Three-Dimensional Infinite-Potential Well

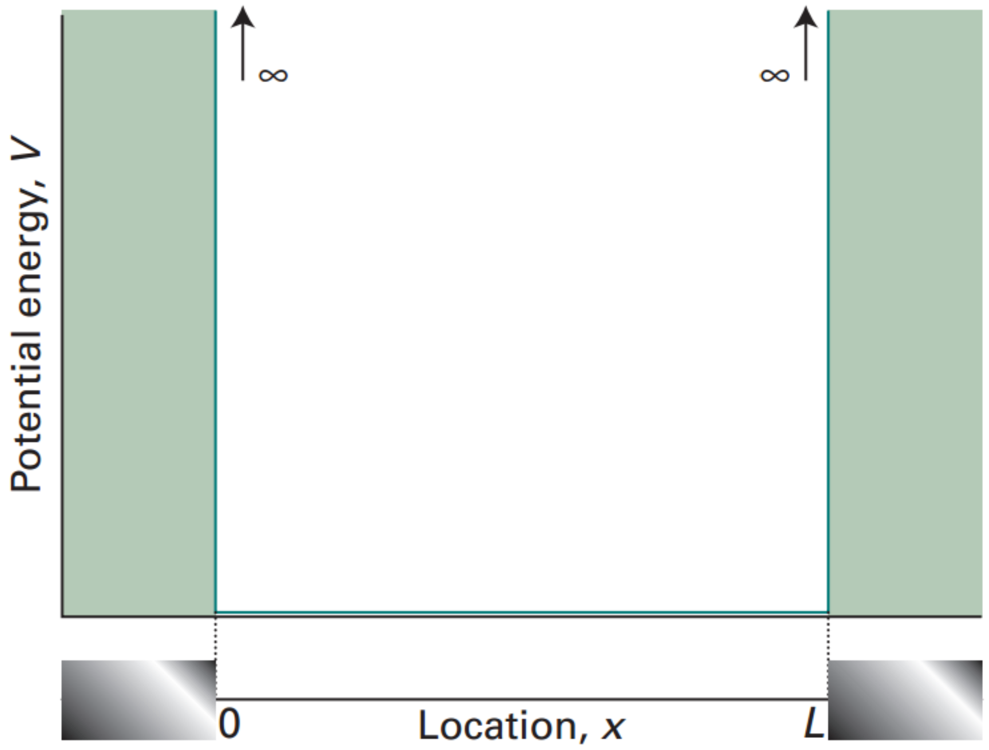
Dr Mohammad Abdur Rashid

Infinite Square-Well Potential

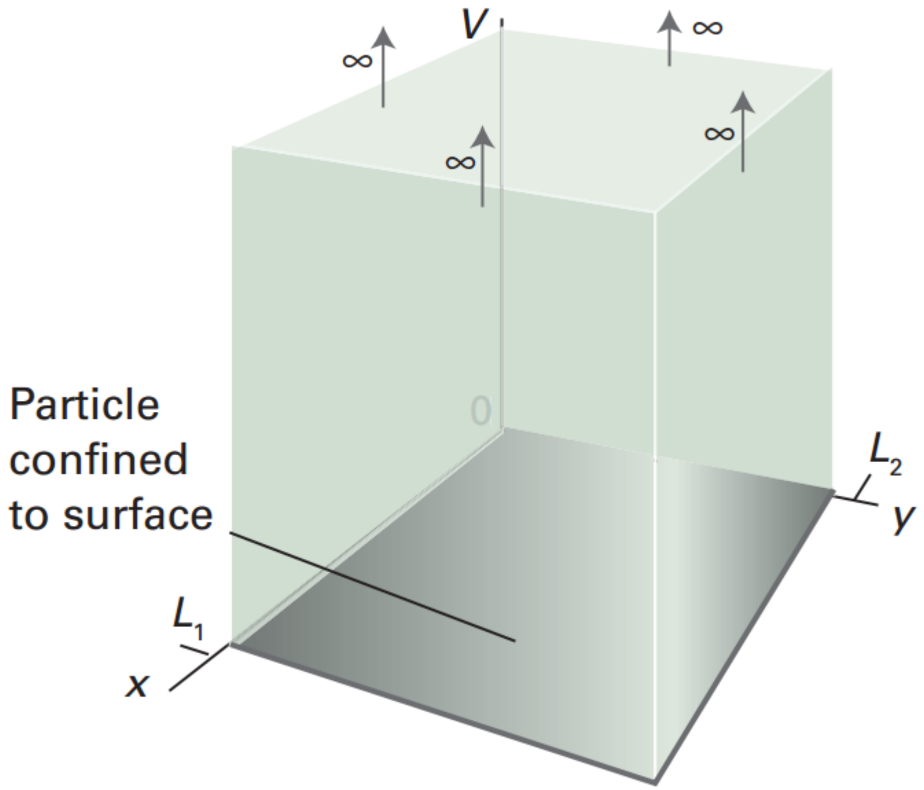
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2}$$

$$(n = 1, 2, 3, 4, \ldots)$$



Two-Dimensional Infinite-Potential Well



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

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

Separation of Variables Technique

The wave function can be written as a product of functions, one depending only on *x* and the other only on *y*:

$$\psi(x,y) = X(x)Y(y)$$

The total energy is given by

$$E = E_X + E_Y$$

Separation of Variables Technique

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2 XY}{\partial x^2} = Y\frac{d^2X}{dx^2}$$

$$\frac{\partial^2\psi}{\partial y^2} = \frac{\partial^2 XY}{\partial y^2} = X\frac{d^2Y}{dy^2}$$

