The Infinite Potential Well in Three Dimensions

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In three dimensions, the Time Independent Schrödinger Equation can be written as:

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

If $V(x,y,z)$ is separable, i.e. if $V(x,y,z) = V(x) + V(y) + V(z)$, then we can write the Hamiltonian as:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + V(y) - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + V(z) = \hat{H}_x + \hat{H}_y + \hat{H}_z \tag{2}$$

Therefore, in this case, we can perform separation of variables to solve the Time Independent Schrödinger Equation.

$$\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z) \tag{3}$$

Therefore,

$$(\hat{H}_x + \hat{H}_y + \hat{H}_z)\psi_x(x)\psi_y(y)\psi_z(z) = E\psi_x(x)\psi_y(y)\psi_z(z) \tag{4}$$

Dividing by $\psi_x(x)\psi_y(y)\psi_z(z)$, we get:

$$\frac{1}{\psi_x}\hat{H}_x\psi_x + \frac{1}{\psi_y}\hat{H}_y\psi_y + \frac{1}{\psi_z}\hat{H}_z\psi_z = E \tag{5}$$

Since each term on the Left Hand Side are all dependent on one variable only, each term, must be a constant, say E_x, E_y and E_z. Therefore, we get three Equations identical to the one dimensional Time Independent Schrödinger Equation.

$$\hat{H}_x\psi_x = E_x\psi_x \tag{6}$$

$$\hat{H}_y\psi_y = E_y\psi_y \tag{7}$$

$$\hat{H}_z\psi_z = E_z\psi_z \tag{8}$$

Now, $E = E_x + E_y + E_z$ and $\psi = \psi_x\psi_y\psi_z$.
In the three dimensional Infinite Potential Well, we have $V(x,y,z) = V(x) + V(y) + V(z)$, where:

$$V(x) = \begin{cases} 0 & x \in [0, L_x] \\ \infty & x \notin [0, L_x] \end{cases} \tag{9}$$

$$V(y) = \begin{cases} 0 & x \in [0, L_y] \\ \infty & x \notin [0, L_y] \end{cases} \tag{10}$$

$$V(z) = \begin{cases} 0 & x \in [0, L_z] \\ \infty & x \notin [0, L_z] \end{cases} \tag{11}$$

Since $V(x, y, z)$ can be written as $V(x) + V(y) + V(z)$, this problem reduces into solving for the Wave Equation of three one dimensional Infinite Potential Wells. And we already know the solution to these!

$$\psi_x = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n_x \pi x}{L_x}\right) \tag{12}$$

$$\psi_y = \sqrt{\frac{2}{L_y}} \sin\left(\frac{n_y \pi y}{L_y}\right) \tag{13}$$

$$\psi_z = \sqrt{\frac{2}{L_z}} \sin\left(\frac{n_z \pi z}{L_z}\right) \tag{14}$$

And

$$E_x = \frac{n_x^2 \pi^2 \hbar^2}{2mL_x^2} \tag{15}$$

$$E_y = \frac{n_y^2 \pi^2 \hbar^2}{2mL_y^2} \tag{16}$$

$$E_z = \frac{n_z^2 \pi^2 \hbar^2}{2mL_z^2} \tag{17}$$

Where n_x, n_y and n_z are positive integers. Therefore,

$$\psi(x, y, z) = \sqrt{\frac{8}{L_x L_y L_z}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right) \sin\left(\frac{n_z \pi z}{L_z}\right) \tag{18}$$

and

$$\boxed{E = \frac{\pi^2 \hbar^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)} \tag{19}$$