Unit-I

QUANTUM PHYSICS & COMPUTING

- **Prerequisite:** Dual nature of radiation, Photoelectric effect, Matter waves-wave nature of particles, de-Broglie relation, Davisson-Germer experiment.
- **Introduction**
- **Matter waves:** De Broglie hypothesis of matter waves; properties of matter waves, Wave packet, phase velocity and group velocity.
- **Heisenberg uncertainty principle:** State & Explain; nonexistence of electron in nucleus.
- **Schrodinger's wave equation:** Schrodinger's time dependent wave equation; time independent wave equation; Particle trapped in one dimensional infinite potential well.
- **Fundamentals of Quantum Computing:**
- Numerical on De Broglie wavelength, Heisenberg uncertainty principle and Particle trapped in one dimensional infinite potential well.

❖ De-Broglie hypothesis

In 1924 De-Broglie extended wave particle parallism of optics to all fundamental particles of physics such as **electrons**, **protons, atoms** etc.

De-Broglie put bold suggestion that "**like radiation matter also has dual nature**" He have been put this hypothesis on the basis of the "nature love symmetry". De-Broglie hypothesis was soon confirmed by diffraction of electrons.

De-Broglie wave (Matter wave): According to De-Broglie hypothesis moving particle is always associated with the wave called as De-Broglie wave or matter wave.

The matter wave travel with the velocity of particle.

❖ De-Broglie wavelength:

The expression for the wavelength of matter wave can be derived on the analogy of light wave as follows'.

According the Plank's theory of radiation, the energy of the photon is given by

$$\mathbf{E = h\upsilon} \qquad \left(\upsilon = \frac{c}{\lambda}\right)$$

$$\mathbf{E} = \frac{hc}{\lambda} \qquad \ldots\ldots. (1)$$

According to Einstein relation

$$\mathbf{E = mc^2} \qquad \ldots\ldots. (2)$$

From equation 1 & 2

$$\mathbf{mc^2} = \frac{hc}{\lambda}$$

$$\lambda = \frac{h}{mc} \qquad \ldots\ldots. (3)$$

Equation 3 represents the wavelength of light wave.

If we consider the case of material particle of mass is '**m'** moving with the velocity of **'v'** then the wavelength associate with the matter wave is given by analogy of equation **3** as follow

$$\lambda = \frac{h}{mv} \qquad \ldots\ldots (4)$$

Equation 4 represents the equation for the wavelength of matter wave

λ = wavelength of matter wave

h = Plank's constant **(6.64×10^{-34}JS)**

m = mass of particle

v = velocity of particle

But momentum of particle is **(p= mv)**

So equation (**4)** become

$$\boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\boldsymbol{p}} \quad \textbf{....... (5)}$$

P = momentum of the particle.

❖ De-Broglie wavelength in terms of kinetic energy (K.E.):

Let us consider the particle of mass **'m'**, moving with the velocity **'v'.** According to De-Broglie hypothesis it exhibit the wave nature & wavelength of matter wave is given by equation (**4)**

$$\boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\boldsymbol{mv}} \quad \textbf{....... (1)}$$

Here particle posses K.E. due to its motion

$$\mathbf{E} = \frac{1}{2}\,\mathbf{mv^2} \quad \textbf{....... (2)}$$

Multiply & divide the equation **(2)** by **'m'**

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

So, $\mathbf{mv} = \sqrt{\boldsymbol{2mE}}$ **...... (3)**

Put the value of **'mv'** from equation **(3)** in equation **(1)**

$$\boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\sqrt{\boldsymbol{2mE}}} \quad \textbf{...... (4)}$$

E = K.E. of the particle

❖ De-Broglie wavelength of electron:

Let us consider the electron subjected to p.d. of '**V**'volt. In this potential the electron will move with the certain velocity & hence possess K.E. The K.E. to electron is provided by electrical energy.

K.E. = electrical energy

$$\frac{\mathbf{1}}{\mathbf{2}}\,\boldsymbol{m}\mathbf{v}^2 = \boldsymbol{eV}$$

$$\frac{\mathbf{1}}{\mathbf{2m}}\,\boldsymbol{m}^2\mathbf{v}^2 = \boldsymbol{eV}$$

So $\boldsymbol{m}\mathbf{v} = \sqrt{\boldsymbol{2me}\mathbf{V}}$ **...... (1)**

But we know that $\boldsymbol{\lambda} = \frac{\mathbf{h}}{\mathbf{mv}}$ **....... (2)**

Put the value of '**mv**' from equation (1) into (2)

$$\boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\sqrt{\boldsymbol{2me}\mathbf{V}}} \quad \textbf{...... (3)}$$

Equation (3) represents the De-Broglie wavelength of electron.\

Here, h = 6.64×10^{-34} JS

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

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

V = Applying voltage

If we put all the value in equation (3) it becomes

$$\boldsymbol{\lambda = \frac{12.26}{\sqrt{V}}\ A^0} \quad \textbf{....... (4)}$$

By using equation (3) & (4) we can calculate the De-Broglie wavelength of electron.

❖ Properties of matter wave (De-Broglie wave):

1) These waves are not electromagnetic waves but are new kind of waves.
2) Velocity of electromagnetic waves is constant where as matter wave is **variable** & it depends upon the velocity of particle.
3) Phase velocity of matter wave is greater than the velocity of light wave **i.e.** $\boldsymbol{u = \frac{c2}{v}}$ **.**
4) They are pilot wave in the sense that they pilot or guide the matter particle.
5) Wavelength of matter wave is given by $\boldsymbol{\lambda = \frac{h}{mv}}$ so Wavelength of matter wave is inversely proportional to **mass** & **velocity** of particle.
6) Lighter is the particle greater is the wavelength associated with it.
7) Smaller is the velocity of the particle greater is the wavelength associated with it.
8) The wave natures of the particle introduce an uncertainty in the location of the position of the particle hence matter wave is the wave of probability.

