Application of Uncertainty Principle:

According to uncertainty principle the position & momentum of the particle cannot be measured with accuracy, while according to classical ideas it is possible to predict exactly the position & momentum of the particle at any instant when its initial position & momentum is known. Moreover new mechanics gives us the laws of probability and hence the probability takes the place of certainty. According to new mechanics the term particle is something ~~made~~ made up a very deep & essential unison of both the corpuscle and the wave resulting in a certain unavoidable uncertainty. The principle of uncertainty explains a large number of facts which could not be explained by classical ideas. Some of its application are discussed here.

(1) **The non existence of the electrons in the nucleus.** The radius of the nucleus of any atom is of the order of 10^{-14} m, so that if an electron is confined with nucleus, the uncertainty in its position must not be greater than 10^{-14} m.

According to uncertainty principle

$$\Delta q\, \Delta p \approx \hbar, \qquad ...(1)$$

where Δq is the uncertainty in the position and Δp is the uncertainty in the momentum and $\hbar = h/2\pi$.

Equation (1) gives

$$\Delta p = \frac{\hbar}{\Delta q}$$

$$\approx \frac{1 \cdot 055 \times 10^{-34}}{2 \times 10^{-14}} \left[\text{since } \hbar = \frac{h}{2\pi} = \frac{6 \cdot 625 \times 10^{-34}}{2 \times 3 \cdot 14} = 1 \cdot 055 \times 10^{-34} \text{ joule—sec. and } \Delta q = 2r = 2 \times 10^{-14} \text{ m.} \right]$$

$$\approx 3 \cdot 275 \times 10^{-21} \text{ kg. m./sec.}$$

It this is the uncertainty in momentum of the electron, the momentum of the electron must be at least comparable with its magnitude, *i.e.*,

$$p \approx 5 \cdot 275 \times 10^{-21} \text{ kg. m./sec.}$$

The kinetic energy of the electron of mass m is given by

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

$$\approx \frac{(5 \cdot 275 \times 10^{-12})^2}{2 \times 9 \times 10^{-31}} \text{ joule} \qquad (\text{since } m = 9 \times 10^{-31} \text{ kg.})$$

$$\approx \frac{(5 \cdot 275 \times 10^{-21})^2}{2 \times 9 \times 10^{-31} \times 1 \cdot 6 \times 10^{-19}} \text{ eV.}$$

$$\approx 9 \cdot 7 \times 10^7 \text{ eV.}$$

$$\approx 97 \text{ MeV.}$$

This means that if the electrons exist inside the nucleus, their kinetic energy must be of the order of 97 MeV. But experimental observations show that no electron in the atom possess energy greater than 4 MeV. Clearly the inference is that the *electrons do not exist in the nucleus.*

(ii) **The radius of the Bohr's First Orbit.** If Δq and Δp are the uncertainties in the position and momentum of the electron in first orbit, then we have

$$\Delta q \Delta p \approx \hbar$$

or

$$\Delta p \approx \frac{\hbar}{\Delta q}$$

The uncertainty in the kinetic energy of the electron may be written as

$$\Delta T = \tfrac{1}{2} m (\Delta v)^2 \qquad ...(2)$$

$$= \tfrac{1}{2} \frac{(m\Delta v)^2}{m}$$

$$= \tfrac{1}{2} \frac{(\Delta p)^2}{m}$$

$$\approx \frac{1}{2m} \left(\frac{\hbar}{\Delta q}\right)^2$$

$$\approx \frac{\hbar^2}{2m (\Delta q)^2}. \qquad ...(3)$$

The uncertainty in the potential energy of the same electron is

$$\Delta V = -\frac{Ze^2}{\Delta q},$$

so that the uncertainty in the total energy is

$$\Delta E = \Delta T + \Delta V$$

$$= \frac{\hbar^2}{2m (\Delta q)^2} - \frac{Ze^2}{\Delta q}. \qquad ...(5)$$

The uncertainty in the energy will be minimum if

$$\frac{d(\Delta E)}{d(\Delta q)} = 0 \text{ and } \frac{d^2 (\Delta E)}{d (\Delta q)^2} = (+) \text{ ve}.$$

