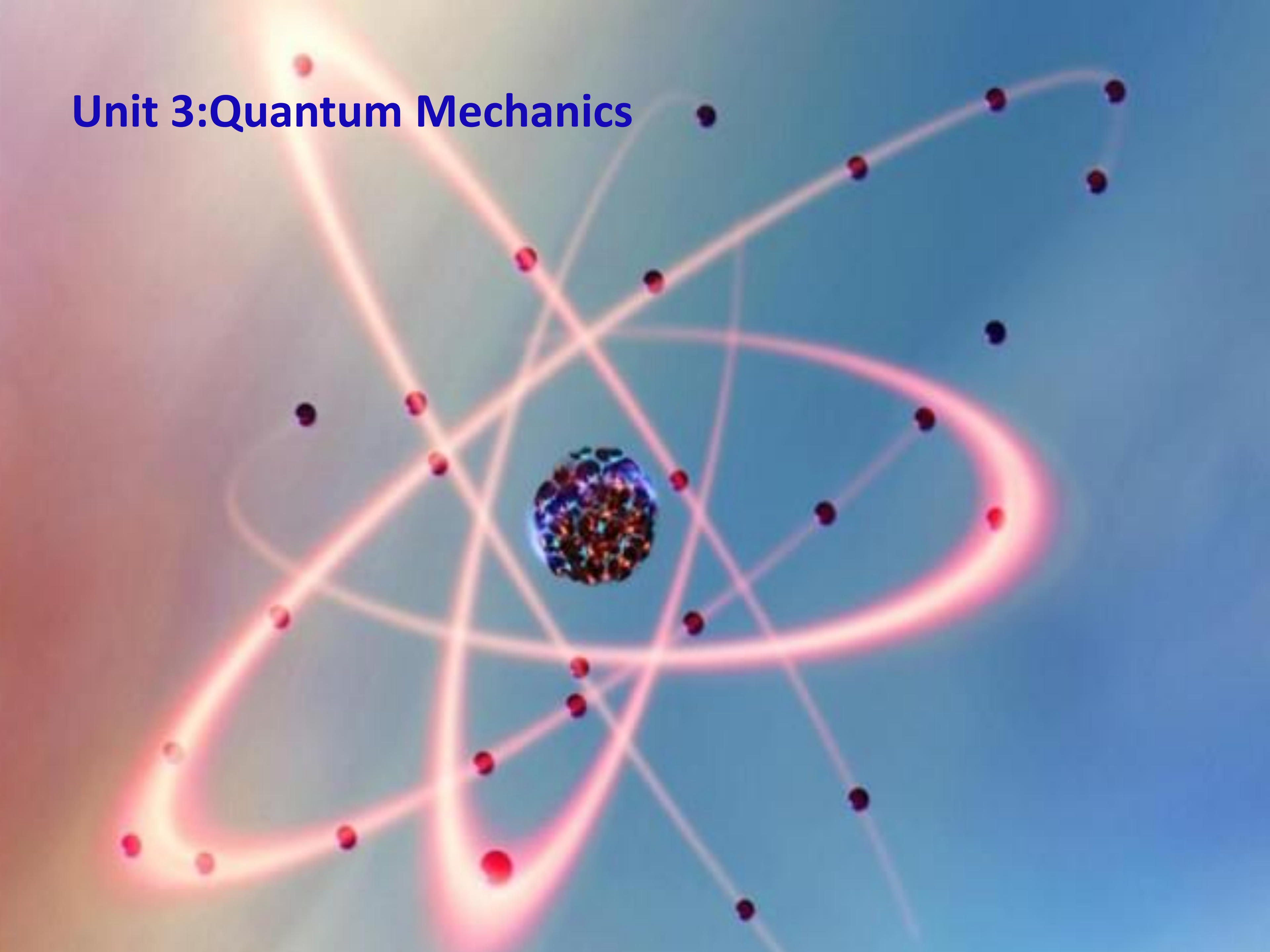
Sinhgad Institutes

Engineering Physics

Unit III

Unit 3:Quantum Mechanics



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Classical Mechanics and Quantum Mechanics

Mechanics: the study of the behavior of physical bodies when subjected to forces or displacements

Scientists W.Heisenberg, E. Schrodinger, P.A.M. Dirac, W. Pauli, M. Born and Neils Bohr

Classical Mechanics: describing the motion of macroscopic objects.

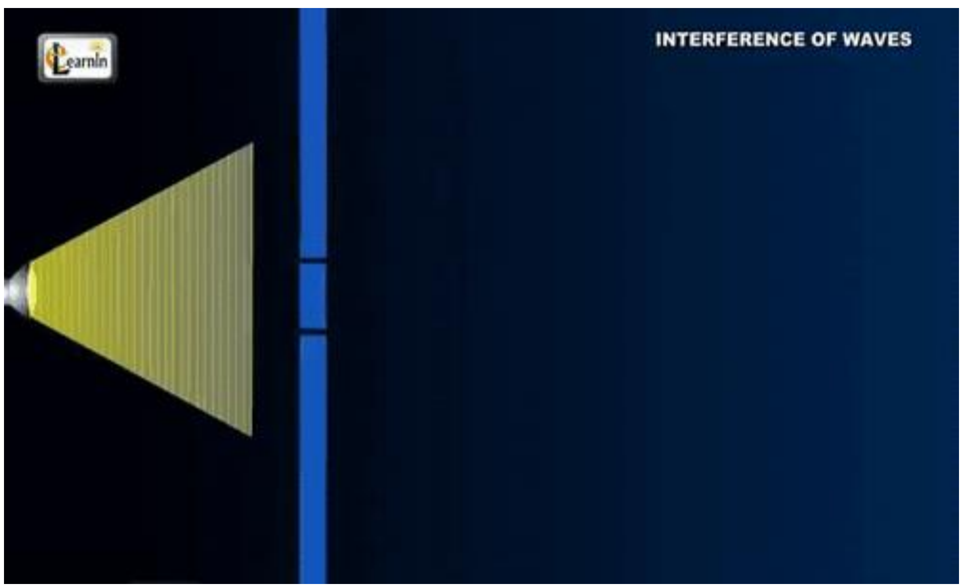
Macroscopic: measurable or observable by naked eyes

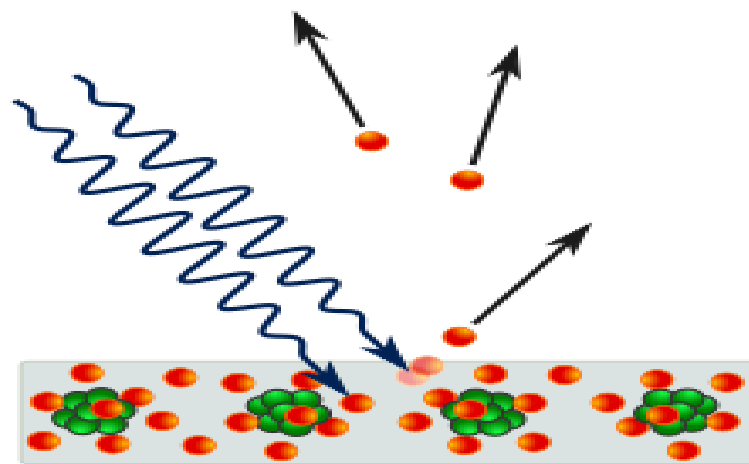
Quantum Mechanics: describing behavior of systems at atomic length scales and smaller .

Wave particle duality of radiation

Radiation (light)

Wave	Interference
	Diffraction
	Polarization
Particle	Photoelectric effect
	Compton Scattering
	Pair production





The emission of electrons from a metal plate caused by light quanta – photons.

De-Broglie hypothesis

- According to Louis de Broglie since radiation such as light exhibits dual nature both wave and particle, the matter must also posses dual nature.
  - The wave associated with matter called matter wave has the wavelength

$$\boldsymbol{\lambda = \frac{h}{p} = \frac{h}{mv}} \quad ----(1)$$ and is called de Broglie wavelength

Scientist	Electron	Experiment
J.J. Thomson	particle	e/m
Davisson and Germer	wave	Davisson-Germer

- Davisson and Germer provided experimental evidence on matter wave when they conducted electron diffraction experiments.
- G.P.Thomson independently conducted experiments on diffraction of electrons when they fall on thin metallic films

De Broglie wavelength by analogy of radiation

By Einstein's mass energy relation we have

$$E = mc^2 \text{ ------- } (2)$$

By Planck's theory of radiation, the energy of a photon is given by

$$E = h\vartheta \text{ -------- } (3)$$

From equation (1) and (2)

$$h\vartheta = mc^2$$

$$\text{But } \vartheta = \frac{c}{\lambda} \quad (\because \quad C = \vartheta\lambda)$$

$$\therefore \; h.\frac{c}{\lambda} = mc^2$$

$$\boldsymbol{\lambda = \frac{h}{mc} = \frac{h}{p}} \text{ ------- } \mathbf{(4)}$$

Where p = mc is the momentum associated with the photon and λ is its wavelength

De Broglie wavelength in terms of K.E of the particle

- The momentum of a particle of mass ‘m’ moving with velocity ‘v’ is given by

P= mv ; and the De Broglie wavelength associated with the particle is given by

$$\boldsymbol{\lambda = \frac{h}{mv} = \frac{h}{p}} \text{ ---------(1)}$$

- The Kinetic Energy of particle is given by

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

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

$$\therefore \mathbf{P} = \sqrt{\boldsymbol{2mE}} \text{ --------- (2)}$$

From equation (1) and (2)

$$\boldsymbol{\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}} \text{------ } \mathbf{(3)}$$

