❖ Evaluation of Average Position, Average Momentum and Determination of Uncertainty in Position and Momentum and Hence Heisenberg's Uncertainty Principle

The third postulate of quantum mechanics states that when the wave-function of a particular quantum mechanical state is multiplied by the operator of an observable quantity, we get a real value multiplied by the wave function itself. However, the value obtained this way can be constant or variable. Mathematically, the constant value of the observable quantity can be reported directly, and the function is called an eigenfunction of the operator under consideration. If the value of the physical property obtained after multiplying the wave function by the corresponding operator is variable i.e. non-eigen, the value can be reported only after averaging it over the whole configurational space.

$$< a > = \frac{\oint \psi^* \hat{O} \psi \, d\tau}{\oint \psi^* \psi \, d\tau} \tag{456}$$

Since the wave function ψ is normalized, the denominator becomes unity; therefore, equation (456) is reduced to the following

$$< a > = \oint \psi^* \hat{O} \psi \, d\tau \tag{457}$$

Since the operation by the Hamiltonian over the symbolic form has already given the absolute expressions for different quantum mechanical states, now we can operate other operators to evaluate their average values. In this section, we will determine the average values of position, position-squared, momentum and momentum-squared; which in turn will be used to prove the Heisenberg's uncertainty finally.

➢ *Evaluation of Average Position*

The quantum mechanical operator for the position of a particle in one-dimensional is $\hat{x}$; while the general form of wave function is

$$\psi_n = \sqrt{\frac{2}{a}} \, Sin \frac{n\pi x}{a} \tag{458}$$

Using this in equation (457), we get

$$< x > = \oint \psi^* x \, \psi \, d\tau \tag{459}$$

or

$$< x > = \oint x \, \psi^2 \, dx \tag{460}$$

$$< x > = \int_0^a x.\ \frac{2}{a} Sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{2}{a}\int_0^a x\ Sin^2\left(\frac{n\pi x}{a}\right) dx \quad (461)$$

$$= \frac{2}{a}\int_0^a x \left[\frac{1 - Cos\left(\frac{2n\pi x}{a}\right)}{2}\right] dx \quad (462)$$

$$= \frac{1}{a}\int_0^a \left(x - x\ Cos\frac{2n\pi x}{a}\right) dx \quad (463)$$

$$= \frac{1}{a}\left[\int_0^a x\ dx - \int_0^a x\ Cos\left(\frac{2n\pi x}{a}\right) dx\right] \quad (464)$$

$$= \frac{1}{a}\left[\frac{a^2}{2} - 0\right] = \frac{a}{2} \quad (465)$$

➢ ***Evaluation of Average Position-Squared***

The quantum mechanical operator for the position-squared of a particle in one-dimensional is $\hat{x}^2$; Using this in equation (457), we get

$$< x^2 > = \oint \psi^*\ x^2\ \psi\ dx \quad (466)$$

$$< x^2 > = \int_0^a x^2.\ \frac{2}{a} Sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{2}{a}\int_0^a x^2\ Sin^2\left(\frac{n\pi x}{a}\right) dx \quad (467)$$

$$= \frac{2}{a}\int_0^a x^2 \left[\frac{1 - Cos\left(\frac{2n\pi x}{a}\right)}{2}\right] dx \quad (468)$$

$$= \frac{2}{a}\left[\frac{a^3}{6} - \frac{a^3}{4n^2\pi^2}\right] = \frac{1}{a}\left[\frac{a^3}{3} - \frac{a^3}{2n^2\pi^2}\right] \quad (469)$$

$$= \frac{a^2}{3} - \frac{a^2}{2n^2\pi^2} \quad (470)$$

➢ ***Evaluation of Average Momentum***

The quantum mechanical operator for the position-squared of a particle in one-dimensional is $\hat{p}_x$; Using this in equation (457), we get

$$< \hat{p}_x > = \oint \psi^* \, \frac{h}{2\pi i}\frac{\partial}{\partial x} \, \psi \, dx \tag{471}$$

$$< \hat{p}_x > = \int_0^a \left[\sqrt{\frac{2}{a}} Sin\left(\frac{n\pi x}{a}\right)\right] \frac{h}{2\pi i}\frac{\partial}{\partial x} \left[\sqrt{\frac{2}{a}} Sin\left(\frac{n\pi x}{a}\right)\right] dx \tag{472}$$

$$= \frac{h}{2\pi i}\left[\frac{2}{a}\right] \int_0^a Sin\left(\frac{n\pi x}{a}\right)\left(\frac{n\pi}{a}\right) \, Cos\left(\frac{n\pi x}{a}\right) dx \tag{473}$$

