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

Schrödinger time-independent wave equations inside box:

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

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

Substituting (2) into (1) and dividing by $\psi(x, y, z)$

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

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

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)

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

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

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

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

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

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

Now eqns. 5, 8, 10 give

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

with $E = E_x + E_y + E_z$.