## Ch. 4 The Schrodinger Equation and its Applications

1. Wave Function: The probability that a particle will be found at a given place in space at a given instant of time is characterised by the function $\Psi(x, y$, $\mathrm{z}, \mathrm{t})$. It is called as wave function. This function can be either real or complex. The only quantity having a physical meaning is the square of its magnitude $\mathrm{P}=$ $|\Psi|^{2}=\Psi \Psi^{*}$ where $\Psi^{*}$ is the complex conjugate of $\Psi$. The quantity P is the probability density. The probability of finding a particle in a volume dxdydz is $|\Psi|^{2}$ dxdy dz.

Further, the particle is certainly to be found somewhere in space

$$
\iiint|\Psi|^{2} \mathrm{dx} \mathrm{dy} \mathrm{dz}=1
$$

A wave function $\Psi$ satisfying this relation is called as a normalised wave function.

There are two types of wave function such as orthogonal wave function and normalised wave function.

If the product of a function $\Psi_{1}(\mathrm{x})$ and the complex conjugate $\Psi_{2} *(\mathrm{x})$ of function $\Psi_{2}(\mathrm{x})$ vanishes, when integrated with respect to x over the internal $-\infty \leq \mathrm{x} \leq \infty$, that is, if $\int_{-\infty}^{\infty} \Psi_{2}^{*}(x) \Psi_{1}(x) d x=0$

Then $\Psi_{1}(\mathrm{x})$ and $\Psi_{2}(\mathrm{x})$ are said to be orthogonal in the interval $(-\infty, \infty)$.
We know that the probability of finding a particle in the volume element dv is given by $\Psi \Psi^{*} \mathrm{dv}$.

The total probability of finding the particle in the entire space is unity i.e. $\int_{-\infty}^{\infty}|\Psi|^{2} d v=1$

This equation can also be written as, $\int_{-\infty}^{\infty} \Psi \Psi^{*} \mathrm{dv}=1$

Any wave function satisfying the above equation is said to be normalised to unity or simply normalised wave function.

Very often $\Psi$ is not a normalised wave function. If we multiply $\Psi$ by A, it gives new wave function which is also a solution of wave equation then,

$$
\begin{aligned}
& \int_{-\infty}^{\infty}(A \Psi)^{*}(A \Psi) \mathrm{dx} \mathrm{dy} \mathrm{dz}=1 \\
& |\mathrm{~A}|^{2} \int_{-\infty}^{\infty} \Psi \Psi^{*} d x d y d z=1 \\
& |\mathrm{~A}|^{2}=\frac{1}{\int_{-\infty}^{\infty} \Psi \Psi^{*} d x d y d z}
\end{aligned}
$$

$|\mathrm{A}|$ is known as normalised constant.

Physical significance of wave function $\Psi$ :
i) $\Psi$ must be single valued and continuous everywhere.
ii) If $\Psi_{1}(\mathrm{x}), \Psi_{2}(\mathrm{x}),-\cdots---\Psi_{\mathrm{n}}(\mathrm{x})$, are solutions of Schrödinger equation then the linear combination $\Psi(x)=a_{1} \Psi_{1}(x)+a_{2} \Psi_{2}(x)+\cdots----+a_{n} \Psi_{n}(x)$ must be a solution.
iii) The wave function $\Psi(x)$ must approach to zero as $x \rightarrow \pm \infty$.

## 2. Time dependent Schrodinger wave equations:

The quantity that characterises the De Broglie waves is called the wave function. It is denoted by $\Psi$.

Let us assume that $\Psi$ is specified in the X-directions by

$$
\begin{equation*}
\Psi=A e^{-i w(t-x / v)} \tag{1}
\end{equation*}
$$

If $v$ is the frequency then $w=2 \pi \nu$ and $v=v \lambda$

$$
\begin{gather*}
\therefore \Psi=A e^{-i 2 \pi v(t-x / v \lambda)} \\
\therefore \Psi=A e^{-i 2 \pi(v t-x / \lambda)-------(2} \tag{2}
\end{gather*}
$$

Let E be total energy and p be momentum of the particle. Then $\mathrm{E}=\mathrm{h} \nu$ and $\lambda=\mathrm{h} / \mathrm{p}$.

