UNIT – I

PRINCIPLES OF QUANTUM MECHANICS

WAVES : A Wave can be described as a disturbance that travel through a medium from one location to another location.

or

The Repeating and periodic disturbance that moves through a medium from one location to another is Referred to as a Wave a medium is a substance or material that carries the Wave.

→ A Particle is a minute fragment or quality of matter.

De - Broglie Hypothesis :

→ According to DB hypothesis when particles are accelerated they will spread like a wave with a Certain Wavelength.

→ Let us consider a photon with fq ν travelling in the Velocity of light c

→ Then the Velocity of light $c = \nu\lambda$ where λ is Wavelength of the light. ⟶ ①

According to Einstein, the Equation of photon

$$E = h\nu \longrightarrow ②$$

Considering the Momentum of the photon subjected to an External force

$$p = \frac{E}{c} \longrightarrow (3)$$

Substituting the Values of $c = v\lambda$ & $E = h\nu$

$$p = \frac{h\nu}{\nu\lambda} \quad \text{or} \quad p = \frac{h}{\lambda}$$

Consider a particle of mass m moving with a Velocity v then the wavelength associated with the particle is $\lambda = \frac{h}{m\nu}$

DBW in terms of KE

Consider a Particle of mass m moving with a Velocity v then the (KE) of the particle is

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

$$= \frac{1}{2m} m^2 v^2 = \frac{p^2}{2m}$$

W.K.T $p = mv$

$$p^2 = 2mE \quad \text{or} \quad p = \sqrt{2mE}$$

the wavelength $\lambda = \frac{h}{\sqrt{2mE}}$

DBW interms of EV:

Consider an e^- of mass m and charge e that is accelarated through a P.D of V volts. then the KE of e^- is equal to the loss of P.E

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

$$m^2V^2 = 2meV$$

the momentum of the Electron $p = mV = \sqrt{2meV}$

$$\text{DBW} \quad \lambda = \frac{h}{mV} = \frac{h}{\sqrt{2meV}}$$

$$\lambda = \frac{6.626\times10^{-34}}{\sqrt{2\times9.1\times10^{-3}\times1.6\times10}} = \frac{12.28\times10^{-10}}{\sqrt{V}}\,m$$

$$\boxed{\lambda = \frac{12.28}{\sqrt{V}}\,A^\circ}$$

Schrodinger's One-dimensional time-Independent WE:

→ According to de-Broglie hypothesis the particle in motion is always associated with a wave.

→ To describe the motion of a particle in terms of its associated wave, Schrodinger derived a wave eqn is termed as Schrodinger Wave eqn

→ Consider a particle a mass m moving with Velocity v along the x direction. It is associated with a Wave

→ The displacement of the Wave is given by the Wave function ψ. For steady state wave motion ψ

is a function of x Coordinate only for 1D Motion.

→ 1D eqn for steady state associated with a particle is

$$\psi(x) = A \sin \frac{2\pi}{\lambda} x \longrightarrow ①$$

where A is the amplitude & λ is Wavelength

diff eqn ① w.r.to x

$$\frac{d\psi}{dx} = A \frac{2\pi}{\lambda} \cdot \cos \frac{2\pi x}{\lambda}$$

$$\frac{d^2\psi}{dx^2} = -\frac{4\pi^2}{\lambda^2} A \sin \frac{2\pi x}{\lambda} = -\frac{4\pi^2}{\lambda^2}\psi \longrightarrow ②$$

de Broglie Wavelength $\lambda = \frac{h}{mv}$

$$\frac{1}{\lambda^2} = \frac{m^2v^2}{h^2} = \frac{2m\left(\frac{1}{2}mv^2\right)}{h^2} \longrightarrow ③$$

Let E be total energy of particle & V be the PE of particle then

$KE = \frac{1}{2}mv^2 = E - V$ substituting eqn ③

$$\frac{d^2\psi}{dx^2} = -\frac{8\pi^2 m}{h^2}(E-V)\psi$$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

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

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

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

Properties of Matter Waves:

→ Matter Waves are produced by the motion of the particles and independent of charge.

→ They can travel through Vaccum and donot require any material medium for their propagation

→ The Smaller the Velocity of the particle, the Longer is the Wavelength of the matter Waves associated with it.

→ The lighter the particle, longer is the Wavelength of the matter Waves associated with it.

→ Velocity of matter waves depends on the Velocity of the material particle and is not a Const. quantity.

→ The Velocity of matter Waves is greater than the Velocity of light

Heisenberg uncertainity Principle:

The HUP states that the stimulated determination of a pair of physical quantities like position and momentum of a particle Cannot be determined with the Required accuracy

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi} \text{ or } \frac{\hbar}{2\pi}$$

$$\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$$

$$\Delta L \cdot \Delta \theta \geq \frac{h}{4\pi}$$

Consequences of Uncertainity Principle :

→ Let Eg E be emitted during the time interval Δt if the Eg in the form of E-M Waves, We cannot measure the fq ν of the Waves accurately in the limited time Available

$$fq = \frac{\text{No of Wave}}{\text{time Interval}} \Rightarrow \Delta \nu \geq \frac{1}{\Delta t}$$

$$\Delta E = h \Delta \nu \quad , \quad \Delta E \geq \frac{h}{\Delta t}$$

$$\Delta E \, \Delta t \geq h \quad , \quad \Delta E \cdot \Delta t \geq \frac{h}{4\pi}$$