Equation (3) is the De broglie wavelength of λ of a moving particle has been expressed in terms of K.E of the particle

De Broglie wavelength for an electron in terms of potential difference

If an electron having velocity 'v' accelerated through a potential difference of 'V' volts then work done on the electron is eV, e is the charge of the electron and this work is converted into Kinetic energy of the electron,

$$\text{i.e } E = \frac{1}{2} mv^2 = eV$$

$\therefore$ equation (3) $\boldsymbol{\lambda = \frac{h}{\sqrt{2mE}}}$ becomes

$$\boldsymbol{\lambda = \frac{h}{\sqrt{2meV}}} \text{------} \quad \textbf{(3)}$$

$$\text{Here , } h = 6.625\times 10^{-34} \text{J.Sec}$$

$$e = 1.6 \times 10^{-19}$$

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

substituting these values in equation (3) we get,

$$\lambda = \frac{6.625\times10^{-34}}{\sqrt{2\times9.1\times10^{-31}\times1.6\times10^{-19}\times V}} \text{ m}$$

$$\therefore \boldsymbol{\lambda = \frac{12.27}{\sqrt{V}} A^o} \text{------}\textbf{(4)}$$

Numerical based on De-Broglie Hypothesis:

Formulae:

1. $\lambda = \frac{h}{p}$
2. $\lambda = \frac{h}{mv}$
3. $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$
4. $\lambda = \frac{h}{\sqrt{2meV}}$
5. $\lambda = \frac{12.27}{\sqrt{V}} A^o$

Numerical based on Heisenberg's uncertainty principle:

6. $\Delta x . \Delta p$=h
7. $\Delta E . \Delta t$=h
8. $E = \frac{n^2 h^2}{8mL^2}$
9. P= $\sqrt{2mE}$

1) What is the De-Broglie wavelength of an electron when accelerated through a pd of 10kv?

Data: V=10000v

Formula: $\boldsymbol{\lambda = \frac{12.27}{\sqrt{V}} A^o}$

$$\lambda = \frac{\mathbf{12.27}}{\sqrt{\mathbf{10000}}}$$
$$= 0.1227\ \boldsymbol{A^o}$$

2) What is the De-Broglie wavelength associated with a 5000kg car having a constant speed of 20m/s ?

Data: m=5000kg, h=6.6x10^{-34}Js

Formula: $\boldsymbol{\lambda = \frac{h}{mv}}$

$$\lambda = \frac{\mathbf{6.6x10^{-34}}}{\mathbf{5000x20}}$$
$$= \mathbf{6.6x10^{-39}}\text{m}$$

3)An electron has kinetics energy equal to the mass energy. Calculate De-Broglie wavelength associated with it.

Data: E=m

Formula: $\boldsymbol{\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2mm}} = \frac{h}{\sqrt{2}\ \mathrm{m}}}$=0.5144x 10^{-3}m

4) Find the De-Broglie wavelength associated with monoenergetic electron beam having momentum 10^{-23} kg m/s.

Data: p=10^{-23} kg m/s, h= 6.6x10^{-34}Js

Formula: $\boldsymbol{\lambda = \frac{h}{p}} = \frac{6.6\text{x}10^{-34}}{10^{-23}}$=0.663 $\boldsymbol{A^o}$

5) In an expt, the wavelength of a photon is measured to an accuracy of one part per million. What is the uncertainty Δx in a simultaneous measurement of the position of the photon having a wavelength of 6000 $\boldsymbol{A^o}$

Data: $\boldsymbol{\lambda}$ =6000 $\boldsymbol{A^o}$=6000x10^{-10} uncertainty in measurement of wavelength is , $\boldsymbol{\Delta\lambda}$/ $\boldsymbol{\lambda}$=1/ 10^6

$\boldsymbol{\Delta\lambda}$=$\boldsymbol{\lambda}$ / 10^6

$\boldsymbol{\Delta\lambda}$ = 6000x10^{-10} / 10^6

$\boldsymbol{\Delta\lambda}$ =6000x 10^{-16}

Formula: $\Delta\boldsymbol{x}.\boldsymbol{\Delta p}$=h and $\boldsymbol{\Delta p = \frac{h}{\lambda}}$

$\boldsymbol{\Delta p = 1.1x}10^{-21}$ $\quad$ $\Delta\boldsymbol{x}$=6x 10^{-16}

6. An electron has a speed of 600m/sec with an accuracy of 0.005%. Calculate the uncertainty with which we can locate the position of the electron.

7. An electron is confined to a box of length 1 A. calculate the minimum uncertainty in its velocity, given mass of electron.

8. Assume that the uncertainty in the location is of particle is equal to its De Broglie wavelength. What will be the uncertainty in its velocity is equal to_ ?

9. At what kinetic energy an electron will have a wavelength of 5000A .

10.Electrons moving with a speed of 7.3 x 10^7m/sec have a wavelength of 0.1A. Calculate the Planck's constant

11. Compute the permitted energy level of an election in an infinite potential well of width 1 A°

12. Lowest energy level of an electron trapped in a potential well is 38 eV. Find the width of the well.

13. An electron is trapped is an rigid box of width 2 A°. Find its lowest energy level and momentum. Hence, find energy of the 3rd energy level.

14. Calculate the energy and momentum of an electron confined in a rigid box of width 3A° for lowest energy state.

Concept of Phase velocity and Group velocity

Phase velocity

The speed with which a crest and trough of wave travels, is called the phase velocity of De-Broglie waves. It is called as wave velocity (u). For wave velocity phase remains constant.

- For a particle of mass m, moving with velocity v, the De-Broglie wavelength is

$$\boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\boldsymbol{mv}} ------ -(1)$$

and energy $E = h\vartheta = mc^2$

$$\therefore \vartheta = \frac{mc^2}{h} \text{ ------------}(2)$$

The equation of motion of a plane wave of frequency ϑ and wavelength $\boldsymbol{\lambda}$ moving in x- direction is,

$$y = a \sin(\omega t - kx)$$

Where $\omega = 2\pi\vartheta$ (angular frequency) ------(3) and

$$K = \frac{2\pi}{\lambda} \text{ (propagation constant)}$$

i.e $\omega t - kx$ = constant ---------(4)

$$u = \frac{dx}{dt} = \frac{\omega}{k} \text{ (By differentiating the above equation)}$$

$$\therefore u = 2\pi\vartheta \times \frac{\lambda}{2\pi} = \vartheta\lambda \text{ ---------- (5)}$$

Substitution of equation (1) and (2) in (5)

$$u = \frac{mc^2}{h} \times \frac{h}{mv}$$

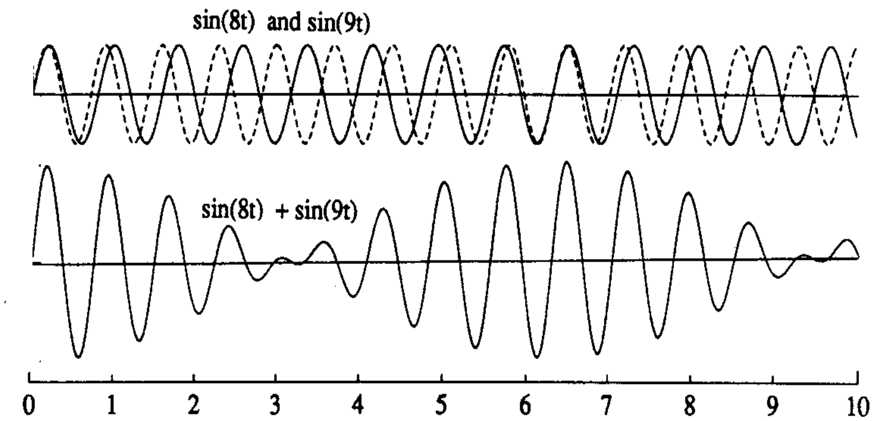
$$\mathbf{V_p = u = \frac{c^2}{v}} \text{ i.e wave velocity}$$

For any particle , v is always less than c

Group velocity

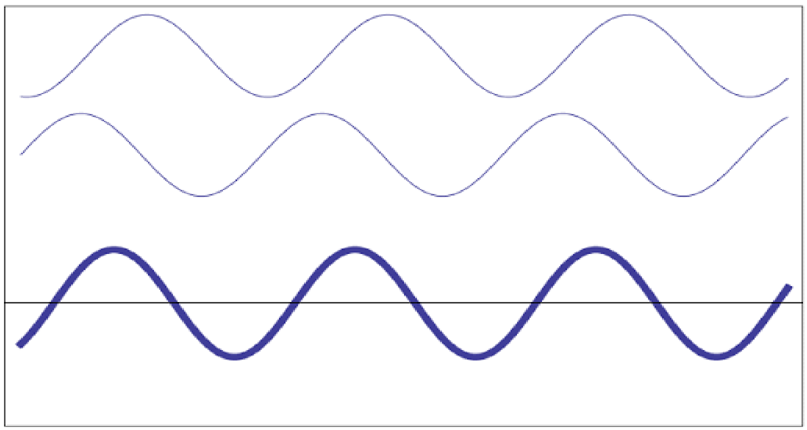
A material particle can be represented by a wave packet or the group of waves and the velocity of wave group is called group or The rate at which the envelope of the wave packet propagates. Envelope of wave packet shows where particle is likely to found