Therefore $\mathrm{eq}^{\mathrm{n}}(2)$ becomes,

$$
\begin{gathered}
\Psi=A e^{-i 2 \pi\left(\frac{E}{h} t-\frac{x p}{h}\right)} \\
\therefore \Psi=A e^{-\frac{i 2 \pi}{h}(E t-x p)}
\end{gathered}
$$

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

$$
\therefore \Psi=A e^{\frac{-i}{\hbar}(E t-x p)}---------(3)
$$

$E q^{n}(3)$ is mathematical description of the wave equivalent to unrestricted particle of total energy E and momentum p moving in positive direction of X axis.

Differentiate $\mathrm{Eq}^{\mathrm{n}}(3)$ with respect to t , we get

$$
\frac{\partial \Psi}{\partial t}=A \cdot e^{\frac{-i}{\hbar}(E t-x p)} \cdot \frac{-i}{\hbar} E=\frac{-i}{\hbar} E \Psi----(4)
$$

Differentiate $\mathrm{Eq}^{\mathrm{n}}(3)$ twice with respect to $x$, we get

$$
\begin{gathered}
\frac{\partial \Psi}{\partial x}=A \cdot e^{\frac{-i}{\hbar}(E t-x p)} \cdot \frac{-i}{\hbar}(-p)=\frac{i p}{\hbar} \Psi \\
\frac{\partial^{2} \Psi}{\partial x^{2}}=\frac{i p}{\hbar} \frac{\partial \Psi}{\partial x}
\end{gathered}
$$

$$
\therefore \frac{\partial^{2} \Psi}{\partial x^{2}}=\frac{i p}{\hbar} \cdot \frac{i p}{\hbar} \Psi=\frac{i^{2} p^{2}}{\hbar^{2}} \Psi=\frac{-p^{2}}{\hbar^{2}} \Psi=---(5)
$$

At small speed compared with that of light, the total energy $E$ of a particle is sum of its kinetic energy and its potential energy V .

Therefore, total energy =Kinetic energy + potential energy

$$
\therefore E=\frac{1}{2} m v^{2}+V=\frac{1}{2} \frac{m^{2} \mathrm{v}^{2}}{m}+V
$$

But $\mathrm{p}=\mathrm{mv}$

$$
\therefore E=\frac{p^{2}}{2 m}+V
$$

Multiplying both side by $\Psi$

$$
\begin{equation*}
\therefore E \Psi=\frac{p^{2} \Psi}{2 m}+V \Psi----- \tag{6}
\end{equation*}
$$

From $\mathrm{Eq}^{\mathrm{n}}(4), E \Psi=\frac{-\hbar}{i} \frac{\partial \Psi}{\partial t}$
From $\mathrm{Eq}^{\mathrm{n}}(5), p^{2} \Psi=-\hbar^{2} \frac{\partial^{2} \Psi}{\partial x^{2}}$

Substituting these values in $\mathrm{Eq}^{\mathrm{n}}$ (6), we get

$$
\begin{gathered}
\frac{-\hbar}{i} \frac{\partial \Psi}{\partial t}=\frac{-\hbar^{2}}{2 m} \frac{\partial^{2} \Psi}{\partial x^{2}}+V \Psi \\
\frac{-\hbar i}{i^{2}} \frac{\partial \Psi}{\partial t}=\frac{-\hbar^{2}}{2 m} \frac{\partial^{2} \Psi}{\partial x^{2}}+V \Psi \\
i \hbar \frac{\partial \Psi}{\partial t}=\frac{-\hbar^{2}}{2 m} \frac{\partial^{2} \Psi}{\partial x^{2}}+V \Psi-----(7)
\end{gathered}
$$

$\mathrm{Eq}^{\mathrm{n}}(7)$ is called as time dependent form of Schrodinger's equation.

Put $\hbar=\frac{h}{2 \pi}$
Therefore $\mathrm{Eq}^{\mathrm{n}}(7)$ becomes,

$$
\frac{i h}{2 \pi} \frac{\partial \Psi}{\partial t}=\frac{-h^{2}}{8 \pi^{2} m} \frac{\partial^{2} \Psi}{\partial x^{2}}+V \Psi----- \text { (8) }
$$

In three dimensions, the time dependent form of Schrodinger equation can be written as,

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

## 3. Expectation Values:

The expectation or average value of a dynamical quantity is defined as it is mathematical average for the result of a single measurement.