→ Explanation for absence of e^- in the Nuclear Uncertainity in momentum of e^- $\Delta p \geq \frac{h}{4\pi \Delta x}$

$$\geq \frac{6.62 \times 10^{-34}}{4\pi \times 10^{-15}} = 0.5266 \times 10^{-19} \text{ Kg/s}$$

$$E^2 = p^2c^2 + m_0^2c^4$$

$$= (0.5266\times10^{-19}\times3\times10^{5})^2 + (9.1\times10^{-31}\times(3\times10^{8})^2)^2$$

$$= 2.4958\times10^{-22}\ J$$

$$E = 10^8\ eV = 100\ MeV.$$

3. Uncertainity in the fq of light emitted by an atom

$\Delta E\cdot\Delta t \geq \frac{h}{4\pi}$ ⇒ from one principle of energy & time relation $\Delta E \geq \frac{h}{4\pi\cdot\Delta t}$

$\Delta E + h\Delta V$, Corresponding fq spread.

$$\Delta V = \frac{\Delta E}{h},\ \Delta V \geq \frac{1}{4\pi\,\Delta t}$$

The life time of e^- in the excited orbit is of the order of 10^{-8} sec. Hence $\Delta V \geq \frac{1}{4\pi\times10^{-8}}$

$$\geq 0.08\times10^{8}\ Hz$$

$$\geq 8\times10^{16}\ Hz.$$

4. energy of an e^- in an atom

To calculate the eq of an e^- in an atom, let us Consider the Case of hydrogen atom the Radius of e^- orbit of hydrogen atom is 5.3×10^{-11} m.

$$\Delta p \geq \frac{h}{4\pi \cdot \Delta x}, \quad \Delta x = 5.3 \times 10^{-11} m$$

$$\Delta p \geq \frac{6.62 \times 10^{-34}}{4 \times \pi \times 5.3 \times 10^{-11}} \geq 0.1 \times 10^{-23} \text{ Kg-m/s.}$$

K.E of e^-. $K = \frac{p^2}{2m} = \frac{(0.1 \times 10^{-23})^2}{2 \times 9.1 \times 10^{-31}} = 0.055 \times 10^{-17} J$

$$= \frac{0.055 \times 10^{-17}}{1.6 \times 10^{-19}} eV = 3.44 eV.$$

Ex: A Microscope using photons is employed to locate an e^- in an atom to within a distance of 0.2 A°. What is the uncertainity in the Momentum of e^- located in this

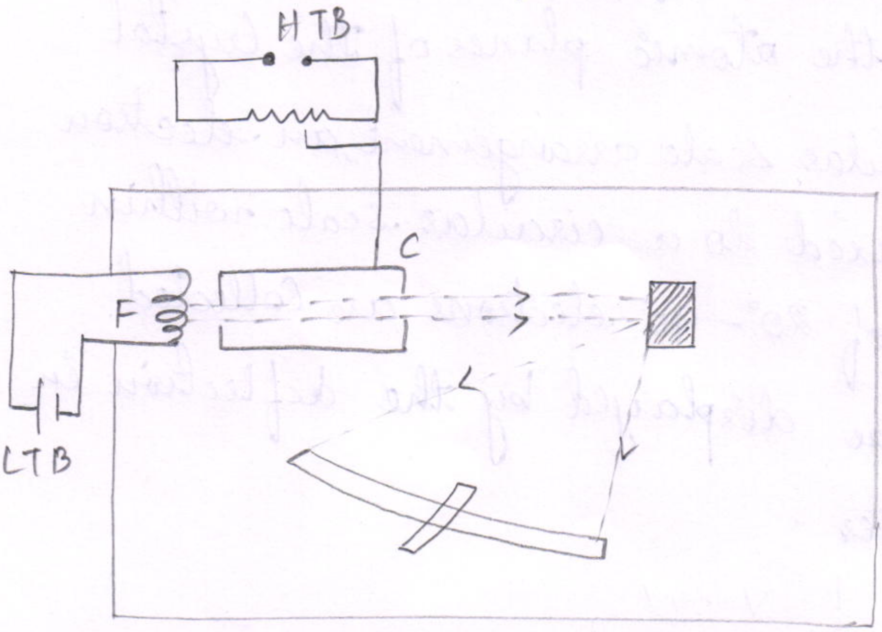
$$\Delta x \cdot \Delta p \sim h$$

$$\Delta x = 0.2 A^\circ = 0.2 \times 10^{-10} m.$$

$$\Delta p = \frac{h}{4\pi \cdot \Delta x} = \frac{6.626 \times 10^{-34}}{4\pi \times 0.2 \times 10^{-10}}$$

$$\simeq 5.27 \times 10^{-24} \text{ Kg.m/s.}$$

Davission - Germer Experiment:



→ In 1927, Davisson and Germer made an attempt to prove the wave nature of atomic Particles.

→ The Entire setup is divided into 3 parts i.e e^- gun, target and circular scale arrangement

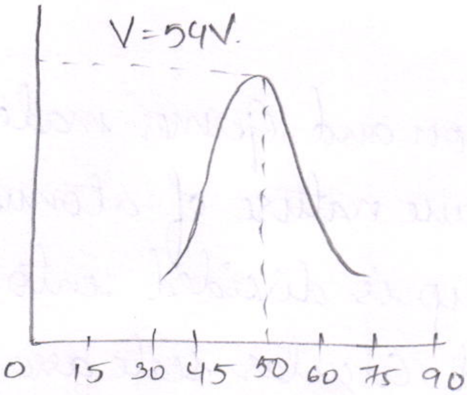
→ When tungsten filament F is heated by a low tension battery (LTB) then Electrons are produced and allowed to pass through Collimated Cylinder

→ These Electrons are accelarated to a required Velocity by applying sufficient potential of 30-600V by high tension Battery

→ The fast moving beam of Electrons is made to incident on the Nickel Crystal/target which can be rotated about an axis perpendicular to the plane of the diagram.