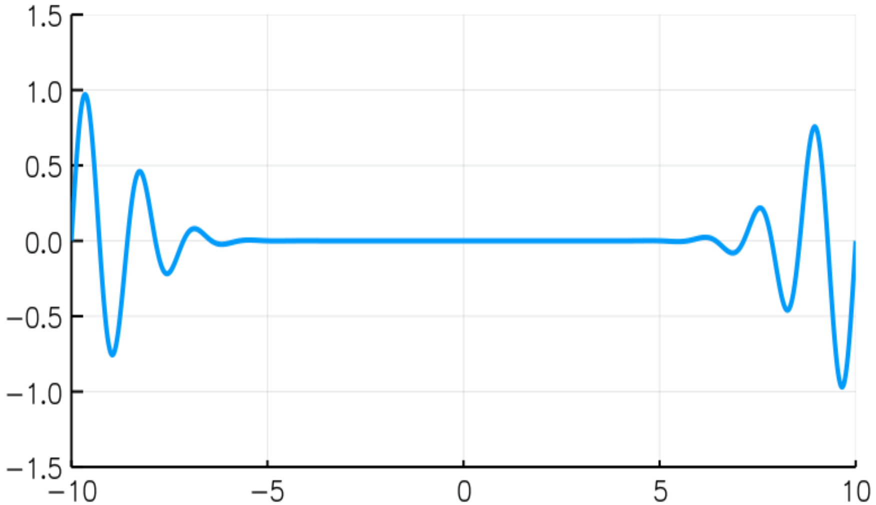
V=Vg



If several of waves of different frequencies (wavelengths) and phases are superimposed together, one would get resultant which is a localized wave packet

A wave packet is localized – a good representation for a particle!





The relation between phase velocity and group velocity:

$Vp = u = c^2 / V$

$V = Vg$

from both this equation we can write,

$\boxed{Vp = c^2 / Vg}$

$C^2 = Vp \times Vg$

Properties of matter waves

Since the De Broglie's wavelength for matter waves $\boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\boldsymbol{mv}}$ and these waves travel with velocity $u = \frac{c^2}{v}$.

- Lighter the particle, greater is the wavelength associated with it

  $\left(\because \lambda \propto \frac{1}{m}, \text{v } is\ const\right)$

- Lesser the velocity of the particle, longer the wavelength associated with it.

  $\left(\because \lambda \propto \frac{1}{v},\ m\ is\ const\right)$

- For *v*= ∞, λ becomes and for v=0, λ becomes infinity and This means that only with moving particle, matter wave is associated.
- Whether the particle is charged or not, matter wave is associated with it. This reveals that these waves are not electromagnetic but a new kind of waves.
- The velocity of matter wave depends on the velocity of particle generating them $\left(u = \frac{c^2}{v}\right)$ and it is not constant
- Matter waves travel faster than the velocity of light because the particle velocity v cannot exceed the velocity of light c. velocity of matter waves $u = \frac{c^2}{v}$ is greater than c .
- A wave is spread out in space and it cannot be localized at any point Thus the wave nature of matter introduces an uncertainty in the location of the position of the particle.

The Heisenberg Uncertainty Principle

- **It is impossible to determine accurately and simultaneously the position and momentum of a particle**

- To examine the uncertainty principle, consider an electron of mass m associated with matter waves of wavelength λ . This electron can be found somewhere within this wave and therefore, the uncertainty in this position measurement Δx is equal to its wavelength

$$\therefore \Delta x = \lambda \text{ ———————— ———————(1)}$$

To observe electron we have to illuminate it with light of wavelength λ,

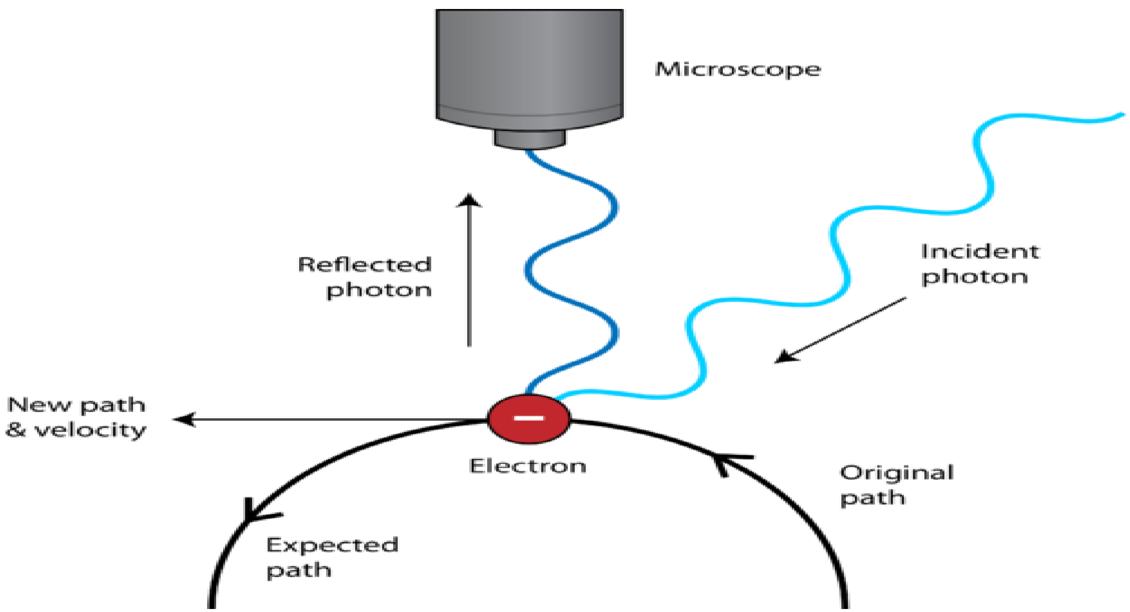


Fig. An electron cannot be observed without changing its momentum by an indeterminate amount

- In this process the photon of light strike the electron and bounce off it. Each photon possesses the momentum $\frac{h}{\lambda}$and when it collides with the electron, original momentum p of the electron is changed
- The precise change of the momentum of the electron cannot be predicted, but it is likely to be the same order of magnitude as the photon momentum $\frac{h}{\lambda}$. Thus the electron cannot be observed without changing its momentum by an indeterminate amount.
- To determine position of the particle introduces an uncertainty in its momentum Δp and this uncertainty in the momentum is at least equal to the momentum of incident photon

$$\therefore \Delta p = \frac{h}{\lambda} ---- -(2)$$

From equation (1) and (2)

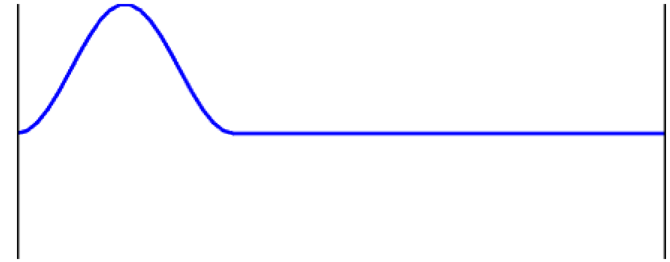
$$\therefore \Delta x . \Delta p = \lambda . \frac{h}{\lambda} = \mathrm{h} ----- -(3)$$

$$\therefore \Delta x . \Delta p = \mathrm{h}$$

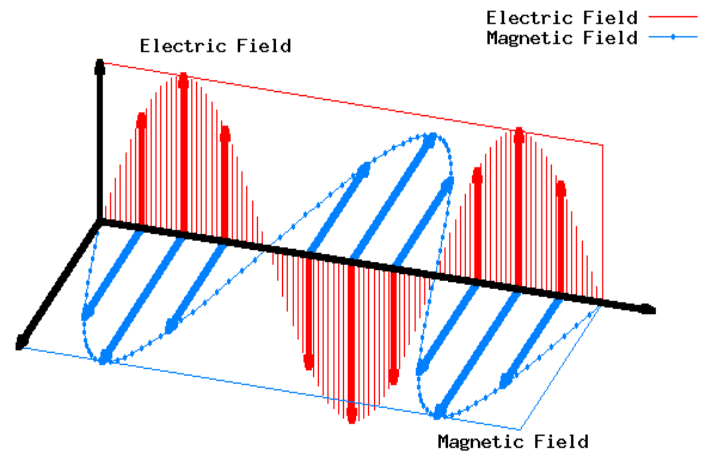
- From equation (3) it is clear that if the position of the electron is known exactly at given instant i.e if $\Delta x = 0$, then the momentum becomes indeterminate and vice-versa. Thus, both position and the momentum cannot be determined accurately and simultaneously.

