QUANTUM PHYSICS

Wave - particle duality
Matter waves (de - Broglie hypothesis)
Wave function
Observables, Operators
Eigen value, eigen functions
Normalization, ~~Epe.~~ Expectation values
Schrodinger's equⁿ's < time dep / time ind.

Particle in box

Wave - Particle Duality

de - Broglie hypothesis explains that a wave is always associated with every moving particle and its corresponding wavelength which is called as de-Broglie's wavelength given by

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

where, $\lambda \rightarrow$ wavelength of a wave
$p \rightarrow$ momentum $= mv$
$h \rightarrow$ Planck's constant

There are different forms of de - Broglie equⁿ :-

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

$$K.E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m} = E \text{ (say)}$$

or $p = \sqrt{2mE}$

1) $$\lambda = \frac{h}{\sqrt{2mE}}$$

where E represents the K.E of an accelerated particle

2) If the particle is accelerated with the help of an electrostatic energy $E = qV \Rightarrow \lambda = \frac{h}{\sqrt{2mqV}}$

3) When the particle is accelerated by thermal energy the Kinetic energy is given by

$$E = \frac{3}{2}KT$$

$$\lambda = \frac{h}{\sqrt{2m \times \frac{3}{2}KT}} = \frac{h}{\sqrt{3mKT}}$$

4) When the particle is moving with a velocity comparable to that of light, then the mass of the particle no longer remains constant but it will vary according to the eq^n

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

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

$$= \frac{h}{\frac{m_0}{\frac{\sqrt{c^2 - v^2}}{\cancel{c}}} \times \cancel{v}v} = \frac{h\sqrt{c^2 - v^2}}{m_0 vc}$$

Q. Distinguish between electromagnetic wave and matter wave

Electromagnetic Waves	Matter Waves
→ These waves have electric and magnetic fields associated with them	→ Matter Waves have no electric and magnetic fields associated with them.
→ These waves can easily pass through the vacuum.	→ These waves cannot pass through the vacuum.
→ These waves have fixed velocities.	→ Matter waves have velocities less than velocities of light and depend on the situation.

Q. Mention the properties of matter wave.

→ Matter wave represents the probability of finding a particle in space.

→ Matter waves are not electromagnetic in nature.

→ Matter wave is independent of the charge on the material particle.

* The wave particle duality of matter wave was experimentally proved by Davisson - Germer expt.

Wave Function

fn. As per the theory of quantum mechanics every physical system is characterized by a wave function which contains all information about the system.

→ Wave functions are the mathematical representations of particles in motion which gives the probabilistic description of the particle.

→ A wave function is a function of space and time coordinates.

$$\psi = \psi(\vec{r}, t)$$

In 1-D, $\psi = \psi(x, t)$

or $\psi(y, t)$

or $\psi(z, t)$

$$\psi = A e^{i(kx - \omega t)}$$

or $\psi = A \sin(kx - \omega t)$

or $\psi = A \cos(kx - \omega t)$

or $\psi = \_\_\_ + \ldots$

ψ = Wave function

A = Amplitude

$i = \sqrt{-1}$

k = Wave propagation vector $= \frac{2\pi}{\lambda}$

λ = wavelength

x = displacement

$\omega = 2\pi\nu$

t = time at any instant

The probability density is given by $\psi\psi^* = |\psi|^2$

ical
pretation
f^n.

→ The wave f^n ψ must be continuous and single-valued.

→ The wave f^n must satisfy Schrodinger's wave eq^n.

→ Acc. to the principle of Superposition the wave function of a system is a linear combination of different possible allowed state which is expressed as

for numerical problems ✓ $\psi = c_1\psi_1 + c_2\psi_2 + c_3\psi_3 + \dots$

where $c_1, c_2, c_3, \dots$ are the coefficients

(eigen functions)

$\psi_1, \psi_2, \psi_3, \dots$ are the wave functions associated with the allowed states.

