Course Code/Name : PH3151 / ENGINEERING PHYSICS
Regulation : 2021 – R

Course Objective:

1. To make the students effectively to achieve an understanding of mechanics.
2. To enable the students to gain knowledge of electromagnetic waves and its applications.
3. To introduce the basics of oscillations, optics and lasers.
4. Equipping the students to successfully understand the importance of quantum physics.
5. To motivate the students towards the applications of quantum mechanics.

UNIT IV BASIC QUANTUM MECHANICS

Photons and light waves - Electrons and matter waves –Compton effect - The Schrodinger equation (Time dependent and time independent forms) - meaning of wave function - Normalization –Free particle - particle in a infinite potential well: 1D,2D and 3D Boxes- Normalization, probabilities and the correspondence principle.

After completion of this course, the students should be able to

COs	OUTCOMES	RBT
C103.1	Remember the concepts of Mechanics and understand the Fundamentals of static and dynamics of bodies.	K1
C103.2	Understand the properties of electro Magnetic waves and its practical applications.	K2 & K3
C103.3	Demonstrate a strong foundational knowledge, and understand the principles of sound, Light and optics with experimental examples.	K2
C103.4	Understand and deduce the basic quantum concepts and equations.	K2
C103.5	Understand the fundamentals of quantum applications	K2
Revised Bloom's Taxonomy **K1**- Remembering, **K2**- Understanding, **K3**- Applying, **K4**- Analyzing, **K5**- Evaluating, **K6**- Creating		

CO-PO Mapping

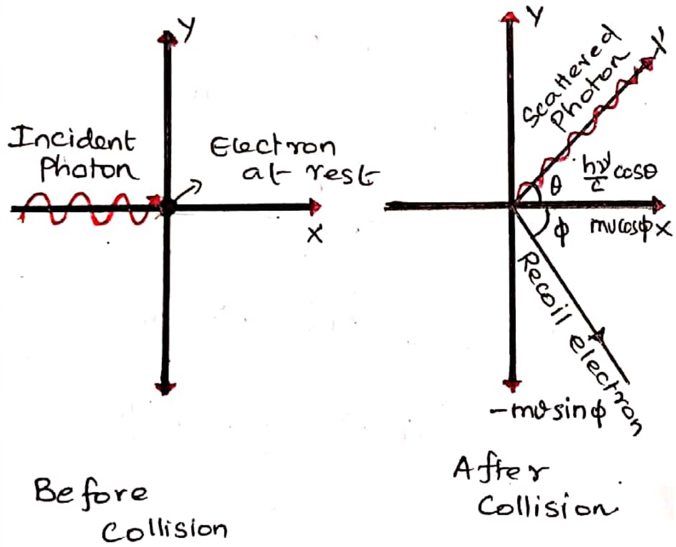
COs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
C103.1	3	2	1									
C103.2	3	2	1									
C103.3	3	2	1									
C103.4	2											
C103.5	1											
Avg	2.4	2	1									

Compton Effect:-

When a beam of x-ray Scattered by a substance, the Scattered x-ray radiation Consists of two Components. One has same wavelength (λ) and other one has longer wavelength (λ').

This change is wavelength is called Compton shift. and this phenomenon is called Compton effect.

Let us consider Collision between a photon with energy $h\nu$ and an electron.



Energy:-

Before Collision:-

Energy of photon $= h\nu$

Energy of electron $= m_0c^2$

Total energy $= h\nu + m_0c^2$

After Collision:-

Energy of electron $= mc^2$

Energy of photon $= h\nu'$

Total energy $= mc^2 + h\nu'$

According to law of conservation of energy.

$$\left.\begin{array}{c}\text{Energy before}\\ \text{collision}\end{array}\right\} = \begin{array}{c}\text{Energy after}\\ \text{Collision}\end{array}$$

$$h\nu + m_0c^2 = mc^2 + h\nu'$$

$$mc^2 = h\nu - h\nu' + m_0c^2$$

$$mc^2 = h(\nu - \nu') + m_0c^2 \quad \text{—} (1)$$

Momentum along X-Axis:-

Before Collision:-

Momentum of electron $= 0$

Momentum of photon $= \frac{h\nu}{c}$

Total momentum $= \frac{h\nu}{c}$

After Collision:-

Momentum of electron $= m\upsilon\cos\phi$

Momentum of photon $= \frac{h\nu'}{c}\cos\theta$

Total momentum $= m\upsilon\cos\phi + \frac{h\nu'}{c}\cos\theta$

According to law of conservation of momentum

$$\left.\begin{array}{c}\text{Momentum before}\\ \text{collision}\end{array}\right\} = \begin{array}{c}\text{Momentum after}\\ \text{Collision.}\end{array}$$

