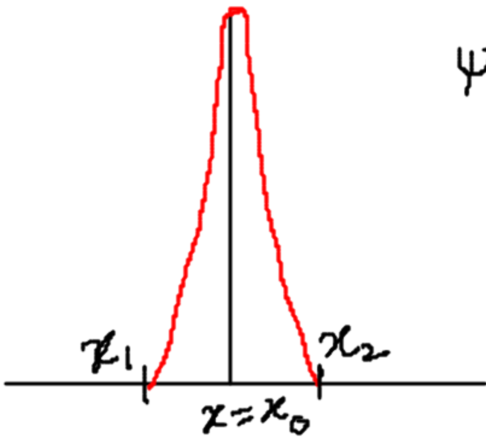
Wave Mechanics (TPH101)

By Dr. Vishal Chauhan

Dirac Delta Function



$$\psi(x) = A\,\delta(x - x_0) \qquad (A = 1)$$

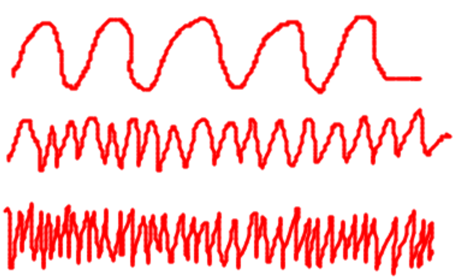
$\psi(x)$ is zero at all places except at $x = x - x_0$

at $x \neq x_0$, $\psi = 0$

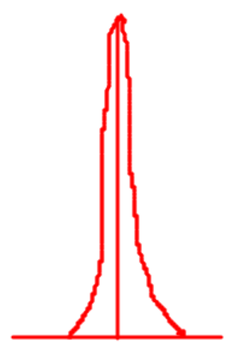
$x = x_0$, $\psi = \infty$

$x_1 < x_0 < x_2$

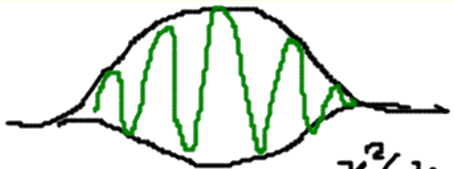
$$\int_{x_1}^{x_2} \psi(x)\,dx = 1$$



Momentum is fixed but not position



position is fixed but not momentum



$$e^{-x^2/a^2} \cdot e^{ikx}$$

$$\downarrow$$

$$\cos kx + i \sin kx$$

probability of finding particle in x-direction

$$[\psi(x)\,\psi^*(x)]\,dx$$

We can not know definite position due to that we talk about probability //

So now there may be two Conditions

① At any instant particle has a definit position but we don't know

② At any instant particle is everywhere having mixed state of different positions

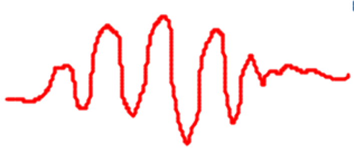
Conditions For realistic wave functions

① wave function should be continuous.
② It should be finite everywhere.
③ It should be square integrable.

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \text{ or finite.}$$

We can make realistic wave functions by mixing different unrealistic wave functions

Now suppose we have a mixed realistic state and we want to know that how many pure states of momentum are inside it



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If H is the operator corresponding to the total energy of the system and is givne a special name, i.e. Hamiltonian of the system, then we can write the Schrodinger wave equation as follows;

$$\left(H = -\frac{\hbar^2}{2m}\cdot\frac{\partial^2}{\partial x^2} + V_x\right)$$

$$H = K + V$$

$$\left(H = i\hbar\frac{\partial}{\partial t}\right)$$

$\therefore$ Schrödinger's wave equation is

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

here $H|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle = -\frac{\hbar^2}{2m}\cdot\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$

For a particle in one dimension, ψ is a function of x & t, then

$$-\frac{\hbar^2}{2m}\cdot\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$

For three dimensions :→

we can replace $\frac{\partial^2}{\partial x^2}$ with $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

and $\psi(x,t)$ as $\psi(x,y,z,t)$ or $\psi(\vec{r},t)$

$V(x)$ as $V(x,y,z)$ or $V(\vec{r})$

$$H = -\frac{\hbar^2}{2m}\cdot\frac{\partial^2}{\partial x^2} + V(x)$$

$$H = -\frac{\hbar^2}{2m}\cdot\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right] + V(\vec{r})$$

$$H = -\frac{\hbar^2}{2m}\cdot\nabla^2 + V(\vec{r})$$

Now schrödinger equation →

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

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Time Independent Schrodinger wave equation

Let at any state if at $t=0$, the wavefunction becomes eigen function of Hamiltonian

then at $t=0$

$$\psi(x,0) = \phi_i(x)$$

[No need to expand like $\psi(x,0)=\sum_i c_i \phi_i(x)$ since c_i is 1 for this wave function & all other will be zero.

$$H\psi(x,0) = E_i \psi(x,0)$$
$$= E_i \phi_i(x)$$

at $\underline{t=t}$

$$\psi(x,t) = e^{-i/\hbar E_i t}\phi_i(x)$$
$$= e^{-i/\hbar E_i t}\psi(x,0)$$

$$\psi(x,t) = e^{-i/\hbar E_i t} H\psi(x,0)$$
$$= \underbrace{e^{-i/\hbar E_i t}}\, E_i\, \underbrace{\psi_i(x,0)}$$

$$H\psi(x,t) = E_i \psi(x,t)$$

$$H\psi(x,t) = E_i \psi(x,t)$$

At this state the energy is definite & constant.
It means its a pure state of energy

It also means that at any time the value of E_i will be same and not dependent on time.

Let observable (a) & expectation value $\langle a \rangle$

$$\langle a \rangle = \langle \psi | A | \psi \rangle$$

$$\langle \psi | A | \psi \rangle = \int \psi^*(x,t) A \psi(x,t)\, dx$$

$$\psi^*(x,t) \rightarrow e^{-i/\hbar E_i t} \psi^*(x,0)$$

$$A\psi(x,t) \rightarrow e^{-i/\hbar E_i t} A\psi(x,0)$$

$$e^{-i/\hbar E_i t} \times e^{i/\hbar E_i t} = 1$$

$$\therefore \langle \psi | A | \psi \rangle = \int \psi^*(x,0) A \psi(x,0)\, dx$$

This equation is independent of time.

We know probability to get a_i

is $|c_i|^2 =$ Prob. of a_i

$$c_i = \langle a_i | \psi(x,t) \rangle$$

It mean wave function is changing but not other parameters

stationary state

$$\boxed{H\phi = E\phi}$$

So this is Time Independent Schrodinger Wave Equation.