LITTLE FLOWER COLLEGE
DEPARTMENT OF CHEMISTRY

TOPIC : SCHRONDINGER WAVE EQUATION (QUANTUM MECHANICS)

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SCHRONDINGER WAVE EQUATION

- He explained particle can be wave and wave can be particle
- He said that a new theory is required to explain the behavior of electron , atoms and molecule.
- Wave equation was introduced for describing subatomic or atomic system
- E = T+V = ½ mv2 =(p2 / 2m) +V
- E = h v
- ג = h / mv

Schrodinger's philosophy

$$\frac{\partial^2\Psi(x,t)}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2\Psi(x,t)}{\partial t^2}$$ Classical Wave Equation

$\Psi(x,t)$ = Amplitude

Schrodinger Equation

Time-dependent Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=\widehat{H}\cdot\Psi(x,t)=\left[\frac{-\hbar^2}{2m}\nabla^2+V(x)\right]\Psi(x,t)$$

$$\widehat{H}\cdot\Psi(x,y,z,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,y,z,t)\ ; \quad \widehat{H}=\frac{-\hbar^2}{2m}\nabla^2+V(x,y,z)$$

H is the Hamiltonian operator

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

OPERATOR

Operator is a mathematical instruction which can be carried out on certain function so that the function get converted into another function.

Operator (function)= new function

eg; differential function , square root, trignometric

$$\widehat{H}\cdot\Psi(x,y,z,t)=i\hbar\frac{\partial}{\partial t}\Psi(x,y,z,t)\ ;\quad \widehat{H}=\frac{-\hbar^2}{2m}\nabla^2+V(x,y,z)$$

$$\Psi(x,y,z,t)=\psi(x,y,z)\cdot\phi(t)\quad\Rightarrow\quad\Psi=\psi\cdot\phi$$

$$\widehat{H}(\psi\cdot\phi)=i\hbar\frac{\partial}{\partial t}(\psi\cdot\phi)$$

$\widehat{H}$ operates only on ψ and $\frac{\partial}{\partial t}$ operates only on ϕ

$$\phi\cdot\widehat{H}\psi=\psi\left(i\hbar\frac{\partial}{\partial t}\phi\right)$$

Divide by $\psi\cdot\phi$

$$\frac{\widehat{H}\psi}{\psi}=\frac{1}{\phi}\left(i\hbar\frac{\partial}{\partial t}\phi\right)$$

$$\frac{\widehat{H}\psi}{\psi}=\frac{1}{\phi}\left(i\hbar\frac{\partial}{\partial t}\phi\right)=W$$

$$\frac{\widehat{H}\cdot\psi}{\psi}=W \qquad\qquad \widehat{H}\psi=W\psi$$

$$\frac{1}{\phi}\left(i\hbar\frac{\partial}{\partial t}\phi\right)=W \qquad\qquad i\hbar\frac{\partial}{\partial t}\phi=W\phi$$

In classical mechanics $\hat{H}$ represents total energy

We can therefore write

$$\widehat{H}\psi = W\psi \quad \text{as} \quad \widehat{H}\psi = E\psi$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E \cdot \psi(x)$$

EIGEN VALUE AND EIGEN FUNCTION

When an operator operates on a well behaved function to give the same function multiplied by a constant.

Then the constant is called as Eigen value and the function is called as Eigen function.

The time independent wave function is Eigen function of Hamiltonian operator

Energy of system is obtained as Eigen value.

STATE FUNCTION OR WAVE FUNCTION POSTULATE

- It states that the state of a system at time t consisting of N particles can be represented as completely as possible by a function called wave function or state function which is the function of all position coordinates and time .
- I.e. $\Psi(x, y, z, t)$
- All the possible information about the system can be obtained from the wave function.
- The value of $\Psi \Psi^* d\tau$ represent the probability of finding the system in the volume element.

The state function Ψq, t can be varied depending on the values of q and t.

Though there are many values for Ψ only the well behaved functions can be chosen so we will apply the boundary condition to the function.

When we apply the boundary condition the phenomena of quantisation arises.

The representation in which the wave function is a function of coordinates and time is called the coordinate representation.

BORN INTERPRETATION OF THE WAVE FUNCTION

- If the wave function of a particle has the value ψ at x then the probability of finding the particle between x and x +dx is proportional to $|\psi 2|$ dx.
- $|\psi 2| = \psi * \psi$

Because $\psi 2$ dx is a dimensionless probability,

$\psi 2$ is the probability density for one dimensions.

