SEPARATION OF VARIABLES IN 3-D PARTICLE-IN-A-BOX

Schrödinger time-independent wave equations inside box:

$$\boxed{\frac{-\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)=E\psi} \tag{1}$$

$$\psi(x,y,z) = X(x)Y(y)Z(z) \tag{2}$$

Substituting (2) into (1) and dividing by ψ(x, y, z)

$$\frac{-\hbar^2}{2m}\left[\frac{1}{X}\frac{\partial^2 X}{\partial x^2}+\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}+\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right]=E \tag{3}$$

$$\underbrace{\frac{-\hbar^2}{2m}\left[\frac{1}{X}\frac{\partial^2 X}{\partial x^2}\right]}_{\| \; E_x} = E + \underbrace{\frac{\hbar^2}{2m}\left[\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}+\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right]}_{\| \; E_x} \tag{4}$$

since left side is function of x and right is function of y, z

$$\frac{-\hbar^2}{2m}\left[\frac{\partial^2 X}{\partial x^2}\right]=E_x X(x) \tag{5}$$

from (4)

$$\frac{-\hbar^2}{2m}\left[\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}+\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right]=E-E_x \tag{6}$$

$$\underbrace{\frac{-\hbar^2}{2m}\left[\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}\right]}_{\| \; E_y} = E - E_x + \underbrace{\frac{\hbar^2}{2m}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right]}_{\| \; E_y} \tag{7}$$

since left is function of y only and right is function of z only (note E_x = constant)

$$\frac{-\hbar^2}{2m}\left[\frac{\partial^2 Y}{\partial y^2}\right]=E_y Y(y) \tag{8}$$

$$\frac{-\hbar^2}{2m}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right] = \underbrace{E-E_x-E_y}_{\substack{\textit{Call this constant} \\ E_z = E-E_x-E_y}} \tag{9}$$

$$\frac{-\hbar^2}{2m}\left[\frac{\partial^2 Z}{\partial z^2}\right] = E_z Z(z) \qquad (10)$$

Now eqns. 5, 8, 10 give

$$\psi(x, y, z) = X(x)Y(y)Z(z), \;\; E_x, \;\; E_y, \;\; E_z$$

$$with \; E = E_x + E_y + E_z.$$