

## **HEISENBERG UNCERTAINTY PRINCIPLE:**

According to Heisenberg, “It is impossible to determine both the exact position and exact momentum of a moving particle at the same time.”

**OR**

It is impossible to determine exactly and simultaneously the values of both the members of pair of physical variables which describes the motion of an atomic system.

**OR**

If momentum of a particle is precisely known the location of the same particle is completely unknown.

If  $\Delta x$  denotes the error (uncertainty) in the measurement of the position of the particle along x-axis and  $\Delta p$  represents the error in the measurement of momentum, then

$$\Delta x \cdot \Delta p = h \text{ ----- (1)}$$

Where  $h$  is plank's constant. The above equation represents the uncertainty involved in the measurement of both the position and momentum of the particle.

In more optimized form the above equation can be written as

$$(\Delta x \cdot \Delta p) \geq \frac{\hbar}{2\pi} \text{ or } \frac{h}{4\pi} \text{ ----- (2)}$$

If the time during which a system occupies a certain state is not greater than  $\Delta t$ , then the energy of the state cannot be known to within  $\Delta E$ , where:

$$(\Delta E) (\Delta t) \geq \frac{\hbar}{2\pi} \text{ ----- (3)}$$

Similarly

$$(\Delta J) (\Delta \theta) \geq \frac{\hbar}{2\pi} \text{ ----- (4)}$$

where  $\Delta J$  and  $\Delta \theta$  are uncertainties in determining the angular momentum and angle.

In the world of very small particles, one cannot measure any property of a particle without interacting with it in some way and this interaction changes related property.

### **Consequence of Uncertainty relation:**

The most important consequence of uncertainty principle is that it is impossible to determine the wave and particle properties exactly at the same time.

According to the complementary principle the wave and particle aspects of matter and light are complementary rather than contradictory, i.e. both aspects are necessary to have a complete picture of the system.

### **APPLICATIONS OF HEISENBERG UNCERTAINTY PRINCIPLE**

#### **a) Nonexistence of electron inside the nucleus**

From  $\alpha$  scattering experiment it is known that the nucleus radius is the order of  $10^{-14}$  m. If an electron exists inside the nucleus the uncertainty in its position must be of this diameter. That is

$\Delta x \cong 2 \times 10^{-14}$  m. Substitute the value of  $\Delta x$  in the equation  $\Delta x \cdot \Delta p \geq h/2\pi$ .

$$\Rightarrow \Delta p \geq \frac{h}{2\pi \times \Delta x} \geq \frac{6.626 \times 10^{-34}}{2 \times 3.14 \times 2 \times 10^{-14}} = 0.527 \times 10^{-20} \text{ kg m/s}$$

Then the momentum of the electron  $p$  must be at least order  $\cong 0.527 \times 10^{-20}$  Kg m/s. when the energy of the electron is very large as compared to its rest energy, then from Einstein mass energy relation  $E = mc^2 = mc \cdot c = pc$ , here  $c$  is the velocity of light  $= 0.527 \times 10^{-20} \times 3 \times 10^8 = 1.581 \times 10^{-12}$  J. Now it is converted in to electron volts  $\Rightarrow 1.581 \times 10^{-12} / 1.6 \times 10^{-19}$  J/eV  $= 0.988 \times 10^7$  eV.  $= 9.88 \times 10^6$  eV.  $\cong 10$  MeV.

This means that if the electron exists inside the nucleus, the energy must be of the order 10 MeV. However the energy of electron emitted in a  $\beta$  decay

experiment is of the order of only 3 to 4 MeV. So electron does not exist in the nucleus.

**b) Zero- point energy of a harmonic oscillator**

**c) Ground state energy and the radius of the hydrogen atom**

**d) Evidence for finite width of the spectral lines**

**e) Binding energy of an electron in atom**

### **WHY 'Ψ' CAME INTO PICTURE:**

- We make use of our knowledge of standing waves i.e. waves confined to a certain region, like waves produced by vibratory strings fixed at two ends, vibrating air columns in a tube, electromagnetic radiation inside a cavity. Larger is the amplitude, more intense is the wave.
- A similar situation exists inside the atom. The electron is situated within a distance of around  $10^8$ - $10^{-10}$  m from the nucleus and is always confined within this distance.
- The matter wave associated with it may be defined in terms of standing waves which have varying amplitudes at different points in the region and practically zero outside the region.
- The first and simple interpretation of  $\Psi$  was given by Schrodinger himself in terms of charge density.
- We know that in any electromagnetic wave system if A is the amplitude of the wave then energy density, i.e., energy per unit volume is equal to  $A^2$ , so that the number of photons per unit volume, i.e., photon density is equal to  $\frac{A^2}{h\nu}$  or the photon density is proportional to  $A^2$  as  $h\nu$  is constant.