what is wave function and its significance

Wave in string- vary wave displacement



Electromagnetic wave – vary electric and magnetic wave



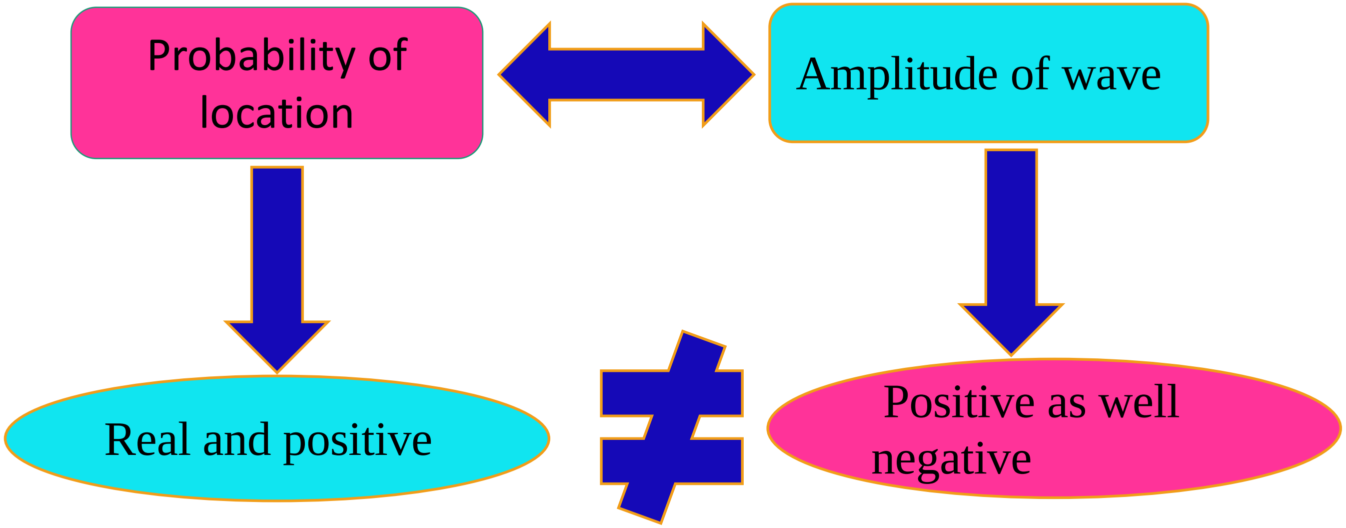
Sound wave – vary Pressure

In the same way , for matter waves wave function ψ varies with space and time

- It is suggested that the De-Broglie or Matter wave also should have a wave variable and should be function of space and time
- the wave variable of matter waves is called the wave function and denoted by ψ
- It is analogous to wave variable electric and magnetic field E and B in electromagnetic wave, pressure P in sound waves but ψ itself unlike E and P has no direct physical significance hence do not experimentally measurable.
- it represents mathematically the motion of particle and value of ψ depend upon x,y,z and t

$$\therefore \psi \rightarrow f(x,y,z,t)$$

- From the concept of wave packet we know that the amplitude of wave packet gives the value of probability of finding the particle.
- The value of wave function $\psi = f(x,y,z,t)$ associated with a moving particle at a particular position in space at a particular time t is related to probability of finding the particle at that time. Hence it is called probability amplitude
- This means the ψ represents the amplitude.



- However probability always real and positive, whereas ψ can be positive or negative therefore ψ^2 is taken which is always positive
- In general ψ is complex, therefore take $|\psi|^2$ instead of ψ^2, where $|\psi|^2 = \psi^*\psi$, ψ^* denoting the complex conjugate of ψ.
- In any case $\psi^*\psi$ always real and positive
- If dv is a volume element located at a point then the probability of finding the particle in the volume element at time t is proportional to $\psi^*\psi dv$. By analogy with ordinary mass density the square of the wave function $\psi^*\psi$ is called the probability density i.e probability per unit volume

Physical significance of wave function

- Schrodinger interpreted ψ in terms of charge density. If A is the amplitude of an electromagnetic wave then the energy per unit volume ie energy density is equal to A^2. Also the photon energy $h\vartheta$ is constant so the number of photons per unit volume i.e the photon density is equal to $\frac{A^2}{h\vartheta}$ and it proportional to the amplitude square.
- Similarly, if ψ is the amplitude of matter waves at any point in space, the particle density at that point may be taken as proportional to $|\psi|^2$. so $|\psi|^2$ is a measure of particle density and multiplying this by the charge of the particle we shall get the charge density. Thus $|\psi|^2$ is a measure of charge density.
- we know that ψ is not real and positive but $|\psi|^2 = \psi^*\psi$ is a real and positive quantity, ψ^* denoting the complex conjugate of ψ hence max born assign some physical meaning to $|\psi|^2$ as follows
- According to max born the wave function $\psi = f(x,y,z,t)$ gives the probability of finding the particle at position (x,y,z) and at time 't' proportional to the value of $|\psi|^2$ at that point at time t. the probability depends on the value of $|\psi|^2$

- If the value of $|\psi|^2$ large, it gives large value of probability of finding the particle there. if the value of $|\psi|^2$ small it gives small value of probability of finding the particle there. $|\psi|^2$ is called as probability density. Therefore probability of finding the particle within the small volume element dv is

$$P = |\psi|^2 dv.$$

Therefore particle is certainly to be found somewhere in space.

$$\iiint |\psi|^2 dx.dy.dz = 1\text{-----------}(1)$$

the wave function satisfying this relation is called a normalized wave function and equation (1) is called normalization condition. Thus has to be normalisable function

ψ must also satisfy the following conditions.

1) ψ must be single valued and finite

2) ψ and its derivatives must be continuous everywhere in the region . Where ψ is defined

Schrodinger's wave equation

- Schrodinger wave equation is a mathematical expression describing the energy and position of the electron in space and time, taking into account the matter wave nature of the electron inside an atom.

There are two types of Schrodinger's wave equation's

1. Schrodinger's time independent wave equation
2. Schrodinger's time dependent wave equation

Schrodinger's time independent wave equation

Consider a system of stationary waves associated with particle. let (x, y, z) be the coordinates of the particle and let ψ denote the wave displacement of matter waves at time 't'.

By analogy with 2D wave equation $\frac{d^2y}{dt^2} = v^2\frac{d^2y}{dx^2}$ we can write the 3D wave equation with wave velocity 'u' as

Represents a periodic changes in the displacement y of a string produce a 2D (in XY plane) wave system in a string having wave velocity 'v'

$$\frac{\partial^2\psi}{\partial t^2} = u^2\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right)$$

Represents a periodic changes in wave function φ produce a 3D (in XYZ plane) wave system called a de broglie wave having wave velocity 'u'

$$i.e\ \frac{\partial^2\psi}{\partial t^2} = u^2\nabla^2\psi ------(1)$$

Where ∇^2 *is a laplacian operator* $\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$

The solution of equation (1) is

i.e $\psi(x, y, z, t) = \psi_{\,0}(x, y, z).\, e^{-i.\omega t}$

i.e $\psi = \psi_{\,0}.\, e^{-i.\omega t} -----(2)$

$where\ \psi_0\ \ is\ wave\ amplitude\ at\ (x, y, z)$

Now from equation (2) ,

$$\frac{\partial\psi}{\partial t} = -i\ \omega\psi_{\,0}.\, e^{-i.\omega t}$$

$$\frac{\partial\psi}{\partial t} = -i\ \omega\psi ----(3) \qquad \because \psi = \psi_{\,0}.\, e^{-i.\omega t}$$

$$\frac{\partial^2\psi}{\partial t^2} = i^2\omega^2\psi_{\,0}.\, e^{-i.\omega t}$$

$\because$ i=$\sqrt{-1}$

$$\frac{\partial^2\psi}{\partial t^2} = -\omega^2\psi ----(4)$$

Comparing equation (1) and (4) becomes

$$u^2\nabla^2\psi = -\omega^2\psi$$

$$\therefore \nabla^2\psi + \frac{\omega^2}{u^2}\psi = 0 ---- (5)$$

But $\omega = 2\pi\vartheta \ and \ u = \vartheta\lambda$ where ϑ is frequency and λ is wavelength of matter wave

Therefore equation (5) becomes

$$\therefore \nabla^2\psi + \frac{4\pi^2\vartheta^2}{\upsilon^2\lambda^2}\psi = 0$$

$$\therefore \nabla^2\psi + \frac{4\pi^2}{\lambda^2}\psi = 0$$

But $\boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\boldsymbol{p}} \therefore \lambda^2 = \frac{h^2}{p^2}$

$$\nabla^2\psi + \frac{4\pi^2p^2}{h^2}\psi = 0 ---- (6)$$

Total energy of the particle represented by ψ is E = K.E +P.E

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

$$\therefore\ p^2 = 2m(E - V) --- (7)$$

Therefore equation (6) becomes

$$\nabla^2\psi + \frac{4\pi^2 2m}{h^2}(E - V)\psi = 0 ---- (8)$$

Taking $\hbar = \frac{h}{2\pi}$ equation (9) becomes

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

Schrodinger's time dependent wave equation

We know that, $\omega = 2\pi\vartheta$ and $\mathrm{E} = h\upsilon \therefore \vartheta = \frac{E}{h} \therefore \omega=2\pi\frac{E}{h}$

Therefore equation (3) becomes, $\frac{\partial\psi}{\partial t} = -i\,\omega\psi ---- (3)$

$$\frac{\partial\psi}{\partial t} = -i\left(2\,\pi\,\frac{E}{h}\right)\psi$$

$$since\ \hbar = \frac{h}{2\pi}$$

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

Multiply both sides by i, we get, $i\frac{\partial\psi}{\partial t} = \frac{E}{\hbar}\psi$

$$E\psi = i\hbar\frac{\partial\psi}{\partial t} ---- (10)$$

Recalling Schrodinger's time independent equation

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

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

Putting the value of Eψ from equation (10) we get,

$$\nabla^2\psi + \frac{2m}{\hbar^2}\left(i\hbar\frac{\partial\psi}{\partial t} - V\psi\right) = 0$$