$$\frac{h\nu}{c} = m\upsilon\cos\phi + \frac{h\nu'}{c}\cos\theta$$

$$m\upsilon c\cos\phi = h\nu - h\nu'\cos\theta$$

$$m\upsilon c\cos\phi = h[\nu - \nu'\cos\theta] \quad \text{—} (2)$$

Momentum along Y-Axis

Before Collision:-

Momentum of electron = 0

Momentum of Photon = 0

Total momentum = 0

After Collision:-

Momentum of electron $= -m\vartheta\sin\phi$

Momentum of photon $= \frac{h\nu'}{c}\sin\theta$

Total momentum $= \frac{h\nu'}{c}\sin\theta - m\vartheta\sin\phi$

According to law of conservation of momentum

$$\left.\begin{array}{l}\text{Momentum before}\\ \text{Collision}\end{array}\right\} = \begin{array}{l}\text{Momentum before}\\ \text{Collision}\end{array}$$

$$0 = \frac{h\nu'}{c}\sin\theta - m\vartheta\sin\phi$$

$$m\vartheta\sin\phi = \frac{h\nu'}{c}\sin\theta$$

$$m\vartheta c\sin\phi = h\nu'\sin\theta \quad —(3)$$

Squarring and adding eqn (2) & (3)

$$m^2\vartheta^2c^2\cos^2\phi + m^2\vartheta^2c^2\sin^2\phi = [h(\nu-\nu'\cos\theta)]^2 + h^2\nu'^2\sin^2\theta$$

$$m^2\vartheta^2c^2 = h^2[\nu-\nu'\cos\theta]^2 + h^2\nu'^2\sin^2\theta$$

$$m^2\vartheta^2c^2 = h^2[\nu^2+\nu'^2\cos^2\theta - 2\nu\nu'\cos\theta] + h^2\nu'^2\sin^2\theta$$

$$m^2\vartheta^2c^2 = h^2\nu^2 + h^2\nu'^2 - 2h^2\nu\nu'\cos\theta$$

$$m^2\vartheta^2c^2 = h^2[\nu^2 - 2\nu\nu'\cos\theta + \nu'^2] \quad —(4)$$

Squaring eqn (4) on both sides

$$m^2c^4 = [h(\nu-\nu') + m_oc^2]^2$$

$$m^2c^4 = h^2[\nu-\nu']^2 + m_o^2c^4 + 2h(\nu-\nu')m_oc^2$$

$$m^2c^4 = h^2[\nu^2+\nu'^2-2\nu\nu'] + m_o^2c^4 + 2h(\nu-\nu')m_oc^2 \quad (5)$$

$$m^2c^4 = h^2\nu^2 + h^2\nu'^2 - 2h^2\nu\nu' + m_o^2c^4 + 2h(\nu-\nu')m_oc^2 \quad —(5)$$

Substract eqn (4) from eqn (5)

$$m^2c^4 - m^2\vartheta^2c^2 = \cancel{h^2\nu^2} + \cancel{h^2\nu'^2} - 2h^2\nu\nu' + m_o^2c^4 + 2h(\nu-\nu')m_oc^2 - \cancel{h^2\nu^2} - \cancel{h^2\nu'^2} + 2h^2\nu\nu'\cos\theta$$

$$m^2c^2[c^2-\vartheta^2] = -2h^2\nu\nu'(1-\cos\theta) + 2h(\nu-\nu')m_oc^2 + m_o^2c^4 \quad —(6)$$

