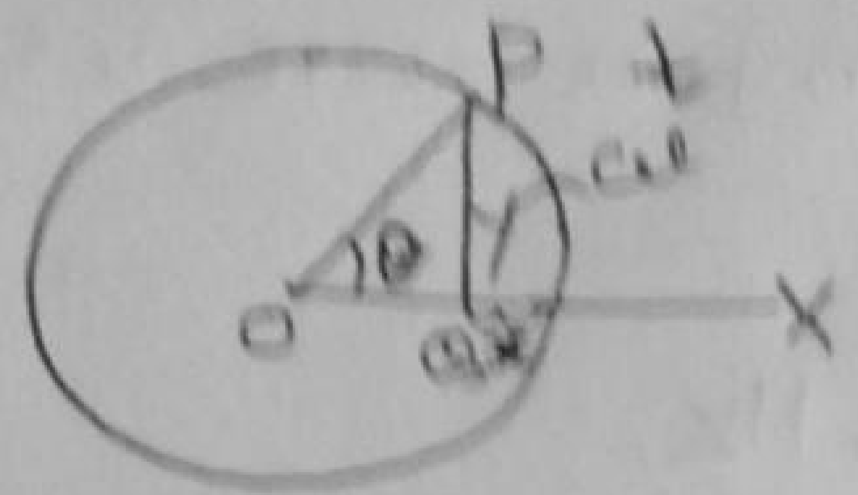
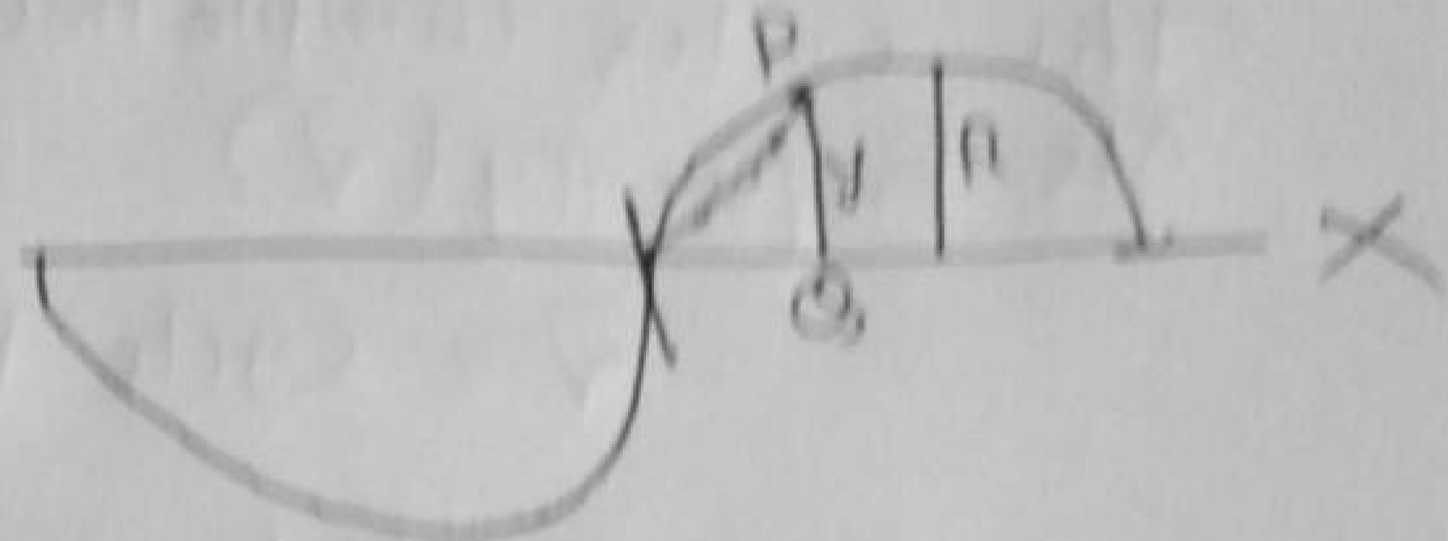
T.D.C. Part III
Physical Chemistry — Wave Mechanics — Dr. Vijay Kumar

# 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

velocity (c) = distance / time

From Δ OPQ

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

PQ = hight 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 ($\nu$)

$\nu$ = cycle per sec = Hz

One complete cycle = $2\pi$ radian.

$\because$ $\omega$ rad. in 1 sec.

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

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

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

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

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 $y = A \sin 2\pi \frac{x}{\lambda}$ ——— (1V

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

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

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

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

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

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

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

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

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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 $\psi$ 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 : $\psi$ = 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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