→ The electrons are reflected in all possible directions by the atomic planes of the crystal.

→ In the circular scale arrangement, an electron collector is fixed to a circular scale within the Range of 20°–90° electrons are collected with can be displayed by the deflection in galvanometer.



→ When a potential of 54V is applied, the first order maximum is observed at an angle of 50° between incident and Reflected Rays.

→ It can also be observed in the plot of Variation of number of scattering electrons with an angle of diffraction of 65°

(since 90-25=65°).

→ The Interplanar spacing (d) of nickel Crystal is 0.91 A° which is measured by the X-Ray diffraction method.

$$2d\sin\theta = n\lambda$$

$$2 \times 0.91 \times \sin\theta = n\lambda$$

$$\boxed{\lambda = 1.65\ A^\circ}$$

→ The Wavelength of Electron wave can be Computed from the accelarating potential V using the de-Broglie equation

$$\lambda = \frac{h}{\sqrt{2meV}}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{2 \times 9.1 \times 10^{-31} \times 1.602 \times 10^{-19} \times 54}$$

$$\boxed{\lambda = 1.66\ A^\circ}$$

→ Davission- Germer experiment gave Conclusive evidence that Electrons exhibit diffraction Property.

Problems :

1. Calculate the de broglie Wavelength associated with a proton moving with a velocity of $1/10$th of Velocity of light (Mass of proton $= 1.67 \times 10^{-27}$ Kg).

Velocity of proton $v = \frac{1}{10} \times c = 3 \times 10^{7}$ m/s.

Mass of proton $m = 1.67 \times 10^{-27}$ Kg

$$D.B.W = \lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34}}{1.67 \times 10^{-27} \times 3 \times 10^{7}}$$

$$= 1.323 \times 10^{-14} \text{ m}.$$

2. Calculate the debroglie Wavelength of an e^- which has been accelarated from rest on application of Potential of 400 Volts

$$\lambda = \frac{12.26}{\sqrt{V}} = \frac{12.26}{\sqrt{400}} A^{\circ} = 0.613 A^{\circ}$$

3. If the KE of neutron is 0.025 eV. Calculate its de-Broglie wavelength. Mass of Neutron $= 1.674 \times 10^{-27}$

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$K.E = \frac{1}{2} m v^{2} = 0.025 \text{ eV}.$$

$$= 0.025 \times 1.6 \times 10^{-19} \text{ J}.$$

$$V = \left(\frac{2 \times 0.025 \times 1.6 \times 10^{-19}}{1.674 \times 10^{-27}} \right)^{1/2}.$$

$$= (0.04779 \times 10^{8})^{1/2} = 0.2186 \times 10^{4} \text{ m/s}$$

$$\lambda = \frac{h}{mV} = 0.181 \text{ nm}.$$

4. Calculate the Wavelength associated with an e^- raised to a potential 1600V.

de Broglie Wavelength $\lambda = \frac{12.26}{\sqrt{V}} A^{\circ}$

$$\lambda = \frac{12.26}{\sqrt{V}} A^{\circ} = \frac{12.26}{\sqrt{1600}} = 0.3065 A^{\circ}$$

Schrodinger's one-dimensional Time Independent WE

→ According to de Broglie hypothesis the particle in motion is always associated with a wave.

→ To describe the motion of a particle in terms of its associated wave. Schrodinger derived a Wave eqn which is termed as Schrodinger Wave eqn.

→ Consider a particle of mass m moving with Velocity V along the x direction. It is associated with a Wave.

→ The displacement of the wave is given by the wave function ψ. For steady state wave motion ψ is a function of x coordinate only for 1D motion.

→ 1D eqn for steady state associated with a particle is

$$\psi(x) = A \sin \frac{2\pi}{\lambda} x \longrightarrow (1)$$

where A is amplitude & λ is wavelength diff. eqn (1) wrt to x.

$$\frac{d\psi}{dx} = A \cdot \frac{2\pi}{\lambda} \cdot \cos \frac{2\pi x}{\lambda}$$

$$\frac{d^2\psi}{dx^2} = -\frac{4\pi^2}{\lambda^2} A \sin \frac{2\pi x}{\lambda} = -\frac{4\pi^2}{\lambda^2} \psi \longrightarrow (2)$$

de Broglie wavelength $\lambda = \frac{h}{mv}$

$$\frac{1}{\lambda^2} = \frac{m^2 v^2}{h^2} = \frac{2m\left(\frac{1}{2}mv^2\right)}{h^2} \longrightarrow (3)$$

Let E be total energy of particle & V be the PE of particle then

$KE = \frac{1}{2}mv^2 = E - V$ substituting eq (3)

$$\frac{d^2\psi}{dx^2} = -\frac{8\pi^2 m}{h^2}(E-V)\psi$$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

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

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

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

Physical significance of Wavefunction:

The Wavefunction is a Variable quantity used to Characterize the matter waves or deBroglie Waves.

