# Quantum Mechanics.

The fundamental difference between classical (or Newtonian) mechanics and quantum mechanics lies in what they describe. In classical mechanics, the future history of a particle is completely determined from its initial position and momentum together with forces that act upon it.

Quantum mechanics also arrives at relationships between observable quantities, but the uncertainity principle also suggests that the nature of observable quantity is different in atomic realm. In quantum mechanics the kind of certainity about the future characteristic of classical mechanics is impossible because the initial state of a particle can not be established with sufficient accuracy. The more we know about the position of a particle now, the less we know about its momentum and hence about its position later.

The quantities whose relationships quantum mechanics explores are probabilities. Instead of asserting for example, that the radius of electron's orbit in ground state of hydrogen atom as always exactly $5.3 \times 10^{-11}$ m, as the Bohr's theory does, quantum mechanics states that, this is the most probable radius.

## Wave function.

For quantum mechanical description, every physical system is characterised by a wave function $\psi(\vec{r}, t)$ are state function which contains information about the system. Just as the wavefunction of a mechanical wave contains information like amplitude, frequency, wavelength etc, the wave function in quantum mechanics contains all information for the probabilistic description of a system. But unlike the wave function of a mechanical or electromagnetic wave the quantum mechanical wave function is not a directly measurable quantity

## Characteristic of the wave function:

① Wave functions are mathematical representation of quantum mechanical particles which contain all the information required for the probabilistic description of the particle.

② The wave function $\psi$ is in general is a mathematical function of space and time i.e $\psi(x, y, z, t)$

③ The wavefunction is, in general, a complex function having both real and imaginary parts. For example $\psi(\vec{r}, t) = Ae^{i(\vec{K}\cdot\vec{r} - \omega t)}$

④ The wave function $\psi$ and its first derivatives $\frac{\partial\psi}{\partial x}$ w.r.t to space coordinate are continuous at all space including boundaries.

⑤ The wave function $\psi$ must be continuous and single valued everywhere.

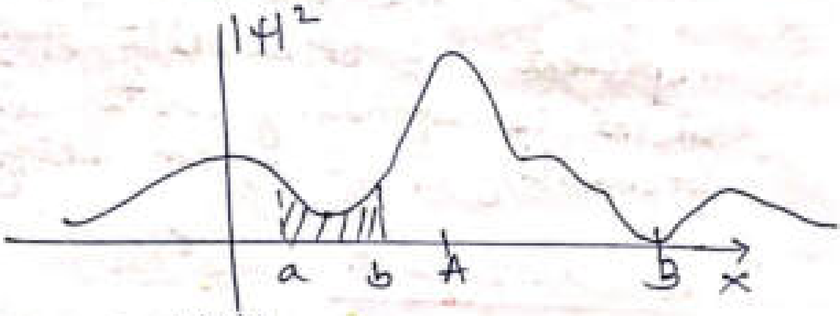
⑥ The wavefunction is a square integrable, i.e the integral of the square of ~~its~~ the wave function over the entire space should be finite quantity and should not diverge to infinity.

⑦ The quantity $|\psi|^2$ represents the probability density or the probability per unit volume of finding the system in the state. So, the wave function $\psi$ is regarded as the probability amplitude.

⑧ The wave function satisfies the Schrödinger equation.

(g) $\psi$ must be normalizable, which means that $\psi$ must go to '0' as $x \to \pm\infty$ in order that $\int |\psi|^2 dV$ over all space be finite.

## The statistical Interpretation:




$$\int_a^b |\psi(x,t)|^2 dx = \left\{ \begin{array}{l} \text{probability of finding the} \\ \text{particle between } a \,\&\, b \text{, at time } t \end{array} \right\}$$

The shaded area represents the probability of finding the particle between a and b. The particle would be relatively likely to be found near A, and unlikely to be found near B.

The probability of finding the particle per unit volume is called probability density and is given by

$$\rho = \psi \psi^* = |\psi|^2$$

## The principle of superposition:

The wave function representing the actual state of a system is a linear superposition of different possible allowed states in which the system can exist.

Scanned with CamScanner

Let $\psi_1, \psi_2, \psi_3$ --- represent the allowed states in which a system can exist. The actual state of the system is a linear ~~combinade~~ combination of these allowed states with different coefficients.

$$\psi = c_1\psi_1 + c_2\psi_2 + c_3\psi_3 + \cdots = \sum c_n \psi_n$$

The squares of the co-efficients represent the probability of the system existing in the corresponding state. For example $|c_2|^2$ is the probability of the system being in the system $\psi_2$.

