4.4 Characteristics of the Schrödinger Equation

The one-dimensional Schrödinger equation for a free particle of mass m is given by,

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} \quad \text{[same as (4.16)]} \tag{4.27}$$

1. A close look into equation (4.27) reveals that $\frac{\partial\psi(x,t)}{\partial t}$ and $\frac{\partial^2\psi(x,t)}{\partial t^2}$ occur only in the first power, i.e., linearly. This implies that, not only harmonic waves of the form $\psi(x,t) = Ae^{-i(\omega t-kx)}$ are the solutions of equation (4.27) but any linear combination or, superposition of harmonic waves such as,

$$\psi(x,t) = \int A(k)e^{-i(\omega t-kx)}dk \tag{4.28}$$

are also the solution of the same equation. This is an important property of Schrödinger equation. According to this principle if, $\psi_1(x,t)$ and $\psi_2(x,t)$ be two wave functions of the system then, $\psi(x,t) = C_1\psi_1(x,t) + C_2\psi_2(x,t)$ will also be a possible wave function of the system satisfying equation (4.27). The equation (4.28) represents a wave packet. Hence, Schrödinger wave equation also has perfectly good wave packet solutions.

2. The wave equation (4.27) is in the first order in time implying that if ψ is known at some point $\vec{r}$ at the initial time t_0 then at any subsequent time t, the wave function $\psi(\vec{r},t)$ at the same point will be uniquely determined.

3. All the partial differential equations of classical physics contains only real parameters. But Schrödinger wave equation contain the imaginary unit i explicitly. This sets apart Schrödinger equation from all other classical partial differential equation.

4. The wave function $\psi(r,t)$ representing the matter wave must be a complex function of x and t.

5. The wave equation (4.27) is consistent with de Broglie's hypothesis and correspondence principle.

(1) Schroedinger time-independent equation — V.U-2003

Let us consider a group of waves associated with a moving
Let $\psi(r,t)$ represents the displacement of these waves at a
any instant t.

The wave motion can be represented by the classical

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

Where v is

To find the solution of the above equation, let us take the

$$\psi(r,t) = \psi(r)\cdot e^{-i\omega t}$$

$$\therefore \frac{\partial^2\psi}{\partial t^2} = -\omega^2\psi \quad \text{——— (2)}$$

Putting in equation (1), we may write,

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

$$= -\frac{(2\pi\nu)^2}{(\nu\lambda)^2}\psi$$

$$= -\frac{4\pi^2}{\lambda^2}\psi$$

$$= -\frac{4\pi^2}{h^2/p^2}\psi \qquad \text{as } \lambda = \frac{h}{p}$$

$$= -\left(\frac{p}{\hbar}\right)^2\psi$$

$$= -\left(\frac{mv}{\hbar}\right)^2\psi \quad \text{——— (3)}$$

If E and V be the total energy and the potential en
particle respectively, then,

$$E = \frac{1}{2}mv^2 + V$$

$$\text{or, } m^2v^2 = 2m(E-V)$$

$$\text{or } mv = \sqrt{2m(E-V)}$$

Putting in equation (3), $\nabla^2\psi = -\frac{2m(E-V)}{\hbar^2}\psi$

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

This is known as Schroedinger time-independent

Schroedinger time dependent equation — from time dependent

Schroedinger time independent equation,

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

or, $\nabla^2\psi - \frac{2mV}{\hbar^2}\psi = -\frac{2mE}{\hbar^2}\psi$

or, $-\frac{\hbar^2}{2m}\left(\nabla^2\psi - \frac{2m}{\hbar^2}V\psi\right) = E\psi$

or, $\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi$ —— (1)

Let the trial solution, $\psi(r,t) = \psi(r)\,e^{-i\omega t}$

or, $\frac{\partial\psi}{\partial t} = -i\omega\psi$

or, $i\hbar\frac{\partial\psi}{\partial t} = \hbar\omega\psi = E\psi$ —— (2)

From equation (1) and (2),

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

This equation is known as Sch. time dependent eqn.

The operator $\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right) = \hat{H}$, called Hamiltonian operator.

