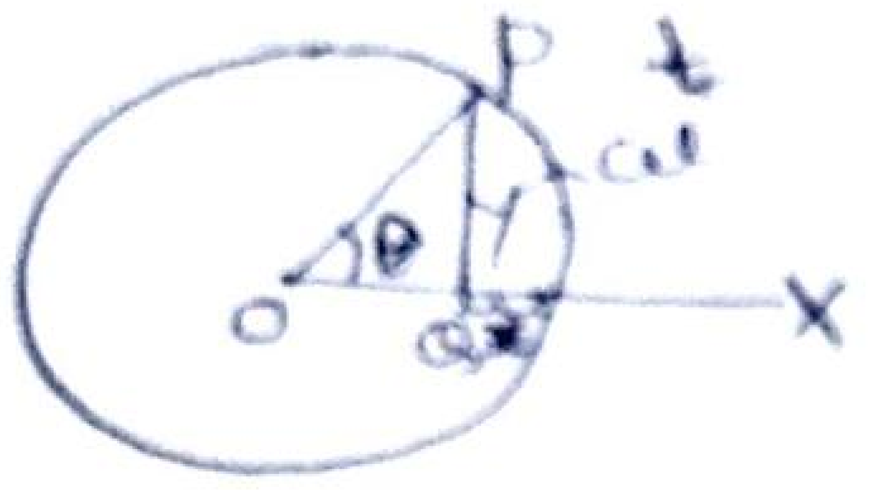
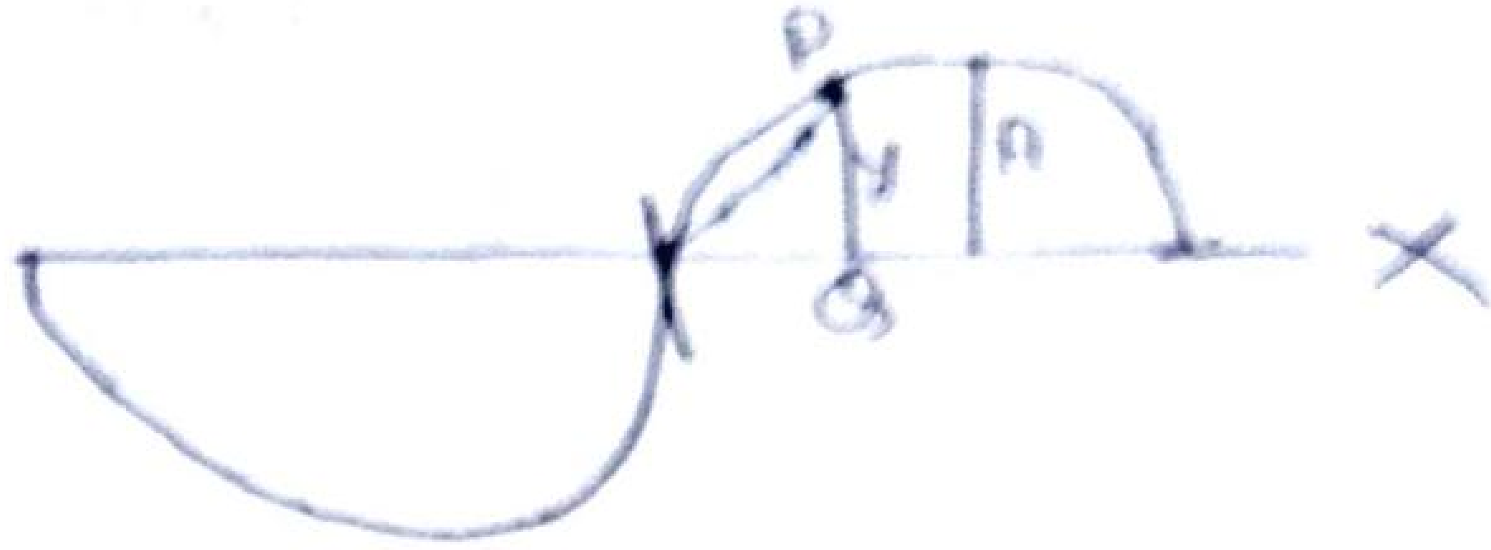
T.D.C. Part III rd   Dr. Vijay Kumar

Physical Chemistry   Wave Mechanics

Schrodinger's Wave Equation





Suppose a wave of a microparticle of mass 'm' moves with angular velocity ω rad./sec and linear velocity 'C' cm/sec.

