## Particle in a 3-Dimensional Box

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}\Psi+\frac{\partial^2}{\partial y^2}\Psi+\frac{\partial^2}{\partial z^2}\Psi\right)+V(x,y,z)\Psi=E\Psi$$

$$\nabla^2=\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi+V(x,y,z)\Psi=E\Psi 1$$

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

$$\frac{E}{h^2/8ma^2} = \frac{12}{10}$$

$$\frac{-222}{113} = -131 = -311$$

$$\frac{1}{3} = -122 = -212 = -221$$

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For Separable Potentials,  $\Psi(x,y,z)$  is a Product of One-Dimensional Wave Functions:  $\Psi(x,y,z) = X(x)Y(y)Z(z)$  for  $0 \le x \le a$ ,  $0 \le y \le b$ , and  $0 \le z \le c$ 

$$\begin{split} \frac{\overline{\partial^2}}{\partial x^2} \Psi &= Y(y) Z(z) \, \frac{d^2 X(x)}{dx^2} \\ - \frac{h^2}{2m} \left( Y(y) Z(z) \, \frac{d^2 X(x)}{dx^2} + X(x) Z(z) \, \frac{d^2 Y(y)}{dy^2} + X(x) Y(y) \, \frac{d^2 Z(z)}{dz^2} \right) = E \, X(x) Y(y) Z(z) \\ - \frac{h^2}{2m} \left( \frac{1}{X(x)} \, \frac{d^2 X(x)}{dx^2} + \frac{1}{Y(y)} \, \frac{d^2 Y(y)}{dy^2} + \frac{1}{Z(z)} \, \frac{d^2 Z(z)}{dz^2} \right) = E = ? \\ - \frac{h^2}{2m} \, \frac{1}{X(x)} \, \frac{d^2 X(x)}{dx^2} = E_x \qquad - \frac{h^2}{2m} \, \frac{1}{Y(y)} \, \frac{d^2 Y(y)}{dy^2} = E_y \qquad - \frac{h^2}{2m} \, \frac{1}{Z(y)} \, \frac{d^2 Z(z)}{dz^2} = E_z \\ - \frac{h^2}{2m} \, \frac{d^2 X(x)}{dx^2} = E_x \, X(x) \qquad - \frac{h^2}{2m} \, \frac{d^2 Y(y)}{dy^2} = E_y \, Y(y) \qquad - \frac{h^2}{2m} \, \frac{d^2 Z(z)}{dz^2} = E_z \, Z(z) \\ X(x) &= \left( \frac{2}{a} \right)^{\frac{1}{2}} \sin \frac{n_x \pi x}{a} \qquad Y \, (y) = \left( \frac{2}{b} \right)^{\frac{1}{2}} \sin \frac{n_y \pi y}{b} \qquad Z(z) = \left( \frac{2}{c} \right)^{\frac{1}{2}} \sin \frac{n_z \pi z}{c} \\ E_x &= \frac{h^2}{8m} \, \frac{n_x^2}{a^2} \qquad E_y = \frac{h^2}{8m} \, \frac{n_y^2}{b^2} \qquad E_z = \frac{h^2}{8m} \, \frac{n_z^2}{c^2} \end{split}$$

$$\overline{\Psi(x,y,z) = \left(\frac{4}{abc}\right)^{1/2} \sin\frac{n_x\pi x}{a} \sin\frac{n_y\pi y}{b} \sin\frac{n_z\pi z}{c}}$$

$$E = E_x + E_y + E_z = \frac{h^2}{8m} \left( \frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$$

square box with side length a:

$$E = \frac{h^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2)$$