Difference between Electromagnetic wave & matter wave:

Electromagnetic wave	Matter wave
i) In electromagnetic wave Electric and magnetic field are perpendicular to the direction of motion.	i) Motion of particle associate with wave known as matter wave.
ii) In electromagnetic wave Electric and magnetic field is periodically vary.	ii) Matter wave shows periodic variation of wave function.
iii) It does not show probability	iii) It is the wave of probability.
iv) Velocity of electromagnetic wave is constant.	iv) Velocity of matter wave is variable & depends on velocity of particle.
v) Ex. X-rays, γ rays, visible rays.	v) Ex. Electron wave, neutron wave, proton wave etc.

❖ Phase Velocity & Group Velocity:

Phase velocity (v_p):

The phase velocity is the velocity with which particular phase of the wave propagated in the medium.

$$\mathbf{v_p = \vartheta\, \lambda} \quad \text{………} \ 1)$$

Let us consider equation of the wave traveling along x direction.

$$\boldsymbol{y} \mathbf{= A \sin(\omega t - kx)}$$

A = amplitude of wave

ω = angular frequency

k = Propagation constant

$$\omega = 2\pi\vartheta \Rightarrow \vartheta = \frac{\omega}{2\pi} \ \ldots\ldots(2)$$

$$k = \frac{2\pi}{\boldsymbol{\lambda}} \Rightarrow \boldsymbol{\lambda} = \frac{2\pi}{\boldsymbol{K}} \ \ldots\ldots \ 3)$$

put equation 2) and 3) in equation 1) we get

$$\mathbf{v_p} = \frac{\omega}{2\pi}\frac{2\pi}{K}$$

$$v_p = \frac{\omega}{K}\ldots\ldots 4)$$

Again $k = \frac{2\pi}{\boldsymbol{\lambda}}$ & $\boldsymbol{\lambda} = \frac{h}{mv} \Rightarrow k = \frac{\mathbf{2\pi}}{\mathbf{h/mv}}$

$$\mathbf{k} = \frac{\mathbf{2\pi mv}}{\mathbf{h}}\ldots\ldots\mathbf{5})$$

We have $E = mc^2$ & $E = h\vartheta$ &

$$mc^2 = h\vartheta$$

$$\vartheta = \frac{mc^2}{h}$$

$$Again\ \omega = 2\pi\vartheta \Rightarrow \boldsymbol{\omega} = \frac{\boldsymbol{2\pi mc^2}}{\boldsymbol{h}}\ldots\ldots\mathbf{6})$$

put equation 5) and 6) in equation 4) we get

$$v_p = \frac{\omega}{k} = \frac{\frac{2\pi mc^2}{h}}{\frac{2\pi mv}{h}}$$

$$\mathbf{v_p} = \frac{\boldsymbol{c^2}}{\mathbf{v}}$$

The phase velocity of a matter wave is greater than velocity of light

Group velocity (v_g):

The velocity with which group of the wave travelling is known as group velocity.

Consider the two progressive wave having wave equation

$$\boldsymbol{y1 = A \sin(\omega t - kx)}$$

$$\boldsymbol{y2 = A \sin[(\omega + d\omega)t - (k + dk)x]}$$

$$\boldsymbol{y = y1 + y2}$$

$$y = 2A\, sin\left(\frac{2\omega + d\omega}{2} t - \frac{2k + dk}{2} x\right) cos\left(\frac{d\omega}{2}\ t - \frac{dk}{2}\ x\right) \dots\dots 3)$$

The sine term represent a wave angular frequency ω & propagation constant k.

The cosine term modulate this wave with angular frequency $\frac{d\omega}{2}$ to produce wave group travelling with velocity

$$\mathbf{v}_g = \frac{\boldsymbol{d\omega}}{\boldsymbol{dk}}\ \dots\dots(\mathbf{1})$$

Divide numerator and denominator by dv

$$\mathbf{v}_g = \frac{\boldsymbol{d\omega/d}\mathbf{v}}{\boldsymbol{dk/d}\mathbf{v}} \dots\dots(\mathbf{2})$$

$$mc^2 = h\vartheta \Rightarrow \vartheta = \frac{mc^2}{h}$$

But $\omega = 2\pi\vartheta$

$$\boldsymbol{\omega = \frac{2\pi mc^2}{h} \Rightarrow \omega = \frac{2\pi c^2}{h}\frac{m_0}{\sqrt{1 - v^2/c^2}}} \qquad \because m = \frac{m_0}{\sqrt{1 - v^2/c^2}}$$

$$\boldsymbol{\omega = \frac{2\pi c^2 m_0}{h}\left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}}}$$

$$\boldsymbol{\frac{d\omega}{dv} = \frac{2\pi c^2 m_0}{h}\ \frac{d}{dv}\left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}}}$$

$$\boldsymbol{\frac{d\omega}{dv} = \frac{2\pi m_0 c^2}{h}\left[-\frac{1}{2}\left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}-1}\left(\frac{-2v}{c^2}\right)\right]}$$

$$\boldsymbol{\frac{d\omega}{dv} = \frac{2\pi m_0 v}{h}\left(1 - \frac{v^2}{c^2}\right)^{-\frac{3}{2}}} \dots\dots(\mathbf{3})$$

$$Again\ k = \frac{2\pi}{\boldsymbol{\lambda}}\ \&\ \boldsymbol{\lambda} = \frac{h}{mv}\ \Rightarrow\ \mathbf{k} = \boldsymbol{\frac{2\pi mv}{h}}$$

$$\boldsymbol{k = \frac{2\pi v}{h}\frac{m_0}{\sqrt{1 - v^2/c^2}}}$$

$$\boldsymbol{k = \frac{2\pi m_0 v}{h}\left(1 - \frac{v^2}{c^2}\right)^{-\frac{1}{2}}}$$

$$\frac{dk}{d\mathbf{v}} = \frac{2\pi m_0}{h}\frac{d}{d\mathbf{v}}\left[\mathbf{v}\cdot\left(1-\frac{\mathbf{v}^2}{c^2}\right)^{-\frac{1}{2}}\right]$$

$$\frac{dk}{d\mathbf{v}} = \frac{2\pi m_0}{h}\left(1-\frac{\mathbf{v}^2}{c^2}\right)^{-\frac{3}{2}} \quad \ldots\ldots (4)$$

From equation 4) & 5) equation 2) becomes

$$\therefore \mathbf{v}_g = \frac{\frac{2\pi m_0 \mathbf{v}}{h}\left(1-\frac{\mathbf{v}^2}{c^2}\right)^{\frac{-3}{2}}}{\frac{2\pi m_0}{h}\left(1-\frac{\mathbf{v}^2}{c^2}\right)^{\frac{-3}{2}}}$$

$$\mathbf{v}_g = \mathbf{v}$$

The group velocity of matter wave is equal to the velocity of the particle.