→ It gives a statistical relationship between the particle and Wave nature

→ It is a Complex quantity and hence it Cannot locate the position of a particle.

→ It is a function of wave and time Coordinate hence it cannot locate

$$= |\psi|^2 dV$$

where $|\psi|^2$ is Known as the probability density or probability function

$$\text{i.e } |\psi|^2 = \psi^* \psi.$$

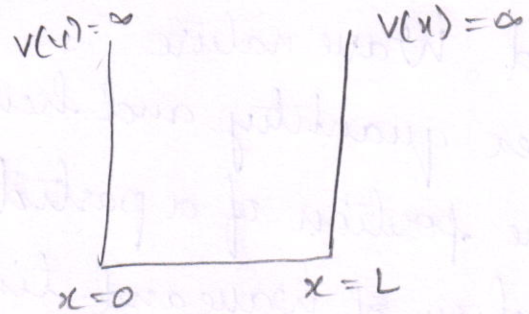
→ Total probability of finding the particle in the entire space is equal to unity and is known as Normalization

$$\int_{-\infty}^{\infty} |\psi|^2 dv = 1.$$

Particle in One dimensional Box Potential Wall.

→ Consider a One dimensional box with width $x=0$ at $x=L$ and infinite height.

→ The Particle of mass m, total energy E is moving freely in the x-direction inside the Potential box with limitations $x=0$ and $x=L$ hence its motion is Restricted by Walls.



→ Schrodinger time independent equation to Obtain wave function and energy of the Particle inside the box is zero.

→ The Particle is inside the box and Hence the Potential energy is zero.

for $0 < x < 2$ $V = 0$

$\therefore$ Wave function for $0 \nless x > 2$ $|\psi|^2 = 0$

$\psi = 0.$

$\rightarrow$ The Particle Cannot be Outside the box and hence the potential energy is infinite

for $0 \geq x \geq L$ $V(x) = \infty$

$\therefore$ the Wavelength $|\psi|^2 \neq 0$ for $0 < x < L$

According to Schrodinger, one-dimensional time-independent Wave equation is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \longrightarrow ③$$

for a freely moving particle $V = 0 \longrightarrow$ We get

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0.$$

$$\boxed{\frac{d^2\psi}{dx^2} + K^2\psi = 0} \longrightarrow ④ \text{ where } K^2 = \frac{2mE}{\hbar^2}$$

Solution of the above equation give the Wave function of the particle inside the box

$$\psi = A \sin Kx + B \cos Kx \longrightarrow ⑤$$

where A is the Amplitude of the electron's wave function Applying the boundary Condition where $x=0$ & $\psi=0$ we get $B=0$

Similarly when $x=L$ and $\psi=0$ we get $0=A\sin KL$

We know that the Electron is present inside the box and hence $A\neq 0$

Therefore $\sin KL=0$

But $\sin KL=0$ only when $KL=n\pi$

$$\therefore K=\frac{n\pi}{L} \longrightarrow (6)$$

$\therefore$ Applying the boundary Condition to the Value of K from (6) in eq (5) we get

$$\boxed{\psi_n = A\sin\frac{n\pi x}{L}} \longrightarrow (7)$$

Problems :

1. Calculate the Velocity & Kinetic energy of an e^- of Wavelength 1.66×10^{-10} m.

deBroglie Wavelength. $\lambda=\frac{h}{mv} \Rightarrow v=\frac{h}{m\lambda}$

$$=\frac{6.626\times10^{-34}}{9.1\times10^{-31}\times1.66\times10^{-10}}$$

$$K.E=\frac{1}{2}mv^2$$

$$=\frac{1}{2}\times9.1\times10^{-31}\times(0.4386\times10^{7})^2$$

$$=0.8754\times10^{-17}\,J$$

$$=\frac{0.8754\times10^{-17}}{1.6\times10^{-19}}=54.71\,eV.$$

2. An e^- is moving under a potential field of 15KV Calculate the wavelength of e^- waves

de Broglie wavelength $\lambda = \frac{12.26}{\sqrt{V}} A^o$

$$= \frac{12.26}{\sqrt{15000}} A^o \Rightarrow \frac{12.26}{22.47} A^o = 0.1 A^o$$

Calculate the wavelength of matter waves associated with a neutron whose kinetic energy is 1.5 times the rest of e^- (Given the mass of neutron $= 1.676 \times 10^{-27}$ Kg, mass of $e^- = 9.1 \times 10^{-31}$ Kg, Planck's const $= 6.62 \times 10^{-34}$ J-sec, Vel of light $= 3 \times 10^{8}$ m/s

For Neutron $\frac{1}{2} mv^2 = 1.5 \times 9.1 \times 10^{-31}$ J

$$v^2 = \frac{2 \times 1.5 \times 9.1 \times 10^{-31}}{1.67 \times 10^{-27}} = 16.288 \times 10^{-4}.$$

$$v = 4.046 \times 10^{-2}.$$

$$\lambda = \frac{h}{mv} = \frac{6.602 \times 10^{-34}}{1.676 \times 10^{-27} \times 4.046 \times 10^{-2}}$$

$$= 0.976 \times 10^{-5} m.$$

4. e^- are accelarated by 344 Volts and equal from a crystal. The first reflection max.

