Num:- What is the ground state energy for an electron which is confined to a potential well (one dimensional box) having a width of 0.2 nm?

Ans:-

$$E = \frac{n^2 h^2}{8ma^2} \quad \text{for ground state } n=1$$

$m = 9.31 \times 10^{-31}$ kg , $h = 6.626 \times 10^{-34}$ Js

$a = 0.2$ nm $= 0.2 \times 10^{-9}$ m

$$\therefore E = \frac{(1)^2 \times (6.626 \times 10^{-34} \text{ Js})^2}{8 \times 9.31 \times 10^{-31} \text{ kg} \times (0.2 \times 10^{-9} \text{ m})^2}$$

$$= \frac{43.904 \text{ J}^2 \text{s}^2 \times 10^{-68}}{2.979 \times 10^{-49} \text{ kg m}^2} = 14.738 \times 10^{-19} \frac{\text{J}^2}{\text{kgm}^2\text{s}^{-2} \text{ (J)}}$$

$$= 1.474 \times 10^{-18} \text{ J}$$

Num:- An electron is confined to move in one dimensional box of width 1 Å. What quantized values of energy can it have? Express them in electron volts & represent them in suitable energy level diagram.

Ans:-

$$E = \frac{n^2 h^2}{8ma^2}, \quad h = 6.626 \times 10^{-34} \text{ Js}$$

$m = 9.31 \times 10^{-31}$ kg, $a = 1$ Å $= 10^{-10}$ m

$$\therefore E = \frac{n^2 (6.626 \times 10^{-34} \text{ Js})^2}{8 \times 9.31 \times 10^{-31} \text{ kg} \times (10^{-10} \text{ m})^2}$$

$E_3 = 329.85$ ev

$$= \frac{n^2 \times 43.904 \times 10^{-68} \text{J}^2 \text{s}^2}{7.448 \times 10^{-50} \text{ kg m}^2} = n^2 \times 5.894 \times 10^{-18} \text{ J}$$

$E_2 = 146.6$ ev

$$= \frac{n^2 \times 5.894 \times 10^{-18}}{1.6 \times 10^{-19}} \text{ ev} \quad [\because 1 \text{ ev} = 1.6 \times 10^{-19} \text{ J}]$$

$E_1 = 36.65$ ev

$$= n^2 \times 36.65 \text{ ev}$$

For n = 1, 2, 3 ... we get the value as 36.65ev, 146.6ev, 329.85ev ...

Num:- Verify that the wave function of a particle in one-dimensional box of width a & infinite height are orthogonal.

Sol— Since for particle in 1-D box.

$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \qquad n = 1, 2, 3 \ldots$$

The orthogonality eqn. require then

$$\int_0^a \psi_m^*(x)\, \psi_n(x)\, dx = 0$$

Here $\psi_m^*(x) = \psi_m(x) = \sqrt{\frac{2}{a}} \sin \frac{m\pi x}{a}$

$$\therefore \int_0^a \sqrt{\frac{2}{a}} \sin \frac{m\pi x}{a} \cdot \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

$$= \frac{2}{a} \int_0^a \frac{1}{2}\left[\cos \frac{(m-n)\pi x}{a} - \cos \frac{(m+n)\pi x}{a} \right] dx$$

$$= \frac{1}{a}\left[\frac{a}{(m-n)\pi} \sin\left[\frac{(m-n)\pi x}{a}\right]_0^a + \frac{a}{(m+n)\pi} \sin\left[\frac{(m+n)\pi x}{a}\right]_0^a \right]$$

$$= 0$$

Num:- Calculate the expectation (average) value of energy of a particle of mass 'm' confined to move in 1-D box of width 'a' & infinite height with P.E zero inside the box.

Sol:- Since Total energy $E = K.E + P.V = \frac{1}{2} m u_x^2 + V(x)$

But $V(x) = 0$

$$\therefore E = \frac{1}{2} m u_x^2 = \frac{1}{2m}(m u_x)^2 = \frac{p_x^2}{2m}$$

but $\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$ $\therefore$ $p_x^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$

Hence $\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$

$\therefore$ expectation value $\langle E \rangle = \int_0^a \psi_m(x)\, \hat{H}\, \psi_m(x)\, dx$

$$= -\frac{\hbar^2}{2m} \int_0^a \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \cdot \frac{d^2}{dx^2} \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \cdot dx$$

$$= -\frac{\hbar^2}{2m} \int_0^a \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \cdot \frac{d}{dx} \sqrt{\frac{2}{a}} \cos \frac{n\pi x}{a} \cdot \frac{n\pi}{a} \cdot dx$$

$$= \frac{-\hbar^2}{2m}\int_0^a \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}\cdot\sqrt{\frac{2}{a}}\left(-\sin\frac{n\pi x}{a}\right)\cdot\frac{n^2\pi^2}{a^2}\cdot dx$$

$$= \frac{+\hbar^2}{\cancel{2}m}\cdot\frac{\cancel{2}}{a}\cdot\frac{n^2\pi^2}{a^2}\int_0^a \sin^2\frac{n\pi x}{a}\,dx$$

$$= \frac{h^2}{4\cancel{\pi^2}m}\cdot\frac{n^2\cancel{\pi^2}}{a^3}\frac{1}{2}\int_0^a\left(1-\cos\frac{2n\pi x}{a}\right)dx$$

$$= \frac{n^2h^2}{8ma^3}\left[x\Big|_0^a - \frac{\sin\frac{2n\pi x}{a}}{\frac{2n\pi}{a}}\Big|_0^a\right]$$

$$= \frac{n^2h^2}{8ma^3}\left[a-0\right]$$

$$\therefore \langle E\rangle = \frac{n^2h^2}{8ma^2}$$