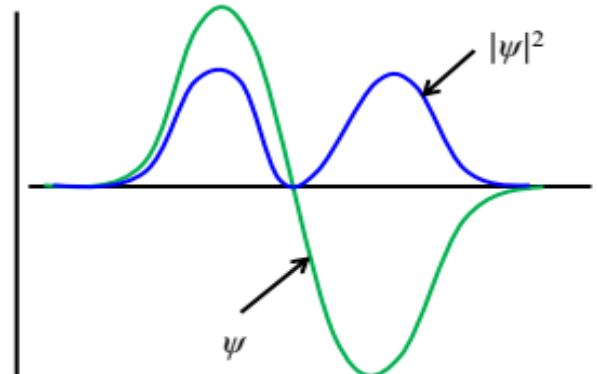
- If  $\Psi$  is the amplitude of matter waves at any point in space, then the particle density at that point may be taken as proportional to  $\Psi^2$ . Thus,  $\Psi^2$  is a measure of particle density.
- When this is multiplied by the charge of the particle, the charge density is obtained. In this way,  $\Psi^2$  is a measure of charge density.

$\Psi$  is appreciably different from zero within some finite region known as wave packet. It is natural to ask, 'where is the particle in relation to wave packet?' In order to explain this, **Max Born** specified a new idea.

- According to **Max Born**  $\psi^* \psi = |\Psi^2|$  gives the probability of finding the particle in the state  $\Psi$ , i.e.,  $\Psi^2$  is a measure of probability density.
- The probability of finding a particle in volume  $d\tau = dx dy dz$  is given by  $|\Psi^2| dx dy dz$ . For the total probability of finding the particle somewhere is, of course, unity i.e., particle is certainly to be found somewhere in space

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

- The sign of a wave function has no direct physical significance
- The positive and negative regions of this wave function both correspond to the same probability distribution.



### PHYSICAL SIGNIFICANCE OF THE WAVE FUNCTION ' $\Psi$ ':

Max Born in 1926 gave a satisfactory explanation for the wave function ' $\Psi$ ' associated with a moving particle. Born postulated that the square of the

magnitude of the wave function  $|\Psi^2|$  or  $(\Psi\Psi^*$  if  $\Psi$  is complex) represents the probability of finding the particle in the given region.  $|\Psi^2|$  is called probability density and  $\Psi$  is probability amplitude.

The probability that a particle will be found at a given place in space at a given instant of time is characterized by the function  $\Psi(x, y, z, t)$  it is called the wave function. The wave function  $\psi$  itself has no direct physical significance. This function can be either real or complex. The only quantity having a physical meaning is the square of its magnitude  $P = |\Psi|^2 = \Psi\Psi^*$  where  $\Psi^*$  is the complex conjugate of  $\Psi$ . The quantity  $P$  is the probability density.  $|\Psi|^2$  the square of the absolute value of the wave function, is also called probability density. The probability of finding a particle in a volume  $dx, dy, dz$ , is  $|\Psi|^2 dx dy dz$ . Further, since the particle is certainly to be found somewhere in space.

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |\Psi|^2 dx dy dz = 1 \quad \text{or} \quad \iiint_V |\Psi|^2 dV = 1$$

the triple integral extending over all possible values of  $x, y, z$ . A wave function that obeys the above equation is called **normalized** wave function.

Every acceptable wave function must be normalizable and should fulfill the following conditions:

1.  $\psi$  must be finite for all values of  $x, y, z$ .
2.  $\psi$  must be continuous in all regions except where the potential energy is infinite. ( $\because \frac{d^2\Psi}{dx^2}$  must be finite everywhere. This possible only when  $\frac{d\Psi}{dx}$  has no discontinuity at any boundary where potential changes. This implies that  $\Psi$  too must be continuous)

3.  $\psi$  must be single valued.
4.  $\psi$  must possess continuous first order derivative everywhere
5.  $\psi$  vanishes at the boundaries.
6. Every wave function must satisfy **normalization condition**.