## Normalization.

Since $|\psi|^2$ is proportional to the probability density $\rho$ of finding the body described by $\psi$, the integral of $|\psi|^2$ over all space must be finite — the body is somewhere, after all. If

$$\int_{-\infty}^{\infty} |\psi|^2 dv = 0$$

, the particle does not exist, and the integral cannot be $\infty$ and still mean anything. Further more $|\psi|^2$ can not be negative or complex because the way it is defined. The only possibility left is that the integral be a finite quantity if $\psi$ to is to describe a real body.

It is usually convinient to have $|\psi|^2$ be equal to the probability density $\rho$ of finding the particle described by $\psi$, rather than merely be proportional to $\rho$. If $|\psi|^2$ is equal to $\rho$, then it must be true that—

$$\int_{-\infty}^{\infty} |\psi|^2 dv = 1 \quad \text{--- } (1)$$

Since if the particle exists somewhere at all times

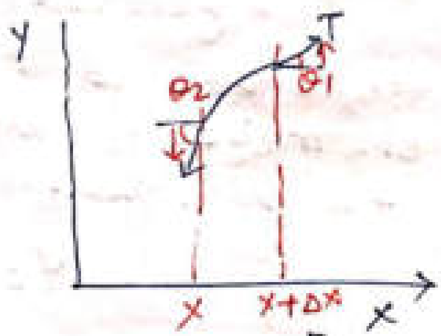
$$\int_{-\infty}^{\infty} \rho \, dv = 1$$

Scanned with CamScanner

A wave function obeying eq$^n$ ① is said to be normalized. Every acceptable wave function can be normalized by multiplying it by an appropriate constant.

## The wave equation:

$$F = ma$$




$$T(\sin\theta_1 - \sin\theta_2) = \mu \Delta x \frac{\partial^2 y}{\partial t^2}$$

In the small angle limit

$$T(\tan\theta_1 - \tan\theta_2) = \mu \Delta x \frac{\partial^2 y}{\partial t^2}$$

$$T\left(\frac{\partial y}{\partial x}\bigg|_{x+\Delta x} - \frac{\partial y}{\partial x}\bigg|_{x}\right) = \mu \Delta x \frac{\partial^2 y}{\partial t^2}$$

[$\mu$ = mass per unit length]

$$T \frac{\partial^2 y}{\partial x^2} \cancel{\Delta x} = \mu \cancel{\Delta x} \frac{\partial^2 y}{\partial t^2}$$

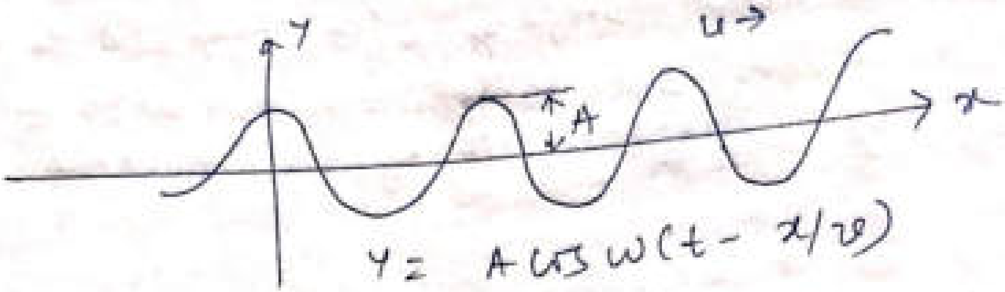
$$\frac{\partial^2 y}{\partial x^2} = \frac{\mu}{T} \frac{\partial^2 y}{\partial t^2}$$

$$\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y}{\partial t^2}} \qquad \because \frac{\mu}{T} = \frac{1}{v^2}$$

Solution $\quad y = F\left(t \pm \frac{x}{v}\right)$

Let us consider the wave equivalent of a "free particle" which is a particle that is not under the influence of any forces and therefore pursues a straight path at constant speed.