Multiplying both sides by $-\frac{\hbar^2}{2m}$ we get,

$$-\frac{\hbar^2}{2m}\nabla^2\psi - \frac{\hbar^2}{2m}\frac{2m}{\hbar^2}\left(i\hbar\frac{\partial\psi}{\partial t} - V\psi\right) = 0$$

$$\text{or } -\frac{\hbar^2}{2m}\nabla^2\psi - i\hbar\frac{\partial\psi}{\partial t} + V\psi = 0 ---- -(11)$$

$$or\ \left(-\frac{\hbar^2}{2m}\nabla^2 + \mathbf{V}\right)\boldsymbol{\psi} = \boldsymbol{i}\hbar\frac{\boldsymbol{\partial\psi}}{\boldsymbol{\partial t}} ----- -(12)$$

This is Schrodinger's time dependent equation

The operator $\left(-\frac{\hbar^2}{2m}\nabla^2\psi + \mathrm{V}\right)$ is called Hamiltonian operator and is represented by ‘H’

Also from equation (10), $E\psi = i\hbar\frac{\partial\psi}{\partial t}$

Therefore equation (12) becomes

$$H\,\psi = i\hbar\frac{\partial\psi}{\partial t}$$

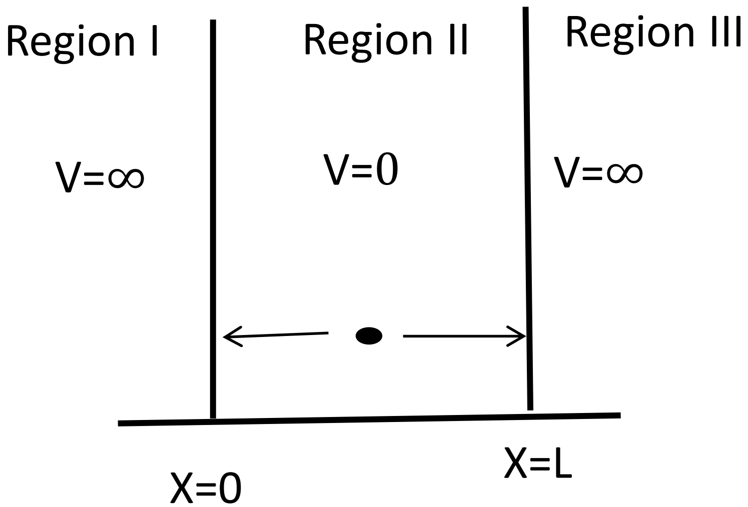
This is Schrodinger's time dependent wave equation

Applications of Schrodinger's time independent wave equation

- **Particle in a rigid box**
- **Particle in a non-rigid box**
- **Tunneling effect**

Particle in a rigid box (Infinite potential well)

Consider a particle of mass 'm' confined to a one dimensional rigid box of length 'L' such that,



V(x) =0 in the region $0< x < L$
V(x) $= \infty$ for x≤ 0 and $x \geq L$

Let ψ be the wave function of the particle

the particle cannot have infinite amount of energy
So it cannot exist outside the box

Hence, ψ(x,t) = 0 for x≤ 0 and x$\geq L$

Now we can find the value of wave function ψ of the particle by using Schrodinger's time independent equation because v is independent of time.

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

Since , V=0 inside the box and particle can move along x- axis only we get,

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

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

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

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

The solution of equation (2) is either sine function or cosine function, Hence the general solution is,

$$\psi(\mathrm{x}) = \mathrm{Asinkx} + \mathrm{Bcoskx} -- -(3)$$

$$or\ \psi(\mathrm{x}) = \mathrm{A}e^{ikx} + \mathrm{B}e^{-ikx}$$

Here A and B are constants whose values can be determined by applying the boundary conditions. The particle is within the box hence boundary conditions on ψ are,

ψ(x) = 0 at x = 0

ψ(x) = 0 at x = L

Applying first boundary condition to equation (3) we get,

$$0 = \mathrm{Asin}\,0 + \mathrm{Bcos}\,0$$

Therefore equation (3),

$$\psi(\mathrm{x}) = \mathrm{Asinkx} --- (4)$$

Now applying 2nd boundary condition to equation (4), we get

$$0 = AsinkL --- (5)$$

It means either A = 0 or Sin kL = 0

In equation no (4) if A = 0 then $\psi(\mathrm{x})$ =0 which is not possible as it would mean that the particle does not exist

Therefore A $\neq$0, thus, Sin kL = 0
$\Rightarrow kL = nL$ where n = 0,1,2,3....etc

Here n =0 is not possible, because when n= 0, kL = 0 i.e either k = 0 or L = 0

$k = \sqrt{\frac{2mE}{\hbar^2}} \neq 0$ as well as L = width of the box $\neq 0$

$$\therefore kL = n\pi \; where \; n = 1,2,3 ---- etc.$$

$$\therefore k = \frac{n\pi}{L} ---- (6)$$

Therefore equation (4) becomes,

$$\psi(x) = A \sin \frac{n\pi}{L} x --- (7)$$

The wave function must be normalized wave function and the condition for normalization is

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

But here is $\psi(x) = 0$ for $x \leq 0 \; and \; x \geq L$ i.e outside the box

Therefore the condition becomes

$$\int_{0}^{L} |\psi(x)|^2 dx = 1$$

Putting the value of $\psi(x)$ from equation (7) we get,

$$i.e \int_{0}^{L} A^2 Sin^2\left(\frac{n\pi}{L}x\right)dx = 1$$

$$\therefore \frac{A^2}{2}\int_{0}^{L}\left[1 - cos\left(\frac{2n\pi}{L}x\right)\right]dx = 1 \qquad \because Sin^2\theta = \frac{1 - cos2\theta}{2}$$

$$\therefore \frac{A^2}{2}\left[x - \frac{sin\frac{2n\pi}{L}x}{\frac{2n\pi}{L}x}\right]_0^L = 1$$

$$\therefore \frac{A^2}{2}L = 1 \qquad \therefore A = \sqrt{\frac{2}{L}} ----(8)$$

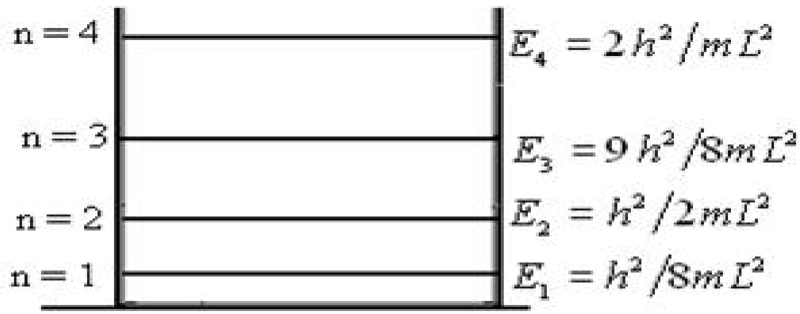
Therefore, the normalized wave function, from equation (7) is

$$\psi_n(x) = \sqrt{\frac{2}{L}} sin\left(\frac{n\pi}{L}\right)x ----(9) \qquad for\ all\ 0 < x < L\ and\ n = 1,2,3 ---etc$$

From equation (1) and (6) we can write, $\frac{2mE}{\hbar^2} = \left(\frac{n^2\pi^2}{L^2}\right)$

$$\therefore E = \frac{n^2\pi^2\hbar^2}{2mL^2} ----(10) \quad since\ \hbar = \frac{h}{2\pi} \quad \therefore \hbar^2 = \frac{h^2}{4\pi^2}$$

$$\therefore E = \frac{n^2h^2}{8mL^2} ----(11) \quad where\ n = 1,2,3 ----etc$$



The energy values for an electron in a potential box

The wave function $\psi_n(x)$ and the probability density i.e probability of finding the particle $|\psi_n(x)|^2$ can be graphically represented as

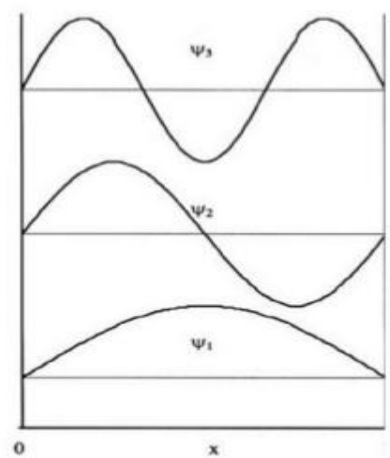


Fig. 3.1. The wave functions for the One-dimensional particle-in-a-box

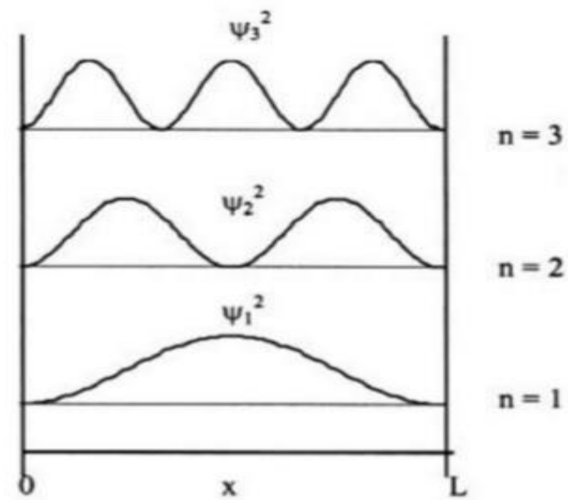


Fig. 3.2. The probability densities in One-dimensional particle-in-a-box

Conclusions

1.The particle can be described by set of wave functions $\psi_n(x)$ called as eigen states with corresponding energies E_n called as eigen energy values for different values of n called as quantum number

2. From this wave can say that, the energy of the particle is quantized i.e the particle can take only discrete values.

3.The lowest energy of particle is $E = \frac{h^2}{8mL^2} \neq 0$ this is direct contradiction with classical concept, that the particle can have any energy including zero.