❖ Heisenberg's uncertainty principle:

In 1927 Heisenberg's proposed a very interesting principle which is direct regarding to the dual nature of matter know as Heisenberg's uncertainty principle.

According to the Classical mechanics a moving particle at any instant has fixed position in a space & definite momentum which can be determine if the initial values are known.

However in wave mechanics the particle is described in terms of wave packet. According to Born probability particle may be found anywhere within wave packet.

Statement: According to Heisenberg's uncertainty principle **"It is impossible to determine simultaneously the position & momentum of the particle which associated with wave to any desired accuracy".**

$\Delta x.\ \Delta p \geq \hbar/2$

$\Delta x.\ m\Delta v \geq \hbar/2$ …… 1)

Δx = uncertainty in the measurement of position.

$\Delta P = m\Delta v$ = uncertainty in the measurement of momentum.

$\hbar = h/2\pi$ = Plank's constant (1.054×10^{-34}JS)

Different forms of Heisenberg's uncertainty principle,

$\Delta E.\ \Delta t \geq \hbar/2$ ……. 2)

ΔE = uncertainty in the measurement of Energy.

Δt = uncertainty in the measurement of time.

$\Delta L.\ \Delta\theta \geq \hbar/2$ ……. 3)

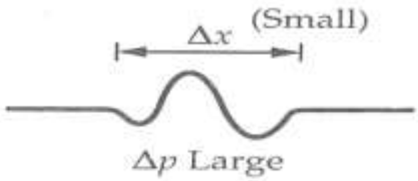
ΔL = uncertainty in the measurement of angular momentum.

Δt = uncertainty in the measurement of angular displacment.

Explanation:

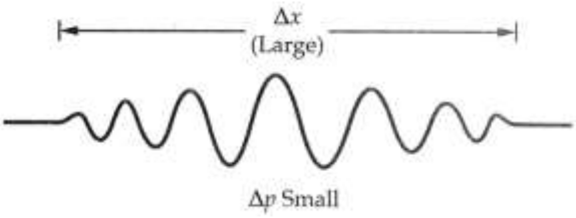
1) Size of the wave packet is small –

When the wave packet is small the position of the particle may be fixed but velocity becomes indeterminate (**p=mv**) means momentum becomes indeterminate.



2) Size of the wave packet is large – On the other hand when the size of the wave packet is large momentum of the particle fixed but position becomes indeterminate.

In this way the certainty in the position involve uncertainty in the momentum & certainty momentum in the involve uncertainty in the position so the statement of the Heisenberg's principle as follows.



❖ Wave Function (ψ):

The variable quantity characterizing the matter waves is called the Wave Function (ψ).

Every wave is characterized by periodic variation in some physical quantity e.g. 1)pressure varies periodically in sound wave 2) electric & magnetic field varies periodically in electromagnetic wave.

Slimily the quantity whose periodic variation makes up the matter wave is called the wave function (ψ).

The value of the Wave Function (ψ) at a particular point (x, y, z) in space at time (t) is related to the probability of finding the particle at a point (x, y, z) & at time (t). The probability of finding the particle at a point (x, y, z) & at time (t) is positive value between 0 & 1. But Wave Function (ψ) can be positive, negative, or complex. Hence Wave Function (ψ) is not observable quantity.

❖ Physical significance of Wave Function (ψ) –

- According to Max Born interpretation probability of finding the particle described by the Wave Function (ψ) at a point (x, y, z) & at time (t) is proportional to the value of $|\boldsymbol{\psi}|^2$ at a point (x, y, z) & at time (t).
- A larger the value of $|\boldsymbol{\psi}|^2$ represents larger probability of finding the particle.
- The probability of finding the particle is '**zero**' at a point (x, y, z) & at time (t) only if $|\boldsymbol{\psi}|^2 = \mathbf{0}$ at that point.
- Even if there is a small value of $|\boldsymbol{\psi}|^2$ at a point (x, y, z) & at time (t), there will be some probability of finding the particle there.
- The probability of finding the particle in certain volume element 'dv = dx.dy.dz' is '$|\boldsymbol{\psi}|^2\,\mathbf{dv}$' is called the probability density.
- As the particle has to exist somewhere in space the total probability of finding the particle is **'1'**

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

❖ Schrodinger's wave equation:

The behavior of matter wave associated with the particle can be represented by an equation proposed by Schrodinger & hence known as Schrodinger's wave equation.