The operator $i\hbar\frac{\partial}{\partial t} = \hat{E}$, called Energy operator.

$$\therefore \quad \hat{H}\psi = \hat{E}\psi$$

4.10 Physical Interpretation of the Wave Function $\psi(\vec{r},t)$

We have seen that the waves associated with a particle are represented by a function $\psi(\vec{r},t)$ called the *wave function*. Regarding $\psi(\vec{r},t)$ several questions arise:

(i) Is $\psi(\vec{r},t)$ a measurable quantity?

(ii) What precisely does $\psi(\vec{r},t)$ describe?

(iii) What feature of the particle is related to $\psi(\vec{r},t)$?

Unless the properties of the waves represented by $\psi(\vec{r},t)$ and the way in which $\psi(\vec{r},t)$ used in the calculations be known, satisfactory answers to the above questions cannot be expected. Still the wave function $\psi(\vec{r},t)$ which describes the space time behaviour of the particle is such that its magnitude is large in the region where the probability of finding the particle is large. In other region where the probability of finding the particle is amll, the magnitude of $\psi(\vec{r},t)$ is small. In otherworld $\psi(\vec{r},t)$ may be regarded as the probability of finding the particle around a particular position in space. Again the probability (P) is a real and non-negative quantity whereas $\psi(\vec{r},t)$ is a complex function, we shall assume that the quantity,

$$\left|\psi(\vec{r},t)\right|^2 d^3r = \psi^*(\vec{r},t)\psi(\vec{r},t)d^3r \tag{4.72}$$

is proportional to the probability of finding the particle in the volume element d^3r around the point r at time t. Here $\psi^*(\vec{r},t)$ is the complex conjugate of $\psi(\vec{r},t)$.

Hence, the total probability of finding the particle anywhere in space is,

$$P(\vec{r},t) \propto \int_{-\infty}^{+\infty} \left|\psi(\vec{r},t)\right|^2 d^3r.$$

The position probability density is defined as,

$$\rho(\vec{r},t) = \frac{\left|\psi(\vec{r},t)\right|^2}{\int_{-\infty}^{+\infty} \left|\psi(\vec{r},t)\right|^2 d^3r}. \tag{4.73}$$

Thus according to Max Born, the most direct physical interpretation of the wave function $\psi(\vec{r},t)$ is that its modulus square determines the probability density of the particle in space.

Since $\left|\psi(\vec{r},t)\right|^2$ is a positive quantity $P(\vec{r},t)$ is always positive. So, the total probability of finding the particle anywhere in space is,

$$P(\vec{r},t) = \int_{-\infty}^{+\infty} \rho(\vec{r},t)d^3r = \frac{\int_{-\infty}^{+\infty} \left|\psi(\vec{r},t)\right|^2 d^3r}{\int_{-\infty}^{+\infty} \left|\psi(\vec{r},t)\right|^2 d^3r} = 1 \tag{4.74}$$

Normalisation :

If we consider a small element of volume dv defined by the co-ordinates $(x, x+dx)$; $(y, y+dy)$; and $(z, z+dz)$ then

Prob. of finding the particle within volume dv is given by,

$$\rho \, dv = \psi^* \psi \, dx\,dy\,dz .$$

Prob. of finding the particle within a finite volume v,

$$\int_v \rho \, dv = \iiint_v \psi^* \psi \, dx\,dy\,dz .$$

The process of integration over all possible locations is uni[ty]. This is called normalisation.

i.e.

$$\boxed{\iiint_{\text{all space}} \psi^* \psi \, dx\,dy\,dz = 1}$$

All space means.

$x \to -\infty$ to

$y \to -\infty$ to

$z \to -\infty$ to

N.B. For 1D case : $\int_{-\infty}^{+\infty} \psi^* \psi \, dx = 1$.

Orthogonality :

Two wave functions ψ_n and ψ_m are said to be orthogonal if they satisfy the condition,

ORTHOGONALITY CONDITION

$$\int_{-\infty}^{+\infty} \psi_n^*(x,t) \cdot \psi_m(x,t) \, dx = 0 \quad \text{for } n \neq m$$

$$\iiint_{-\infty}^{+\infty} \psi_n^*(x,y,z,t) \cdot \psi_m(x,y,z,t) \, dx\,dy\,dz = 0 \quad \text{for } n \neq m$$

