:- Quantum mechanism :-

According to newton corpuscular theory light travels in form of tiny particle called corpuscle.

when these particles falls on the retina sensation of region take place.

by particle theory we can explain phenomena of reflection refraction of light but

phenomena of interference, diffraction, polarisation can be explain by Huygens wave theory.

Whereas Maxwell's EMT says light is a EMW but phenomenon of PEE, compton effect absorption ~~spectra~~, or radiation cannot be explain by above these theory.

these can be explain by quantum theory. According to this quantum theory vibrating atomic particle with different frequency radiate energy in discrete manner not in continuous manner. And it is given by

$$\boxed{E = nh\nu}$$

Where n is an integer and h is plank constant ν - frequency.

by Quantum theory we can explain the transition of atom and emission of energy.

and energy radiated during transition will be integral multiple of '$h\nu$'

Particle → mass, velocity, P, Position
wave → λ, T, amplitude, intensity

Failure of classical mechanics:-

→ A classical mechanics can be applied on motion of bodies which observable or can be observe by some instrument.

→ As we know that negatively charged particle revolve around the positively charged nucleus there will be attractive force between e and nucleus therefore, the e should collapse into nucleus classically.

→ As the e experiences centripetal acceleration and we know that accelerated charged particle radiates energy classically, there is decrease in E and again it should collapse in nucleus but it doesn't happen.

Such motion can be explain by quantum mechanics considering vibration of electron.

Dual nature:-

De-broglie concept:- According to debroglie concept when a particle is moving in space a wave is associated with it. If a particle of mass 'm' is moving with velocity v,

then wavelength of wave associated with particle

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

Date
Page

$$\boxed{\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2meV}} = \frac{h}{\sqrt{3mkT}}}$$

Schrodinger's equation :- If a particle of mass 'm' is moving with velocity 'v' at any instant If its potential energy is 'V' then

$$T.E = K.E + PE$$

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

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

$$p = \sqrt{2m(E-V)}$$

$$\lambda = \frac{h}{(2m(E-V))^{1/2}} \quad \text{—— (A)}$$

$$\nabla^2 \phi = \frac{1}{v^2}\frac{\partial^2 \phi}{\partial t^2} \quad \text{—— (3)}$$

$$\phi = \phi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \phi}{\partial t^2} = -\omega^2 \phi_0 e^{-i\omega t}$$

$$\frac{\partial \phi}{\partial t^2} = -\omega^2 \phi$$

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

$$\nabla^2\phi = \frac{-(2\pi\nu)^2}{\left(\frac{v}{\lambda}\right)^2}$$

$$\cancel{\nabla^2\phi = -4\pi\lambda^2}$$

$$\cancel{\nabla^2\phi = \frac{-4\pi h^2}{(2m(E-V))}}$$

$$\nabla^2\phi = \frac{-4\pi}{h^2}(2m(E-V))\cancel{\phi}$$

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

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

(time independent equation)

time dependent

$$\phi = \phi_0 e^{-i\omega t}$$

$$\frac{\partial\phi}{\partial t} = -\phi_0 i\omega e^{-i\omega t}$$

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

$$\frac{\partial\phi}{\partial t} = \frac{\omega\phi}{i} \qquad \omega = 2\pi\frac{E}{h}$$

$$\frac{\partial\phi}{\partial t} = \frac{2\pi E\phi}{hi}$$

$$\left(\frac{\partial\phi}{\partial t}\right)\frac{hi}{2\pi} = E\phi = i\hbar\frac{\partial\phi}{\partial t} \quad (5)$$

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

$$\nabla^2\phi - \frac{2mV\phi}{\hbar} = -\frac{2m}{\hbar}E\phi$$

$$-\left(\nabla^2\phi - \frac{2mV\phi}{\hbar}\right)\frac{\hbar}{2m} = E\phi$$

$$\cancel{2m}\ V\phi - \frac{\hbar}{2m}\nabla^2\phi = E\phi$$

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

$$\phi\left(-\frac{\hbar}{2m}\nabla^2 + V\right)$$

$$H\phi = E\phi$$

$$H \Rightarrow \left(-\frac{\hbar}{2m}\nabla^2 + V\right)$$ Hemitonian Operator

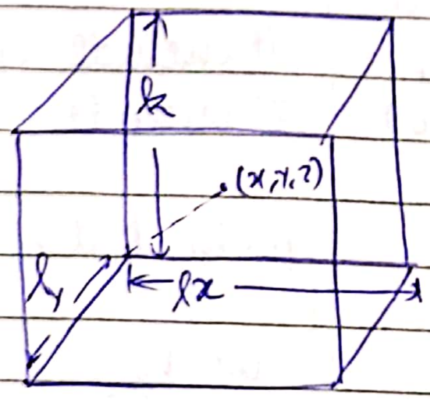
$$\nabla x \cdot \Delta p \geq \frac{h}{4\pi}$$

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

$$\nabla \theta \cdot \Delta w \geq h/4w$$

Date
Page

Let us consider a particle in 3-D Box



and $\frac{\partial^2\psi}{}$

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

Let us consider a particle of mass 'm' confined in a 3-D box of edge lengths l_x, l_y and l_z

Let at any instant if position of particle is 'P' with co-ordinate (x, y, z),

inside the box let potential $V=0$, it rises suddenly to a very high value at the boundaries and it is infinity at outside the boundaries. Therefore as a particle reaches the boundary it rebound back simultaneously so the speed of particle at the boundaries is zero.

