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* Schrodinger's time dependent wave equation :-

Q. Derive Schrodinger's eqn. of time dependent & write the significance of wave function.

Sol: In order to derive time dependent Schrodinger wave eqn., Schrodinger introduced a mathematical function which associates characteristics of the DeBroglie waves called as wave function denoted by ψ , which is a complex function.

The differential eqn representing one dimensional wave motion expressed mathematically,

$$\frac{\partial^2 \psi}{\partial t^2} = v^2 \frac{\partial^2 \psi}{\partial x^2}$$

in generally $\frac{\partial^2 \psi}{\partial t^2} = v^2 \nabla^2 \psi$ — (1)

the solution of eqn (1) assumed to be in the x-direction by a wave function

$$\therefore \psi = A \cdot e^{-i\omega(t - \frac{x}{v})} \quad \text{--- (2)}$$

$$\text{(or)} \quad \psi = A \cdot e^{-i(\omega t - i\omega \frac{x}{v})}$$

where ν = frequency $\omega = 2\pi\nu$ & $v = \nu\lambda$

$$\Rightarrow \psi = A \cdot e^{-i(2\pi\nu) \left[t - \frac{x}{\nu\lambda} \right]}$$

$$\psi = A \cdot e^{-2\pi \left[i\nu t - i\nu \cdot \frac{x}{\nu\lambda} \right]}$$

$$\psi = A \cdot e^{-2\pi i \left[\nu t - \frac{x}{\lambda} \right]} \quad \text{--- (3)}$$

Let E be total energy & P be the momentum of the particle then Quantum energy $E = h\nu$ and $\lambda = \frac{h}{P} \Rightarrow \nu = \frac{E}{h}$.

Substituting in eqm (2) we get

$$\psi = A \cdot e^{-2\pi i \left[\frac{E}{h} \cdot t - \frac{x \cdot P}{h} \right]}$$

$$\psi = A \cdot e^{-\frac{2\pi}{h} [Et - Px]}$$

$$\left[\because \hbar = \frac{h}{2\pi} \right]$$

$$\left[\frac{2\pi}{h} = \frac{1}{\hbar} \right]$$

$$\Rightarrow \psi = A \cdot e^{-i/\hbar [Et - Px]} \quad \text{--- (4)}$$

diff. eqm (4) w.r.t "x"

$$\frac{\partial \psi}{\partial x} = A \cdot e^{-i/\hbar [Et - Px]} \cdot \left[\frac{i}{\hbar} P \right]$$

Again diff. w.r.t "x"

$$\frac{\partial^2 \psi}{\partial x^2} = A \left[\frac{i}{\hbar} \cdot p \right] \cdot e^{-i/\hbar (\epsilon t - p x)} \cdot \left(\frac{i p}{\hbar} \right)$$

$$\frac{\partial^2 \psi}{\partial x^2} = A \left[\frac{i^2 p^2}{\hbar^2} \right] \cdot e^{-i/\hbar (\epsilon t - p x)}$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{(-1) p^2}{\hbar^2} \cdot A \cdot e^{-i/\hbar (\epsilon t - p x)}$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{-p^2 (4\pi^2)}{\hbar^2} \cdot A \cdot e^{-\frac{2\pi i}{\hbar} (\epsilon t - p x)}$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2}{\hbar^2} p^2 \psi^2 \quad \text{--- (5)}$$

At speeds the eqn (5) is the result of position of a particle in terms of its momentum.

differentiating eqn (4) w.r.t 'time' we get,

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= \frac{\partial}{\partial t} (e^{at}) \\ &= a \cdot e^{at} \end{aligned}$$

$$\frac{\partial \psi}{\partial t} = A \cdot e^{-\frac{2\pi i}{h}(Et - Px)} \left[-\frac{2\pi i}{h} E \right]$$

$$\frac{\partial \psi}{\partial t} = - \left[\frac{2\pi i}{h} E \right] \psi \quad \text{--- (6)}$$

The Speed of particle is very Small as Compared to Speed of light. then, the total energy E of particle is

$$E = K.E + P.E.$$

$$E = \left(\frac{p^2}{2m} + V \right)$$

here p^2 & V are position & time.

