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QUANTUM MECHANICS

WAVE FUNCTION

All the objects have both wave & particle like nature. So does the $\bar{e}$ & photon. In both cases it interacts with other materials as particles, but probability of its being found at a place is governed by the wave that always accompanies the object. But wave associated with with $\bar{e}$ is very abstract & does not corresponds to any measurable physical quantity.

So when we consider any material particle like $\bar{e}$, we say that there is a wave function $\psi(\vec{r},t)$ associated with it. $\psi(r,t)$ represent the state of a particle. At a given $\vec{r}$ & t, $\psi(r,t)$ has a definite value which may be complex.

The multiplication of $\psi(r,t)$ by a constant does not change the form of the wave function. So the state of a particle is related to the form of the wave function and not its value. Thus $\psi(r,t)$ & $c\psi(r,t)$ represent same state of the particle.

So if $\psi(r,t)$ is known we can get all the information about the quantum system.

Time dependent Schrödinger Equation

consider one dimensional motion of free particle of mass m moving in x dirn with momentum p & energy E. The monochromatic plane wave is described by

$$\psi(\vec{x},t) = A e^{i(px-Et)/\hbar} \quad (1)$$

Differentiating it w.r.t to t

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

$$\Rightarrow i\hbar \frac{\partial \psi}{\partial t} = E\psi \quad - (2)$$

Diff. twice ① w.r.t x, we have

Derive it from Register

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

$$\Rightarrow -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} = p^2 \psi \quad — ③$$

$$\Rightarrow \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = \frac{p^2}{2m} \psi \quad — ④$$

For a non-relativistic free particle,

$$E = \frac{p^2}{2m}$$

$\Rightarrow$ Put value of E in eqⁿ ② & then compare with eqⁿ ④ we have

$$\Rightarrow \boxed{i\hbar \frac{\partial \psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2}}$$

- TIME DE[PENDENT] SCHORDI[NGER] EQUATIO[N]

This equation tells us how the quantum system evolves with time.

Postulates of Quantum Mechanics:

Postulate 1: The state of a QM system is completely described by a wave function

$$P(x,t) = \psi^*(x,t)\,\psi(x,t) = |\psi(x,t)|^2$$

For ~~finding~~ measuring the probablity of finding a particle the wavefunction $\psi(x,t)$ should be normalisable, finite, single valued & continuo[us]

Postulate 2: For every measurable prope[rty] of a system there exist a corresponding operator. All CM properties have corr. QM operator.

OBSERVABLE	OPERATOR
x $(\hat{x})$	$\hat{x}$
P_x $(\hat{P}_x)$	$-i\hbar \frac{\partial}{\partial x}$
K.E. $(\hat{K})$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
P.E $(\hat{V})$	$V(x)$
Hamiltonian $(\hat{H})$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$
E	$i\hbar\frac{\partial}{\partial t}$

Properties of these operators.

Hermitian $\Rightarrow$ E. values are real.

Order dep. $\Rightarrow$ $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

Operate from left.

Postulate 3: For any measurement involving an observable corr. to operator, the only values that will be measurable will be E. values of operators

for. eg. $\hat{H}\,\psi_n(x) = E_n\,\psi_n(x)$

Postulate 4: Expectation values of an observable is the average value & if system is described by normalised wavefunction then $\langle x \rangle = \int_{-\infty}^{+\infty} \psi^* \hat{x}\, \psi\, dx.$

If ψ is not normalised then

$$\langle x \rangle = \frac{\int_{-\infty}^{+\infty} \psi^* \, x\, \psi\, dx}{\int_{-\infty}^{+\infty} \psi^* \psi\, dx}$$

Postulate 5: The time evolution of QM system is given by TDSE.

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

$$E = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + T$$

If we consider the particle in 3-D then

$$\psi(\vec{r},t) = A\, e^{i(\vec{p}\cdot\vec{r} - Et)/\hbar}$$

where the operator p is now rep.

$$P_x = -i\hbar \frac{\partial}{\partial x} \quad P_y = -i\hbar \frac{\partial}{\partial y} \quad P_z = -i\hbar$$

So, $\hat{P} = -i\hbar \nabla$

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

Particle in a force field: If the particle is not a free particle but is acted upon by a force which is derivable from pot. $V(\vec{r})$ then

$$E = \frac{p^2}{2m} + V(r,t)$$

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

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

Time Dep. S.E. in 3-D for bound particle.

where $-\frac{\hbar^2}{2m}\nabla^2 + V = \hat{H}$ = The Hamilto operator.

Condition for Acceptable wave function (3)

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

This 1-D TDSE is true if the wave function for this satisfies the following condition.

) $\psi(x)$ must ~~be~~ exist & satisfy the S.E.

) $\psi(x)$ & $\frac{d\psi}{dx}$ must be continuous since Prob. of finding a particle cannot vary discontinuously from point to point.

$\psi(x)$ & $\frac{d\psi}{dx}$ must be finite & single valued.

) $\psi(x) \to 0$ fast enough as $x \to \pm\infty$ so that particle remains bounded & solution does not shoot up.

$\psi(x)$ should be square integrable or normalisable i.e.

$$\int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = 1.$$

This is because physically reliable state corr. to square int. sol^n.

Note: S.E. automatically preserves the normalisation of wave fun^n. in future times.

onsider $\psi(x)$ to be normalised at $t=0$
hen

$$\frac{d}{dt} \int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = \int_{-\infty}^{+\infty} \frac{\partial}{\partial t} |\psi|^2 dx$$

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