Schrodinger's wave equation having two types

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

❖ Schrodinger's time independent wave equation:

According to De-Broglie hypothesis, particle of mass 'm', move with velocity 'v' it shows wave nature & the wavelength of matter wave is

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

Where m = Mass of moving particle
v = Velocity of particle

Let us consider a system of stationary waves associated with moving particle. The wave equation is given by

$$\Psi = \Psi_0 \sin 2\pi \vartheta t \quad \dots\dots\dots \quad (1)$$

Where Ψ = wave function of stationary wave
Ψ_0 = amplitude of stationary wave

Differentiate equation (1) w.r.t. time 2 times, we get

$$\frac{\partial \Psi}{\partial t} = \Psi_0 \cos 2\pi \vartheta t \ (2\pi \vartheta)$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -\Psi_0 \sin 2\pi \vartheta t \ (2\pi \vartheta) \ (2\pi \vartheta)$$

$$\frac{\partial^2 \Psi}{\partial t^2} = (-4\pi^2 \vartheta^2) \Psi_0 \sin 2\pi \vartheta t \quad \dots\dots\dots \quad (2)$$

But from equation (1), equation (2) becomes

$$\frac{\partial^2 \Psi}{\partial t^2} = -4\pi^2 \vartheta^2 \Psi \quad \dots\dots\dots \quad (3)$$

But we know that $(\vartheta = \frac{v}{\lambda})$ so equation (3) becomes

$$\frac{\partial^2 \Psi}{\partial t^2} = -4\pi^2 \frac{v^2}{\lambda^2} \Psi \quad \dots\dots\dots \quad (4)$$

According to differential form of equation for progressive wave having wave velocity 'v' is given by

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = v^2 \frac{\partial^2 \Psi}{\partial x^2} \quad \dots\dots\dots \quad (5)$$

Compare equation (4) & (5) we get

$$v^2 \frac{\partial^2 \Psi}{\partial x^2} = -4\pi^2 \frac{v^2}{\lambda^2} \Psi \quad \dots\dots\dots \quad (6)$$

Put the value of 'λ' from equation (1), equation (6) becomes

$$\frac{\partial^2 \Psi}{\partial x^2} = -4\pi^2 \frac{m^2 v^2}{h^2} \Psi \quad \dots\dots\dots \quad (7)$$

T.E. = K.E. + P.E.

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

$$m^2 v^2 = 2m (E - V) \ \dots\dots \ (8)$$

Put the value of 'm^2v^2' from equation (8) in (7) we get

$$\frac{\partial^2\Psi}{\partial x^2} = -4\pi^2 \frac{2m\,(E - V)}{h^2}\,\Psi \quad \dots\dots\dots \quad (9)$$

Put the $\hbar = \frac{h}{2\pi}$ equation (9) become

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

$$\mathbf{\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\,\Psi = 0} \quad \dots\dots\dots. \quad (10)$$

Equation (10) is known as the Schrodinger's time independent wave equation.

❖ Schrodinger's time dependent wave equation:

Schrodinger's time dependent equation can be obtain from Schrodinger's time independent wave equation. Let us consider a system of stationary waves associated with moving particle. The differential equation of a progressive wave with a velocity u is given by

$$\frac{\partial^2\Psi}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2\Psi}{\partial t^2} \quad \dots\dots\dots (1)$$

Where ψ wave function and the solution of above equation is,

$$\Psi = \Psi_0 e^{-i\omega t} \quad \dots\dots\dots (2)$$

Differentiating equation (2) with respect to t, we get,

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

But, $\boldsymbol{\omega = 2\pi\vartheta}$

$$\frac{\partial\Psi}{\partial t} = -i\,2\pi\vartheta\,\Psi$$

But we know that $E = h\vartheta$ so ($\vartheta = \frac{E}{h}$) above equation becomes

$$\frac{\partial\Psi}{\partial t} = -i2\pi\frac{E}{h}\psi \quad \dots\dots\dots (3)$$

$$\frac{\partial\Psi}{\partial t} = -i2\pi\frac{E}{h}\psi \qquad (\because \hbar = \frac{h}{2\pi})$$

Multiply both side by $-\,\frac{\hbar}{i}$

$$-1\,\frac{\hbar}{i}\frac{\partial\Psi}{\partial t} = E\Psi \qquad (\because i^2 = -1)$$

$$\therefore E\Psi = i\,\hbar\frac{\partial\Psi}{\partial t} \quad \dots\dots\dots \quad (5)$$

From Schrodinger's time independent equation we get,

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

Multiply above equation by $\frac{\hbar^2}{2m}$

$$\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + E\Psi - V\Psi = 0$$

$$-\frac{\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi = E\Psi$$

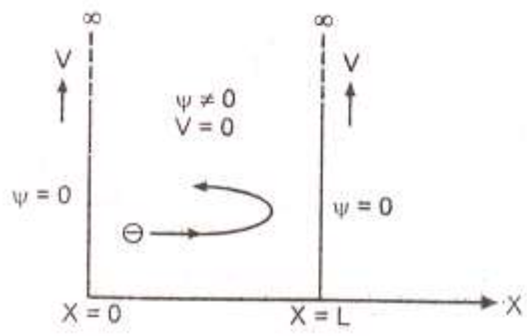
Then, putting the value of EΨ in above equation we get,

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

It is Schrodinger's time dependent equation

❖ Application of Schrodinger's wave equation:

(1-D infinite potential well OR particle in a rigid box**)**



In Quantum mechanics the fundamental description of the state of system is given in terms of wave function for that system. Schrodinger's equation when applied to any system determines the wave function for that system. It can also determine possible energy state of the system.
Consider a particle (electron) of mass m, which is restricted to move along x-axis between **'x=0 to x=L'** inside the box bounded by infinitely rigid walls. The particle bounce back & forth between the walls & the collision is perfectly elastic so total energy of the particle remain constant.
From quantum mechanics point of view P.E. of the particle infinite on the both side of the box & inside the box P.E. is constant, for our convenience we take **'V = 0'** inside the box.
So probability of the finding the particle outside the box is '**zero'** so **ψ = 0** for $X \leq 0$ and $x \geq L$
Consider Schrodinger's time independent

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0 \quad \dots\dots\dots \quad (1)$$

But the box is 1-D & V = 0 inside the box so equation (1) within box is

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m}{\hbar^2}E\Psi = 0 \quad \dots\dots\dots (2)$$

Putting, $\frac{2mE}{\hbar^2} = K^2 \quad \dots\dots\dots (3)$

$$\frac{\partial^2\Psi}{\partial x^2} + K^2\Psi = 0 \quad \dots\dots\dots (4)$$

The solution of above equation is

ψ = A sin (Kx + B) ------ (5)

Applying boundary conditions to the equation,

(1) **ψ = 0 at x = 0**

Equation (5) becomes

∴ A sin B = 0

But A ≠ 0 because amplitude never be zero

∴ sin B = 0

Since B= 0, π, 2π, 3π, …..