4. If the particle is free to move anywhere in the space then we have, $L \to \infty$ $i.e\ E \to 0\ for\ any\ n$

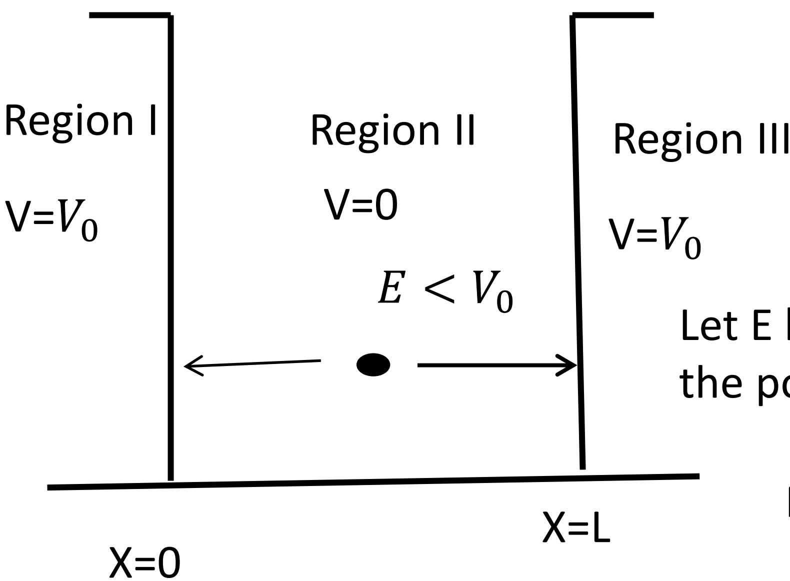
This shows that the only bound particle take discrete energy values.

5. Here quantum mechanically the probability of finding the particle is not only location dependent but also energy dependent. Classically probability of finding the particle anywhere in the box is equal.

Particle in a Non rigid box (finite potential well)

Consider a particle of mass 'm' confined to a one dimensional non rigid box of length 'L' such that,

V(x) $=V_0$ at x≤ 0 and x$\geq L$
V(x) $= 0\ for\ 0 < x < L$ as shown in figure



The walls of the box is non rigid hence it is represented by potential well of finite depth

Let E be the total energy of particle inside the box and V be the potential energy assumed to be zero inside the box

Potential outside the box is finite say V_0 and $E < V_0$

Classically particle cannot appear outside the box

In this problem we shall check this possibility quantum mechanically.

Let $\psi_{I,}\ \psi_{II}$ and ψ_{III} *be the wave functions in the region I, II and III respectively*

The Schrodinger's time independent wave equation is

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

In region II, V = 0 and the particle having wave function ψ_{II} is moving along x- axis only. Therefore the equation becomes

$$\frac{d\psi_{II}{}^2}{dx^2} + \frac{2mE}{\hbar^2}\psi_{II} = 0$$

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

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

This equation is same as the rigid box ; we know that there is general solution.

$$\psi(\mathrm{x}) = Pe^{ikx} + Qe^{-ikx} --- -(2) \qquad for\ 0 < x < L$$

In region I, V = V_0 and wave function of the particle is ψ_I. Therefore the Schrodinger's equation becomes

$$\frac{d\psi_I{}^2}{dx^2} + \frac{2m(E - V_0)}{\hbar^2}\psi_I = 0 \qquad but\ E < V_0$$

$$\frac{d\psi_I{}^2}{dx^2} - \frac{2m(V_0 - E)}{\hbar^2}\psi_I = 0$$

Let, $\frac{2m(V_0-E)}{\hbar^2} = k'^2$

$$\frac{d\psi_I{}^2}{dx^2} - k'^2\psi_I = 0 \text{ ----- } -(3)$$

Hence the there general solution of equation 3 is

$$\psi_I = Ae^{ik'x} + Be^{-ik'x}$$

Now ψ should be finite in the region is the defined in region I $x \leq 0$

In region I as $x \to -\infty$ the term, $Be^{-ik'x} \to -\infty$

This is not possible , therefore B = 0

$$\psi_I = Ae^{ik'x} \text{ --- } -(4)$$

The situation in region III is identical to that in region I, we have,

$$\psi_{III} = Ce^{ik'x} + De^{-ik'x}$$

In region III, as $x \to \infty$, the term, $Ce^{ik'x} \to \infty$

This is not possible, therefore C=0

$$\psi_{III} = De^{-ik'x} --- (5)$$

The constants P,Q, A and D from equations (2), (4) and (5) can be determined by applying boundary conditions by considering that the wave function ψ and its derivative ${}^{d\psi}/_{dx}$ should be continuous in the region where ψ is defined

The boundary conditions on the left side are,

1.$\psi_I(x) = \psi_{II}$ $\quad at\ x = 0$ $\quad$ the result $\mathrm{A = P + Q} ---- (6)$

2.$\frac{d\psi_I}{dx}$ =$\frac{d\psi_{II}}{dx}$ $--- \mathrm{at\ x = 0}$ $\quad$ the result $\mathrm{Ak' = iPk - iQk} ---- (7)$

3. $\psi_{II}(x) = \psi_{III} \qquad at\ x = \mathrm{L}$

the result is $Pe^{ik'L} + Qe^{-ik'L} = De^{-k'L} ---- (8)$

4. $\frac{d\psi_{II}}{dx} = \frac{d\psi_{III}}{dx} --- \text{at x} = \mathrm{L}$

the result is $Pike^{ikL} - Qike^{-ikL} = -Dk'e^{-k'L} ---- (9)$

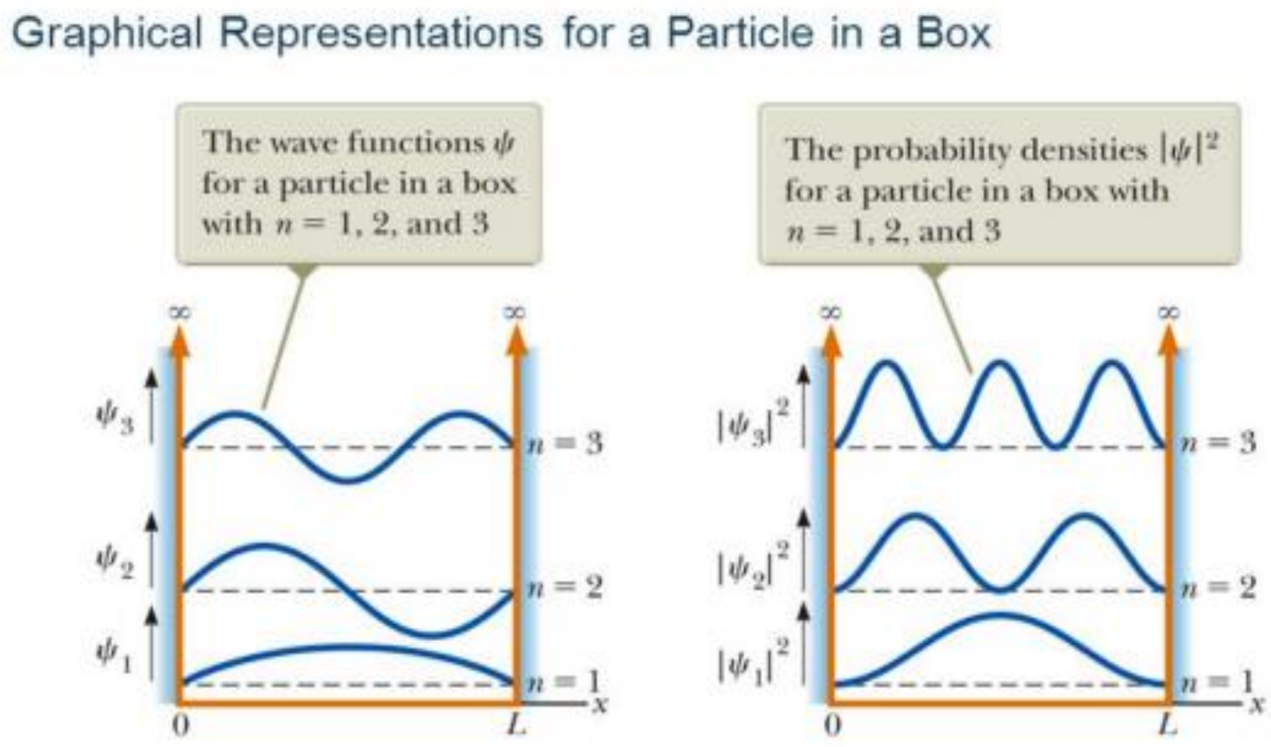
These equations (6), (7), (8) and (9) can be solved to find the four unknowns P, Q,A and D

In the process, we also get conditions that should be satisfied by *k* and *k' and therefore by E,* because they are related by

$$\mathrm{k} = \sqrt{\frac{2mE}{\hbar^2}} \text{ or } \mathrm{k'} = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

These conditions relate to a certain quantum number n such that the energy E has certain discrete allowed for n =1,2,3,….etc. in other words total energy of the particle quantized.

