

Heisenberg's Uncertainty principle:-

Classical Theory: The position and momentum of a moving particle can be determined with very high accuracy at the same time.

If we consider electron to be a wave i.e. if electron is exhibiting dual nature (wave and particle), is it possible to know the exact position of the electron in space?

According to this principle it is impossible to specify precisely and simultaneously the values of both members of particular pairs of physical variables that describe the behavior of an atomic system.

$$\boxed{\Delta x \Delta p \geq \frac{h}{4\pi}} = \frac{\hbar}{2}$$

where $\hbar = \left(\frac{h}{2\pi}\right)$

uncertainty in momentum uncertainty in position

$$\Delta x \times \Delta p \geq \frac{h}{4\pi}$$
$$\Rightarrow \Delta p \geq \left(\frac{h}{4\pi \Delta x}\right)$$

The more accurately you know the position (i.e., the smaller Δx is), the less accurately you know the momentum (i.e., the larger Δp is); and vice versa

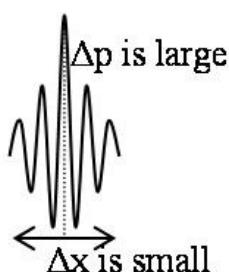


Figure 1.2a : Narrow wave Packet

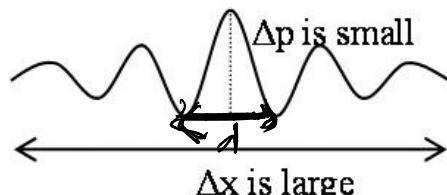


Figure 1.2b : Wide wave

$$\# \quad \lambda = \frac{h}{P} \Rightarrow P = \frac{h}{\lambda}$$

$$\frac{dP}{d\lambda} = -\frac{h}{\lambda^2} \Rightarrow dP = -\frac{h}{\lambda^2} \cdot d\lambda$$

dP = Uncertainty in momentum

$d\lambda$ = Uncertainty in DeBroglie wavelength of e^-

$$\Rightarrow \Delta x \cdot \Delta P \geq \frac{h}{4\pi}$$

$$\Delta x \cdot \frac{h}{\lambda^2} \cdot \Delta \lambda \geq \frac{h}{4\pi}$$

$$\boxed{\Delta x \cdot \Delta \lambda \geq \frac{\lambda^2}{4\pi}}^*$$

Schrodinger wave Eqn :-

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m}{h^2} [E - V] \psi = 0$$

Where ψ = Wave function of e^- # $\psi^2 = \psi \cdot \psi^*$
 h = plank's cont

m = mass of e^-

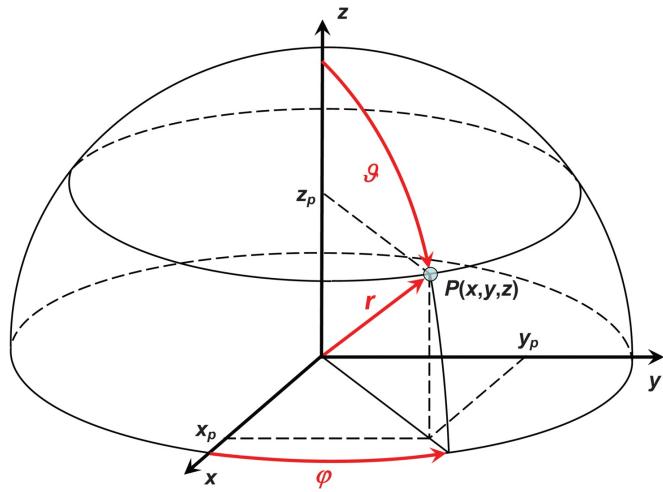
E = Total energy of e^-

V = PE of e^-

Significance of the wave function, ψ . The wave function ψ in Schrodinger equation, by itself, has no physical significance except that it represents the *amplitude of the electron wave*. However, the square of the wave function, viz., ψ^2 , gives the **probability of finding an electron of a given energy E , from place to place in a given region around the nucleus**. Just as the intensity of light is proportional to the *square of the amplitude* of the light wave at that point, similarly, the *probability of finding a particle at a particular point* is proportional to the *square of the wave function* at that point.

It is thus possible to identify regions of space around the nucleus where there is *high probability* of locating an electron associated with a specific energy. This space is called an *atomic orbital*. An **atomic orbital**, thus, represents a *definite region in three-dimensional space around the nucleus where there is high probability of finding an electron of a specific energy E* .