Suppose we have find average or mean positions of all particles along xaxis. If $\mathrm{N}_{1}$ number of particles is at $\mathrm{x}_{1}, \mathrm{~N}_{2}$ number of particles is at $\mathrm{x}_{2}$ and so on, then the average position $\bar{x}$ in this case is similar to the centre of mass of the distribution

$$
\begin{align*}
& \text { i.e. } \quad \bar{x}=\frac{N_{1} x_{1}+N_{2} x_{2}+N_{3} x_{3}+\ldots \ldots \ldots \ldots \ldots \ldots . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . ~}{N_{1}+N_{2}+N_{3}+\ldots}=\frac{\sum_{i=1}^{n} N_{i} x_{i}}{\sum_{i=1}^{n} N_{i}} \\
& \text { or } \tag{1}
\end{align*}
$$

Quantum mechanically, this expression can be modified for a single particle, by replacing the number $\mathrm{N}_{\mathrm{i}}$ of particles at $\mathrm{x}_{\mathrm{i}}$ by the probability $\mathrm{P}_{\mathrm{i}}$. The probability that the particle may found in an interval dx at $x_{i}$ may be given as

$$
\begin{equation*}
P_{i}=\left|\psi_{i}\right|^{2} d x \tag{2}
\end{equation*}
$$

where $\psi_{i}$ is wave function associated with the particle. Substituting (2) in (1) and taking integral between limits $-\infty$ to $+\infty$ instead of the summation, we have

$$
\begin{equation*}
\bar{x}=\frac{\int_{-\infty}^{\infty} x|\psi|^{2} d x}{\int_{-\infty}^{\infty}|\psi|^{2} d x} \tag{3}
\end{equation*}
$$

If the wave function is normalized, then

$$
\int_{-\infty}^{\infty}|\psi|^{2} d x=1
$$

Thus, equation (3) becomes

$$
\begin{equation*}
\bar{x}=\int_{-\infty}^{\infty} x|\psi|^{2} d x \tag{4}
\end{equation*}
$$

The equation (4) is more conveniently written as

$$
\begin{equation*}
\overline{\mathrm{x}}=\int_{-\infty}^{\infty} \psi^{*} \mathrm{x} \psi \mathrm{dx} \tag{5}
\end{equation*}
$$

where $\psi^{*}$ is complex conjugate of $\psi$.
The expectation value $G(x)$ of any quantity which is a function of the position $x$ of a particle and is described by a wave function $\psi$ may be expressed as

$$
\begin{equation*}
\bar{G}=\int_{-\infty}^{\infty} \psi^{*} G(x) \psi d x \tag{6}
\end{equation*}
$$

The expression (6) holds even if $G(x)$ changes with time, since $\psi$ is function of time t .
4. Operators: An operator is a rule by means of which a given function is changed into another function.

However the choice of operator is arbitrary in quantum mechanics, when an operator operates on a wave function it must give observable quantity times the wave function. It is necessary condition for an operator.

The wave function of a particle is

$$
\therefore \Psi=A e^{\frac{-i}{\hbar}(E t-x p)}
$$

Differentiate with respect to $x$ and $t$, we get

$$
\frac{\partial \Psi}{\partial x}=A \cdot e^{\frac{-i}{\hbar}(E t-x p)} \cdot \frac{-i}{\hbar}(-p)=\frac{i p}{\hbar} \Psi
$$

and

$$
\frac{\partial \Psi}{\partial t}=A \cdot e^{\frac{-i}{\hbar}(E t-x p)} \cdot \frac{-i}{\hbar} E=\frac{-i}{\hbar} E \Psi
$$

This equation can be written as,

$$
p \Psi=\frac{\hbar}{i} \frac{\partial \Psi}{\partial x} \text { and } E \Psi=\frac{\hbar}{-i} \frac{\partial \Psi}{\partial t}=i \hbar \frac{\partial \Psi}{\partial t}
$$

The dynamical quantity p in some sense corresponds to the differential operator $\frac{\hbar}{i} \frac{\partial}{\partial x}$ and dynamical quantity E corresponds to the differential operator $i \hbar \frac{\partial}{\partial t}$.