From theory of relativity

$$m = \frac{m_o}{\sqrt{1-\frac{\vartheta^2}{c^2}}}$$

Squarring on bothsides $m^2 = \frac{m_o^2}{1-\vartheta^2/c^2}$

$$m^2 = \frac{m_o^2}{\frac{c^2-\vartheta^2}{c^2}} \Rightarrow m^2 = \frac{m_o^2c^2}{c^2-\vartheta^2}$$

$$m^2(c^2-\vartheta^2) = m_o^2c^2$$

Multiply by c^2 on bothsides

$$m^2c^2[c^2-\vartheta^2] = m_o^2c^4 \quad —(7)$$

Compare eqn (6) & (7)

$$m_o^2c^4 = -2h^2\nu\nu'(1-\cos\theta) + 2h(\nu-\nu')m_oc^2 + m_o^2c^4$$

$$2h^2\nu\nu'(1-\cos\theta) = 2h(\nu-\nu')m_oc^2$$

$$\frac{h}{m_oc^2}(1-\cos\theta) = \frac{\nu-\nu'}{\nu\nu'}$$

$$\frac{h}{m_oc^2}[1-\cos\theta] = \frac{\lambda'-\lambda}{c}$$

$$\boxed{d\lambda = \frac{h}{m_oc}[1-\cos\theta]} \quad —(8)$$

Eqn (8) is called Compton Shift

Case (i)

When $\theta = 0°$

$$d\lambda = \frac{h}{m_0 c}[1-\cos 0°]$$

$$= \frac{h}{m_0 c}[1-1]$$

$$\boxed{d\lambda = 0}$$

Case (ii)

When $\theta = 90°$

$$d\lambda = \frac{h}{m_0 c}[1-\cos 90°]$$

$$= \frac{h}{m_0 c}(1-0)$$

$$d\lambda = \frac{h}{m_0 c}$$

$$\boxed{d\lambda = 0.0243 Å}$$

Compton wavelength

Case (iii)

When $\theta = 180°$

$$d\lambda = \frac{h}{m_0 c}[1-\cos 180°]$$

$$= \frac{h}{m_0 c}[1-(-1)]$$

$$d\lambda = \frac{2h}{m_0 c}$$

$$\boxed{d\lambda = 0.0486 Å}$$

Schroedinger's Wave Equation:

Schroedinger's wave eqn is a mathematical equation to describe the dual nature of matter wave.

There are two forms of eqn.

(i) Time independent wave Equation

(ii) Time dependent wave Equation.

Time Independent Wave Equation:-

Let us consider a system of stationary waves associated with a moving particle.

If ψ be the wave function along the axes x, y, z at any time 't'.

then the differential wave equation of the wave velocity 'v' can be written interms of cartesian coordinates is

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \quad \text{—(1)}$$

$$\text{(or)} \quad \nabla^2\psi = \frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} \quad \text{—(1)}$$

Where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

↳ Laplacian Operator

The solution of eqn (1) is of the form

$$\psi = \psi_0 e^{-i\omega t} \quad \text{—(2)}$$

$\omega \rightarrow$ Angular frequency

Differentiate eqn (2) with respect to 't'.

$$\frac{\partial\psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t}$$

$$\frac{\partial^2\psi}{\partial t^2} = -i\omega \cdot -i\omega\, \psi_0 e^{-i\omega t}$$

$$\frac{\partial^2\psi}{\partial t^2} = -\omega^2\psi \quad \text{—(3)}$$

Substituting eqn (3) in eqn (1) we have

$$\nabla^2\psi = \frac{-\omega^2}{v^2}\psi$$

$$\nabla^2\psi + \frac{\omega^2}{v^2}\psi = 0 \quad \text{—(4)}$$

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

$$\nabla^2\psi + \frac{4\pi^2}{\lambda^2}\psi = 0 \quad \text{—(5)}$$

$\omega = 2\pi\nu$

$\omega = \frac{2\pi v}{\lambda}$

$\frac{\omega}{v} = \frac{2\pi}{\lambda}$

By de-Broglie wave length

$\lambda = \frac{h}{mv}$ eqn (5) becomes

$$\nabla^2\psi + \frac{4\pi^2}{h^2/m^2v^2}\psi = 0$$

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

WKT

Total Energy = Kinetic Energy + Potential Energy

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

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

$$2(E-V) = mv^2$$

Multiply by 'm' on bothsides

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

Substituting eqn (7) in eqn (6) we get

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

Let $\hbar = \frac{h}{2\pi}$; $\hbar^2 = \frac{h^2}{4\pi^2}$; $\frac{1}{\hbar^2} = \frac{4\pi^2}{h^2}$

$\therefore$ eqn (8) $\Rightarrow$ $\boxed{\nabla^2\psi + \frac{2m}{\hbar^2}[E-V]\psi = 0}$ $-(9)$

Eqn (9) known as Schroedinger's time independent wave equation.