multiplying ~~on~~ b.s on ψ

$$E \psi = \left[\frac{p^2}{2m} + V \right] \psi$$

$$E \psi = \frac{p^2}{2m} \psi + V \cdot \psi \quad \text{--- (7)}$$

Observing the eqms (6) and (5). we get from eqm (6).

$$\frac{\partial \psi}{\partial t} = -\frac{2\pi i}{h} E \psi$$

$$\frac{-h}{2\pi i} \cdot \frac{\partial \psi}{\partial t} = E \psi \quad \text{--- (8)}$$

$$i. \frac{h}{2\pi} \cdot \frac{\partial \psi}{\partial t} = E \psi$$

(or)

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

$$\text{from eqn (5)} \Rightarrow \frac{\partial^2 \psi}{\partial x^2} = - \frac{4\pi^2}{h^2} \cdot p^2 \psi$$

$$\frac{h^2}{4\pi^2} \cdot \frac{\partial^2 \psi}{\partial x^2} = -p^2 \psi$$

$$\frac{-h^2}{2m(4\pi^2)} \cdot \frac{\partial^2 \psi}{\partial x^2} = + \frac{p^2}{2m} \psi$$

$$\frac{-h^2}{8m\pi^2} \cdot \frac{\partial^2 \psi}{\partial x^2} = \frac{p^2}{2m} \psi \quad \text{--- (9)}$$

Substituting eqn (8) & (9) in eqn (7).

we get,

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

$$\frac{-h}{2\pi i} \cdot \frac{\partial \psi}{\partial t} = - \frac{h^2}{8\pi^2 m} \cdot \frac{\partial^2 \psi}{\partial x^2} + V \psi$$

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The above as Schrodinger

'+' x-direction
 \Rightarrow In 3-d

$$-\frac{h}{2\pi i}$$

$$\frac{-h}{2\pi i} \cdot \frac{\partial \psi}{\partial t}$$

$$\frac{-h}{2\pi i}$$

$$\frac{h}{2\pi i}$$

The above wave

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The above eqm is called are known as Schrodinger's dependent wave eqm. in '+' x-direction.

⇒ In 3-dimensions

$$-\frac{h}{2\pi i} \cdot \frac{\partial \psi}{\partial t} = \frac{h^2}{8\pi^2 m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V\psi$$

$$-\frac{h}{2\pi i} \cdot \frac{\partial \psi}{\partial t} = \frac{h^2}{8\pi^2 m} \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] \psi + V\psi$$

$$\boxed{-\frac{h}{2\pi i} \cdot \frac{\partial \psi}{\partial t} = \frac{h^2}{8\pi^2 m} \nabla^2 \psi + V\psi}$$

$$i^2 = -1$$

$$\boxed{\frac{h \cdot i}{2\pi} \cdot \frac{\partial \psi}{\partial t} = \frac{h^2}{8\pi^2 m} \nabla^2 \psi + V\psi}$$

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

$$\hbar^2 = \frac{h^2}{4\pi^2}$$

The above eqm. is known as Schrodinger's wave eqm.

* Schrodinger's time independent wave eqn. (or) steady state form of

Schrodinger's wave equation :-

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Q. Derive an expression for Schrodinger's time independent wave equation and write the significance of wave function.

Sol: In many cases potential energy of a particle does not depend on time. Thus, potential is a function of position of a particle only. Hence, Schrodinger's time dependent wave eqn. may be simplified by removing all references to time.

⇒ From the one dimensional wave function expressed as $\psi = A \cdot e^{-\frac{2\pi i}{h}(Et - Px)}$ along one direction.

$$\psi = A \cdot e^{-\frac{2\pi i}{h} i Et} \cdot e^{-\frac{2\pi i}{h} i (-Px)}$$

$$\psi = A \cdot e^{\frac{-2\pi i}{h}(Et)} \cdot e^{\frac{2\pi i}{h}(Px)} \quad \text{--- (IA)}$$

$$\psi = A \cdot e^{2\pi i/h (Px)} \cdot e^{-\frac{2\pi i}{h} (Et)}$$

$$\psi = A \cdot e^{-\frac{2\pi i}{h} (Et)}$$

→ In eqn position differentiating

$$\frac{\partial \psi}{\partial t}$$

Again

$$\frac{\partial \psi}{\partial x}$$

$$\frac{\partial^2 \psi}{\partial x^2}$$

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Sub

we get

⇒ In eqn (1B), ψ is the product of position dependent and time dependent. Differentiating (1B) w.r.t time (t).