Let $\mathrm{P}_{\text {op }}$ is operator that corresponds to momentum p and $\mathrm{E}_{\mathrm{op}}$ is operator that corresponds to total energy E .

$$
\therefore P_{o p}=\frac{\hbar}{i} \frac{\partial}{\partial x}-----(1)
$$

And

$$
E_{o p}=i \hbar \frac{\partial}{\partial t}-----(2)
$$

The total energy of a particle with the operator equation is sum of kinetic energy T and potential energy V i.e. $\mathrm{E}=\mathrm{T}+\mathrm{V}$.

Since kinetic energy in terms of momentum P is

$$
\begin{gathered}
T=\frac{P^{2}}{2 m} \\
\therefore T_{o p}=\frac{1}{2 m}\left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right)^{2}=\frac{-\hbar^{2}}{2 m} \frac{\partial^{2}}{\partial x^{2}}
\end{gathered}
$$

Total energy operator is,

$$
\begin{gathered}
E_{o p}=T_{o p}+V \\
i \hbar \frac{\partial}{\partial t}=\frac{-\hbar^{2}}{2 m} \frac{\partial^{2}}{\partial x^{2}}+V
\end{gathered}
$$

Multiplying both side by $\Psi$,

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

This is Schrödinger equation.
We can use operators to obtain expectation values for p and E . Thus, expectation values for p is,

$$
\bar{p}=\int_{-\infty}^{\infty} \Psi^{*} P_{o p} \Psi d x=\int_{-\infty}^{\infty} \Psi^{*}\left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right) \Psi d x=\frac{\hbar}{i} \int_{-\infty}^{\infty} \Psi^{*}\left(\frac{\partial \Psi}{\partial x}\right) d x
$$

And expectation value for E is

$$
\bar{E}=\int_{-\infty}^{\infty} \Psi^{*} E_{o p} \Psi d x=\int_{-\infty}^{\infty} \Psi^{*}\left(i \hbar \frac{\partial}{\partial t}\right) \Psi d x=i \hbar \int_{-\infty}^{\infty} \Psi^{*}\left(\frac{\partial \Psi}{\partial t}\right) d x
$$

## 5. Time Independent form of Schrodinger Equation (Steady state form):-

In many problems potential energy of a particle depends only on its position, Schrodinger equation may be obtained by removing all references to time $t$. The wave function of a particle may be written in the form as

$$
\begin{gather*}
\Psi=A e^{\frac{-i}{\hbar}(E t-x p)}------(  \tag{1}\\
\Psi=A e^{\frac{-i E t}{\hbar}} \cdot e^{\frac{i p x}{\hbar}}
\end{gather*}
$$

Put $\Psi_{0}=A e^{\frac{i p x}{\hbar}}$ is the position dependent function

$$
\Psi=\Psi_{0} e^{\frac{-i E t}{\hbar}}-------(2)
$$

Differentiate with respect to $t$ we get,

$$
\begin{equation*}
\frac{\partial \Psi}{\partial t}=\Psi_{0} e^{\frac{-i E t}{\hbar}} \cdot \frac{-i E}{\hbar}=\frac{-i E \Psi_{0}}{\hbar} e^{\frac{-i E t}{\hbar}} \tag{3}
\end{equation*}
$$

Differentiate eq ${ }^{\mathrm{n}}(2)$ twice with respect to $x$ we get,

$$
\begin{equation*}
\frac{\partial \Psi}{\partial x}=\frac{\partial \Psi_{0}}{\partial x} e^{\frac{-i E t}{\hbar}}----- \tag{4}
\end{equation*}
$$

And

$$
\begin{equation*}
\frac{\partial^{2} \Psi}{\partial x^{2}}=\frac{\partial^{2} \Psi_{0}}{\partial x^{2}} e^{\frac{-i E t}{\hbar}}------- \tag{5}
\end{equation*}
$$

Now time dependent form of Schrodinger equation is

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

By substituting values of $\frac{\partial \Psi}{\partial t}, \frac{\partial^{2} \Psi}{\partial x^{2}}$ and $\Psi$ we get

$$
\begin{gathered}
i \hbar\left(\frac{-i E \Psi_{0}}{\hbar} e^{\frac{-i E t}{\hbar}}\right)=\frac{-\hbar^{2}}{2 m} \frac{\partial^{2} \Psi_{0}}{\partial x^{2}} e^{\frac{-i E t}{\hbar}}+V \Psi_{0} e^{\frac{-i E t}{\hbar}} \\
-i^{2} E \Psi_{0}=\frac{-\hbar^{2}}{2 m} \frac{\partial^{2} \Psi_{0}}{\partial x^{2}}+V \Psi_{0} \\
E \Psi_{0}=\frac{-\hbar^{2}}{2 m} \frac{\partial^{2} \Psi_{0}}{\partial x^{2}}+V \Psi_{0} \\
\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \Psi_{0}}{\partial x^{2}}+(E-V) \Psi_{0}=0 \\
\frac{\partial^{2} \Psi_{0}}{\partial x^{2}}+\frac{2 m}{\hbar^{2}}(E-V) \Psi_{0}=0-----(6)
\end{gathered}
$$

