## Numerical Based on Schrödinger's Equation

① A particle limited to the x-axis has the wave function $\psi = ax$ between $x = 0$ and $x = 1$, $\psi = 0$ elsewhere.

a) Find the probability that particle can be found between $x = 0.45$ and $x = 0.55$.

b) Find the expectation value $\langle x \rangle$ of particle's position

Soln:- a) Here, $\psi = ax$

$\therefore$ probability, $P = \int_{0.45}^{0.55} |\psi|^2 dx$

$$= a^2 \int_{0.45}^{0.55} x^2 dx = a^2 \left[\frac{x^3}{3}\right]_{0.45}^{0.55}$$

$$\Rightarrow \boxed{P = 0.0251 a^2}$$

b) The expectation value is,

$$\langle x \rangle = \int_0^1 x |\psi|^2 dx$$

$$= a^2 \int_0^1 x^3 dx = a^2 \left[\frac{x^4}{4}\right]_0^1$$

$$\Rightarrow \boxed{\langle x \rangle = \frac{1}{4} a^2}$$

② Find the values of momentum and energy for an electron in a box of length $1\text{Å}$ for $n = 1, 2$.

Ans:- Length of box, $a = 1\text{Å} = 1 \times 10^{-10}$ m

$\therefore$ Momentum, $P_n = n\hbar\pi/a$

$\therefore$ for $n = 1$, $P_1 = \hbar\pi/a = \frac{h}{2\pi} \cdot \frac{\pi}{a} = \frac{h}{2a}$

$$= 6.63 \times 10^{-34}\ \text{J-s} / 2 \times 10^{-10}\ \text{m} = 3.3 \times 10^{-24}\ \text{kgm/sec}$$

for $n = 2$, $P_2 = 2\hbar\pi/a = \frac{2h}{2\pi} \cdot \frac{\pi}{a} = \frac{h}{a} = 6.63 \times 10^{-24}\ \text{kgm/s}$

$\therefore$ Energy, $E_n = n^2 \cdot \hbar^2 \pi^2 / 2ma^2$.

For $n = 1$, $E_1 = \hbar^2\pi^2/2ma^2 = \frac{h^2}{4\pi^2} \cdot \frac{\pi^2}{2ma^2} = \frac{h^2}{8ma^2}$

$$= \frac{(6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (10^{-10})^2} = 60.4 \times 10^{-10}\ \text{J}$$

& Similarly, $E_2 = 241.6 \times 10^{-10}\ \text{J}$