Initially

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}(E_x + E_y + E_z)\psi = 0$$

$$(\vec{E} = E_x\hat{i} + E_y\hat{j} + E_z\hat{k})$$

multiply and divided by $\psi = X(x)\,Y(y)\,Z(z)$

$$\left\{\frac{1}{X}\frac{\partial^2 X}{\partial x^2}+\frac{1}{Y}\frac{\partial^2 Y}{\partial x^2}+\frac{1}{Z}\frac{\partial^2 Z}{\partial x^2}+\frac{2m}{\hbar}(E_x+E_y+E_z)\right.$$

$$\left.\begin{aligned}
&\frac{1}{X}\frac{\partial^2 X}{\partial x^2}+\frac{2m}{\hbar^2}E_x X=0\\
&\frac{1}{Y}\left(\frac{\partial^2 Y}{\partial y^2}\right)+\frac{2m}{\hbar^2}E_y Y=0\\
&\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}+\frac{2m}{\hbar^2}E_z Z=0
\end{aligned}\right\}$$

Solution of such differential equation

$$X(x) = A\sin(Bx+C)$$

A, B, C are constant

boundary consideration

at $x=0$

Here $|\psi(x)|^2$ is probability of finding of particle but it is zero at the boundaries.

therefore

$|\psi|^2=0$ at $x=0$ and $x=l_x$

at $x=0$

$$0 = A\sin(B\times 0+C)$$

$$\boxed{C=0}$$

at $x=l_x$ $\quad 0 = A\sin(Bl_x)=0$

$$A\sin(Bl_x)=0$$

$$Bl_x = n_x\pi$$

$$\boxed{B=\frac{n_x\pi}{l_x}}$$

$$\boxed{X = A\sin\left(\frac{n_x\pi}{l_x}x\right)}$$

Appling normalization condition

$$\int_0^{l_x} |\psi(x)|^2 dx = 1$$

$$\int_0^{l_x} X^2 dx = 1$$

$$\int_0^{l_x} A^2 \sin^2\left(\frac{n_x\pi}{l_x}x\right) dx$$

$$A^2\int\left(\frac{1-\cos(2\omega)}{2}\right)dx$$

$$\frac{A^2}{2}\int\left(1-\cos\left(\frac{2n_x\pi x}{l_x}\right)\right)dx = 1$$

$$\frac{A^2}{2}\left[x - \sin\left(\frac{2n_x\pi x}{l_x}\right) \times \frac{l_x}{2n_x\pi}\right]_0^{l_x}$$

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

$$\boxed{A = \sqrt{\frac{2}{l_x}}}$$

$$X(x) = \sqrt{\frac{2}{l_x}} \sin\left[\left(\frac{n_x \pi}{l_x}\right) x\right]$$

$$Y(y) = \sqrt{\frac{2}{l_y}} \sin\left[\frac{n_y \pi}{l_y} \cdot x\right]$$

$$Z(z) = \sqrt{\frac{2}{l_z}} \sin\left[\frac{n_z \pi}{l_z} \cdot z\right]$$

therefore

$$\psi(x) = X(x) \cdot Y(y) \cdot Z(z)$$

$$\boxed{\sqrt{\frac{2}{l_x}} \sqrt{\frac{2}{l_y}} \sqrt{\frac{2}{l_z}} \sin\left(\frac{n_x \pi}{l_x} x\right) \sin\left(\frac{n_y \pi}{l_y} \cdot y\right) \sin\left(\frac{n_z \pi}{l_z} \cdot z\right)}$$

$$\frac{\partial^2 X}{\partial x^2} + \frac{2m}{\hbar^2} E_x X = 0 \quad \text{—— (1)}$$

$$X = \sqrt{\frac{2}{l_x}} \sin\left(\frac{n_x \pi}{l_x} \cdot x\right)$$

$$\frac{\partial X}{\partial x^2} = \sqrt{\frac{2}{l_x}} \cos\left(\frac{n_x \pi}{l_x} \cdot x\right) \times \frac{n_x \pi}{l_x}$$

$$\frac{\partial^2 X}{\partial x^2} = -\sqrt{\frac{2}{l_x}} \times \left(\frac{n_x \pi}{l_x}\right)^2 \sin\left(\frac{n_x \pi \cdot x}{l_x}\right)$$

$$\frac{\partial^2 X}{\partial x^2} = -\left(\frac{n_x \pi}{l_x}\right)^2 X$$

Putting in ①

$$-\left(\frac{n_x \pi}{l_x}\right)^2 \cancel{X} + \frac{2m}{\hbar^2} E_x \cancel{X} = 0$$

$$\frac{2m}{\hbar^2} E_x = \left(\frac{n_x \pi}{l_x}\right)^2$$

$$\boxed{E_x = \frac{\hbar^2}{2m}\left(\frac{n_x \pi}{l_x}\right)^2}$$