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In this equation (6) $\Psi_{0}$ is a function of $x$ only, therefore this equation being independent of time. This is steady state form of Schrodinger wave equation.

In three dimensions, this equation is written as

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

Usually it is written in the form as

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

## 6. Particle in one dimensional box- Energy quantization:

Consider a particle moving inside a box along the X -direction. The particle is bouncing back and forth between the walls of the box i.e. $x=0$ and $x=L$ by infinitely hard walls. The box is supposed to have walls of infinite height at $x=0$ and $x=L$ as shown in figure. The particle has a mass $m$ and its position $x$ at any instant is given by $0<x<L$.

The potential energy V of particle is infinite on both sides of the box. The potential energy V of the particle can



Fig. A particle confined to a box of width L be assumed to be zero between $x=0$ and $x=L$ i.e. inside the box. Interms of boundary conditions imposed by problem, the potential function is

$$
\begin{align*}
& V=0 \text { for } 0<x<L \\
& V=\infty \text { for } x \leq 0 \text { and } x \geq L \tag{1}
\end{align*}
$$

The particle cannot exist outside the box and so it's wave function $\Psi$ is zero for $\mathrm{x} \leq 0$ and $\mathrm{x} \geq \mathrm{L}$.

The Schrodinger wave equation is,

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

Inside the box $\mathrm{V}=0$,

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

$\operatorname{Put} \frac{2 m}{\hbar^{2}} E=k^{2}$
The above equation becomes,

$$
\frac{d^{2} \Psi}{d x^{2}}+k^{2} \Psi=0
$$

The general solution of this equation is,

$$
\Psi=A \sin K x+B \cos k x------(3)
$$

Where A and B are arbitrary constants. The boundary conditions can be used to evaluate the constants A and B is $\Psi=0$ at $\mathrm{x}=0$.
$\therefore$ eqn(3) becomes,

$$
0=A \sin 0+B \cos 0=B \quad \text { i.e. } B=0
$$

And $\Psi=0$ at $\mathrm{x}=\mathrm{L}$,

$$
\begin{aligned}
& 0=A \operatorname{sink} L+0 \\
& \therefore A \operatorname{sink} L=0
\end{aligned}
$$

$$
\text { Since } \mathrm{A} \neq 0, \therefore \operatorname{sinkL}=0
$$

$\therefore \mathrm{kL}=\mathrm{n} \pi$ where n is integer.

$$
\therefore k=\frac{n \pi}{L}
$$

Putting value of $B$ and $k$ in $q^{n}(3)$,

$$
\Psi_{n}=A \sin \frac{n \pi x}{L}-------(4)
$$

As the particle is certainly within the box, the normalization condition is,

$$
\begin{gathered}
\int_{0}^{L} \Psi \Psi^{*} d x=1 \\
\therefore \int_{0}^{L}\left(A \sin \frac{n \pi x}{L}\right)\left(A \sin \frac{n \pi x}{L}\right) d x=1 \\
\therefore A^{2} \int_{0}^{L} \sin ^{2} \frac{n \pi x}{L} d x=1 \\
\therefore A^{2} \int_{0}^{L} \frac{1-\cos \frac{2 n \pi x}{L}}{2} d x=1 \\
\therefore \frac{A^{2}}{2}\left[x-\frac{\sin \frac{2 n \pi x}{2 n \pi}}{2 n}\right]_{0}^{L}=1 \\
\frac{A^{2}}{2}\left[L-\frac{L}{2 n \pi} \sin 0-0\right]=1 \\
\frac{A^{2} L}{2}=1 . \therefore A^{2}=\frac{2}{L} \quad \therefore A=\sqrt{\frac{2}{L}}
\end{gathered}
$$

