The Schrodinger Equation

The Schrodinger equation is the fundamental equation of quantum mechanics, which is a wave equation in the variable ψ

Consider a particle moving freely in the +ve X-direction. The wavefunction ψ for a free particle is given by,

$$\psi = Ae^{-i\omega(t - x/v)} \longrightarrow (1)$$

$$\psi = Ae^{-2\pi i(\nu t - x/\lambda)} \longrightarrow (2)$$

We have
$\omega = 2\pi\nu$
$v = \lambda\nu$.

Converting λ and ν in terms of energy and momentum,

$E = h\nu = 2\pi\hbar\nu$ $\quad \lambda = \frac{h}{p} = \frac{2\pi\hbar}{p}$

$$\therefore \psi = Ae^{-i/\hbar(Et - px)} \longrightarrow (3)$$

$Ae^{-i2\pi\nu(t - \frac{x}{\lambda\nu})}$
$Ae^{-2\pi i(\nu t - \frac{x\cancel{\nu}}{\lambda\cancel{\nu}})}$
$Ae^{-2\pi i(\nu t - x/\lambda)}$

$$\boxed{\hbar = \frac{h}{2\pi}}$$

$Ae^{-2\pi i(\frac{E}{2\pi\hbar}t - \frac{xp}{2\pi\hbar})}$
$= Ae^{-i/\hbar(Et - px)}$

Eqn (3) represents a free particle in terms of its energy E and momentum p.

Differentiating (3) twice w.r.t. t

$$\frac{d^2\psi}{dx^2} = \frac{-p^2}{\hbar^2} Ae^{-i/\hbar(Et - px)}$$

$$\frac{d^2\psi}{dx^2} = \frac{-p^2}{\hbar^2}\psi \longrightarrow (4)$$

$$p^2\psi = -\hbar^2 \frac{\partial^2\psi}{\partial x^2}.$$

Differentiating ③ ~~twice~~ w.r.t t

$$\frac{\partial\psi}{\partial t} = -\frac{iE}{\hbar}\psi$$

$$E\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t}$$

At speeds small compared with that of light, the total energy E of a particle is the sum of its kinetic energy $p^2/2m$ and its potential energy U, where U is in general a function of position x and time

$$E = \frac{p^2}{2m} + U(x,t) \longrightarrow ⑤$$

Xing both sides by ψ

$$E\psi = \frac{p^2\psi}{2m} + U(x,t)\psi.$$

substituting value of $E\psi$ and $p^2\phi$

$$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = -\hbar^2\frac{\partial^2\psi}{\partial t^2} + U\psi$$

~~xing throughout by~~

$$-\frac{\hbar}{i}\times\frac{i}{i}$$

$$i\hbar\frac{\partial\psi}{\partial t} = -\hbar^2\frac{\partial^2\psi}{\partial t^2} + U\psi.$$

$$= -\frac{i\hbar}{+i^2} =$$

$$i^2 = -1$$

$$= i\hbar$$

Thus the time dependent Schrodinger equation is given by

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\hbar^2\frac{\partial^2\psi}{\partial t^2} + U\psi}$$

Schrodinger's Equation : Steady State form

Time independent Schrodinger Equation

In many situations the potential energy of a particle doesnot depend on time explicitly, the forces that act on it and hence U vary with position of the particle only.

The wave function of a free particle,

$$\Psi = Ae^{-i/\hbar (Et - px)}$$

$$= Ae^{-i/\hbar Et} \times e^{\frac{ip}{\hbar}x}$$

Taking $\psi = \cancel{Ae^{-i/\hbar Et}}\ Ae^{\frac{ip}{\hbar}x}$

$$\Psi = \psi e^{-i/\hbar Et} \longrightarrow (1)$$

$\Psi = \psi_{(x)} \psi_{(t)}$

$\psi_{(x)} = Ae^{\frac{ip}{\hbar}x}$

$= \psi$

Substituting (1) in time dependent Schrodinger equation,

$$E\Psi = \frac{-p^2}{2m}\Psi + U\Psi$$

$p^2\psi = -\hbar^2 \frac{\partial^2\psi}{\partial x^2}$

$$E\psi e^{-i/\hbar Et} = \frac{-\hbar^2}{2m} \frac{\partial^2\Psi}{\partial x^2} + U\Psi$$

$$E\psi e^{-i/\hbar Et} = -\frac{\hbar^2}{2m} e^{-i/\hbar Et} \frac{\partial^2\psi}{\partial x^2} + U\psi e^{-i/\hbar Et}$$

$\div$ throughout by $e^{-i/\hbar Et}$

$$\boxed{E\psi = \frac{-\hbar^2}{2m} \frac{\partial^2\psi}{\partial x^2} + U\psi}$$

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

xing throughout by $-\frac{2m}{\hbar^2}$

$$-\frac{2m}{\hbar^2} E\psi = \frac{\partial^2\psi}{\partial x^2} + -\frac{2m}{\hbar^2}U\psi$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}E\psi - \frac{2m}{\hbar^2}U\psi$$

Schrodingers time independent Equation

$$\boxed{\frac{\partial^2\psi}{\partial x^2}+\frac{2m}{\hbar^2}(E-U)\psi=0}$$

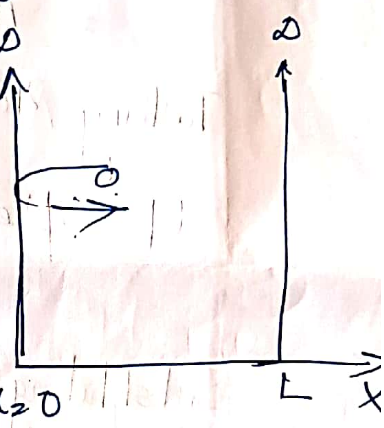
Infinite Square Well

Consider a particle trapped in a box with infinitely hard walls

$U=0$ inside the box

$U=\infty$ at the sides

$\therefore \psi=0 \quad x\le 0 \quad x\ge L.$



The time independent Schrodinger equation is given by

$$\frac{\partial^2\psi}{\partial x^2}+\frac{2m}{\hbar^2}(E-U)\psi=0 \longrightarrow (1)$$