Suppose in time 't' sec., the particle wave comes to point 'P' forming angle θ radian at the centre and covering linear distance x along x-axis.

So, $$\theta = \omega t$$

and $$x = ct$$

Ang. vel. (ω) = Angle (θ) / time (t)
velocity (c) = distance (x) / Time (t)

From Δ OPQ

$$\frac{PQ}{OP} = \sin\theta.$$

PQ = height of wave at point 'Q' which is called amplitude function (or wave function) of the wave which is function of x and t. Let the amplitude function be represented by y

So, $$y = f(x, t)$$

OP = Maximum amplitude which is constant for a particular wave.

Let it be represented by 'A'

So, $$\frac{y}{A} = \sin\theta$$

or $y = A \sin \theta$

or $y = A \sin \omega t$ ——— (1)

The cycles completed in 1 sec by a wave is called its frequency (ν)

ν = cycle per sec. = Hz.

One complete cycle = 2π radian.

$\because$ ω rad. in 1 sec

$\therefore$ 2π rad. in $\frac{2\pi}{\omega}$ sec.

$\because$ $\frac{2\pi}{\omega}$ sec = 1 cycle

$\therefore$ 1 sec = $\frac{\omega}{2\pi}$ cycles

$$\therefore \quad \nu = \frac{\omega}{2\pi}$$

or, $\omega = 2\pi\nu$

So, from equation (1)

$y = A \sin 2\pi\nu t$ ——— (11)

$\because$ $x = c \cdot t$ $\therefore$ $t = \frac{x}{c}$

So, from equation (11).

$y = A \sin 2\pi\nu \frac{x}{c}$ ——— (111)

$\because$ $\nu = \bar{\nu} c = \frac{c}{\lambda}$

So, $y = A \sin 2\pi \frac{\cancel{c}}{\lambda} \cdot \frac{x}{\cancel{c}}$

or $y = A \sin 2\pi \frac{x}{\lambda}$ ——— (IV)

Schrodinger's equation with the double differentiation of equation (IV) which is given as

$$y = A \sin 2\pi \frac{x}{\lambda}$$

$$\frac{d \sin mx}{dx} = m \cos mx$$

$$\frac{\partial y}{\partial x} = A \cdot \frac{2\pi}{\lambda} \cdot \cos 2\pi \frac{x}{\lambda}$$

$$\frac{\partial^2 y}{\partial x^2} = -A \frac{4\pi^2}{\lambda^2} \sin 2\pi \frac{x}{\lambda}$$

or $$\frac{\partial^2 y}{\partial x^2} = -\frac{4\pi^2}{\lambda^2} \cdot A \sin 2\pi \frac{x}{\lambda}$$

or $$\frac{\partial^2 y}{\partial x^2} = -\frac{4\pi^2}{\lambda^2} \cdot y \qquad \text{(V)}$$

Now, from de-Broglie's equation,

$$\lambda = \frac{h}{mv} \qquad \therefore \lambda^2 = \frac{h^2}{m^2 v^2}$$

or, $$\frac{\partial^2 y}{\partial x^2} = -\frac{4\pi^2 m^2 v^2}{h^2} \cdot y(x)$$

or, $$\frac{\partial^2 y}{\partial x^2} = -\frac{4\pi^2 m \cdot 2 \times \frac{1}{2} m v^2}{h^2} \cdot y(x)$$

or, $$\frac{\partial^2 y}{\partial x^2} = -\frac{8\pi^2 m \cdot K.E}{h^2} \cdot y(x)$$

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

Total energy, $E = K.E + P.E$

$\therefore K.E = E - P.E$

$= E - V$

or, $$\frac{\partial^2 y}{\partial x^2} = \frac{-8\pi^2 m (E - V)}{h^2} \cdot y(x)$$

or, $$\frac{\partial^2 y}{\partial x^2} + \frac{8\pi^2 m (E - V)}{h^2} y(x) = 0 \qquad \text{(VI)}$$

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Equation (VI) is schrodinger's wave equation along y axis only.

But wave is free to propagate along all the three axis x, y and z

So, $y_{(x)}$ may be replaced by a wave function ψ which is function of x, y and z.

So, equation (VI) comes to be —

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi_{(x,y,z)} = 0 \quad \text{(VII)}$$

Equation (VII) is schrodinger's equation for three dimensional wave

Terms : ψ = Amplitude function or wave function which is function of x, y and z variables along x, y and z axis.

m = mass of microparticle (electron)

h = plank's constant.

E = Total energy.

V = potential energy.

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