For our convince we assume **B = 0**

(2) ψ **= 0 at x=L**

Equation (5) become

∴ 0 = A sin KL

again A ≠ 0 because amplitude never be zero

∴ sin KL = 0

It is possible only when KL = nπ

Or $K=\frac{n\pi}{L}$ where n = 1,2,3,……. ----- (6)

Substituting value of K in equation (3),

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2} \quad \dots\dots\dots \quad (7)$$

$$E = \frac{n^2\pi^2}{L^2}\frac{\hbar^2}{2m} = \frac{n^2\pi^2}{L^2}\frac{h^2}{4\pi^2 2m} \quad (\because \hbar = \frac{h}{2\pi})$$

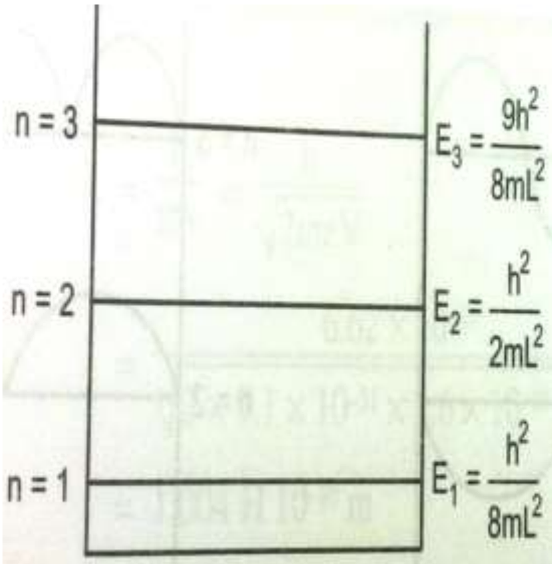
$$E_n = \frac{n^2h^2}{8mL^2} \quad \dots\dots\dots (8)$$

For electron h = 6.63 x 10^{-34}Js, m = 9.1 x 10^{-31}kg, L = $1A^0$, equation (8) becomes

E_n = 38n^2 eV ----- (9)

The meaning of above equation is that the particle in box has discrete value of energy. Here n≠0 because the particle cannot have zero energy. If the energy of particle zero i.e. n=0 then wave function ψ is zero inside the box that is, particle never exist inside the box. Therefore E=0 is not permissible in this case.

The energy level diagram for an electron in one dimensional box is,



Derive the expression for probability of finding a particle confined in a box of width L.

The solution of Schrodinger time independent equation is

$$\Psi_n = A\sin Kx ----(1) \quad \text{where, } K = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\therefore \Psi_n = A\sin\sqrt{\frac{2mE}{\hbar^2}}\ x \quad (\because \hbar = \frac{h}{2\pi})$$

$$\therefore \Psi_n = A\sin\sqrt{\frac{2mE4\pi^2}{h^2}}\ x \quad (\because E = \frac{n^2h^2}{8mL^2})$$

$$\Psi_n = A\sin\sqrt{\frac{8m\pi^2}{h^2}\frac{n^2h^2}{8mL^2}}\ x$$

$$\therefore \Psi_n = A\sin\sqrt{\frac{n^2\pi^2}{L^2}}\ x$$

$$\therefore \Psi_n = A\sin\left(\frac{n\pi x}{L}\right) \quad ----(2)$$

The probability of finding a particle confined in a box of width L is given as,

$$\int_{-\infty}^{\infty}|\Psi_n|^2\,dx = \int_0^L|\Psi_n|^2\,dx$$

$$= A^2\int_0^L \sin^2\frac{n\pi x}{L}\,dx \quad (\because \sin^2\theta = \frac{1-\cos^2\theta}{2})$$

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

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

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

$$= \frac{A^2}{2}\left[(L-0)-\frac{L}{2n\pi}(\sin 2n\pi - \text{Sin } 0)\right]$$

$$\int_{-\infty}^{\infty}|\Psi_n|^2\,dx = \frac{A^2}{2}\left[L-\frac{L}{2n\pi}(0-0)\right] = \frac{A^2 L}{2} \quad ----(3)$$

For normalize wave equation,

$$\int_{-\infty}^{\infty}|\Psi_n|^2\,dx = 1 \quad ----(4)$$

From equation (3) & (4) we get,

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

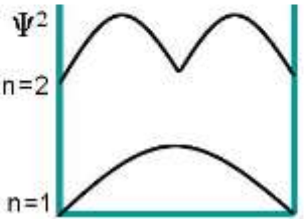
$$\therefore \Psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad ----(5)$$

Particle in the box is a problem under quantum mechanical conditions. The most probable location of the particle in the box and its energies we can write eign function Ψ_1, Ψ_2, Ψ_3 of particle in a box by putting n = 1, 2, 3, ---

Case 1: for n = 1

$$\therefore \Psi_1 = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}\right)x$$

Here, $\Psi_1 = 0$ for both x = 0 and x = L, but Ψ_1 has maximum value for x = L/2



Quantum Computing:

- Developing a computer that uses quantum mechanical phenomenon to perform operation on data through devises such as superposition and entanglement.
- **Quantum superposition** states that, much like waves in classical physics, any two (or more) quantum states can be added together (“superposed”) and the result will be another valid quantum state.
- **Quantum entanglement** is a quantum mechanical phenomenon in which the quantum states of two or more objects have to be described with reference to each other, even though the individual objects may be spatially separated.
- **Quantum bits (Qubits):** Quantum computers use Quantum bits (Qubits) i.e. bits 0, 1 & both of them simultaneously to run machine faster.
- Quantum computing uses the power of atoms and molecules to perform memory and processing tasks.
- It is high speed parallel computer based on quantum mechanics.
- The information storage in quantum computer is in Quantum bit based on direction of an electron spin.

Advantages of Quantum Computing:

- Very high speed can be achived.
- Use of Qubit allows handeling number of calculations.
- Classical algorothms calculations are also performed.
- Very small size.
- Less power consumes.