Scanned with CamScanner




$$Y = A \cos \omega(t - x/v)$$

general solution of wave equation for undamped (i.e. constant amplitude A), monochromatic (constant ω) harmonic waves in the +x direction

$$Y = A e^{-i\omega(t - x/v)}$$

$$e^{-i\theta} = \cos\theta - i\sin\theta$$

$$Y = A\cos\omega(t - x/v) - iA\sin\omega(t - x/v)$$

## Schrödinger's equation: Time-dependent form

In quantum mechanics, the wave function $\psi$ corresponds to the wave variable $Y$ of the wave motion in general. However, $\psi$ unlikely $Y$, is not itself a measurable quantity and may therefore be complex. For this reason we assume that $\psi$ for a particle moving freely in the +x direction is specified by

$$\psi = A e^{-i\omega(t - x/v)}$$

$\because$ $\omega = 2\pi\nu$ and $v = \lambda\nu$

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

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

$$\psi = A e^{-(i/\hbar)(Et - px)} \quad \text{- - - (1)}$$

This describes the wave equivalent of a unrestricted particle of total energy 'E' and momentum 'p' moving in the +x direction

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

$$p^2\psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} \quad \text{- - - - (2)}$$

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

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

At speeds small compared with that of light, the total energy E of a particle is the sum of its K-E $\frac{p^2}{2m}$ and its potential energy U, where U is in general a function of position x and time t:

$$E = \frac{p^2}{2m} + U(x, t) \quad \text{- - - - (3)}$$

The function U represent the influence of the rest of the universe on the particle.

Putting (1) & (2) in equation

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

In three dimensions the time-dependent form of Schrödinger's equation is

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}\right) + U\psi$$

where the particle's potential energy $U$ is some function of $x, y, z$ and $t$.

## Expectation values.

The study of quantum mechanics involves an observable/measurable physical quantity which is associated with mathematical operators. Once Schrödinger equation has been solved for a particle in a given physical situation, the resulting wave function $\psi(x,y,z,t)$ contains all the information about the particle that is permitted by the uncertainity principle.

As an example, let us calculate the expectation value $\langle x \rangle$ of the position of a particle confined to the $x$-axis that is described by the wave function $\psi(x,t)$. This is the value of '$x$' we would obtain if we measured the positions of a great many particles described by the same wave function at some instant '$t$' and then averaged the result.

For example let us consider the average position $\bar{x}$ of a number of identical particles distributed along the $x$-axis in such a way that there are $N_1$ particles at $x_1$, $N_2$ particles at $x_2$, and so on.

Scanned with CamScanner

The average position in this case is the same as the centre of mass distribution system

$$\bar{x} = \frac{N_1 x_1 + N_2 x_2 + \cdots}{N_1 + N_2 + \cdots} = \frac{\sum N_i x_i}{\sum N_i}$$

When we are dealing with a single particle, we must replace the number $N_i$ of particles $x_i$ by the probability $P_i$ that the particle be found in an interval $dx$ at $x_i$

$$P_i = |\psi_i|^2 dx$$

$\psi_i$ is the wave function evaluated at $x = x_i$

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x |\psi|^2 dx}{\int |\psi|^2 dx}$$

If $\psi$ is normalized

Expectation value for position

$$\boxed{\langle x \rangle = \int_{-\infty}^{\infty} x |\psi|^2 dx}$$

In general

$$\langle G(x) \rangle = \int_{-\infty}^{\infty} G(x) |\psi|^2 dx$$

## Observables

An observable is a quantity obtained by the process of observation or measurement on physical system. An observable is a quantity expressed by a number. It is always a real entity as it is the result of actual measurement.

A physical system is disturbed by the act of measurement. Therefore, the value of an observable depends upon the interaction between the system and measuring device and thus spread around some mean value.

## Operators

An observable is a mathematical rule or prescription. Every physical quantity is associated with a quantum mechanical operator.

$$\psi = Ae^{-\frac{i}{\hbar}(Et-px)}$$

$$\frac{\partial\psi}{\partial x} = \frac{i}{\hbar} p\psi \Rightarrow p\psi = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi$$

Momentum operator

$$\boxed{\begin{aligned}\hat{p} &= \frac{\hbar}{i}\frac{\partial}{\partial x} \\ &= \frac{\hbar}{i}\nabla\end{aligned}}$$

(in one dimension)

$\left(\nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}\right)$ in three dimension

Similarly

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

$$\boxed{\hat{E} = i\hbar\frac{\partial}{\partial t}}$$

Kinetic energy $K.E = \frac{p^2}{2m}$

$$= \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Total energy $\hat{E} = K \cdot E + \hat{U}$     $\hat{U}$ = potential energy

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

which is nothing but the Schrödinger equation.