One dimensional Schroedinger's time independent wave equation is

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

Time Dependent wave Equation:

We know that the Solution of the classical differential equation of wave system is

$$\psi = \psi_0 e^{-i\omega t} \quad -(1)$$

Differentiate eqn (1) with respect to 't' we have

$$\frac{\partial\psi}{\partial t} = -i\omega\psi$$

$$\frac{\partial\psi}{\partial t} = -i2\pi\nu\psi \quad -(2)$$

Where $\omega = 2\pi\nu$

wkt $E = h\nu$; $\nu = \frac{E}{h}$

Eqn (2) $\Rightarrow$ $\frac{\partial\psi}{\partial t} = -i\frac{2\pi E}{h}\psi$

$$\frac{\partial\psi}{\partial t} = -\frac{iE}{\hbar}\psi \qquad \because \frac{1}{\hbar} = \frac{2\pi}{h}$$

$$E\psi = i\hbar\frac{\partial\psi}{\partial t} \quad -(3)$$

From Schroedinger's time independent wave equation

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

$$\nabla^2\psi + \frac{2m}{\hbar^2}E\psi - \frac{2m}{\hbar^2}V\psi = 0 \quad -(4)$$

Substituting eqn (3) in eqn (4) we get

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

Multiply the above equation by $\frac{\hbar^2}{2m}$ on bothsides we have

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

$$i\hbar\frac{\partial\psi}{\partial t} = V\psi - \frac{\hbar^2}{2m}\nabla^2\psi$$

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = \left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\psi} \quad -(5)$$

Eqn (5) can be written as

$$\boxed{E\psi = H\psi}$$

Where $E = i\hbar \frac{\partial}{\partial t}$ → Energy Operator

$H = -\frac{\hbar^2}{2m}\nabla^2 + V$ → Hamiltonian operator

Eqn ⑤ and eqn ⑥ are called as Schroedinger's time dependent wave equation.

Application of Schroedinger's Equation:

Particle in a 1D Rigid Box

Consider a particle of mass 'm' moving between two rigid walls of a box at $x=0$ and $x=l$ along x axis.

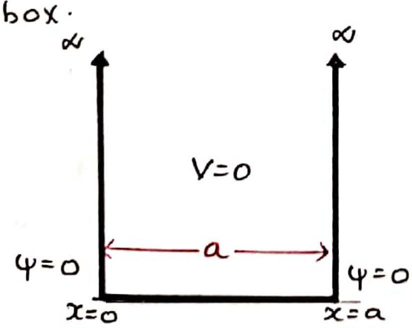
The potential function is given by

$V(x) = 0$ for $0 < x < a$

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

This function is called square well potential.

The wave function ψ is '0' for $x \leq 0$ and $x \geq a$. Let us calculate the value of ψ with in the box.



Schroedinger's wave equation in one dimension is given by

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

Since $V=0$ between the walls the eqn reduces to

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

Substituting $\frac{2mE}{\hbar^2} = k^2$ in eqn ①

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

The general solution of eqn ② is given by

$$\psi(x) = A\sin kx + B\cos kx \quad \text{—③}$$

Here A and B are two constants A&B can be determined by boundary conditions.

Boundary Condition-(i)

$\psi = 0$ at $x = 0$

③ ⇒ $0 = A\sin 0 + B\cos 0$

$0 = 0 + B \times 1$

Hence $B = 0$.

Boundary Condition-(ii)

$\psi = 0$ at $x = a$

Eqn ③ ⇒ $0 = A\sin ka + 0$ $\quad \because B = 0$

$A\sin ka = 0$

It is found that either $A = 0$ or $\sin ka = 0$

Since $B=0$, 'A' cannot be zero

$\therefore \sin ka = 0$

(ie) $Ka = n\pi$

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

$$k^2 = \frac{n^2\pi^2}{a^2} \quad -④$$

We know that

$$k^2 = \frac{2mE}{\hbar^2} = \frac{2mE\,4\pi^2}{h^2}$$

$$k^2 = \frac{8\pi^2 mE}{h^2} \quad -⑤$$

Comparing eqns ④ & ⑤ we have

$$\frac{n^2\pi^2}{a^2} = \frac{8\pi^2 mE}{h^2}$$

$$\boxed{E_n = \frac{n^2h^2}{8ma^2}} \quad -⑥$$

Substituting $k = \frac{n\pi}{a}$ in eqn ③

$$\psi_n(x) = A \sin \frac{n\pi x}{a} \quad -⑦$$

$n = 1, 2, 3 \ldots$

The energy of the particle can only have discrete energy values specified by eqn ⑥.