$$\frac{\partial \psi}{\partial t} = -\frac{2\pi i E}{h} \psi_0 \cdot e^{-\left(\frac{2\pi i E}{h}\right)t} \quad \text{--- (2)}$$

Again differentiating (1B) w.r.t "x". we get

$$\frac{\partial \psi}{\partial x} = e^{-\frac{2\pi i}{h}(Et)} \frac{\partial \psi_0}{\partial x}$$

$$\frac{\partial^2 \psi}{\partial x^2} = e^{-\frac{2\pi i}{h}(Et)} \frac{\partial^2 \psi_0}{\partial x^2} \quad \text{--- (3)}$$

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Schrodinger time dependent wave eqn.

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

Sub the eqn (2) & (3) in the abv. eqn.

we get, $\left(\frac{h i}{2\pi}\right) \left(-\frac{2\pi i}{h} \cdot E\right) \psi = \frac{h^2}{8\pi^2 m} \left(e^{-\left(\frac{2\pi i}{h}\right)Et}\right)$

$$\frac{\partial^2 \psi}{\partial x^2} + \psi$$

$$E\psi - V\psi = \frac{h^2}{8\pi^2 m} \left[\frac{\partial^2 \psi}{\partial x^2}\right]$$

$$\frac{8\pi^2 m}{h^2} (E - V)\psi = -\frac{\partial^2 \psi}{\partial x^2}$$

$$\boxed{\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - V)\psi = 0} \quad \text{--- (4)}$$

⇒ eqn (4) gives study form of Schrodinger's time independent wave eqn. along '+' x-direction of propagation.

⇒ For 3D Schrodinger time independent wave eqn.

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} (\epsilon - V) \psi = 0.$$

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] \psi + \frac{8\pi^2 m}{h^2} (\epsilon - V) \psi = 0$$

$$\boxed{\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (\epsilon - V) \psi = 0}$$

The above eqn shows the Schrodinger time independent wave eqn.

Method 2 : Schrodinger time independent wave eqn :

⇒ Schrodinger eqn. is diff. eqn. for deBroglie waves associates with the particle which describe its motion.

⇒ For the moving particle the Variable motion of a particle expressed mathematically by a function called wave function denoted as ' ψ ' for a Steady State Systems

(time independent)

1D eqn :

Here A = amplitude

λ = wavelength

$$\text{diff. w.r.t "x"} \quad \frac{\partial \psi}{\partial x} = A \left(\frac{2\pi}{\lambda} \right) \cos \left(\frac{2\pi x}{\lambda} \right)$$

again diff w.r.t 'x'.

$$\frac{\partial^2 \psi}{\partial x^2} = -A \frac{4\pi^2}{\lambda^2} \sin \left(\frac{2\pi x}{\lambda} \right)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{4\pi^2}{\lambda^2} \psi \quad \text{--- (2)}$$

\Rightarrow The wavelength associated with the particle mass ' m ' moving with velocity ' v ' expressed from de Broglie's waves.

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

$$\frac{1}{\lambda} = \frac{mv}{h}$$

$$\frac{1}{\lambda^2} = \frac{m^2 v^2}{h^2}$$

$$\frac{1}{\lambda^2} = \frac{2m \left(\frac{1}{2} mv^2 \right)}{h^2} \quad \text{--- (3)}$$

⇒ For non relativistic approach $\frac{1}{2}mv^2$ is the K.E of the particle.

$$\Rightarrow \text{Thus } K.E = \frac{1}{2}mv^2 = (E - V)$$

$$= (\because E = K.E + P.E = \frac{1}{2}mv^2 + V \Rightarrow E - V = \frac{1}{2}mv^2)$$