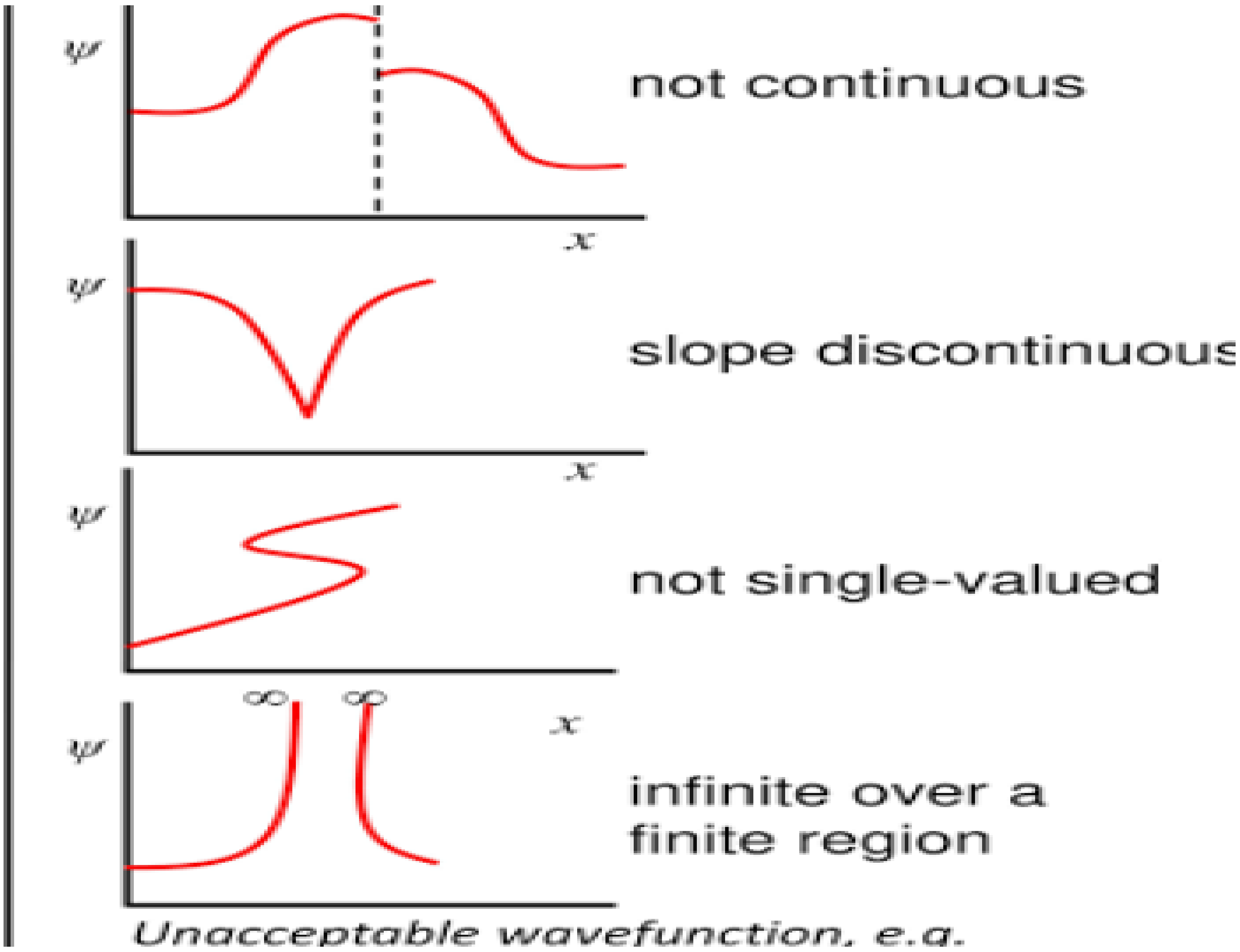
The wave function ψ itself is called the probability amplitude.

WELL BEHAVED FUNCTION

- It must be single valued at all points i.e, it must have one and only one value at a particular point. e.g: y= mx+c is a single valued function but y2 =1 is not a single value function.
- The function must be continuous i.e. their value must not change abruptly at any point.
- The function must be finite i.e., it must not take infinite values.

For e.g: y=mx+c is not a finite function because x can take infinite values .but the exponential functions are finite function

•It must have a first continuous derivative .



ORTHONORMALITY OF WAVE FUNCTION

- A function f which satisfy the condition $\int_{-\infty}^{+\infty} ff^2 d\tau = 1$

Is said to be a normalised function and the condition is called normalisation condition .

- If $\int_{-\infty}^{+\infty} ff^2 d\tau = N$ then the function has to be normalised so divide both sides by N then

$$\frac{1}{N}\int_{-\infty}^{+\infty} ff^* d\tau = 1$$

$$\int_{-\infty}^{+\infty} \left(\frac{1}{\sqrt{N}} f\right)\left(\frac{1}{\sqrt{N}} f^*\right) d\tau = 1$$

here $\frac{1}{\sqrt{N}}$ is called the normalisation factor and the normalised function is $\frac{1}{\sqrt{N}}$ f

- Every finite function is normalised.

Orthogonality of function

- Suppose we have a series of functions f1, f2, f3,…… then the condition for orthogonality is

$$\int_{-\infty}^{+\infty} f_m{}^{*}\ f_n{}^{*} d\tau = 0$$

- Then the function fm and fn are said to be orthogonality is the relationship between two function while normality is property of a single function

$$\int_{-\infty}^{+\infty} f_m{}^{*}\ f_n{}^{*} = \delta_{m,n}$$

Where δm ,n is called kronecker delta.

- If δm,n =1 then the function is normalised
- If δm,n =0 then the functions are orthogonal.

THANK YOU