocity of the particle reduces and it will gets retordation. (-ve acceleration) i.e; the negatively charged electron can behave as the positively charged 'hole', which is the concept of hole.