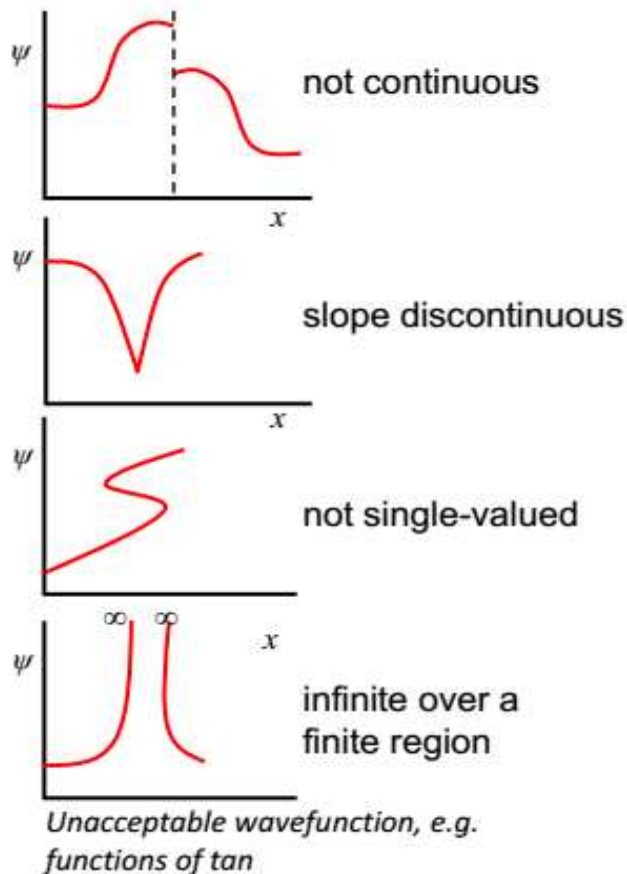
$$\iiint |\Psi|^2 dx dy dz = 1$$

7. A wave function satisfying the following condition is called **orthogonal wave function**.

$$\int_{-\infty}^{\infty} \Psi^* \Psi dx = 0 \quad (or) \quad \int_a^b \Psi_2^* \Psi_1 dx = 0$$

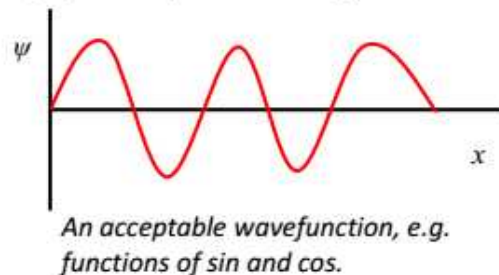
Then  $\Psi_1$  and  $\Psi_2$  are said to be orthogonal in the interval (a, b).

**Examples:**



An acceptable wavefunction must:

- (i) be continuous,
- (ii) have a continuous slope,
- (iii) be single-valued,
- (iv) be square-integrable.



## OPERATORS:

An operator is a mathematical operation which may be applied to a function  $f(x)$  which changes the function to another function  $g(x)$ . This can be represented as

$$\hat{O} f(x) = g(x)$$

So, an operator is a rule by means of which, from a given function, we can find another function.

$$\frac{d}{dx} f(x) = f'(x)$$

i.e., when the operator  $\frac{d}{dx}$  operates on the function  $f(x)$ , it gives the first derivative of  $f(x)$  obtained by the rules of differential calculus.

Example:

$$\frac{d}{dx}(x^3) = 3x^2$$

When the differential operator  $\frac{d}{dx}$  operates on the function  $x^3$ , the function  $x^3$  is changed to another function  $(3x^2)$ .

The operators used in Quantum mechanics are linear operators.

### Operators in tabular form:

$f(x)$	Any function of position, such as $x$ , or potential $V(x)$	$f(x)$
$p_x$	$x$ component of momentum ( $y$ and $z$ same form)	$\frac{\hbar}{i} \frac{\partial}{\partial x}$
$E$	Hamiltonian (time independent)	$\frac{p_{op}^2}{2m} + V(x)$
$E$	Hamiltonian (time dependent)	$i\hbar \frac{\partial}{\partial t}$
$KE$	Kinetic energy	$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
$L_z$	$z$ component of angular momentum	$-i\hbar \frac{\partial}{\partial \phi}$

## EIGEN FUNCTIONS AND EIGEN VALUES:

The values of energy  $E_n$  for which Schrodinger steady state equation can be solved are called **Eigen values** and the corresponding wave functions  $\Psi_n$  are called **Eigen functions**.

- There is a class of well-behaved functions  $\Psi$  which when operated by an Operator  $\mathbf{O}$  are merely multiplied by some constant say  $\lambda$ , i.e.,

$$\mathbf{O} \Psi(x) = \lambda \Psi(x)$$

Then we can say that the number  $\lambda$  is an eigen value of the Operator  $\mathbf{O}$  and operand  $\Psi(x)$  is an Eigen function of  $\mathbf{O}$ .

- In operator form, Schrodinger wave equation can be written as,

$$\hat{\mathbf{H}} \Psi = E \Psi$$

$$\text{where } \hat{\mathbf{H}} = -\frac{\hbar^2}{2m} \nabla^2 + V \text{ and } E = i\hbar \frac{\partial}{\partial t}$$

- **Example:**

$$-\frac{d^2}{dx^2} \sin 4x = 16 \sin 4x$$

Since, the operand  $\sin 4x$  is well behaved function and as it is operated by an Operator  $(-\frac{d^2}{dx^2})$  gives the result as  $16 \sin 4x$ .

We can say then the number 16 is an Eigen value of the operator  $(-\frac{d^2}{dx^2})$  and the operand  $\sin 4x$  is an Eigen function of the operator  $(-\frac{d^2}{dx^2})$ .

$$\hat{Q} \psi_n = \omega_n \psi_n$$

eigenvalue equation

$(\text{operator})(\text{function}) = (\text{constant factor}) \times (\text{function})$

↖  
eigenfunction,  
eigenstate or  
eigenvector

↖  
eigenvalue