Disadvantages of Quantum Computing:

- Technology required to implement a quantum computer is not avilable at present.
- Consistent electron is damaged as soon as it is affected by its environment and that electron is very much essential for the functioning of quantum computers.
- The research on this problem is still going on and require time, efforts and high cost.

Difference between Classical and Quantum Computer:

Sr. No	Classical Computer	Sr. No	Quantum Computer
1.	It is Large Scale integrated multi purpose computer.	1.	It is high speed parallel computer based on quantum mechanics.
2.	Information storage is bit based on voltage or charge etc.	2.	Information storage is Quantum bit based on direction of an electron spin.
3.	Information processing is carried out by logic gates. Ex. NOT, AND, OR etc.	3.	Information processing is carried out by Quantum logic gates.
4.	Circuit behavior is governed by classical physics.	4.	Circuit behavior is governed explicitly by quantum mechanics.
5.	Classical computers use binary codes i.e. bits 0 or 1 to represent information.	5.	Quantum computers use Qubits i.e. bits 0, 1 & both of them simultaneously to run machine faster.
6.	Operation are defined by Boolean Algebra.	6.	Operation are defined by linear algebra over Hilbert Space & can be represented by unitary matrices with complex element.
7.	No restriction exist on copying or measuring signals.	7.	Severe restriction exist on copying or measuring signals.
8.	Circuit are easily implemented in fast, scalable and macroscopic technologies such as CMOS.	8.	Circuit must use macroscopic technologies that are slow, fragile and not yet scalable e.g. NMR (Nuclear Magnetic Resonance).

Numerical of De Broglie wavelength:

1) A bullet of mass 40 gm. and electron both travel with the velocity of 1100 m/s. What wavelength can be associate with them?

- **For Electron:**

  $h = 6.63 \times 10^{-34}\, Js,$

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

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

  $v = 1100\, m/s$

  $\lambda = ?$

  $$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 1100}$$

  $\boldsymbol{\lambda = 0.0006623 \times 10^{-3} m}$

  $\boldsymbol{\lambda = 6.623 \times 10^{-7} m}$

  $\boldsymbol{\lambda = 6623 \times 10^{-10} = 6623\, A^{o}}$

- **For Bullet:**

  $h = 6.63 \times 10^{-34}\, Js,$

$m = 40\ gm = 40\ \times 10^{-3}\ Kg,$
$v = 1100\ m/s$
$\lambda = \ ?$

$$\lambda = \frac{h}{mv} = \frac{6.63\ \times 10^{-34}}{40\ \times 10^{-3}\ \times 1100}$$

$$\boldsymbol{\lambda = 0.0001507 \times 10^{-31} m}$$

$$\boldsymbol{\lambda = 1.507 \times 10^{-35} m}$$

2) Calculate the De-Broglie wavelength of the proton moving with a velocity equal to $\frac{1}{20}$ th of velocity of light. Mass of proton is $1.6\ \times 10^{-27}\ Kg$.

Given:

$h = 6.63\ \times 10^{-34}\ Js,$
$m = 1.6\ \times 10^{-27}\ Kg,$

$$v = \frac{1}{20} \times 3 \times 10^{8}\ m/s$$

$\lambda = \ ?$

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

$$\lambda = \frac{6.63\ \times 10^{-34}}{1.6\ \times 10^{-27}\ \times \frac{1}{20} \times 3 \times 10^{8}}$$

$$\boldsymbol{\lambda = 2.763\ \times 10^{-14}\ m}$$

3) Calculate the wavelength of the wave associate with a neutron moving with energy 0.025 eV. Mass of neutron is $1.676\ \times 10^{-27}\ Kg$.

Given:

$h = 6.63\ \times 10^{-34}\ Js,$
$m = 1.676\ \times 10^{-27}\ Kg,$
$E = 0.025\ eV$
$= 0.025 \times 1.6\ \times 10^{-19}\ J$
$\lambda = \ ?$

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

$$\lambda = \frac{6.63\ \times 10^{-34}}{\sqrt{2 \times 1.676\ \times 10^{-27} \times 0.025 \times 1.6\ \times 10^{-19}}}$$

$$\boldsymbol{\lambda = 1.811\ \times 10^{-10}\ m}$$

4) Calculate the De-Broglie wavelength associate with an α-particle accelerated by a potential difference of 100 KV. Mass of α-particle is $1.68\ \times 10^{-27}\ Kg$.

Given:

$h = 6.63\ \times 10^{-34}\ Js,$
$m = 1.68\ \times 10^{-27}\ Kg,$
$V = 100\ KV$
$= 100 \times 10^{3}$ Volts
$q = 2e = 2 \times 1.6 \times 10^{-19} C$
$q = 3.2 \times 10^{-19} C$

$\lambda = ?$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2meV}} \; \ldots\ldots\ldots (\mathbf{1\ marks})$$

$$\lambda = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 1.68 \times 10^{-27} \times 3.2 \times 10^{-19} \times 100 \times 10^{3}}}$$

$$\boldsymbol{\lambda = 3.206 \times 10^{-14}\ m}$$

5) Calculate group velocity and kinetic energy for a fast moving electron associate with a de-Broglie wavelength of 0.3 nm.

Given: $h = 6.63 \times 10^{-34}\ Js, m = 9.1 \times 10^{-31}\ Kg, E = ?$

$\lambda = 0.3\ nm = 0.3 \times 10^{-9}$ m, v = ?