For such systems the probability $= |C_i|^2$, $i = 1, 2, 3, \dots$

Normalization

It is expressed as $N = \dfrac{1}{\sqrt{\int_V |\psi|^2 dV}}$

where N is the Normalization constant

$Cond^n$ for normalization : $\int_V |\psi|^2 dV = 1$

Observables and Operators

Any dynamic quantity like position, co-ordinates, energy, linear momentum, angular momentum etc: which can be observed or measured is known as observables which can further be explained as follows :

Observables	Operators in 3D	Operators in 1D
Total Energy (E)	$i\hbar \frac{\partial}{\partial t}$	$i\hbar \frac{\partial}{\partial t}$
Linear momentum (p)	$-i\hbar \vec{\nabla}$	$-i\hbar \frac{\partial}{\partial x}$
Kinetic energy $\left(\frac{p^2}{2m}\right)$	$\frac{-\hbar^2}{2m} \nabla^2$	$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
Position	r	x
Potential energy	V	V
Hamiltonian	$\frac{-\hbar^2}{2m} \nabla^2 + V$	$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial t^2} + V$

Eigen functions and Eigen Values

In quantum mechanics a system can be defined by a number of definite states which are called as eigen states and are represented by eigen functions.

→ The actual state of a system is a linear combination of these eigen states with different relative probabilities. So each observable property of a physical system can have a set of definite allowed values called as eigen values.

Expectation Values

If q_1, q_2, q_3 etc. are the eigen values of a physical quantity then the expectation value is given by

$$\langle Q \rangle = \frac{P_1 q_1 + P_2 q_2 + P_3 q_3 + \cdots}{P_1 + P_2 + P_3 + \cdots} = \frac{\sum_n P_n q_n}{\sum_n P_n}$$

where $P_1, P_2, P_3, \ldots$ are different relative probabilities of a system.

What are the characteristic features of a wave function?

→ A wave function is a function of space and time co-ordinates.

→ The wave function must be continuous and single-valued.

→ The wave function must satisfy Schrodinger's wave eqn.

Schrodinger's Wave Equation

Schrodinger eqn is one of the most fundamental eqn required to explain different quantum mechanical principles & theories. It gives the info. about the physical system.

To derive Schrodinger's Wave eqn the wave particle duality principle is used:

Schrodinger's wave eqn has two forms < Time Dependent / Time Independent

Time Dependent Schrodinger's Eqn

Let us consider a particle of mass 'm' moving with a velocity 'v'. The behaviour of the particle is explained through a wave function given by

$$\psi = \psi(x,t) = Ae^{i(kx-\omega t)} \quad \text{—(1)}$$

where A = Amplitude

$K = \frac{2\pi}{\lambda}$

$i = \sqrt{-1}$

$\omega = 2\pi\nu$

Differentiating equn (1) w.r.t x

$$\frac{\partial \psi}{\partial x} = ikAe^{i(kx-\omega t)} = ik\psi \quad \text{—(2a)}$$

On further differentiation of equ^n (2a) w.r.t x, we get.

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial \psi}{\partial x}\right) = -K^2 A e^{i(Kx-\omega t)} = -K^2\psi \quad \text{—(2b)}$$

Differentiating equ^n (1) w.r.t 't' we get

$$\frac{\partial \psi}{\partial t} = -i\omega A e^{i(Kx-\omega t)} = -i\omega\psi \quad \text{—(2c)}$$

The energy of a particle is given by

$$E = h\nu$$

As $\omega = 2\pi\nu$

$\Rightarrow \nu = \frac{\omega}{2\pi}$

$$= \frac{h\omega}{2\pi} = \frac{h}{2\pi}.\omega = \hbar\omega \quad \text{—(3)}$$

where, $\hbar = \frac{h}{2\pi}$ reduced Planck's constant

From de-Broglie's hypothesis on wave particle duality, we know that

$$\lambda = \frac{h}{p} \Rightarrow p = \frac{h}{\lambda}$$

On dividing the numerator & denominator of the above equ^n by 2π, we have.

$$p = \frac{h/2\pi}{\lambda/2\pi} = \frac{h}{2\pi} \times \frac{2\pi}{\lambda} = \hbar K \quad \text{—(4)}$$