The wave function $\psi_n(x)$ and the probability density i.e probability of finding the particle $|\psi_n(x)|^2$ can be graphically represented as

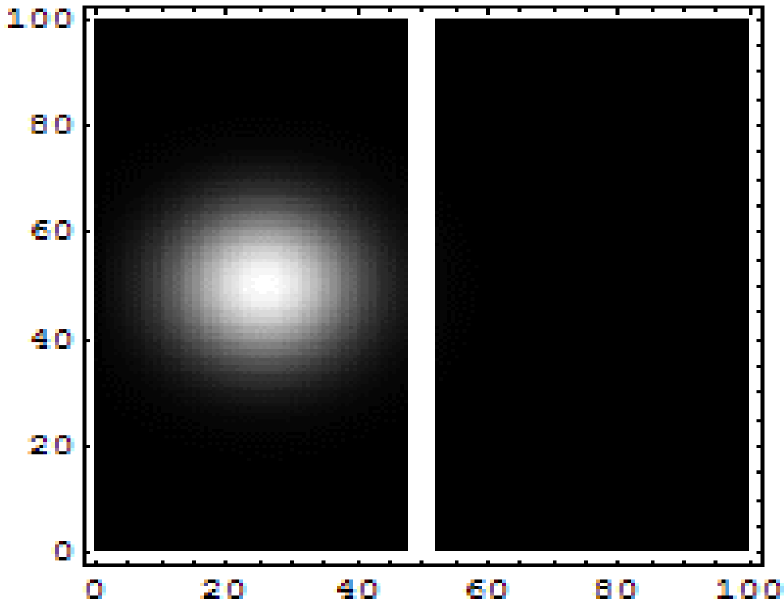


Conclusions :

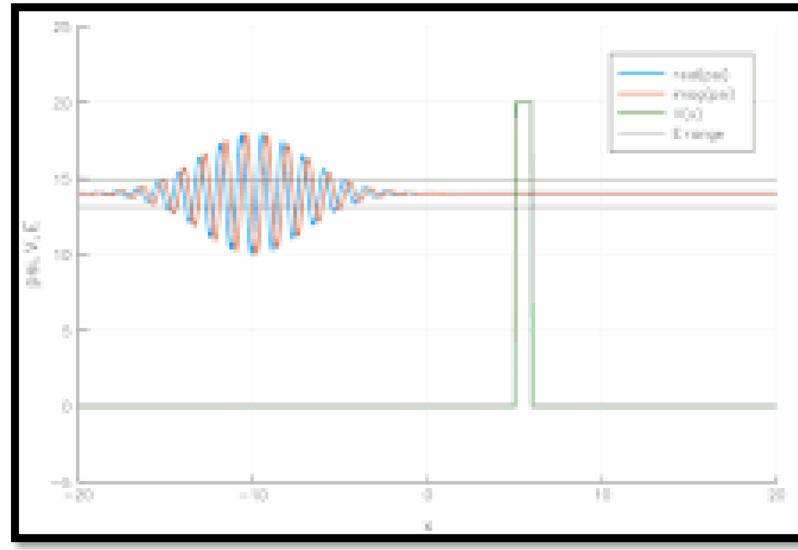
1. The particle can be described by set of wave functions $\psi_n(x)$ called as eigen states with corresponding energies E_n called as energy eigen values for different values of n called as quantum number.
2. From this we can say the energy of the particle is quantized i.e the particle can take only discrete energy values.
3. There is non zero probability of finding the particle outside the non rigid box. Classically the particle with energy less than the potential barrier can never appear outside the region II, however quantum mechanically this possibility is allowed.

What is Quantum Tunneling?

- At the quantum level, matter has corpuscular and wave-like properties
- Tunneling can only be explained by the wave nature of matter as described by quantum mechanics
- Classically, when a particle is incident on a barrier of greater energy than the particle, reflection occurs
- When described as a wave, the particle has a probability of existing within the barrier region, and even on the other side of it.
- If the particle incident on the potential barrier with potential barrier with energy less than the height of the potential barrier, there is always some probability of transmission through the barrier. This phenomenon of crossing the barrier is called as tunneling effect.



An electron [wavepacket](#) directed at a potential barrier. Note the dim spot on the right that represents tunneling electrons.



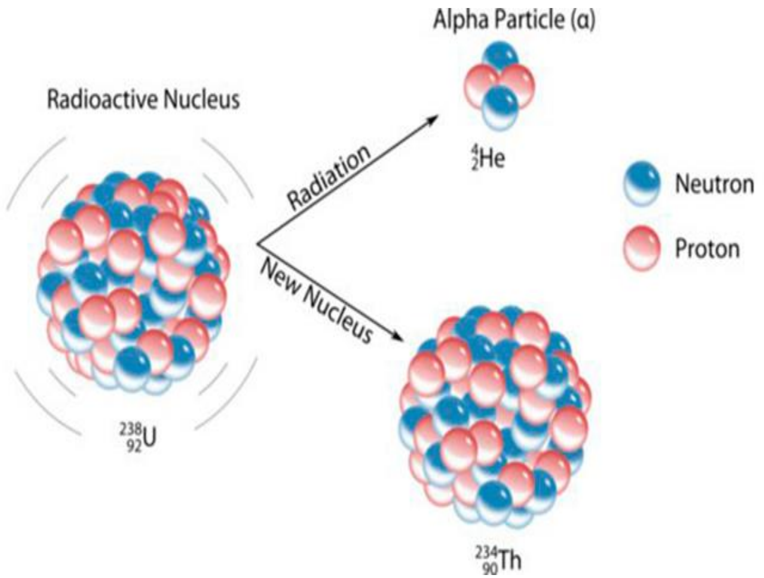
A simulation of a wave packet incident on a potential barrier. In relative units, the barrier energy is 20, greater than the mean wave packet energy of 14. A portion of the wave packet passes through the barrier.

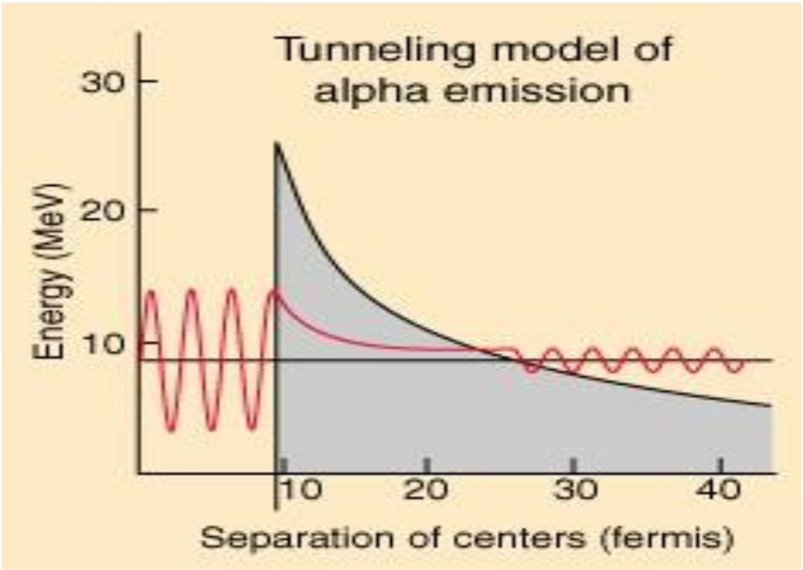
Tunneling Effect

The phenomenon of the particles penetrating the potential barrier is called as tunneling effect e.g tunnel diode, alpha decay, scanning tunneling microscope.

Examples of tunneling effect

1. Alpha decay: The α particle does not have enough kinetic energy to escape the nucleus. There is a chance, due to it’s wave function, that it will escape the potential barrier of the nucleus boundary.