N.B. For time independent wave function,

ORTHOGONALITY CONDITION :

$$\int_{-\infty}^{+\infty} \psi_n^*(x) \cdot \psi_m(x) \, dx = 0 \qquad \text{for } n \neq m$$

$$\iiint \psi_n^*(x,y,z) \cdot \psi_m(x,y,z) \, dx\,dy\,dz = 0 \cdot \text{ for } n \neq m$$

Shortly

$$\boxed{\int \psi_n^* \psi_m \, dv = 0}$$

EXAMPLE 4.2. *Normalised the one-dimensional wave function given by*

$$\psi(x) = \begin{cases} A\sin\left(\frac{\pi x}{l}\right), & 0 < x < l \\ 0, & \textit{outside} \end{cases}$$

[BU(Hons) 1998, 2001; HPU 1995]

Solution: The wave function $\psi(x)$ is said to be normalised if it satisfies the relation

$$\int_{-\infty}^{+\infty} \psi^*(x)\psi(x)dx = 1. \tag{1}$$

As the wave function $\psi(x)$ exists only in the region $0 < x < l$ and is zero outside, we have from equation (1)

$$\int_0^l \psi^*(x)\psi(x)dx = 1$$

$$\text{or, } \int_0^l A^* \sin\left(\frac{\pi x}{l}\right) A\sin\left(\frac{\pi x}{l}\right) dx = 1$$

$$\text{or, } A^*A \int_0^l \sin^2\left(\frac{\pi x}{l}\right) dx = 1$$

$$\text{or, } A^*A \int_0^l \frac{1}{2}\left[1 - \cos\left(\frac{2\pi x}{l}\right)\right] dx = 1$$

$$\text{or, } A^*A \left[\int_0^l dx - \int_0^l \cos\frac{2\pi x}{l} dx\right] = 2$$

$$\text{or, } |A|^2 \left[x - \frac{l}{2\pi} \left\{ \sin\left(\frac{2\pi x}{l}\right) \right\}_0^l \right] = 2$$

$$\text{or, } |A|^2 \, [l - 0 + 0] = 2 \text{ or, } |A|^2 = \frac{2}{l}$$

$$\text{or, } |A| = A = \sqrt{\frac{l}{2}} \text{ [assuming } A \text{ to be real]}$$

Hence the normalised wave function is

$$\psi(x) = \sqrt{\frac{2}{l}} \sin\left(\frac{\pi x}{l}\right).$$ (2

EXAMPLE 4.3. *A particle is represented by the wavefunction* $\psi(x) = e^{-|x|} \sin \alpha x$. *What is the probability that its position to the right of the point* $x = 1$*?*

Solution: Here,

$$\text{let, } \psi_1(x) = e^x \sin \alpha x, \text{ for } x < 0$$
$$\text{and } \psi_2(x) = e^{-x} \sin \alpha x, \text{ for } x > 0$$

$$\therefore \int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx = 1/C^2, \quad \text{where } C \text{ is the normalisation constant}$$

$$\text{or, } \int_{-\infty}^{0} |\psi_1(x)|^2 \, dx + \int_0^{\infty} |\psi_2(x)|^2 \, dx$$

$$= \int_{-\infty}^{0} e^{2x} \sin^2 \alpha x \, dx + \int_0^{\infty} e^{-2x} \sin^2 \alpha x \, dx$$

$$= \int_{-\infty}^{0} e^{2x} \left[\frac{1 - \cos 2\alpha x}{2}\right] dx + \int_0^{\infty} e^{-2x} \left[\frac{1 - \cos 2\alpha x}{2}\right] dx$$

$$= \frac{1}{2} - \frac{1}{2} \int_{-\infty}^{0} e^{2x} \cos 2\alpha x \, dx - \frac{1}{2} \int_0^{\infty} e^{-2x} \cos 2\alpha x \, dx$$

$$= \frac{1}{2} - \frac{1}{4(1+\alpha^2)} - \frac{1}{4(1+\alpha^2)} = \frac{\alpha^2}{2(1+\alpha^2)} = 1/C^2,$$

$$\therefore C = \sqrt{\frac{2(1+\alpha^2)}{\alpha^2}}$$

So, the normalised wave function is,

$$\psi(x) = \sqrt{\frac{2(1+\alpha^2)}{\alpha^2}} e^{-|x|} \sin \alpha x$$