Inside the box, $U=0$

$$\therefore \frac{\partial^2\psi}{\partial x^2}+\frac{2mE}{\hbar^2}\psi=0 \longrightarrow (2)$$

The solution of (2) is

$$\psi = A\sin\frac{\sqrt{2mE}}{\hbar}x+B\cos\frac{\sqrt{2mE}}{\hbar}x \longrightarrow (3)$$

where A and B are constants

Subjecting boundary conditions to obtain the value of A and B

At $x = 0$ $\psi = 0$

$$0 = A \sin 0 + B \cos 0$$

$$0 = 0 + B, \quad B = 0.$$

At $x = L$ $\psi = 0$

$$0 = A \sin \frac{\sqrt{2mE}}{\hbar} L.$$

$$\frac{\sqrt{2mE}}{\hbar} L = n\pi \qquad n = 1, 2, 3 \ldots$$

$$\frac{2mE}{\hbar^2} L^2 = n^2\pi^2.$$

$$\boxed{E^2 = \frac{n^2\pi^2\hbar^2}{2mL^2}}$$

From this it is clear that particle trapped in an infinite square well potential can have only certain values of energy.

Wave function

$$\frac{\sqrt{2mE_n}\, L}{\hbar} = n\pi$$

$$\psi_n = A \sin \frac{\sqrt{2mE_n}}{\hbar} x.$$

$$\sqrt{2mE_n} = \frac{n\pi\hbar}{L}$$

$$\psi_n = A \sin \frac{n\pi x}{L}$$

$$\frac{n\pi\hbar x}{L\hbar}$$

In order to find the value of A we can use normalization condition

$$\int_{-\infty}^{\infty} \psi_n^* \psi_n \, dx = 1 \longrightarrow (1)$$

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

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

$$= \frac{A^2}{2}\times L.$$

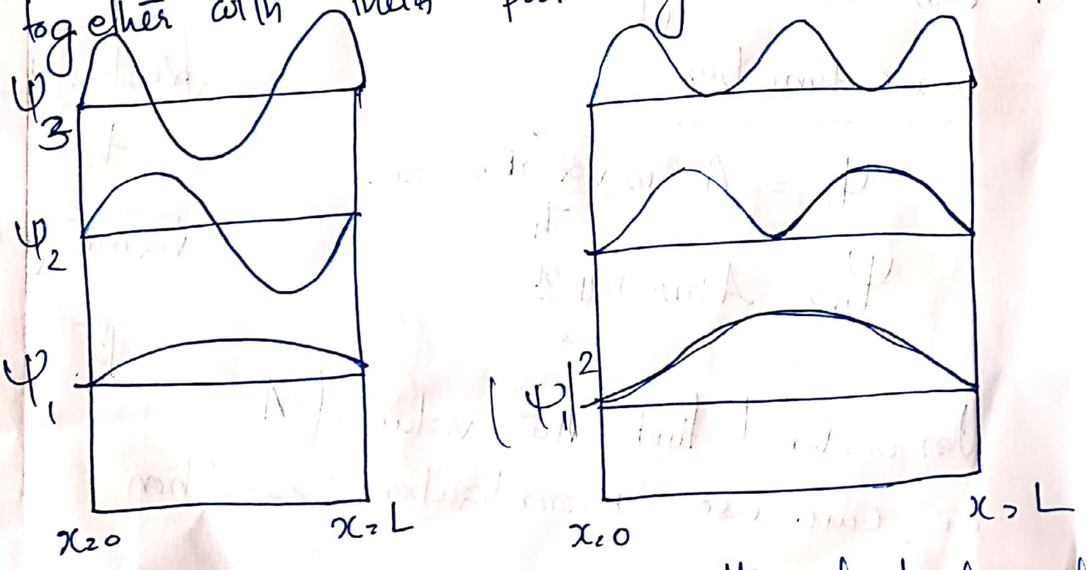
$$\int_{-\infty}^{\infty} \psi_n^* \psi_n\,dx = \int \psi_n^2\,dx = 1$$

$$\frac{A^2}{2}L = 1$$

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

$$\psi_n = \sqrt{\frac{2}{L}}\,\sin\frac{n\pi x}{L} \qquad n = 1, 2, 3$$

The normalized wave functions ψ_1, ψ_2 and ψ_3 are plotted together with their probability densities



$|\psi_1^2|$ has its maximum at middle of the box while $|\psi_2|^2 = 0$ at that place. A particle in the lowest energy level of $n=1$ is most likely to be in the middle of the box while particle in the next ~~lev~~

higher state of $n=2$ is never there. Classical physics ofcourse suggests the same probability for the particle being anywhere in the box.

Stationary states

The time independent Schrodinger equation

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

where $\psi_n = \psi_{(r)} e^{-\frac{iEt}{\hbar}}$

The probability density, $P(r,t) = |\psi_n(r,t)|^2$ = Constant in time

The states for which the probability density is constant in time are called stationary states.

It can be seen ~~that~~ in stationary states, the expectation value of an observable whose operator doesnot depend on time explicitly is a constant in time. Stationary states are the states on which physical measurements are performed. Spectral transitions are induced between such states.

A stationary state is a bound one if the corresponding wave function $\psi(r)$ or probability density $|\psi(r)|^2$ vanishes at ∞

$$\lim_{r\to\infty} \psi(r) = 0$$