## Operators Associated with various Observable quantities:

| Quantity | Operator |
|---|---|
| Position, $x$ | $x$ |
| Linear momentum $p$ | $\frac{\hbar}{i}\frac{\partial}{\partial x}$ |
| Potential energy $U(x)$ | $U(x)$ |
| Kinetic energy $K \cdot E = \frac{p^2}{2m}$ | $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ |
| Total energy $E$ | $i\hbar \frac{\partial}{\partial t}$ |
| Total energy (Hamiltonian form) $H$ | $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U(x)$ |

## Operators and Expectation values:

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi \, dx = \int_{-\infty}^{\infty} \psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \psi \, dx$$

$$= \frac{\hbar}{i}\int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} \, dx$$

$$\langle E \rangle = \int_{-\infty}^{\infty} \psi^* \hat{E} \psi \, dx = i\hbar \int \psi^* \frac{\partial \psi}{\partial t} \, dx$$

$$\langle G(x, p) \rangle = \int_{-\infty}^{\infty} \psi^* \hat{G} \psi \, dx \quad \text{[In general]}.$$

## Eigenvalues and Eigenfunction

The values of energy $E_n$ for which Schrödinger steady-state equation can be solved are called **eigenvalues** and the corresponding wave function $\psi_n$ are called eigenfunctions. ~~The condition~~

Eigenvalue equation: $\hat{G}\psi_n = G_n \psi_n$ where $\hat{G}$ is the operator that corresponds to $G$ and each $G_n$ is a real number

## Time-independent Schrödinger equation:

Schrödinger wave equation in time dependent form

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \quad - - - - (1)$$

where $\psi = \psi(x,t)$

& $V = V(x,t)$

For time independent solution $V$ is a function of space co-ordinates only i.e. $V = V(x)$ and in that case we can use the method of separation variables

$$\psi(x,t) = \alpha(x)\,\phi(t)$$

where $\alpha(x)$ is function of position only and $\phi$ is a function of time only

Now
$$\frac{\partial \psi}{\partial t} = \alpha(x) \frac{d\phi(t)}{dt} \quad - - (2)$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{d^2\alpha(x)}{dx^2}\phi(t) \quad \text{———} \quad (3)$$

Scanned with CamScanner

Putting ② and ③ in equation ①

$$i\hbar\,\alpha(x)\frac{d\phi(t)}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\alpha(x)}{dx^2}\phi(t) + U(x)\,\alpha(x)\,\phi(t)$$

dividing both side by $\alpha(x)\,\phi(t)$

$$i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\alpha(x)}\frac{d^2\alpha(x)}{dx^2} + U(x) \quad \text{④}$$

Now, the left side is a function of 't' alone, and right side is a function of x alone. The only way this can possibly be true is if both side are ~~in~~ fact constant — otherwise, by varying t, one could change the left side without touching the right side, and the two would no longer be equal.

So we shall call the separation constant $E$.

$$i\hbar\frac{1}{\phi(t)}\frac{d\phi(t)}{dt} = E$$

$$\frac{d\phi(t)}{dt} = -\frac{i}{\hbar}E\,\cancel{\phi}\,\phi(t)$$

or $$\cancel{\phi}\,\frac{d\phi(t)}{\phi(t)} = -\frac{iE}{\hbar}\,dt$$

Integrating both side.

$$\cancel{\phi(t)}\ \ln\phi(t) = -\frac{iE}{\hbar}t$$

$$\phi(t) = e^{-iEt/\hbar}$$

So from ④

$$-\frac{\hbar^2}{2m}\frac{1}{\alpha(x)}\frac{d^2\alpha(x)}{dx^2} + U(x) = E$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\alpha(x)}{dx^2} + U(x)\,\alpha(x) = E\,\alpha(x)}$$

As $\alpha(x)$ is any arbitrary function of $x$ we may choose $\alpha(x) = \psi(x)$

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

Schrödinger wave equation for time-independent potential ~~or~~ also called as steady state solution.

## Wave packets.

Single contineous waves with sharply defined frequencies and wave length ~~was~~ have rare occurrance. Usually one observes wave trains of finite extensions formed by superposition of many harmonic waves having different amplitudes, frequencies. Wave packet is formed when a large number of harmonic waves with varying amplitudes, frequencies superpose ~~to~~ such that the resulting wave function vanishes everywhere except for a finite region of space. The range of wavelength & frequencies of the component harmonic wave needed to form the wave packet depends on its spatial extension ($\Delta x$) and duration in time ($\Delta t$).

