Assignment 7 Particle in 3D Box

Considering a particle of mass m in a 3D Box

V = 0 inside the Box
V = ∞ outside the Box

Schrodinger time independent equation may be written as,

$$-\frac{h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi = E\psi$$

Assuming ψ can be resolved as it doesn't depends on the coordinates x, y and z.

$$\psi = \psi_{(x)} \cdot \psi_{(y)} \cdot \psi_{(z)}$$

The corresponding Hamiltonians will be

$$\hat{H}_x = \frac{-h^2}{8\pi^2 m}\frac{\partial^2}{\partial x^2}$$

$$\hat{H}_y = \frac{-h^2}{8\pi^2 m}\frac{\partial^2}{\partial y^2}$$

$$\hat{H}_z = \frac{-h^2}{8\pi^2 m}\frac{\partial^2}{\partial z^2}$$

$$\hat{H}\Psi = E\Psi$$

$$\hat{H}_x \Psi_{(x)}\Psi_{(y)}\Psi_{(z)} + \hat{H}_y \Psi_{(x)}\Psi_{(y)}\Psi_{(z)} + \hat{H}_z \Psi_{(x)}\Psi_{(y)}\Psi_{(z)}$$
$$= E\Psi_{(x)}\Psi_{(y)}\Psi_{(z)}$$

Dividing throughout by $\Psi = \Psi_{(x)}\Psi_{(y)}\Psi_{(z)}$ we get,

$$\frac{\hat{H}_x \Psi_{(x)}}{\Psi_{(x)}} + \frac{\hat{H}_y \Psi_{(y)}}{\Psi_{(y)}} + \frac{\hat{H}_z \Psi_{(z)}}{\Psi_{(z)}} = E \text{ (const)}$$

If a particle is moving parallel to any particular axis, then the other two terms in the eqn corresponds to the other 2 axes will be constant.

$$\frac{\hat{H}_x \Psi(x)}{\Psi_{(x)}} + \text{const} + \text{const.} = E_x$$

$$\Rightarrow \quad E_x = \frac{\hat{H}_x \Psi_{(x)}}{\Psi_{(x)}}, \quad E_y = \frac{\hat{H}_y \Psi_{(y)}}{\Psi_{(y)}}$$

$$E_z = \frac{\hat{H}_z \Psi_{(z)}}{\Psi_{(z)}}$$

$$\Rightarrow E = E_x + E_y + E_z$$

And $\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z$

$$\Rightarrow \hat{H}_x \Psi_{(x)} = E_x \Psi_{(x)}, \quad \hat{H}_y \Psi_{(y)} = E_y \Psi_{(y)}, \quad \hat{H}_z \Psi_{(z)} = E_z \Psi_{(z)}$$

Now the particle in 3 dimensional box is converted into 3 - particle in 1 D problem

Considering three particle in 1 D box with length A, B and C

$$\Psi = \Psi_{(x)} \Psi_{(y)} \Psi_{(z)} = \sqrt{\frac{2}{A}} \sin\left(\frac{n_x \pi x}{A}\right) \cdot$$

$$\sqrt{\frac{2}{B}} \sin\left(\frac{n_y \pi x}{B}\right) \cdot \sqrt{\frac{2}{C}} \sin\left(\frac{n_z \pi x}{C}\right)$$

$$E = E_x + E_y + E_z = \frac{h^2}{8m}\left(\frac{n_x^2}{A} + \frac{n_y^2}{B} + \frac{n_z^2}{C}\right)$$