Sub the above eqn. is eqn (3)

$$\frac{1}{\lambda^2} = \frac{2m}{h^2} (E - V) \quad \text{--- (4)}$$

Using the value of $\frac{1}{\lambda^2}$ from eqn (2) in eqn (4) we get, from eqn (2)

$$-\left(\frac{1}{4\pi^2}\right) \frac{\partial^2 \psi}{\partial x^2} = \frac{1}{\lambda^2} \psi.$$

$$\left[-\left(\frac{1}{4\pi^2}\right) \frac{\partial^2}{\partial x^2} \right] = \frac{2m}{h^2} (E - V)$$

$$-\frac{\partial^2}{\partial x^2} = \frac{8\pi^2 m}{h^2} (E - V).$$

$$-\frac{\partial^2 \psi}{\partial x^2} = \frac{8\pi^2 m}{h^2} (E - V) \psi$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0 \quad \text{--- (5)}$$

⇒ The eq (steady a particle 'E' and for a Sp independent

$$\left(\frac{\partial^2 \psi}{\partial x^2} + \dots \right)$$



* Physical

Properti

⇒ In interpret associat defining ⇒ wave existe identity

⇒ The eqn (5) give time independent (steady state) Schrodinger eqn. for a particle of mass 'm', total energy 'E' and P.E 'V' moving along x-direction for a Space (3D) Schrodinger time independent wave eqn.

$$\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0$$

$$\boxed{\nabla^2 \psi + \frac{8\pi^2 m}{h^2} (E - V) \psi = 0.}$$

* Physical Significance of Wave Function :-

(or)

Properties of wave function :-

⇒ In 1926, Max Bohr gave a satisfactory interpretation of a wave function. ψ associated a particle relation by defining wave packet.

⇒ wave packet :- A finite region exisistency of a particle gives its identity.

⇒ The Square of magnitude of

wave function also called probability density which interprets the probability of finding a particle within a volume $dx dy dz$.

$$1. |\psi|^2 = \psi \psi^*$$

$$\text{Mathematically } |\psi|^2 = \psi \psi^*$$

$$\iiint |\psi|^2 dv = \iiint \psi \psi^* dx dy dz = 1.$$

This eqn. is called probability finding function.

This condition is known as Normalized Condition.

⇒ Here the function ψ is also called Amplitude function.

⇒ The wave function ψ must be finite everywhere. it violates uncertainty principle (or zero value at any point).

⇒ ψ must be single value integration of

$$\int_a^b \int_{\phi_1}^{\phi_2} \psi^*(x) \psi(x) dx = 0.$$

This function is called Orthogonal function.

$\Rightarrow A\psi$ is a wave function multiplied by a constant gives new function its complex conjugate $(A\psi)^*$ then its normalised function $\iiint (A\psi)^* (A\psi) \cdot dx \cdot dy \cdot dz = 1$.

$$\int (A\psi)^* (A\psi) \cdot dx = 1$$

$$|A|^2 \int \psi^* \psi \cdot dx = 1$$

$$A = \frac{1}{\int \psi^* \psi \cdot dx}$$

In the above eqn. the function ψ or interms becomes solutions of Schrodinger wave equations.

\Rightarrow The function ψ must be continuous across the boundary.

\Rightarrow The function ψ always gives characteristics (or) properties of eigen values (allowed energy states of a given function).

Mathematically expressed as $f(\psi)$.

* Application of Schrodinger wave equation
to the organic oscillator :-

L.A.O

Q. Estimate the energy of simple harmonic oscillator from Schrodinger wave mechanics.
(or)

Harmonic oscillator is a parabolic potential well. Support this phenomenon from Quantum wave mechanics.

(or)

Solve the linear harmonic oscillator problem quantum mechanically and obtain its eigen values.

(or)

Establish Schrodinger's equation for a linear harmonic oscillator and solve it to obtain its eigen values and eigen functions.

Sol :- A simple harmonic oscillator is a particle executing simple harmonic motion along x-direction (1D) under a restoring force 'F' acting for a unit displacement.

$$\therefore F = -kx \quad \text{--- (1)}$$