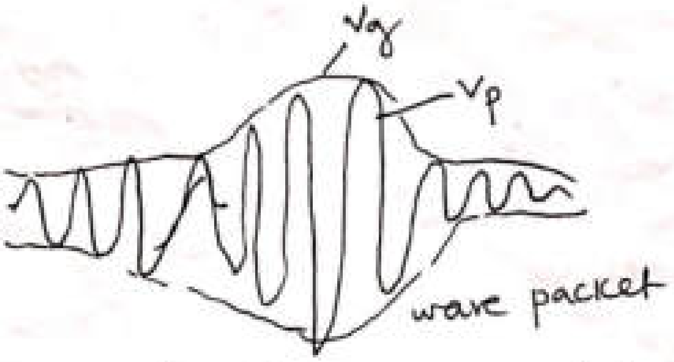
For quantum mechanical description of a particle, the matter wave associated with a moving particle is represented by a wave packet.

A wave packet formed by the superposition of many harmonic waves can be represented by the wave function

$$\psi(\vec{r}, t) = \sum_i A_i \sin(\vec{k}_i \cdot \vec{r} - \omega_i t)$$

If the wave vector angular frequency of the component waves vary continuously, the sum is replaced by the integral

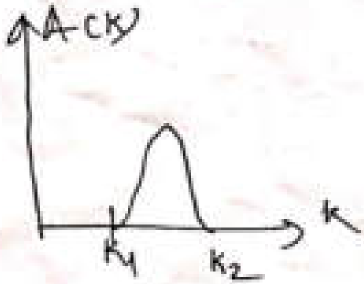
$$\psi(r,t) = \int A(K) \sin(K \cdot x - \omega t)\, dK$$




If the wave vector of the component harmonic waves are spread over a narrow range (say from $k_1$ to $k_2$) the amplitude $A(K)$ has non zero value only within that range of wave vector and vanishes beyond the range.

$$A(K) \neq 0, \quad \text{to} \quad K_1 < K < K_2$$
$$= 0 \qquad K < K_1 \ \& \ K > K_2$$

so $$\psi(x,t) = \int_{K_1}^{K_2} A(K) \sin(Kx - \omega t)\, dK$$




Scanned with CamScanner

## The Free particle.

The simplest system in quantum mechanics has the potential energy V equal to zero everywhere. This is called a free particle since it has no forces acting on it. Let us consider the one-dimensional case, with motion only in the x-direction, giving the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \qquad \text{--- (1)}$$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0 \qquad \text{--- (2)}$$

$$\text{let} \quad k^2 = \frac{2mE}{\hbar^2} \qquad \text{--- (3)}$$

Possible solution of equation (2)

$$\psi(x) = \text{Const}\begin{cases} \sin kx \\ \cos kx \\ e^{\pm ikx} \end{cases} \qquad \text{--- (4)}$$

There is no restriction on the value of K. Thus a free particle, even in quantum mechanics can have any non-negative value of energy.

$$E = \frac{\hbar^2 K^2}{2m} \geq 0 \qquad \text{--- (5)}$$

The energy levels in this case are not quantized and correspond to the same continuum of kinetic energy shown by classical particle

It is also of intense interest to consider the $x$-component of linear momentum for the free-particle solutions. According to the eigen value equation

$$\hat{p}_x \psi(x) = -i\hbar \frac{d\psi(x)}{dx} = p\,\psi(x) \quad \text{—⑥}$$

here we have denoted the momentum eigen value as $p$. It can easily be shown that neither $\sin kx$ or $\cos kx$ from equation ④ is an eigen function of $\hat{p}_x$. [Check it yourself] However, $e^{\pm ikx}$ are both eigen functions with eigen values $p = \pm\hbar k$, respectively. Evidently the momentum $p$ can take on any real values between $-\infty$ and $+\infty$. The kinetic energy, equal to $E = \frac{p^2}{2m}$, can correspondingly have any values between $0$ and $\infty$.