Solution of schrodinger, wave equation:-



$$x = r \sin\theta \cos\phi$$

$$y = r \sin\theta \sin\phi$$

$$z = r \cos\theta$$

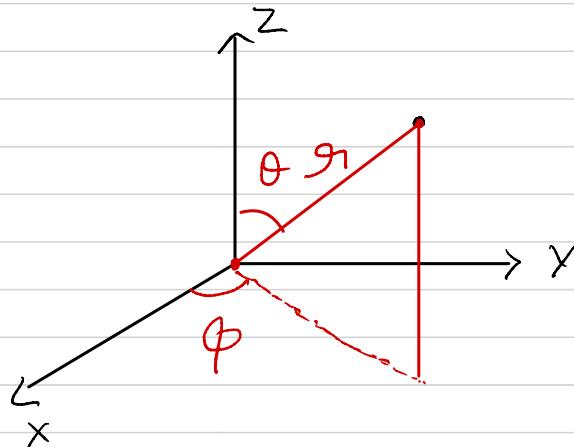
$\Psi_{(l=0)} = \Psi_{(n=1, m)}$

$$\Psi = f(x, y, z)$$



Polar coordinate

$$\Psi = f(r, \theta, \phi)$$



$$\Psi = R(r) Y(\theta, \phi)$$

Radial Wave Function

Angular Wave Function

Node :- Spaces where probability of finding e^- is zero are called as nodes

Nodes are divided in two types.

① Radial nodes (Spherical nodes)

Space where radial wave function change its sign from +ve to -ve (or from -ve to +ve).

Value of Radial wave function is zero at this pt.

$R(r) = 0$ at radial node

No of radial node = $(n-l-1)$

② Angular node

Spaces where angular wave function change its sign at its value is zero are called angular nodes

No of angular nodes = 1

Total No of nodes = $(n-1)$

* nucleus and infinite one not taken as node.

Radial wave function:-

for S-orbital $\Rightarrow \begin{cases} R(r) = +ve & \text{at } r=0 \\ R(r) = 0 & \text{at } r=\infty \end{cases}$

for other orbitals $\Rightarrow \begin{cases} R(r) = 0 & \text{at } r=0 \\ R(r) = 0 & \text{at } r=\infty \end{cases}$

General form :

$$R_{n\ell}(r) = K \cdot e^{-\sigma/2} \cdot \sigma^\ell \quad (\text{Polynomial of order } n - \ell - 1)$$

where $\sigma = \frac{2Zr}{na_0}$ $a_0 = 1^{\text{st}} \text{ Bohr's radius} = 0.529 \text{ \AA}$

#

1s $(n = 1, \ell = 0) : R_{1s}(r) = 2 \cdot \left(\frac{Z}{a_0} \right)^{3/2} \cdot e^{-\sigma/2}$

$$\sigma^l = l \Rightarrow l = 0$$

$$n-l-1 = 0$$

$$n = 1$$

1(s)

where $\sigma = \frac{2Zr}{na_0}$ $a_0 = 1^{\text{st}} \text{ Bohr's radius} = 0.529 \text{ \AA}$

2s $(n = 2, \ell = 0) : R_{2s}(r) = \frac{1}{2\sqrt{2}} \cdot \left(\frac{Z}{a_0} \right)^{3/2} \cdot (2-\sigma)e^{-\sigma/2}$

$$\sigma^l = l \Rightarrow l = 0$$

$$n-l-1 = 1$$

$$n = 2 \Rightarrow 2(s)$$

2p $(n = 2, \ell = 1) : R_{2p}(r) = \frac{1}{2\sqrt{6}} \cdot \left(\frac{Z}{a_0} \right)^{3/2} \cdot \sigma \cdot e^{-\sigma/2}$

$$\sigma^l = l \Rightarrow l = 1$$

$$n-l-1 = 0 \Rightarrow n = 2 \Rightarrow (2p)$$

3s $(n = 3, \ell = 0) : R_{3s}(r) = \frac{1}{9\sqrt{3}} \cdot \left(\frac{Z}{a_0} \right)^{3/2} \cdot (6-6\sigma+\sigma^2)e^{-\sigma/2}$

$$\sigma^l = l \Rightarrow l = 0$$

$$n-l-1 = 2$$

$$n = 3 \Rightarrow 3(s)$$

3p $(n = 3, \ell = 1) : R_{3p}(r) = \frac{1}{9\sqrt{6}} \cdot \left(\frac{Z}{a_0} \right)^{3/2} \cdot \sigma(4-\sigma)e^{-\sigma/2}$

$$\sigma^l = l \Rightarrow l = 1$$

$$n-l-1 = 1 \Rightarrow n = 3$$

(3p)

3d $(n = 3, \ell = 2) : R_{3d}(r) = \frac{1}{9\sqrt{30}} \cdot \left(\frac{Z}{a_0} \right)^{3/2} \cdot \sigma^2 \cdot e^{-\sigma/2}$

$$\sigma^2 = l \Rightarrow l = 2$$

$$n-l-1 = 0 \Rightarrow n = 3$$

(3d)