

3D Particle in a Box

Using separation of variables $[\Psi(x, y, z) = X(x)Y(y)Z(z)]$ to solve the 3D Schrodinger Equation for a particle in a (cubic) box, we find:

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{X''}{X} &= W_1 \\ -\frac{\hbar^2}{2m} \frac{Y''}{Y} &= W_2 \\ -\frac{\hbar^2}{2m} \frac{Z''}{Z} &= W_3 \end{aligned}$$

Where each equation is equivalent to that describing a 1D particle in the box with the same boundary conditions ($[X(0), Y(0), Z(0)] = 0$ and $[X(a), Y(a), Z(a)] = 0$) Therefore, we can write:

$$\begin{aligned} X(x)_n &= \sqrt{\frac{1}{2a}} \sin\left(\frac{n_x \pi}{a} x\right) \\ Y(y)_n &= \sqrt{\frac{1}{2a}} \sin\left(\frac{n_y \pi}{a} y\right) \\ Z(z)_n &= \sqrt{\frac{1}{2a}} \sin\left(\frac{n_z \pi}{a} z\right) \end{aligned}$$

The overall wavefunction is then:

$$\Psi(x, y, z)_n = \sqrt{\frac{8}{a^3}} \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{a} y\right) \sin\left(\frac{n_z \pi}{a} z\right)$$

The energies are:

$$\begin{aligned} W_{1n} &= \frac{n_x^2 \pi^2 \hbar^2}{2ma^2} \\ W_{2n} &= \frac{n_y^2 \pi^2 \hbar^2}{2ma^2} \\ W_{3n} &= \frac{n_z^2 \pi^2 \hbar^2}{2ma^2} \end{aligned}$$

We observe what is formally known as degeneracy, where different combinations of n_x, n_y, n_z , bring about the same total energy of the system.

$$W_n = W_{1n} + W_{2n} + W_{3n}$$

$\frac{W}{W_{1n}}$	(n_x, n_y, n_z)	Degeneracy
1	(1,1,1)	1
3	(2,1,1), (1,2,1), (1,1,2)	3
9	(2,2,1), (2,1,2), (1,2,2)	3
11	(3,1,1), (1,3,1), (1,1,3)	3
12	(2,2,2)	1