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

$$\boldsymbol{E = \frac{h^2}{2m\lambda^2}} \quad \ldots\ldots (\mathbf{1\ marks})$$

$$E = \frac{6.63 \times 10^{-34}}{2 \times 9.1 \times 10^{-31} \times (0.3 \times 10^{-9})^2}$$

$$\boldsymbol{E = 2.683 \times 10^{-18}\ \mathrm{J}} \quad \ldots\ldots (\mathbf{2\ marks})$$

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

$$\mathbf{v} = \sqrt{\frac{2E}{m}} = \sqrt{\frac{2 \times 2.683 \times 10^{-18}}{9.1 \times 10^{-31}}} = \sqrt{5.896 \times 10^{12}} \ldots\ldots (\mathbf{1\ marks})$$

$$\boldsymbol{v = 2.428 \times 10^{6}\ \mathrm{m/s}} \quad \ldots\ldots (\mathbf{1marks})$$

The group velocity of an electron is $\boldsymbol{v_g = v = 2.428 \times 10^{6}\ m/s}$

Numerical of Heisenberg Uncertainty Principle:

6) Using Heisenberg uncertainty principle show that electron does not exist in nucleus:

Consider approximate radius of nucleus = r = 0.5 x 10^{-14} m

Let imaging that electron exist in nucleus.

∴ Uncertainty in position if electron exist in nucleus = $\Delta x = 2r = 2 \times 0.5$ x 10^{-14}

∴ $\boldsymbol{\Delta x = 1 \text{ x } 10^{-14}}$ **m ……. (1)**

According to Heisenberg's uncertainty principle

$$\boldsymbol{\Delta x \,.\, \Delta P_x \geq \frac{\hbar}{2}}$$

$$\therefore \boldsymbol{\Delta P_x} = \frac{\hbar}{2\Delta x} = \frac{1.055 \times 10^{-34}}{2 \times 10^{-14}} = \mathbf{0.5275 \times 10^{-20}}\ \ kgm/s$$

$$E = mc^2 = p.c = 0.5275 \times 10^{-20} \times 3 \times 10^{8} = 1.5825 \times 10^{-12}\ \mathrm{J}$$

$$E = \frac{1.5285 \times 10^{-12}}{1.6 \times 10^{-19}}\ eV = 0.989 \times 10^{7}\ eV$$

Energy of Electron can be calculate as:

$E = mc^2$

$E = 9.1 \times 10^{-31} \times (3 \times 10^{8})^2$

$E = 81.9 \times 10^{-15}$ J

$$E = \frac{81.9 \times 10^{-15}}{1.6 \times 10^{-19}}\ \mathrm{eV}$$

$E = 51.187 \times 10^{4}\ eV$

$E = 0.51 \times 10^{6}\ eV$

$E = 0.51\ MeV \approx \boldsymbol{0.5\ MeV}$

$E = 9.89 \times 10^{6}\ eV = 9.89\ MeV$

$\boldsymbol{E \approx 10\ MeV}$

If the electron exist in a nucleus, it must have energy 10 MeV. But electron have energy 0.5 MeV. Therefore electron cannot exist in nucleus.

7) **An electron has a speed of 400 m/s with uncertainty of 0.01%. Find the accuracy in its position.**

Given:

v = 400 m/s

% error = 0.01 %

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

$\mathrm{h} = 6.63 \times 10^{-34}$ JS

$\Delta \mathrm{x} = ?$

$\Delta \mathrm{v} = \mathrm{v} \times \%\mathrm{error}$

$$\Delta v = 400 \times \frac{0.01}{100}$$

$\boldsymbol{\Delta v = 0.04\ \ \mathrm{m/s}}$

$\Delta p = m\Delta v = 9.1 \times 10^{-31} \times 0.04$

$\Delta p = 0.364 \times 10^{-31}\ \ kgm/s$

$\boldsymbol{\Delta p = 3.64 \times 10^{-32}\ \ kgm/s}$

According to Heisenberg uncertainty principle,

$$\Delta x\ .\ \Delta P_x \geq \frac{\hbar}{2} \qquad \because \hbar = \frac{h}{2\pi}$$

$$\therefore \Delta x\ .\ \Delta P_x \geq \frac{h}{4\pi}$$

$$\therefore \Delta x \geq \frac{h}{4\pi} \times \frac{1}{\Delta P_x} = \frac{6.63 \times 10^{-34}}{4 \times 3.142 \times 3.64 \times 10^{-32}}$$

$\therefore$ $\boldsymbol{\Delta x = 0.1449 \times 10^{-2}\ \ m}$

$\therefore$ $\boldsymbol{\Delta x = 1.449 \times 10^{-3}\ \ m}$

8) **An electron has a speed of 900 m/s with uncertainty of 0.001%. Calculate the uncertainty in the position of the electron.**

Given:

v = 900 m/s

% error = 0.001 %

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

$\mathrm{h} = 6.63 \times 10^{-34}$ JS

$\Delta \mathrm{x} = ?$

$\Delta \mathrm{v} = \mathrm{v} \times \%\mathrm{error}$

$$\Delta v = 900 \times \frac{0.001}{100}$$

$\Delta v = \mathbf{0.009\ m/s}$

$\Delta p = m\Delta v = 9.1 \times 10^{-31} \times 0.009$

$\Delta p = 0.0819 \times 10^{-31}\ \ kgm/s$

$\boldsymbol{\Delta p = 8.19 \times 10^{-33}\ \ kgm/s}$

According to Heisenberg uncertainty principle,

$\Delta x\ .\ \Delta P_x \geq \frac{\hbar}{2} \qquad \because \hbar = \frac{h}{2\pi}$

$\therefore \Delta x\ .\ \Delta P_x \geq \frac{h}{4\pi}$

$\therefore \Delta x\ \geq \frac{h}{4\pi} \times \frac{1}{\Delta P_x} = \frac{6.63 \times 10^{-34}}{4 \times 3.142 \times 8.19 \times 10^{-33}}$

$\therefore \boldsymbol{\Delta x = 0.0644 \times 10^{-1}\ \ m}$

$\therefore \boldsymbol{\Delta x = 6.44 \times 10^{-3}\ \ m}$

9) **The speed of an electron is measured to within an uncertainty of 2×10^4 m/s. What is the minimum space required by the electron to be confined to an**

Given:

$\Delta v = 2 \times 10^4$

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

$h = 6.63 \times 10^{-34}$ JS

$\Delta x = ?$

According to Heisenberg uncertainty principle,

$\Delta x\ .\ \Delta P_x \geq \frac{\hbar}{2} \qquad \because \hbar = \frac{h}{2\pi}$