Each value of E_n is called eigen value, and the corresponding ψ_n is called eigen function.

Normalisation of wave function:-

Probability density is given by $\psi^*\psi$.

We know that

$$\psi_n(x) = A \sin \frac{n\pi x}{a}$$

$$\psi^*\psi = A^2 \sin^2\left[\frac{n\pi x}{a}\right] \quad -⑧$$

The probability of finding the particle inside the box of length 'a' is given by

$$\int_0^a \psi^*\psi \, dx = 1 \quad -⑨$$

Substituting $\psi^*\psi$ from eqn ⑧ in eqn ⑨

$$\int_0^a A^2 \sin^2\left[\frac{n\pi x}{a}\right] dx = 1$$

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

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

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

$$\frac{A^2}{2}\left[a - 0\right] = 1$$

$$\frac{A^2 a}{2} = 1 \Rightarrow A^2 = \frac{2}{a}$$

$$A = \sqrt{\frac{2}{a}} \quad -⑩$$

Substituting eqn ⑩ in eqn ⑦

$$\boxed{\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}} \quad -⑪$$

The eqn ⑪ is known as normalised eigen function.

Special Cases:-

Case (i)

For $n=1$

$$E_1 = \frac{h^2}{8ma^2}$$

$$\psi_1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$$

ψ_1 is maximum at middle of the box

Case (ii)

For $n=2$

$$E_2 = \frac{4h^2}{8ma^2} = 4E_1$$

$$\psi_2 = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)$$

ψ_2 is maximum at quarter distance from either sides of the box.

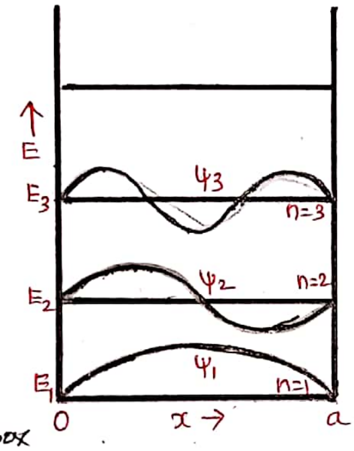
Case (iii)

For $n=3$

$$E_3 = \frac{9h^2}{8ma^2} = 9E_1$$

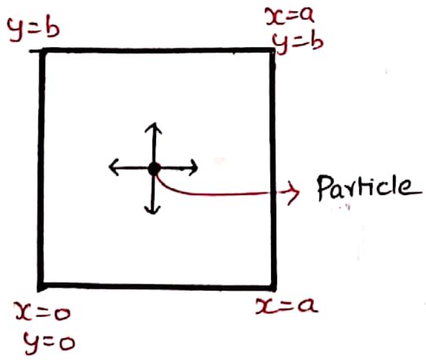
$$\psi_3 = \sqrt{\frac{2}{a}} \sin \frac{3\pi x}{a}$$

ψ_3 is maximum at exactly middle & $\frac{1}{6}$th distance from either sides of the box



Particle in 2D Potential Box:

Consider a particle of mass m' moving two dimensionally in a box of lengths a & b as shown in the figure



The potential function is given by

$$V(x,y) = 0 \quad \text{for} \quad 0<x<a, \quad 0<y<b$$

$$V(x,y) = \infty \quad \text{for} \quad 0 \geq x \geq a, \quad 0 \geq y \geq b.$$

The solution of one-dimensional potential well is extended for a two dimensional potential well.

In 2D potential well, instead of one quantum number 'n', we have to use two quantum numbers n_x and n_y corresponding to the two coordinate axes namely x and y respectively.

1 The Eigen function and eigen value of a particle moving in a one dimensional potential well can be derived as follows.

One dimensional Schroedinger's time independent wave equation of a free particle is given by

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad \text{--- (1)}$$

Substituting $\frac{2mE}{\hbar^2} = k^2$ in equation (1)

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

The general solution of equation (2) is given by

$$\psi(x) = A\sin kx + B\cos kx \quad \text{--- (3)}$$

Where A and B are two constants. A & B can be determined by boundary conditions.