Equation (5) yields

$$\frac{d(\Delta E)}{d(\Delta q)} = -\frac{\hbar^2}{m (\Delta q)^3} + \frac{Ze^2}{(\Delta q)^2}. \qquad ...(6)$$

If E is minimum, we must have

$$0 = -\frac{\hbar^2}{m (\Delta q)^3} + \frac{Ze^2}{(\Delta q)^2}$$

or

$$\frac{\hbar^2}{m (\Delta q)^3} = \frac{Ze^2}{\Delta q^2}$$

or

$$\Delta q \approx \frac{\hbar^2}{m Ze^2} \qquad ...(7)$$

Differentiating equation (6), we get

$$\frac{d^2 (\Delta E)}{d(\Delta q)^2} \approx + \frac{3\hbar^2}{m (\Delta q)^4} - 2 \frac{Ze^2}{(\Delta q)^3}$$

$$\approx \frac{3\hbar^2}{m(\Delta q)^3\left(\frac{\hbar^2}{Zme^2}\right)} - \frac{2Ze^2}{(\Delta q)^3} \text{ using (7)}$$

$$\approx \frac{3Ze^2}{(\Delta q)^3} - \frac{2Ze^2}{(\Delta q)^3} \approx \frac{Ze^2}{(\Delta q)^3}$$

$$=(+)\text{ve}.$$

i.e., equation (7) represents the condition of minimum in the first orbit. Therefore the radius of the first orbit is given by

$$r = \Delta q = \frac{\hbar^2}{mZe^2} = \frac{h^2}{4\pi^2 mZe^2}, \qquad \ldots(1)$$

which is just the radius of Bohr's is first orbit.

2.5. THE EHRENFEST THEOREM

Ehrenfest's theorem states that in *quantum mechanics the expectation or average values of observables behave in the same manner as the observables themselves do in classical mechanics*. This theorem furnishes an example of the correspondence principle.

Consider for simplicity a one-dimensional case where the dynamical system is confined to the x-axis only. The velocity is the rate of change of the expectation value of the position coordinate x with respect to time t.

Therefore,

$$\frac{d<x>}{dt} = \frac{d}{dt}\int_{-\infty}^{\infty} \psi^* (x, t)\, x\psi (x, t)\, dx$$

$$= \int_{-\infty}^{\infty} \psi^* x \frac{\partial \psi}{\partial t} dx + \int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial t} x \psi\, dx \qquad ...(2.24)$$

The value of $\frac{\partial \psi}{\partial t}$ is obtained from the one-dimensional form of Eq. (2.15). The quantity $\frac{\partial \psi^*}{\partial t}$ is also obtained from the Schrödinger wave equation as follows:

The wave function can be written as the sum of its real and imaginary parts;

$$\psi (x, t) = u (x, t) + iv (x, t) \qquad ...(2.25)$$

Substituting this in Eq. (2.15) and equating the real and the imaginary parts we get

$$-\hbar \frac{\partial v}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 u + Vu \qquad ...(2.26)$$

and

$$\hbar \frac{\partial u}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 v + Vv \qquad ...(2.27)$$

Multiplying Eq. (2.27) by $-i$ and adding to Eq. (2.26) we get a wave equation for $\psi^*(=u-iv)$:

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi^* + V\psi^* \qquad ...(2.28)$$

In one-dimension we have

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + V\psi^* \qquad ...(2.28a)$$

Putting the values of $\frac{\partial \psi}{\partial t}$ and $\frac{\partial \psi^*}{\partial t}$ in Eq. (2.24) we get

$$\frac{d}{dt}\langle x\rangle = -\frac{i}{\hbar}\left[\int_{-\infty}^{\infty} \psi^* x\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi\right)dx - \int_{-\infty}^{\infty}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + V\psi^*\right)x\psi dx\right]$$

$$= \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left[\psi^* x\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2}x\psi\right]dx \qquad ...(2.29)$$