occurs when the glancing angle is 60°. Determine the Spacing of the Crystal

de Broglie Wavelength $\lambda = \frac{12.26}{\sqrt{V}} A^{0}$

$$= \frac{12.26}{\sqrt{344}} \times 10^{-10} m = 0.661 \times 10^{-10} m$$

Acc to Bragg's law $2d\sin\theta = n\lambda$

Max Reflection $n=1$, $\sin\theta = \sin 60^{\circ} = 0.866$

$$d = \frac{n\lambda}{2\sin\theta} = \frac{0.661 \times 10^{-10}}{2 \times 0.866} = 0.3816 \times 10^{-10} m.$$

$$= 0.3816 A^{0}$$

5. Calculate the Wavelength associated with a energy 2000 eV ?

$$\lambda = \frac{h}{\sqrt{2mE}}, \quad h = 6.626 \times 10^{-34} J.sec$$

$$m = 9.1 \times 10^{-31} Kg$$

$$E = 2000 \times 1.6 \times 10^{-19} J$$

$$\lambda = \frac{6.626 \times 10^{-34}}{(2 \times 9.1 \times 10^{-31} \times 2000 \times 1.6 \times 10^{-19})^{1/2}}$$

$$= \frac{6.626 \times 10^{-9}}{241.33} = 0.0275 nm.$$

Normalisation: One can determine the Value of A by considering the definite Existence of Electrons inside the box i.e normalization of the Wave function

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1 \longrightarrow (8)$$

$$\int_{0}^{L} A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1 \longrightarrow (9)$$

Rearranging the above equations

$$\int_{0}^{L} \sin^2\left(\frac{n\pi x}{L}\right) dx = 1 \longrightarrow (9')$$

$$\frac{1}{A^2} = \int_{0}^{L} \left[\frac{1-\cos\left(\frac{2\pi n x}{L}\right)}{2}\right] dx.$$

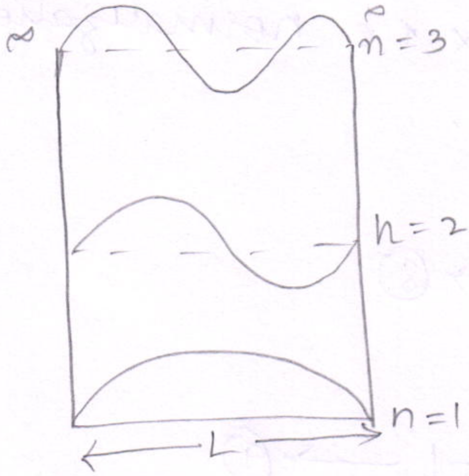
Integrating and substituting the limits in the above equation we get

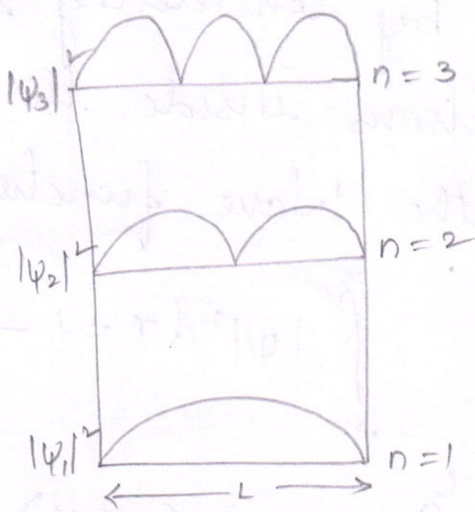
$$\frac{1}{A^2} = \frac{L}{2} \quad \text{or} \quad \boxed{A = \sqrt{\frac{2}{L}}} \longrightarrow (10)$$

substituting eq (10) in eq (7)

$$\boxed{\varphi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}}$$

normalized wave function for an electron in a One dimensional Potential Wall





Calculation of Eigen Values:

wave number $K^2 = \dfrac{2mE}{\hbar^2}$

from eqn 6 $K = \dfrac{n\pi}{L} \Rightarrow K^2 = \dfrac{n^2\pi^2}{L^2}$

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2} \rightarrow \boxed{E_n = \frac{n^2h^2}{8mL^2}}$$

→ It is not possible for the particle to have any arbitary definite energy instead only discrete definite energy levels are allowed and is known as energy equation.

→ The lowest possible energy level of the particle called the zeropoint energy is non-zero

→ Energy levels at nodes employing positions at which the particle can never be found

Problems.

1) Find the lowest energy of an e^- confined in a box of side 0.1 nm each.

The Possible energies of a particle in a Cubical box of each side L are given by.

$$E_{n_1, n_2, n_3} = \frac{h^2}{8mL^2}(n_1^2 + n_2^2 + n_3^2)$$

For lowest energy level $n_x = n_y = n_z = 1$

$$E = \frac{3h^2}{8mL^2} = \frac{3 \times (6.62 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (0.1 \times 10^{-9})^2}$$

$$= 18.06 \times 10^{-18} \text{ J} \quad \text{or} \quad 112.9 \text{ eV}.$$

2) Calculate the energy of e^- in the energy level, immediately after the lowest energy level, Confined in a Cubical box of side 0.1nm

$$E_{n_x, n_y, n_z} = \frac{h^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2).$$

when for lowest eg level $n_x = n_y = n_z = 1$ for level next to lowest $n_x = n_y = 1, n_z = 2$

$$E_{112} = \frac{h^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2) = \frac{6h^2}{8mL^2}$$

$$E_{112} = 36.12 \times 10^{-18} \text{ J} \quad \text{or} \quad 225.75 \text{ eV}$$