Therefore eq ${ }^{\mathrm{n}}(4)$ becomes,

$$
\Psi_{n}=\sqrt{\frac{2}{L}} \sin \frac{n \pi x}{L}------(5)
$$

Differentiate with respect to $x$ twice,

$$
\begin{gathered}
\frac{d \Psi_{n}}{d x}=\sqrt{\frac{2}{L}} \cos \frac{n \pi x}{L} \cdot \frac{n \pi}{L}=\frac{n \pi}{L} \sqrt{\frac{2}{L}} \cos \frac{n \pi x}{L} \\
\frac{d^{2} \Psi_{n}}{d x^{2}}=\frac{n \pi}{L} \sqrt{\frac{2}{L}} \cdot-\sin \frac{n \pi x}{L} \cdot \frac{n \pi}{L}=-\left(\frac{n \pi}{L}\right)^{2} \sqrt{\frac{2}{L}} \cdot \sin \frac{n \pi x}{L} \\
\frac{d^{2} \Psi_{n}}{d x^{2}}=-\left(\frac{n \pi}{L}\right)^{2} \Psi
\end{gathered}
$$

Substituting these values in $\mathrm{eq}^{\mathrm{n}}(2)$,

$$
\begin{gathered}
\therefore-\left(\frac{n \pi}{L}\right)^{2} \Psi_{n}+\frac{2 m}{\hbar^{2}} E \Psi_{n}=0 \\
\therefore\left[-\left(\frac{n \pi}{L}\right)^{2}+\frac{2 m}{\hbar^{2}} E\right] \Psi_{n}=0 \\
\text { i.e. }-\left(\frac{n \pi}{L}\right)^{2}+\frac{2 m}{\hbar^{2}} E=0 \\
\frac{2 m}{\hbar^{2}} E=\frac{n^{2} \pi^{2}}{L^{2}} \\
\therefore E=\frac{n^{2} \pi^{2} \hbar^{2}}{2 m L^{2}} \quad \text { i.e. } E_{n}=\frac{n^{2} \pi^{2} \hbar^{2}}{2 m L^{2}}--(6)
\end{gathered}
$$

Where $n=1,2,3, \cdots-----$
For each value of $n$, there is an energy level and corresponding wave function is given by eq ${ }^{n}(5)$. Each value of $E_{n}$ is called as eigen value and corresponding $\Psi_{n}$ is called as eigen functions. Thus inside the box, the particle can only have the
discrete energy. It may be also noted that the particle in box cannot have zero energy.

## Particle in One-Dimensional Box: Momentum quantization

The energy values of a particle trapped in one-dimensional box are given by

$$
\begin{equation*}
E_{n}=\frac{n^{2} \pi^{2} \hbar^{2}}{2 m L^{2}}, \quad \mathrm{n}=1,2,3, \ldots \ldots \ldots \ldots \tag{1}
\end{equation*}
$$

The wavefunctions representing the particle for various states are given by

$$
\begin{equation*}
\psi_{n}=\sqrt{\frac{2}{L}} \operatorname{Sin}\left(\frac{n \pi}{L} x\right) \tag{2}
\end{equation*}
$$

The relation between energy and momentum is

$$
E_{n}=\frac{P_{n}^{2}}{2 m}
$$

which gives

$$
P_{n}= \pm \sqrt{2 m E_{n}}= \pm \sqrt{\frac{2 m n^{2} \pi^{2} \hbar^{2}}{2 m L^{2}}}= \pm \frac{n \pi \hbar}{L}
$$

Thus there are two momentum values of the particle, denoting by $P_{n}^{+}$and $P_{n}{ }^{-}$, we write

$$
\begin{equation*}
P_{n}^{+}=+\frac{n \pi \hbar}{L} \tag{3a}
\end{equation*}
$$

and $\quad P_{n}^{-}=-\frac{n \pi \hbar}{L}$
When the particle moves along + ve direction of x -axis, it has $P_{n}{ }^{+}$momentum and when it moves along -ve direction it has $P_{n}{ }^{-}$momentum. Clearly, the average value of the momentum is zero.

