

Schrodinger time independent wave equation:

From the classical mechanics, the amplitude of a particle wave moving along x axis can be written as

$$\psi_{(x)} = 2A \sin(2\pi x/\lambda)$$

Differentiating the wave function w.r.t x,

$$\frac{d}{dx} \psi_{(x)} = 2A \cos(2\pi x/\lambda) \times 2\pi/\lambda$$

$$\Rightarrow \frac{d^2}{dx^2} \psi_{(x)} = 2A (-\sin(2\pi x/\lambda)) \times (2\pi/\lambda)^2$$

$$\Rightarrow \frac{d^2}{dx^2} \psi_{(x)} = -\frac{4\pi^2}{\lambda^2} \psi_{(x)}$$

For a microparticle, according to de Broglie equation,

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

So,

$$\frac{d^2}{dx^2} \psi_{(x)} = -\frac{4m^2 v^2 \pi^2}{h^2} \psi_{(x)}$$

The total energy(E) of the particle is the sum of kinetic energy $1/2mv^2$ and potential energy V. Therefore,

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

$$\Rightarrow m^2 v^2 = 2m(E - V)$$

Substituting this to above equation,

$$\frac{d^2}{dx^2} \psi_{(x)} = -\frac{8m\pi^2}{h^2} (E - V) \psi_{(x)}$$

$$\Rightarrow \frac{d^2}{dx^2} \psi_{(x)} + \frac{8m\pi^2}{h^2} (E - V) \psi_{(x)} = 0$$

This is the Schrodinger equation for a single particle of mass m moving in x direction.

For three dimensions,

$$\frac{d^2}{dx^2} \psi + \frac{d^2}{dy^2} \psi + \frac{d^2}{dz^2} \psi + \frac{8m\pi^2}{h^2} (E - V) \psi = 0$$

Where ψ and V are functions of coordinates x,y, and z and ψ is known as wave function.

The above equation can be rearranged as

$$\frac{h^2}{8\pi^2 m} \left(\frac{d^2}{dx^2} \psi + \frac{d^2}{dy^2} \psi + \frac{d^2}{dz^2} \psi \right) + V \psi = -E \psi$$

$$\Rightarrow \left[\frac{-h^2}{8\pi^2m} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) + V \right] \psi = E\psi$$

$$\Rightarrow \hat{H}\psi = E\psi$$

Where

$$\hat{H} = \frac{-h^2}{8\pi^2m} \left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right) + V$$

$$\Rightarrow \hat{H} = \frac{-h^2}{8\pi^2m} \nabla^2 + V$$

is called Hamiltonian operator and

$$\nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$$

Condition for a physically accepted, well behaved, realistic wave function:

1. $\psi(x)$ should be finite, single-valued and continuous everywhere in space.
2. $\frac{dy}{dx} \psi(x)$ should be continuous everywhere in space.
3. $\psi(x)$ should be square integrable i.e. $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \text{finite number}$.

Physical significance of wave function

Generally, $\psi(x)$ is a complex quantity. It can be multiplied by any complex number without affecting its physical significance. In general, $\psi(x)$ has no direct physical significance. But the quantity $\psi^*(x)\psi(x)$ is real, physically significant and is defined as position probability density i.e. probability of finding the particle per unit length at time 't'. Therefore, for 1-D motion the probability of finding the particle between x to $x + dx$ at time 't' is given by

$$\psi^*(x)\psi(x)dx = |\psi(x)|^2 dx$$

Now, $\psi(x)$ should be chosen such that total probability of finding the particle in the entire space should be equal to unity i.e.

$$\int \psi^*(x) \psi(x) dx = 1$$

This is called the normalization condition of the wave function.

Condition for Normalization: Normalization constant

If $\phi(x)$ is unnormalized wave function and if $\psi(x) = N\phi(x)$, then N is normalization constant if

$$\int \psi^*(x) \psi(x) dx = 1$$

$$\Rightarrow \int N \varphi^*(x) N \varphi(x) dx = 1$$

$$\Rightarrow N^2 \int \varphi^*(x) \varphi(x) dx = 1$$

$$\Rightarrow N^2 = \frac{1}{\int \varphi^*(x) \varphi(x) dx}$$

$$\Rightarrow N = \sqrt{\frac{1}{\int \varphi^*(x) \varphi(x) dx}}$$

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