$$= \frac{h}{2\pi i}\left[\frac{2}{a}\right]\left(\frac{n\pi}{a}\right) \int_0^a Sin\left(\frac{n\pi x}{a}\right) \, Cos\left(\frac{n\pi x}{a}\right) dx \tag{474}$$

$$< \hat{p}_x > = 0 \tag{475}$$

- ***Evaluation of Average Momentum-Squared***

The quantum mechanical operator for the position-squared of particle in one-dimensional is $\hat{p}_x^2$; Using this in equation (457), we get

$$< \hat{p}_x^2 > = \oint \psi^* \left(-\frac{h^2}{4\pi^2}\frac{\partial^2}{\partial x^2}\right) \psi \, dx \tag{476}$$

$$< \hat{p}_x^2 > = \int_0^a \left[\sqrt{\frac{2}{a}} Sin\left(\frac{n\pi x}{a}\right)\right] \left(-\frac{h^2}{4\pi^2}\frac{\partial^2}{\partial x^2}\right) \left[\sqrt{\frac{2}{a}} Sin\left(\frac{n\pi x}{a}\right)\right] dx \tag{477}$$

$$= -\frac{h^2}{4\pi^2}\left(\frac{2}{a}\right) \int_0^a Sin\left(\frac{n\pi x}{a}\right)\left[(-)\left(\frac{n\pi}{a}\right)^2 Sin\left(\frac{n\pi x}{a}\right)\right] dx \tag{478}$$

$$= \frac{h^2}{4\pi^2}\left(\frac{2}{a}\right)\left(\frac{n\pi}{a}\right)^2 \int_0^a Sin^2\left(\frac{n\pi x}{a}\right) dx \tag{479}$$

$$= \frac{n^2 h^2}{2a^3} \int_0^a Sin^2\left(\frac{n\pi x}{a}\right) dx \tag{480}$$

$$= \frac{n^2 h^2}{2a^3} \int_0^a \left[\frac{1 - Cos\left(\frac{2n\pi x}{a}\right)}{2}\right] dx \tag{481}$$

$$= \frac{n^2h^2}{2a^3}\left[\frac{x - Sin\left(\frac{2n\pi x}{a}\right)}{\frac{2n\pi}{a}}\right]_0^a \tag{482}$$

or

$$= \frac{n^2h^2}{2a^3}\left(\frac{a}{2}\right) \tag{483}$$

or

$$< \hat{p}_x^2 > = \frac{n^2h^2}{4a^2} \tag{484}$$

➢ ***The Heisenberg's Uncertainty***

In order to prove the Heisenberg's uncertainty principle from for the quantum mechanical system of a particle in one-dimensional box, we first need to find the uncertainties in position and momentum. Once both uncertainties are known, we can simply multiply both to yield final result.

1. Uncertainty in position: The uncertainty in position is simply the difference between the square root of the uncertainty in the position-squared. Mathematically, we can say that

$$\Delta x = (< x^2 > - < x >^2)^{1/2} \tag{485}$$

After putting the values of average position and position-squared from equation (465) and (470) in equation (485), we get

$$\Delta x = \left[\left(\frac{a^2}{3} - \frac{a^2}{2n^2\pi^2}\right) - \left(\frac{a}{2}\right)^2\right]^{1/2} \tag{486}$$

or

$$\Delta x = \left[\left(\frac{a^2}{12} - \frac{a^2}{2n^2\pi^2}\right)\right]^{1/2} \qquad (487$$

or

$$\Delta x = a\left(\frac{1}{12} - \frac{1}{2n^2\pi^2}\right)^{1/2} \tag{488}$$

2. Uncertainty in momentum: The uncertainty in momentum is simply the square root of the difference between the uncertainty in momentum and uncertainty in the momentum-squared. Mathematically, we can say that

$$\Delta p_x = (< p_x^2 > - < p_x >^2)^{1/2} \quad (489)$$

After putting the values of average position and position-squared from equation (475) and (484) in equation (489), we get

$$\Delta p_x = \left[\left(\frac{n^2h^2}{4a^2}\right) - (0)^2\right]^{1/2} \quad (490)$$

or

$$\Delta p_x = \frac{nh}{2a} \quad (491)$$

Now multiplying equation (488) and (491), we get

$$\Delta x.\Delta p_x = \left[a\left(\frac{1}{12} - \frac{1}{2n^2\pi^2}\right)^{1/2}\right]\left(\frac{nh}{2a}\right) \quad (492)$$

or

$$= \frac{nh}{2}\left(\frac{1}{12} - \frac{1}{2n^2\pi^2}\right)^{1/2} \quad (493)$$