The momentum eigenvalue equation is given by

$$
\begin{equation*}
\hat{P} \psi_{n}=P_{n} \psi_{n} \tag{4}
\end{equation*}
$$

The momentum operator is given by

$$
\begin{equation*}
\hat{P}=-i \hbar \frac{d}{d x} \tag{5}
\end{equation*}
$$

Using equations (2), (4) and (5), we get

$$
\begin{aligned}
& \hat{P} \psi_{n}=-i \hbar \frac{d}{d x}\left[\sqrt{\frac{2}{L}} \operatorname{Sin}\left(\frac{n \pi}{L} x\right)\right]=-i \hbar \sqrt{\frac{2}{L} \frac{d}{d x} \operatorname{Sin}\left(\frac{n \pi}{L} x\right)} \\
& \hat{P} \psi_{n}=-i \hbar \frac{n \pi}{L} \sqrt{\frac{2}{L}} \operatorname{Cos}\left(\frac{n \pi}{L} x\right) \neq p_{n} \psi_{n}
\end{aligned}
$$

Thus the energy eigen fuction $\psi_{n}$ given by equation (2) cannot be momentum eigen function.

To obtain the correct momentum eigenfunction, we use the following identity,

$$
\operatorname{Sin} \theta=\frac{e^{i \theta}-e^{-i \theta}}{2 i}
$$

Using it in equation (2), we get

$$
\psi_{n}=\sqrt{\frac{2}{L}} \operatorname{Sin}\left(\frac{n \pi}{L} x\right)=\sqrt{\frac{2}{L}} \frac{e^{i\left(\frac{n \pi}{L} x\right)}-e^{-i\left(\frac{n \pi}{L} x\right)}}{2 i}
$$

which gives two eigenfunctions. Denoting by $\psi_{n}{ }^{+}$and $\psi_{n}{ }^{-}$, we write

$$
\begin{equation*}
\psi_{n}^{+}=\frac{1}{2 i} \sqrt{\frac{2}{L}} e^{i\left(\frac{n \pi}{L} x\right)} \tag{6a}
\end{equation*}
$$

Let us check whether they satisfy equation (4). Therefore,

$$
\hat{P} \psi_{n}^{+}=-i \hbar \frac{d}{d x}\left(\frac{1}{2 i} \sqrt{\frac{2}{L}} e^{i\left(\frac{n \pi}{L} x\right)}\right)=-i \hbar \frac{1}{2 i} \sqrt{\frac{2}{L}} i \frac{n \pi}{L} e^{i\left(\frac{n \pi}{L} x\right)}
$$

or $\quad \hat{P} \psi_{n}{ }^{+}=\frac{n \pi \hbar}{L}\left(\frac{1}{2 i} \sqrt{\frac{2}{L}} e^{i\left(\frac{n \pi}{L} x\right)}\right)$
or $\quad \hat{P} \psi_{n}{ }^{+}=+\frac{n \pi \hbar}{L} \psi_{n}{ }^{+}$
Similarly, we obtain

$$
\begin{equation*}
\hat{P} \psi_{n}^{-}=-\frac{n \pi \hbar}{L} \psi_{n}^{-} \tag{7b}
\end{equation*}
$$

Thus, we get $P_{n}^{+}=+\frac{n \pi \hbar}{L}$ and $P_{n}^{-}=-\frac{n \pi \hbar}{L}$.
Therefore $\psi_{n}{ }^{+}$and $\psi_{n}{ }^{-}$given by equations (6a) and (6b) are the momentum eigen functions corresponding to the momentum eigen values $p_{n}{ }^{+}$and $p_{n}{ }^{-}$. Also, it is clear that the momentum eigen values are quantized.