Condition - 1

$\psi = 0$ at $x = 0$

③ ⇒ $0 = A\sin 0 + B\cos 0$

$0 = 0 + B \times 1$

Hence $B = 0$

Condition - 2

$\psi = 0$ at $x = a$

③ ⇒ $0 = A\sin ka + 0$ $\quad \because B = 0$

$A\sin ka = 0$

It is found that either $A = 0$ or $\sin ka = 0$

Since $B = 0$, 'A' cannot be zero

$\therefore \sin ka = 0$

(ie) $ka = n\pi$

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

$$k^2 = \frac{n^2\pi^2}{a^2} \quad —④$$

We know that

$$k^2 = \frac{2mE}{\hbar^2} = \frac{2mE \cdot 4\pi^2}{h^2}$$

$$k^2 = \frac{8\pi^2 mE}{h^2} \quad —⑤$$

Comparing eqns ④ & ⑤ we get

$$\frac{n^2\pi^2}{a^2} = \frac{8\pi^2 mE}{h^2}$$

$$E_n = \frac{n^2h^2}{8ma^2} \quad —⑥$$

Substituting $k = \frac{n\pi}{a}$ in eqn ③

$$\psi_n(x) = A\sin\frac{n\pi x}{a} \quad —⑦$$

The constant 'A' can be determined by normalisation of wave function.

The value of 'A' is given by

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

$\therefore$ eqn ⑦ ⇒ $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a} \quad —⑧$

The eqn ⑥ and eqn ⑧ give eigen value and eigen function of a particle moving in one dimensional potential well.

These two equations can be extended to two dimensional potential well as follows.

Energy of the particle

$$E = E_{n_x} + E_{n_y}$$

ie. $$E_{n_x n_y} = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8mb^2}$$

$$\boxed{E_{n_x n_y} = \frac{h^2}{8m}\left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2}\right]} \quad —⑨$$

The corresponding normalised wave function of the particle in the two dimensional well is written as

$$\psi_{n_x n_y} = \sqrt{\frac{2}{a}}\sin\left(\frac{n_x\pi x}{a}\right) \times \sqrt{\frac{2}{b}}\sin\left(\frac{n_y\pi y}{b}\right)$$

$$\psi_{n_x n_y} = \sqrt{\frac{2}{a}} \times \sqrt{\frac{2}{b}}\sin\left[\frac{n_x\pi x}{a}\right]\sin\left[\frac{n_y\pi y}{b}\right]$$

$$\boxed{\psi_{n_x n_y} = \sqrt{\frac{4}{ab}}\sin\left[\frac{n_x\pi x}{a}\right]\sin\left[\frac{n_y\pi y}{b}\right]} \quad —⑩$$

The eqns ⑨ & ⑩ give the eigen value and eigen function of a particle in 2D Box.

For Square box $a=b$.

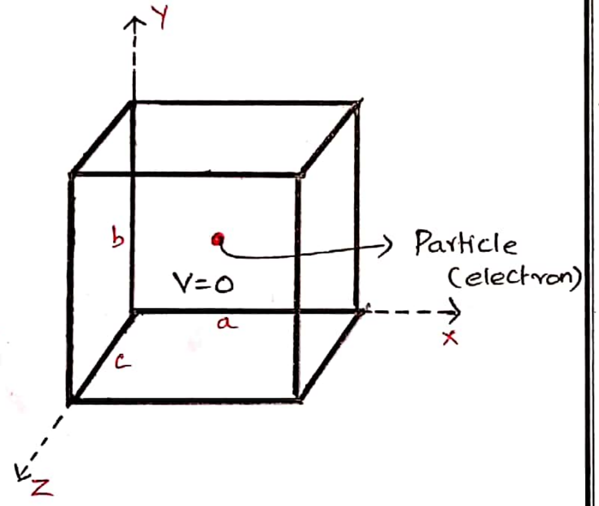
$\therefore$ The eigen value and eigen function is given by

$$\boxed{E_{n_x n_y} = \frac{h^2}{8ma^2}\left[n_x^2+n_y^2\right]}$$

$$\boxed{\psi_{n_x n_y} = \sqrt{\frac{4}{a^2}}\,\sin\left[\frac{n_x \pi x}{a}\right]\sin\left[\frac{n_y \pi y}{a}\right]}$$

Particle in 3D Potential Well:

Consider a particle of mass 'm' moving three dimensionally in a box of lengths a, b & c as shown in the figure.



The potential function is given by

$$V(x,y,z) = 0 \quad \text{for} \quad 0<x<a,\ 0<y<b,\ 0<z<c$$

$$V(x,y,z) = \infty \quad \text{for} \quad 0\geq x \geq a,\ 0\geq y\geq b,\ 0\geq z\geq c$$

The solution of one dimensional potential well is extended for a three dimensional potential well.