Since the kinetic energy is given by

$$E = \frac{p^2}{2m} = \frac{1}{2}mv^2 = \frac{\hbar^2 K^2}{2m} \quad \text{—(5)}$$

Multiplying equ^n (3) by $i\hbar$, we get

$$i\hbar E = i\hbar^2\omega$$

Multiplying equ^n (2c) with $i\hbar$, we get

$$i\hbar\frac{\partial \psi}{\partial t} = (i\hbar)(-i\omega\psi)$$

$$= -i^2\hbar\omega\psi = \hbar\omega\psi$$

$$= E\psi \quad (\text{using } ③)$$

Thus we find $i\hbar\frac{\partial \psi}{\partial t} = E\psi$ —(6)

Using equⁿ (5) in equⁿ (6) we get

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar^2 K^2}{2m} \psi \quad \text{--- (7)}$$

As it was found that $\frac{\partial^2 \psi}{\partial x^2} = -K^2 \psi$ from (2b)

$$\Rightarrow K^2 \psi = -\frac{\partial^2 \psi}{\partial x^2} \quad \text{--- (8)}$$

Using equⁿ (8) in the R.H.S of equⁿ (7), we get

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

$$\therefore \boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}} \quad \text{--- (9)}$$

Time Dependent Schrodinger's equⁿ

Equⁿ (9) holds good for a free particle where the potential energy, $V = 0$.

* Special Case

1) For any particle with potential energy, V the time dependent form of Schrodinger equⁿ (9) can be modified as

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \quad \text{--- (10)}$$

2) In 3-D, eqⁿ (9) can be expressed as

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \quad \text{--- (11)}$$

where, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

Time Independent Schrodinger's Equation

The Schrodinger's eqn in time dependent form is given by

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

but $i\hbar\frac{\partial\psi}{\partial t} = E\psi$ (Refer equn ⑥)

Hence $$E\psi = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$$

or $$(E-V)\psi = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$

or $$\frac{2m}{\hbar^2}(E-V)\psi = -\frac{\partial^2\psi}{\partial x^2}$$

or $$\boxed{\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0} \quad \text{—(12)}$$ Time independent S.E in 1-D

* **In 3-D**

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

In general equation (12) is taken as the reference equation to derive different ~~app~~ appⁿ equns for quantum physics.

Free Particle in a Box.

Let us consider a particle of mass 'm' moving freely in a box. For a free particle, $V=0$

The time ind. S.E in 1-D

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \text{—(1)}$$

Since, $V=0$ $\Rightarrow$ $$\frac{\partial^2\psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad \text{—(2)}$$

Let $$\frac{2mE}{\hbar^2} = K^2 \quad \text{—(3)}$$

Using eqⁿ (3) in eqⁿ (2) we get

$$\frac{\partial^2 \psi}{\partial x^2} + K^2 \psi = 0 \quad \text{— (4)}$$

Equⁿ (4) is a second order differential equⁿ.

Taking $\frac{\partial^2}{\partial x^2} = D^2$

(4) $\rightarrow$ $D^2\psi + K^2\psi = 0$

Auxiliary equⁿ: $D^2 + K^2 = 0$ or $m^2 + K^2 = 0$

or $m^2 = -K^2 = i^2K^2$

Roots $= \pm iK$, $m_1 = iK$, $m_2 = -iK$

Solⁿ: $\psi = Ae^{m_1 x} + Be^{m_2 x}$

So $\psi = Ae^{iKx} + Be^{-iKx}$ — (5)

Eqⁿ (5) represents the solⁿ of the 2nd order differential eqⁿ of the free particle moving inside the box.

In eqⁿ (5), A and B are the arbitrary constants whose values can be found out by putting the boundary conditions.

The eigen functions of eqⁿ (5) are Ae^{iKx} and Be^{-iKx}.
The corresponding eigen values $E = \frac{\hbar^2 K^2}{2M}$

Since both the eigen functions have the same eigen value as explained above so it satisfy the condition of degeneration.