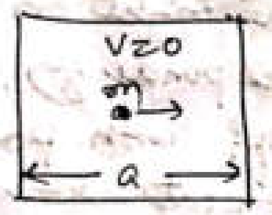
The eigen function $e^{ikx}$ for $k>0$, represents the particle moving from left to the right on the $x$-axis, with momentum $p>0$. Correspondingly, $e^{-ikx}$ represents motion from right to left with $p<0$. The functions $\sin kx$ & $\cos kx$ represents standing waves, obtained by superpositions of opposing wave motions.

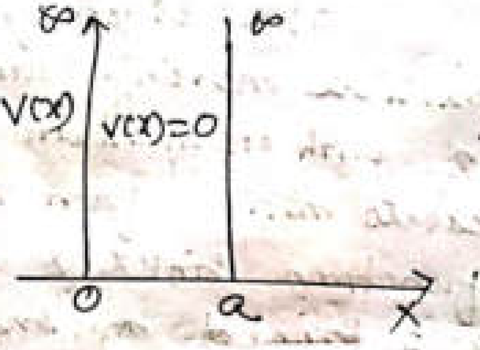
# Particle in a one-dimensional box.

Let us consider the motion of a particle in a hollow rectangular box along the X-axis in a non-relativistic region. We assume that (i) the walls of the box are rigid, hard and elastic. Then the particle will rebound in the box without any loss of kinetic energy. (ii) the walls of the box are non penetrable. The particle then remain confined in the box as the energy of the particle is less than the potential energy outside the box.

$$V(x) = 0 \qquad 0 < x < a$$
$$V(x) = \infty \quad \text{in} \quad x \leq 0 \;\&\; x \geq a$$

where $a$ is the length of the box in the x-direction




The above potential energy curve is also called square well potential of infinite depth.

Since inside the box $V(x)=0$, the particle is free. The Schrödinger time-independent equation for the particle is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

$E$ is the total energy of the particle and $\hbar = \frac{h}{2\pi}$

or $$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad \text{—— (1)}$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \text{when } k^2 = \frac{2mE}{\hbar^2} \qquad (2)$$

The solution of equation (2) can be written like

$$\psi(x) = A\sin kx + B\cos kx \qquad (3)$$

where A and B are constants to be found out from the boundary condition of the problem (a) $\psi(x) = 0$ at $x = 0$ & $x = a$

(i) $\psi(x) = 0$ at $x = 0$

$$0 = A \cdot 0 + B \cdot 1 \text{ or } B = 0$$

thus $\psi(x) = A\sin kx$ ——— (4)

Again at $x = a$

$$\psi(a) = 0 = A\sin ka$$

$$A \neq 0 \therefore \sin ka = 0 \text{ or } ka = n\pi$$

$$\text{so } k = \frac{n\pi}{a}, \quad n = 1, 2, 3 \ldots \qquad (5)$$

But $n = 0$ is not possible because for $n = 0$, $k = 0$ & $E = 0$ so $\psi(x) = 0$ everywhere in the box.

$\therefore$ Thus the wavefunction for the particle is $0 < x < a$

$$\psi_n(x) = A\sin\frac{n\pi x}{a}$$

## Energy eigen values:

From equation (2) & (5)

$$k^2 = \frac{2mE}{\hbar^2}$$

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

$$\text{or } \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}} \qquad (6)$$

or $E_n \propto n^2$ that is energy eigen values are discrete.

Scanned with CamScanner

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2} \quad \text{------} \quad (7)$$

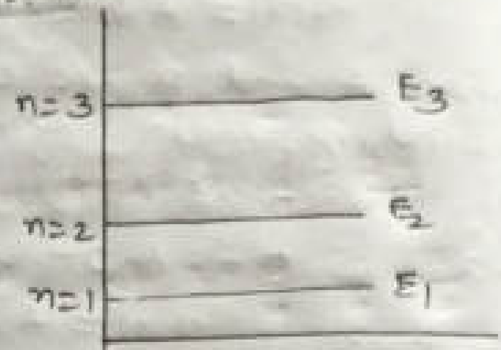
$E_1$ is called the ground state energy of the particle

(ii) The energy for $n = 2, 3, 4$ --- are

$$E_2 = \frac{4\pi^2\hbar^2}{2ma^2}$$

$$E_3 = \frac{9\pi^2\hbar^2}{2ma^2}$$

$$E_4 = \frac{16\pi^2\hbar^2}{2ma^2}$$




which are clearly discrete

## Normalisation of $\psi(x)$

Here we have

$$\psi_n(x) = A\sin\frac{n\pi x}{a} \qquad 0 < x < a$$
$$= 0 \qquad \text{elsewhere.}$$