## Multiple Choice Question:

1) Which of the following is the correct expression for the time dependent form of Schrödinger wave equation?
a) $i \hbar \frac{\partial \Psi}{\partial t}=-\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \Psi}{\partial x^{2}}+V \Psi$
b) $i \hbar \frac{\partial \Psi}{\partial t}=\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \Psi}{\partial x^{2}}-V \Psi$
c) $\frac{\partial \Psi}{\partial t}=\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \Psi}{\partial x^{2}}+V \Psi$
d) $\frac{\partial^{2} \Psi}{\partial x^{2}}+\frac{2 m}{\hbar^{2}}(E-V) \Psi=0$
2) Which of the following is the correct expression for the time independent form of Schrödinger wave equation?
a) $i \hbar \frac{\partial \Psi}{\partial t}=-\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \Psi}{\partial x^{2}}+V \Psi$
b) $i \hbar \frac{\partial \Psi}{\partial t}=\frac{\hbar^{2}}{2 m} \frac{\partial^{2} \Psi}{\partial x^{2}}-V \Psi$
c) $\frac{\partial^{2} \Psi}{\partial x^{2}}-\frac{2 m}{\hbar^{2}}(E+V) \Psi=0$
d) $\frac{\partial^{2} \Psi}{\partial x^{2}}+\frac{2 m}{\hbar^{2}}(\boldsymbol{E}-\boldsymbol{V}) \Psi=\mathbf{0}$
3) Which of the following is not a characteristic of wave function?
a) Continuous
b) single valued
c) differentiable
d) Physically significant
4) Any wave function can be written as a linear combination of
a) Eigen values
b) Eigen functions
c) eigen vectors
d) Operators
5) Which function is considered independent of time to achieve the steady state form?
a) $\Psi$
b) $\frac{\partial \Psi}{\partial t}$
c) $\frac{\partial^{2} \Psi}{\partial t^{2}}$
d) V
6) The values of Energy for which Schrodinger's steady state equation can be solved is called as $\qquad$
a) Eigen vectors
b) Eigen values
c) Eigen function
d) operators
7) For a box with infinitely hard walls, the potential is maximum at $\qquad$
a) $\mathbf{L}$
b) 2 L
c) $\mathrm{L} / 2$
d) 3 L
8) For normalized wave function $\psi \rightarrow 0$ as $x \rightarrow-----$
a) 0
b) 1
c) -1
d) $\infty$
9) The square of the magnitude of the wave function is called $\qquad$
a) Current density
b) volume density
c) probability density
d) zero density
10) The walls of a particle in a box are supposed to be $\qquad$
a) Small but infinitely hard
b) Infinitely large but soft
c) Soft and Small
d) Infinitely hard and infinitely large
11) The Energy of the particle in one dimensional box is proportional to $\qquad$
a) $n$
b) $n^{-1}$
c) $\mathbf{n}^{2}$
d) $n^{-2}$
12) The Eigen value of a particle in a box is $\qquad$
a) $\frac{L}{2}$
b) $\frac{2}{L}$
c) $\sqrt{\frac{2}{L}}$
d) $\sqrt{\frac{L}{2}}$
13) What is the minimum Energy possessed by the particle in a box?
a) Zero
b) $\frac{\pi^{2} \hbar^{2}}{2 m L^{2}}$
c) $\frac{\pi^{2} \hbar^{2}}{m L^{2}}$
d) 1
14) The wave function of a particle in a box is given by $\qquad$
a) $\sqrt{\frac{2}{L}} \operatorname{Sin} \frac{\pi x}{L}$
b) $\sqrt{\frac{2}{L}} \operatorname{Sin} \frac{\pi x}{n L}$
c) $\sqrt{\frac{2}{L}} \operatorname{Sin} \frac{n \pi x}{L}$
d) $\sqrt{\frac{2}{L}} \operatorname{Sin} \frac{n \pi x}{2 L}$
15) For Normalised wave function, $\int_{-\infty}^{\infty} \Psi \Psi^{*} \mathrm{~d} v=-----$
a) 0
b) 1
c) -1
d) $\infty$
16) For orthogonal wave function, $\int_{-\infty}^{\infty} \Psi \Psi^{*} d v=-----$
a) 0
b) 1
c) -1
d) $\infty$
17) which of the following represent operator of energy?
a) $-i \hbar \frac{\partial}{\partial x}$
b) $i \hbar \frac{\partial}{\partial x}$
c) $-i \hbar \frac{\partial}{\partial t}$
d) $i \hbar \frac{\partial}{\partial t}$
18) which of the following represent operator of momentum?
a) $\frac{\hbar}{i} \frac{\partial}{\partial x}$
b) $i \hbar \frac{\partial}{\partial x}$
c) $-i \hbar \frac{\partial}{\partial t}$
d) $\frac{\hbar}{i} \frac{\partial}{\partial t}$
19) For a quantum wave particle, $\mathrm{E}=$ $\qquad$
a) $\hbar \mathrm{k}$
b) $\hbar \omega$
c) $\hbar \omega / 2$
d) $\hbar \mathrm{k} / 2$
20) For a quantum wave particle, $\mathrm{P}=$ $\qquad$
a) $\hbar \mathrm{k}$
b) $\hbar \omega$
c) $\hbar \omega / 2$
d) $\hbar \mathrm{k} / 2$