An e^- is bond is 1D box of size 4×10^{-10} m what will be its minimium energy

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

For mi energy $n=1$ $E = \frac{h^2}{8mL^2} = 0.0346\times10^{-17}$

$= 0.346\times10^{-18}$ J

4. An e^- is bound in 1D infinite wall of width 1×10^{-10} m Find the energy values in ground state & first 2 excited states

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

$E_1 = 0.6031\times10^{-17}$

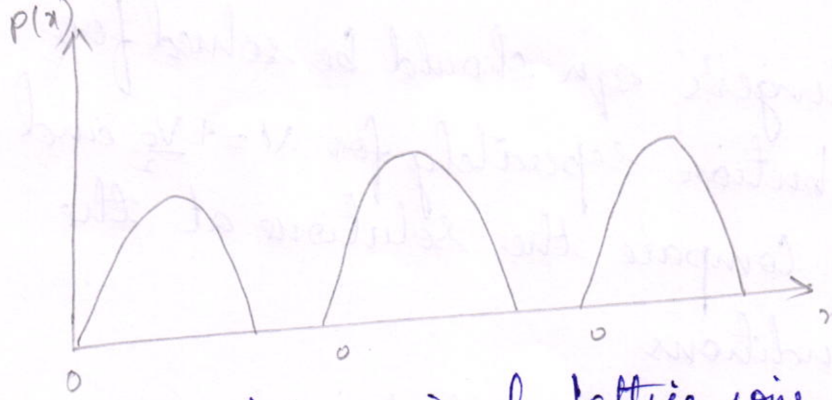
$E_2 = 4\times0.6031\times10^{-17}$

$= 2.412\times10^{-17}$

$E_3 = 9\times0.6031\times10^{-17} = 5.428\times10^{-17}$

Kronig – Penney Model

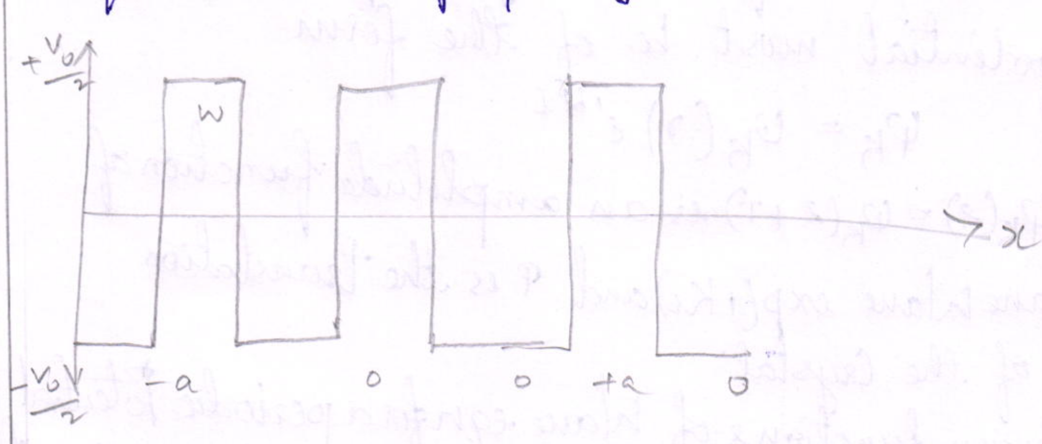
→ KP Model is used to illustrate many Consequences of the Periodic potential.



→ A One-dimensional lattice ions seperated by lattice parameter a is Considered.

→ It is assumed that potential is higher between the ions and lower near the lattice ion.

→ The potential distribution is quite Complicated and for mathematical Solution of schrodinger equation, Kronig-penny model is used.



→ The ions are located at $x = 0, a, 2a, 3a$ etc

→ The potential walls are seperated from each other by potential barrier of height V_0 and Width w.

→ The Schrodinger's eqn should be solved for Potential distribution seperately for $V = +\frac{V_0}{2}$ and $V = -V_0/2$ and Compare the solutions at the boundary Conditions.

Electrons in a Periodic Potential:

→ The Potential energy of e^- in a Crystal are a Result of the +vely charged atomic cores producing a Coulombic attraction.

→ Bloch Theorem specifies the form of levels in a Periodic crystal.

→ The solutions of Schrodinger's equation for a Periodic potential must be of the form

$$\varphi_K = \varphi_K(r)\, e^{iKx}$$

where $\varphi_K(r) = \varphi_K(r+T)$ is an amplitude function of the plane Wave $\exp(iKr)$ and T is the translation Vector of the Crystal.

→ The Eigen functions of Wave eqn for a periodic Potential are the product of plane Wave $\exp(iKr)$ times $\varphi_K(r)$ with Periodicity of a lattice.

→ Wavefunctions of this form are called Bloch functions.

→ In the limit $p \to \infty$ the allowed band Reduces to one single eg level.