Multiply and divide the above equation by $2n\pi$

$$\Delta x.\Delta p_x = \frac{nh}{2}.\frac{2n\pi}{2n\pi}\left(\frac{1}{12} - \frac{1}{2n^2\pi^2}\right)^{1/2} \quad (493)$$

or

$$= \frac{nh}{2}.\frac{1}{2n\pi}\left(\frac{4n^2\pi^2}{12} - \frac{4n^2\pi^2}{2n^2\pi^2}\right)^{1/2} \quad (494)$$

or

$$\Delta x.\Delta p_x = \frac{h}{4\pi}\left(\frac{n^2\pi^2}{3} - 2\right)^{1/2} \quad (495)$$

Since $n^2\pi^2/3$ is always greater than 2, we can conclude that

$$\Delta x.\Delta p_x > \frac{h}{4\pi} \quad (496)$$

Which is the famous Heisenberg's uncertainty principle.

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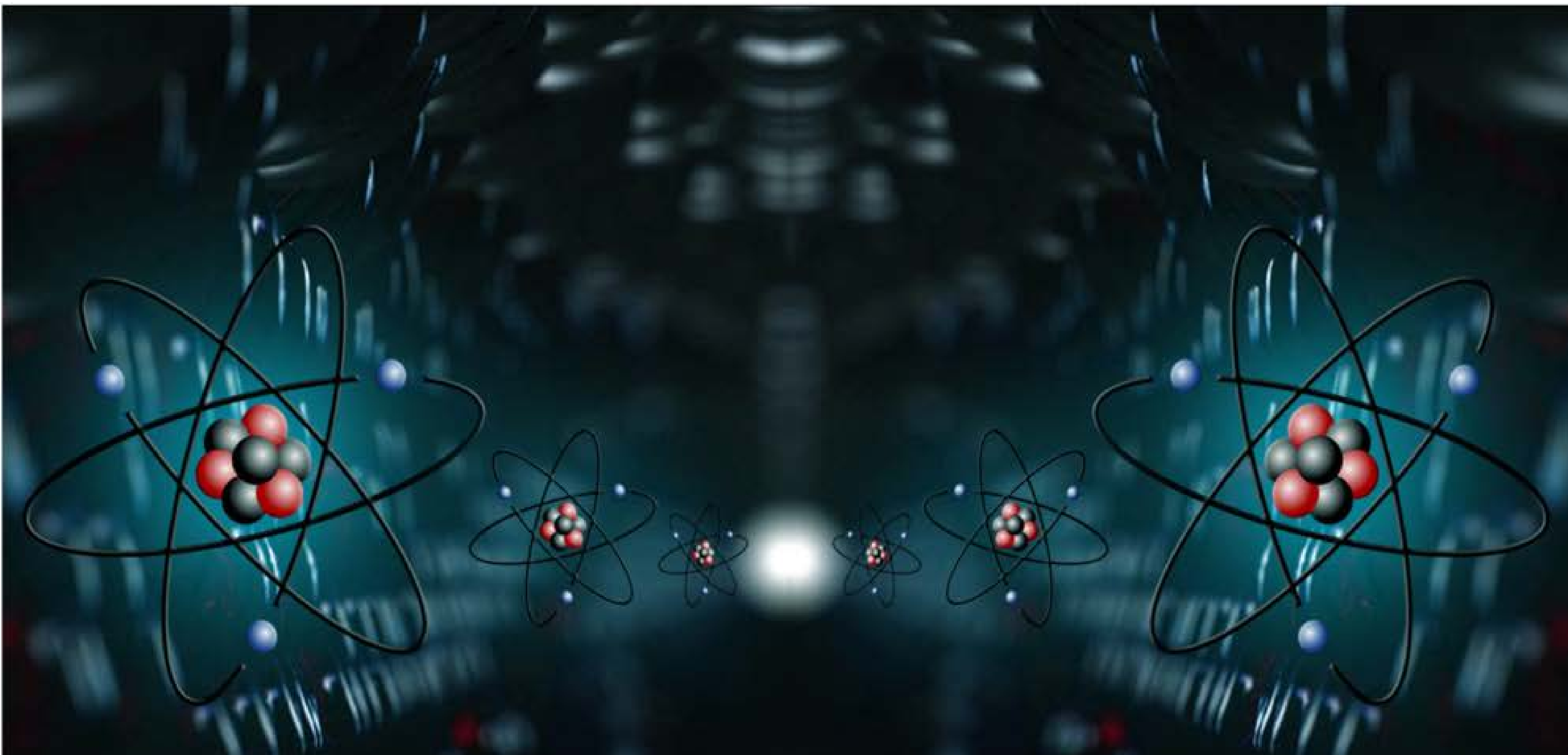

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