$\therefore \Delta x\ .\ m\ \Delta v \geq \frac{h}{4\pi}$

$\therefore \Delta x\ \geq \frac{h}{4\pi} \times \frac{1}{m\ \Delta v}$

$\therefore \Delta x = \frac{6.63 \times 10^{-34}}{4 \times 3.142 \times 9.1 \times 10^{-31} \times 2 \times 10^4}$

$\therefore \boldsymbol{\Delta x = 0.02898 \times 10^{-7}\ \ m}$

$\therefore \boldsymbol{\Delta x = 2.898 \times 10^{-9}\ \ m}$

10) **A position and momentum of 1 KeV electron are simultaneously measured. If position is located within 10 nm then what is the percentage uncertainty in its momentum?**

Given:

$E = 1\ \text{KeV} = 1000 \times 1.6 \times 10^{-19}$ J

$E = 1600 \times 10^{-19}$ J

$\Delta x = 10\ nm = 10 \times 10^{-9}\ m$

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

$h = 6.63 \times 10^{-34}$ JS

$\frac{\Delta p}{p} \times 100 = ?$

$p = \sqrt{2mE}$

$$p = \sqrt{2 \times 9.1 \times 10^{-31} \times 1600 \times 10^{-19}}$$

$$\boldsymbol{p = 1.706 \times 10^{-23} \quad kgm/s}$$

According to Heisenberg uncertainty principle,

$$\therefore \Delta x \,.\, m\,\Delta v \geq \frac{h}{4\pi}$$

$$\therefore \Delta p \geq \frac{h}{4\pi} \times \frac{1}{\Delta x}$$

$$\therefore \Delta p = \frac{6.63 \times 10^{-34}}{4 \times 3.142 \times 10 \times 10^{-9}}$$

$$\therefore \boldsymbol{\Delta p = 5.275 \times 10^{-27} \;\; Kg\, m/s}$$

$$\frac{\Delta p}{p} \times 100 = \frac{5.275 \times 10^{-27}}{1.706 \times 10^{-23}}$$

$$\boldsymbol{\frac{\Delta p}{p} \times 100 = 0.0309\,\%}$$

Numerical of 1-D infinite potential well OR particle in a rigid box:

11) Find the lowest energy of a neutron confined to a nucleus of size 10^{-14} m in eV. Given the mass of neutron is $1.676 \times 10^{-27}\ kg$ and $h = 6.63 \times 10^{-34}\ JS$.

Given:

$L = 10^{-14}\ m$

For lowest energy, n=1

$m = 1.676 \times 10^{-27}$ kg

$h = 6.63 \times 10^{-34}$ JS

$E_1 = ?$

The formula for energy of particle is,

$$\mathbf{E_n = \frac{n^2 h^2}{8 m L^2}}$$

$$E_1 = \frac{1^2 \times (6.63 \times 10^{-34})^2}{8 \times 1.676 \times 10^{-27} \times (10^{-14})^2}$$

$$E_1 = 3.278 \times 10^{-13} \quad \mathrm{J}$$

$$E_1 = \frac{3.278 \times 10^{-13}}{1.6 \times 10^{-19}} \quad \mathrm{eV}$$

$$\mathbf{E_1 = 2.048 \times 10^{6} \quad eV}$$

$$\mathbf{E_1 = 2.048 \quad MeV}$$

12) Calculate the lowest three energy states of an electron confined in potential well of width 10 A°. Given the mass of electron is $9.1 \times 10^{-31}\ kg$ and $h = 6.63 \times 10^{-34}\ JS$.

Given:

$L = 10\ \text{A°} = 10 \times 10^{-10}\ m$

For lowest three energy,

n=1, n=2, and n=3

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

$h = 6.63 \times 10^{-34}$ JS

$E_1 = ?$

$E_2 = ?$

$E_3 = ?$

The formula for energy of particle is,

$$\mathbf{E_n = \frac{n^2h^2}{8mL^2} = \boldsymbol{n^2E_1}}$$

$$E_1 = \frac{h^2}{8mL^2} = \frac{1^2 \times (6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (10 \times 10^{-10})^2}$$

$$E_1 = \frac{43.9569 \times 10^{-17}}{7280} = \mathbf{6.0380 \times 10^{-20}\ J}$$

$$E_2 = n^2E_1 = 2^2 \times 6.0380 \times 10^{-20} = \mathbf{24.152 \times 10^{-20} J}$$

$$E_3 = n^2E_1 = 3^2 \times 6.0380 \times 10^{-20} = \mathbf{54.342 \times 10^{-20} J}$$

13) The lowest energy of an electron trapped in a one dimensional box is 3.2 X 10^{-18} J. Calculate the width of the box. Also calculate the next two energies in eV the particle can have?

Given:

$$E_1 = 3.2 \times 10^{-18} J = \frac{3.2 \times 10^{-18}}{1.6 \times 10^{-19}}\ eV = 20\ eV$$

$L = ?$

$m = 3.1 \times 10^{-31}$ kg

$h = 6.63 \times 10^{-34}$ JS

$E_2 = ?$

$E_3 = ?$

The formula for energy of particle is,

$$\mathbf{E_1 = \frac{h^2}{8mL^2} = \boldsymbol{n^2E_1}}$$

$$L = \sqrt{\frac{h^2}{8mE_1}} = \sqrt{\frac{1^2 \times (6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times 3.2 \times 10^{-18}}}$$

$$L = \sqrt{\frac{43.9569 \times 10^{-20}}{23.296}} = \mathbf{1.3736 \times 10^{-10}}\ m$$

$$\mathbf{L = 13.736 \times 10^{-10}\ m = 13.736\ A^\circ}$$

$$E_2 = n^2E_1 = 2^2 \times 20 = \mathbf{80\ eV}$$

$$E_3 = n^2E_1 = 3^2 \times 20 = \mathbf{180\ eV}$$