→ If $p \to 0$

$$\cos Ka = \cos \alpha a$$

$$K = \alpha \text{ or } K^2 = \alpha^2 = \frac{8\pi^2 mE}{h^2}$$

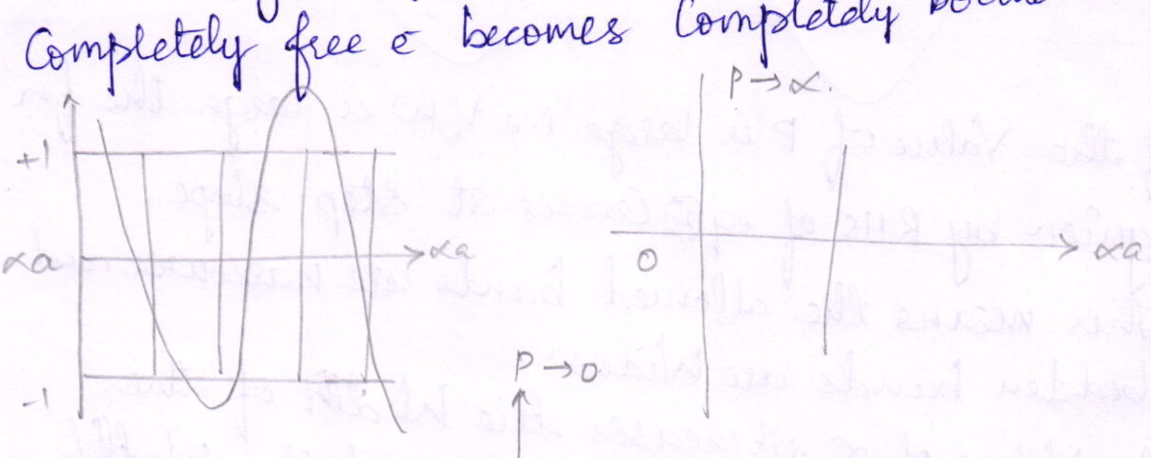
$$\text{or } E = \frac{h^2 K^2}{8\pi^2 m}$$

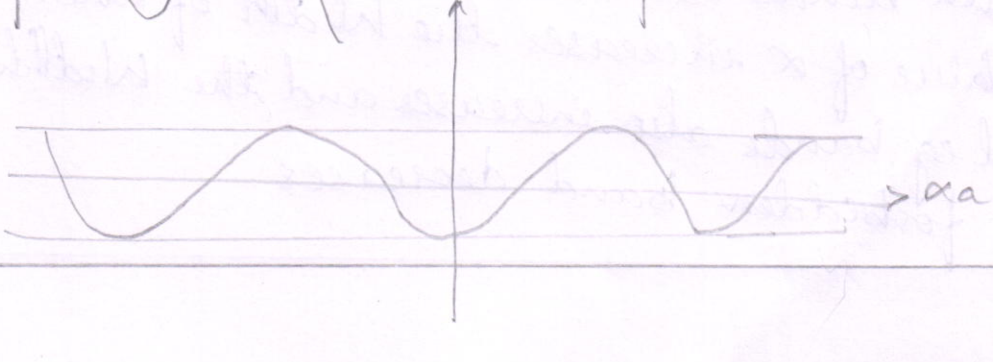
$$E = \frac{h^2}{8\pi^2 m} \cdot \left(\frac{2\pi}{\lambda}\right)^2 = \frac{h^2}{2m}\left(\frac{1}{\lambda^2}\right)$$

$$E = \frac{h^2}{2m}\left(\frac{p^2}{h^2}\right) = \frac{p^2}{2m} \text{ or } \frac{1}{2}mV^2$$

→ This indicates that the particle is completely free and no energy levels exist.

→ Thus by varying p from 0 to α we find the completely free e becomes completely bound.





→ The assumed Wavefunctions has the form.

$$\psi(x) = U_K(x)\, e^{+iKx} \longrightarrow (1)$$

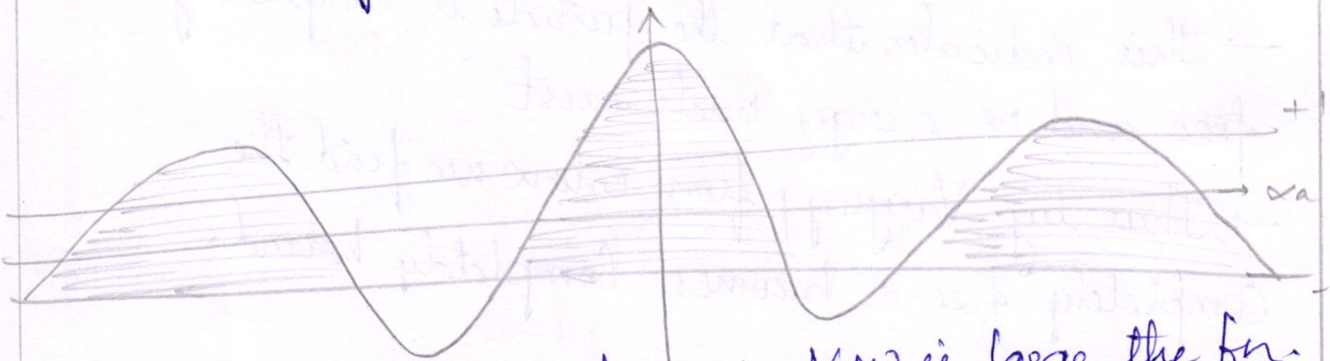
where $U_K(x)$ is a periodic fn with same period as the Lattice.

→ The Solution for the above eqn exists if K is Related to energy E by the following eqn and assuming that $w \to 0$, $V \to \infty$, wV = const

$$\cos Ka = \frac{P \sin \alpha a}{\alpha a} + \cos \alpha a \longrightarrow (2)$$

→ To find exact energy and Wavefunction plot RHS of eq (2) as a function of αa and then by LHS b/w Maximum +1 and minimum Value of -1.

→ Hence only Certain range of Values of α are Allowed.



→ If the Value of P is large i.e $V_0 w$ is large the fn. is given by RHS of eq (2) Crosses at step slope.