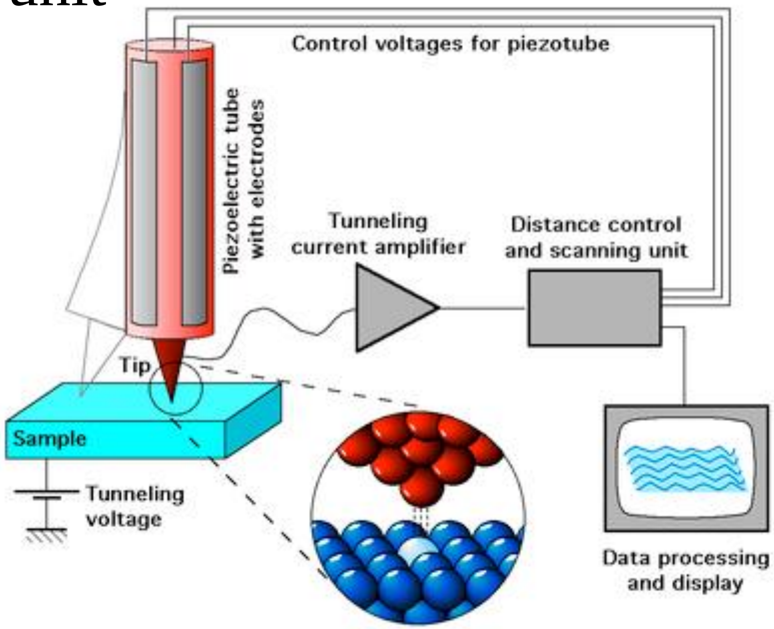




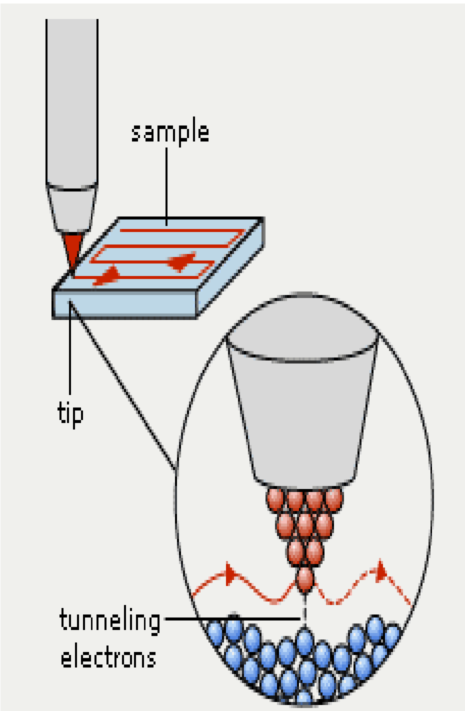
2. Scanning Tunneling Microscope (STM)

STM includes;

- Scanning tip
- Piezoelectric controlled scanner
- Distance control and scanning unit
- Vibration isolation system
- Computer



HOW TO OPERATE STM?..



Based on a phenomenon called
Quantum Mechanical Tunneling

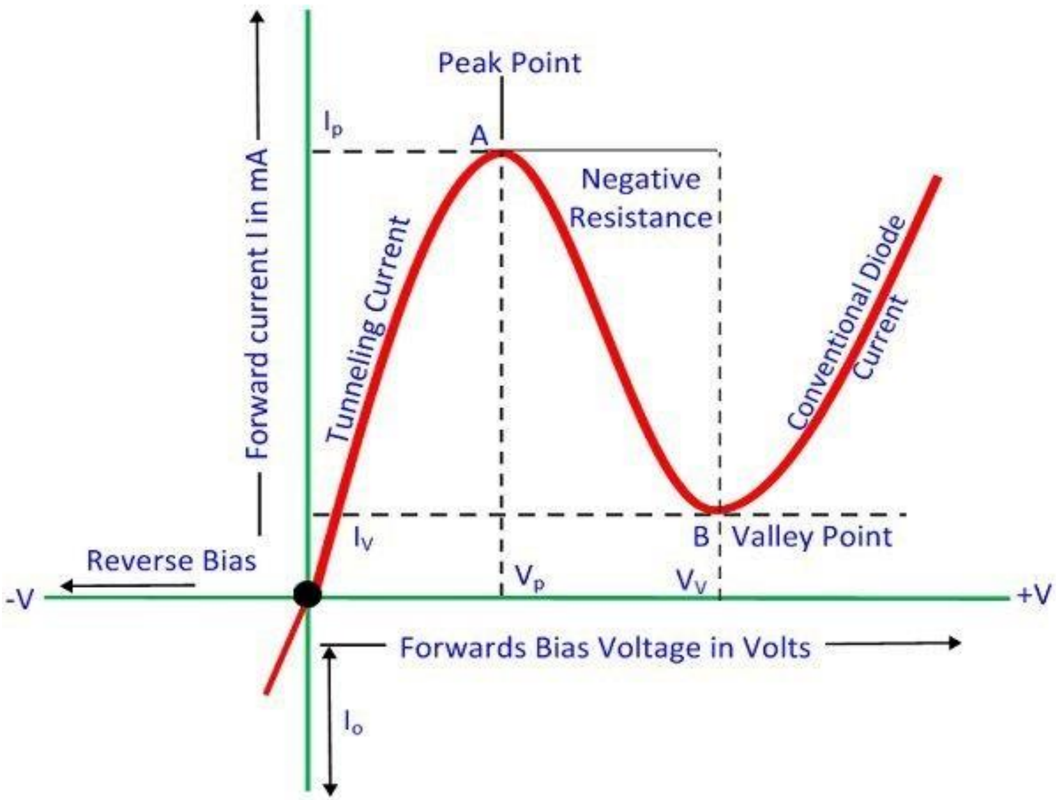
Applied voltage between the sharp tip and the surface

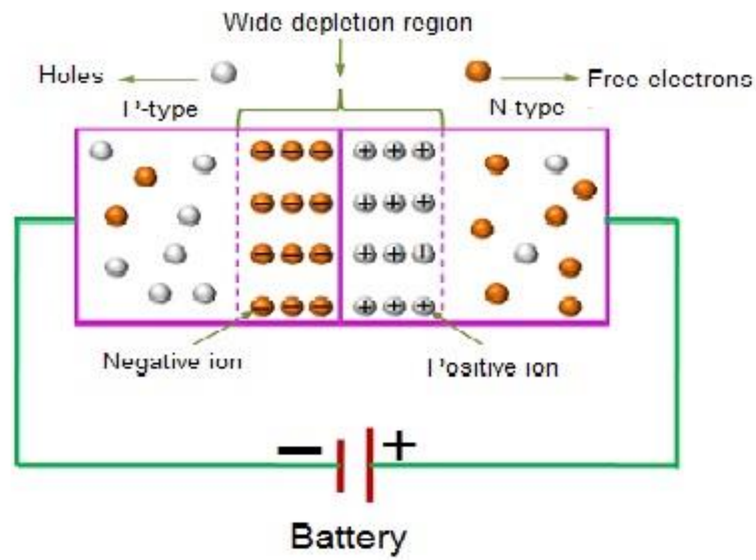
Small tunneling current produced

Small electric current under the circumstances without the need for the tip to touch the surface

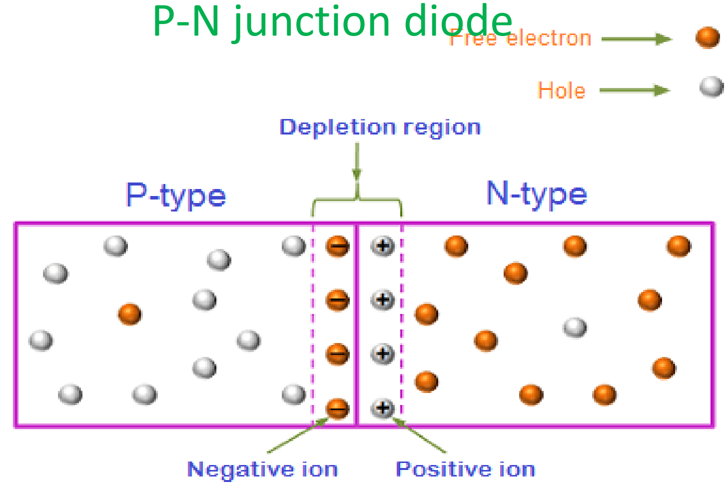
"I think I can safely say that nobody understands Quantum Mechanics." Richard Feynman

3.Tunnel Diode: A Tunnel Diode is a heavily doped p-n junction diode. The tunnel diode shows negative resistance. When voltage value increases, current flow decreases. Tunnel diode works based on Tunnel Effect.





P-N junction diode



Tunnel diode

Applications of Tunnel Diode

•Tunnel diode can be used as a switch, amplifier, and oscillator.

•Since it shows a fast response, it is used as high frequency component.

•Tunnel diode acts as logic memory storage device.

•They are used in oscillator circuits, and in FM receivers. Since it is a low current device, it is not used more.

Introduction to quantum computing

➢ Classical Computer (Binary) :

A computer that uses voltages flowing through circuits and gates, which can be calculated entirely by classical mechanics.

What is a Quantum Computer?

➢Quantum Computer:

A computer that uses quantum mechanical phenomena to perform operations on data through devices such as superposition and entanglement. A number of elemental particles such as electrons or photons can be used, with either their charge or polarization acting as representation of 0 and or 1. each of these particles is known as quantum bit, or qubit. A qubit is a unit of quantum information.

Superposition and Entanglement

- A qubit can hold both values (0 and 1) at the same time known as a superposition state. Thus the number of computations that a quantum computer could undertake is ‘2’ where n is the number of qubits used e.g a quantum computer comprised of 500 qubits have a potential to do 2500 calculations in a single step.
- Entanglement is correlation between particles acting as q- bits such as photons, electrons. By knowing the spin state of one entangled particles up or down. We can know the spin of opposite direction. Quantum entanglement allows qubits separated by distances to interact with each other instantaneously. When multiple qubits options simultaneously. This allows them to process information within a fraction of time.

Applications of quantum computing

- **Artificial intelligence**
- **Drug design**
- **Financial optimization**
- **Development of new material**
- **Logistic and scheduling**
- **Cyber security**
- **Dealing and encryption**
- **Software testing and fault Simulation**