Integrating by parts, the integral on the right -hand side of Eq. (2.29) reduces to

$$\left[\psi^* x\frac{\partial \psi}{\partial x}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left[\frac{\partial \psi^*}{\partial x}x\frac{\partial \psi}{\partial x} + \psi^*\frac{\partial \psi}{\partial x}\right]dx - \left[\frac{\partial \psi^*}{\partial x}x\psi\right]_{-\infty}^{\infty}$$

$$+ \int_{-\infty}^{\infty}\left[\frac{\partial \psi^*}{\partial x}x\frac{\partial \psi}{\partial x} + \frac{\partial \psi^*}{\partial x}\psi\right]dx$$

Since both ψ and $\frac{\partial \psi}{\partial x}$ vanish as $x \to \infty$ or $x \to -\infty$, the above integral

reduces to

$$\int_{-\infty}^{\infty}\left[\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}\right]dx$$

Again, $\int_{-\infty}^{\infty}\frac{\partial \psi^*}{\partial x}\psi dx = \left[\psi^*\psi\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\psi^*\frac{\partial \psi}{\partial x}dx = -\int_{-\infty}^{\infty}\psi^*\frac{\partial \psi}{\partial x}dx$

Therefore we obtain from Eq. (2.29)

$$\frac{d}{dt}\langle x\rangle = \frac{i\hbar}{2m}\left[-2\int_{-\infty}^{\infty}\psi^*\frac{\partial \psi}{\partial x}dx\right] = -\frac{i\hbar}{m}\int_{-\infty}^{\infty}\psi^*\frac{\partial \psi}{\partial x}dx = \frac{\langle p_x\rangle}{m} \qquad ...(2.30)$$

That is, the velocity is equal to the expectation value of the momentum divided by the mass. This corresponds to the classical equation $dx/dt = p_x/m$.

In a similar way we can calculate the time rate of change of x component of the momentum as follows:

$$\frac{d}{dt}\langle p_x\rangle = -i\hbar\frac{d}{dt}\int_{-\infty}^{\infty}\psi^*(x,t)\frac{\partial}{\partial x}\psi(x,t)\,dx$$

$$= -i\hbar\left(\int_{-\infty}^{\infty}\psi^*\frac{\partial}{\partial x}\frac{\partial \psi}{\partial t}dx + \int_{-\infty}^{\infty}\frac{\partial \psi^*}{\partial t}\frac{\partial \psi}{\partial x}dx\right) \qquad ...(2.31)$$

Putting the values of $\frac{\partial \psi}{\partial t}$ and $\frac{\partial \psi^*}{\partial t}$ we get

$$\frac{d}{dt}\langle p_x\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left[\frac{\partial^2\psi}{\partial x^2}\frac{\partial\psi}{\partial x} - \psi^*\frac{\partial^3\psi}{\partial x^3}\right]dx$$

$$+\int_{-\infty}^{\infty}\left[V\psi^*\frac{\partial\psi}{\partial x} - \psi^*\frac{\partial}{\partial x}(V\psi)\right]dx$$

$$= -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left[\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x} - \psi^*\frac{\partial^2\psi}{\partial x^2}\right)\right]dx$$

$$-\int_{-\infty}^{\infty}\psi^*\frac{\partial V}{\partial x}\psi dx$$

$$= -\frac{\hbar^2}{2m}\left[\frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x} - \psi^*\frac{\partial^2\psi}{\partial x^2}\right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\psi^*\frac{\partial V}{\partial x}\psi\, dx$$

$$= -\int_{-\infty}^{\infty}\psi^*\frac{\partial V}{\partial x}\psi\, dx = \langle -\frac{\partial V}{\partial x}\rangle = \langle F_x\rangle, \qquad ...(2.32)$$

which is Newton's second law of motion $\left(\frac{dp_x}{dt} = F_x\right)$. Thus we find that the classical mechanics agrees with the quantum mechanics so far as the expectation values are concerned. However, the measured values of the observables fluctuate over their expectation values. This is the characteristic feature of the quantum theory.