→ This means the allowed bands are narrower and forbidden bands are Wider.

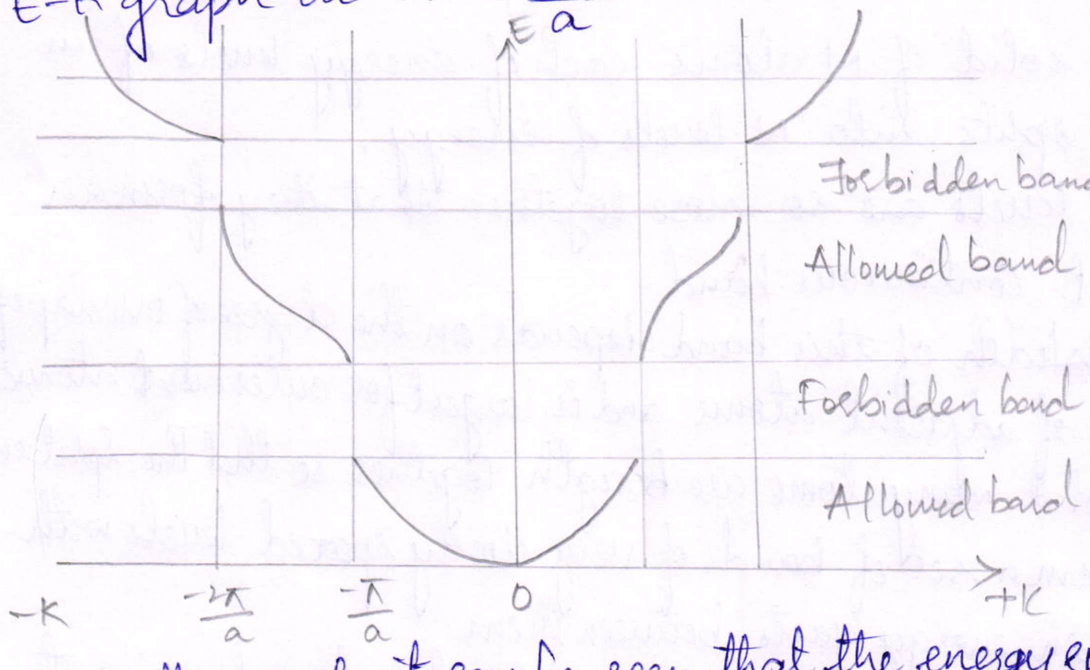
→ As Value of α increases the Width of the allowed eg bands also increases and the Width of the forbidden band decreases.

E-K Curve:

→ From equation $\frac{P \sin \alpha a}{\alpha a} + \cos \alpha a = \cos Ka$ it is Possible to plot a Curve showing the energy E as a function of K.

→ It is Clear from the plot that the energy of e⁻s Continuously increasing from K=0 to π/a

→ The R.H.S of the eqn becomes +1 or -1 for Values of $K = \pm \frac{n\pi}{a}$ and hence discontinuity appeares in the E-K graph at $K = \pm \frac{n\pi}{a}$



→ From the graph it can be seen that the energy spectrum of electrons is Consisting allowed regions and Forbidden Regions.

→ Allowed Region extended from $-\frac{\pi}{a}$ to $+\frac{\pi}{a}$ and is Known as first Brillioun Zone.

→ After a discontinuity in energy Called forbidden gap another allowed region or zone extended form $-\frac{2\pi}{a}$ to $-\frac{\pi}{a}$ & $\frac{\pi}{a}$ to $\frac{2\pi}{a}$ is Known as II Brilliance zone

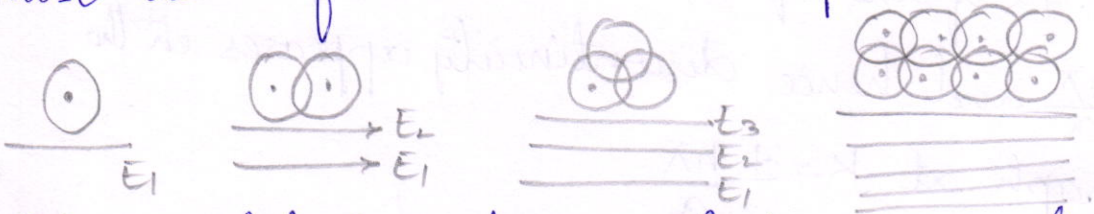
→ Using this graph the Velocity of $\bar{e}$ can be Calculated

→ Velocity of e is zero at the bottom of the energy band

→ As the Value of K increases the Velocity of $\bar{e}$ increases and Reaches to Maximum

Origin of Energy band formation in Solids:

→ When two identical atoms are brought closer the Outer most Orbits of these atoms overlap and Interact.



→ For a solid of N atoms each of energy levels of an atoms splits into N levels of energy.

→ The levels are so close together that they form an almost Continuous band.

→ The Width of this band depends on the degree of overlap of electrons of adjacent atoms and is largest for outer most atomic $\bar{e}$

→ In solid many atoms are bougth together so that the Split energy levels form a set of bands of very closely spaced levels with forbidden energy gaps between them.

→ $\bar{e}$ first occupy the lower energy bands and are of no importance in determining many of $\bar{e}$ properties of solids and next higher eg band determines physical properties

→ Those two allowed energy bands Called Valance & Conduction band gap b/w these two allowed bands is Called forbidden energy gap.