Since the probability of finding the particle in $0 < x < a$ is unity

$$\int_0^a |\psi_n(x)|^2 dx = 1 \quad \text{or} \quad \int_0^a A^2 \sin^2\frac{n\pi x}{a}\, dx = 1$$

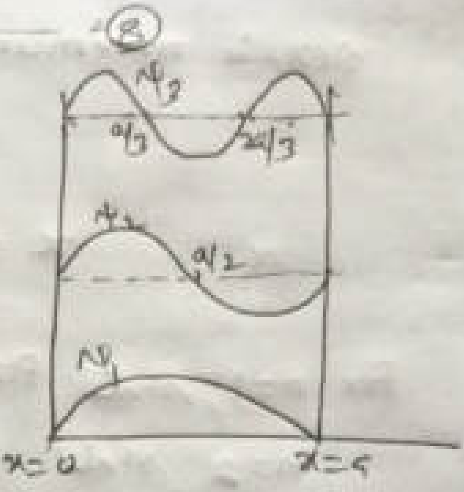
$$\text{or} \quad A^2 \int_0^a \frac{1}{2}\left[1 - \cos\frac{2\pi n x}{a}\right] dx = 1$$

$$\frac{A^2}{2}\left[x - \frac{\sin 2\pi n x/a}{(2\pi n/a)}\right]_0^a = 1$$

$$\text{or} \quad \frac{A^2}{2} a = 1 \quad \text{or} \quad A = \frac{\sqrt{2}}{\sqrt{a}}$$

So the normalized wave function

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \quad \text{--- (8)}$$




$\psi_1(x) = 0$ for $x = 0$ & $x = a$

so $\psi_1(x)$ has two nodes at $x=0$, $x=a$

$\psi_2(x)$ has three nodes at $x=0$, $x=\frac{a}{2}$ & $x=a$

so it is clear that $\psi_n(x)$ has $(n+1)$ nodes. The nature of $\psi_1(x)$, $\psi_2(x)$ & $\psi_3(x)$ are shown in the figure.

## Eigen values of momentum:

For the $n$th state, the momentum $p_n$ is given by $p_n^2 = 2mE_n = 2m \times \frac{n^2\pi^2\hbar^2}{2ma^2}$

$$\text{or} \quad p_n^2 = \frac{n^2\pi^2\hbar^2}{a^2} \quad \text{--- (9)}$$

$$p_n = \pm \frac{n\pi\hbar}{a} \qquad \left[\because \hbar = \frac{h}{2\pi}\right]$$

$$\text{or} \quad p_n = \pm \frac{nh}{2a}$$

The $\pm$ sign before $\frac{nh}{2a}$ is due to the fact that the particle moves back and forth in the box.

## Probability of location of particle:

The probability of finding the particle in the small distance $dx$ is

$$P(x)\,dx = |\psi_n(x)|^2 dx = \frac{2}{a} \sin^2 \frac{n\pi x}{a}\, dx$$

or the probability density

$$P(x) = \frac{2}{a} \sin^2 \frac{n\pi x}{a}$$

Scanned with CamScanner

$P(x)$ is minimum when $\frac{n\pi x}{a} = (2n+1)\frac{\pi}{2}$

$= \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2} \cdots$

or $\quad x = \frac{a}{2n}, \frac{3a}{2n}, \frac{5a}{6}$

For $n=1$, state $P(x)$ is maximum at $x = a/2$

$n=2$ state $P(x)$ is maximum at $x = \frac{a}{4}, \frac{3a}{4}$

$n=3$ " " " at $x = \frac{a}{6}, \frac{3a}{6}, \frac{5a}{6}$

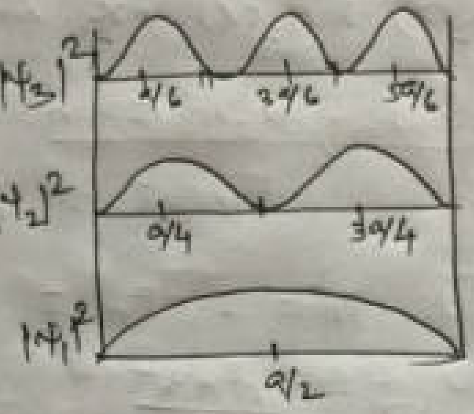



Figure shows the probability density.