In 3D potential well, instead of one quantum number 'n', we have to use three quantum numbers n_x, n_y and n_z corresponding to the three coordinate axes namely x, y and z respectively.

The Eigen function and eigen value of a particle moving in a one dimensional potential well can be derived as follows.

One dimensional schroedinger's time independent wave equation of a free particle is given by

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad \text{--- (1)}$$

Substituting $\frac{2mE}{\hbar^2} = k^2$ in eqn (1)

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

The general solution of equation (2) is given by

$$\psi(x) = A\sin kx + B\cos kx \quad \text{--- (3)}$$

Where A and B are two constants A & B can be determined by boundary conditions.

Condition-1

$\psi = 0$ at $x = 0$

$(3) \Rightarrow \quad 0 = A \sin 0 + B \cos 0$

$0 = 0 + B \times 1$

Hence $B = 0$

Condition-2

$\psi = 0$ at $x = a$

$(3) \Rightarrow \quad 0 = A \sin ka + 0$

$A \sin ka = 0$

It is found that either $A = 0$ or $\sin ka = 0$

Since $B = 0$, 'A' cannot be zero

$\therefore \sin ka = 0$

ie $ka = n\pi$

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

$$k^2 = \frac{n^2\pi^2}{a^2} \quad \text{--- (4)}$$

We know that

$$k^2 = \frac{2mE}{\hbar^2} = 2mE \cdot \frac{4\pi^2}{h^2}$$

$$k^2 = \frac{8\pi^2 mE}{h^2} \quad \text{--- (5)}$$

Comparing eqn (5) & (4) we get

$$\frac{n^2\pi^2}{a^2} = \frac{8\pi^2 mE}{h^2}$$

$$E_n = \frac{n^2h^2}{8ma^2} \quad \text{--- (6)}$$

Substituting $k = \frac{n\pi}{a}$ in eqn (3)

$$\psi_n(x) = A \sin \frac{n\pi x}{a} \quad \text{--- (7)}$$

The constant 'A' can be determined by normalisation of wave function.

The value of 'A' is given by

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

$$\therefore \text{Eqn (7)} \Rightarrow \psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \quad \text{--- (8)}$$

The eqn (6) and eqn (8) give eigen value and eigen function of a particle moving in an one dimensional potential well.

These two equations can be extended to three dimensional potential well as follows.

Energy of the particle

$$E_{n_x n_y n_z} = E_{n_x} + E_{n_y} + E_{n_z}$$

$$E_{n_x n_y n_z} = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8mb^2} + \frac{n_z^2 h^2}{8mc^2}$$

$$\boxed{E_{n_x n_y n_z} = \frac{h^2}{8m}\left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right]} \quad \text{--- (9)}$$

The corresponding normalised wave function of the particle in the three dimensional well is given by

$$\psi_{n_x n_y n_z} = \sqrt{\frac{2}{a}} \sin\left(\frac{n_x \pi x}{a}\right) \sqrt{\frac{2}{b}} \sin\left(\frac{n_y \pi y}{b}\right) \sqrt{\frac{2}{c}} \sin\left(\frac{n_z \pi z}{c}\right)$$

$$\psi_{n_x n_y n_z} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{b}}\sqrt{\frac{2}{c}} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{b}\right) \sin\left(\frac{n_z \pi z}{c}\right)$$

$$\boxed{\psi_{n_x n_y n_z} = \sqrt{\frac{8}{abc}} \sin\left[\frac{n_x \pi x}{a}\right] \sin\left[\frac{n_y \pi y}{b}\right] \sin\left[\frac{n_z \pi z}{c}\right]} \quad \text{--- (10)}$$

The eqns (9) & (10) give the eigen value and eigen function of a particle in 3D Box.

For <u>cubical box</u> $a=b=c$

$\therefore$ The eigen value and eigen function is given by

$$\boxed{E_{n_x n_y n_z} = \frac{h^2}{8ma^2}\left[n_x^2+n_y^2+n_z^2\right]}$$

$$\boxed{\psi_{n_x n_y n_z} = \sqrt{\frac{8}{a^3}}\sin\left[\frac{n_x\pi x}{a}\right]\sin\left[\frac{n_y\pi y}{a}\right]\sin\left[\frac{n_z\pi z}{a}\right]}$$