

Class of 11 Jan.: tying up loose ends

Narayanan Kurur

Department of Chemistry
IIT Delhi

Jan. 12, 2011

de Broglie hypothesis

For photons,

$$E = pc \quad E = h\nu = \frac{hc}{\lambda}$$

implies

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

- de Broglie showed that this relation **also** applies to material particles
- Confirmed later experimentally by Davisson and Germer and G. P. Thomson

A classical plane wave satisfies the DE $\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y}{\partial t^2}$

Plane wave solution $y = A \sin(kx - \omega t)$

$$\frac{\partial y}{\partial x} = kA \cos(kx - \omega t)$$

$$\frac{\partial y}{\partial t} = -\omega A \cos(kx - \omega t)$$

One differential equation satisfied by the plane wave is

$$\frac{\partial y}{\partial x} = -\frac{k}{\omega} \frac{\partial y}{\partial t}$$

Symmetrical opposite going wave $A \sin(kx + \omega t)$ not a solution of this DE Taking second derivatives of y we find the differential equation

$$\frac{\partial^2 y}{\partial x^2} = \frac{k^2}{\omega^2} \frac{\partial^2 y}{\partial t^2}$$

Schrödinger eq. is analogous to the classical wave eq.

Consider a free particle ($V = 0$) of momentum p .

$$E = \frac{\hbar^2 k^2}{2m} = \hbar\omega$$

By analogy with the plane wave its solution is $\Psi = A \sin(kx - \omega t)$

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A \sin(kx - \omega t)$$

Because $\omega = \frac{\hbar k^2}{2m}$ take only the first derivative with respect to t

$$\frac{\partial \Psi}{\partial t} = -\omega A \cos(kx - \omega t)$$

Unfortunately because of the use of sin and cos

$$\frac{\partial^2 \Psi}{\partial x^2} \neq \frac{2m}{\hbar} \frac{\partial \Psi}{\partial t}$$

Using a complex $\Psi(x, t)$ gives Schrödinger equation

Use $\Psi(x, t) = A \exp(i(kx - \omega t))$.

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2 A \exp(i(kx - \omega t)) = -\frac{p^2}{\hbar^2} \Psi$$

$$\frac{\partial \Psi}{\partial t} = -i\omega A \exp(i(kx - \omega t)) = -\frac{iE}{\hbar} \Psi$$

or

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{2mE}{\hbar^2} \Psi = -\frac{2m}{\hbar} \frac{\partial \Psi}{\partial t}$$

DE of a particle experiencing a potential

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

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

which can be written as

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

or

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