Substituting these results to the Schrödinger Equation

$$-\frac{\hbar^2}{2m}\left(Y\frac{d^2X}{dx^2} + X\frac{d^2Y}{dy^2}\right) = EXY$$

Separation of Variables Technique

$$\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{Y}\frac{d^2Y}{dy^2}=-\frac{2mE}{\hbar^2}$$

The first term on the left is only dependent on *x*, similarly the second term on the left is only dependent on *y* and their sum is a constant. Therefore, we can write

$$\frac{1}{X}\frac{d^2X}{dx^2}=-\frac{2mE_X}{\hbar^2} \qquad \frac{1}{Y}\frac{d^2Y}{dy^2}=-\frac{2mE_Y}{\hbar^2}$$

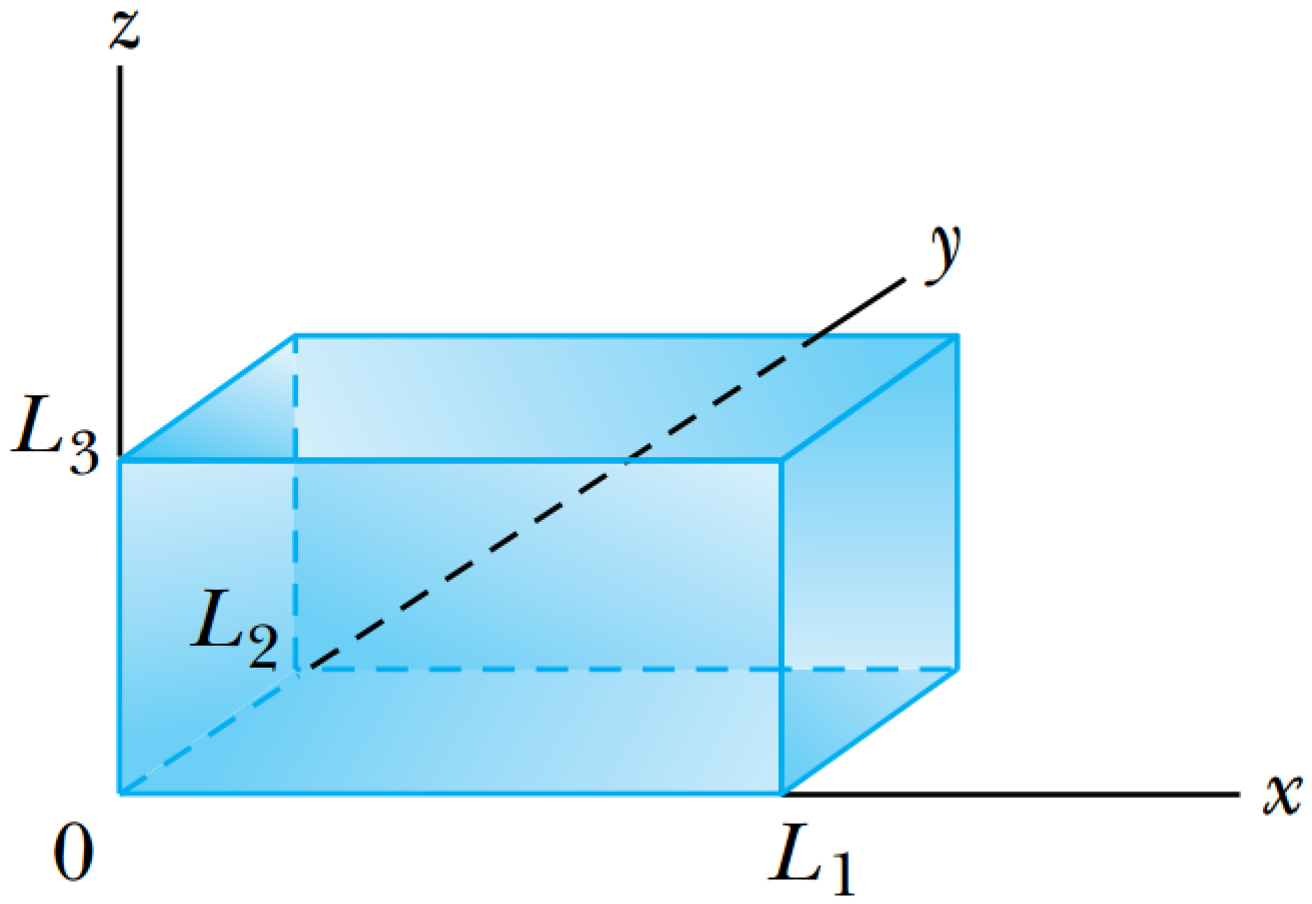
Two-Dimensional Infinite-Potential Well

Finally we have two ordinary (that is, single-variable) differential equations to solve

$$-\frac{\hbar^2}{2m}\frac{d^2X}{dx^2}=E_X X \qquad -\frac{\hbar^2}{2m}\frac{d^2Y}{dy^2}=E_Y Y$$

$$\psi(x,y)=X(x)Y(y)=A\sin(k_1x)\sin(k_2y)$$

3D Infinite-Potential Well



Inside the box

$$V = 0$$

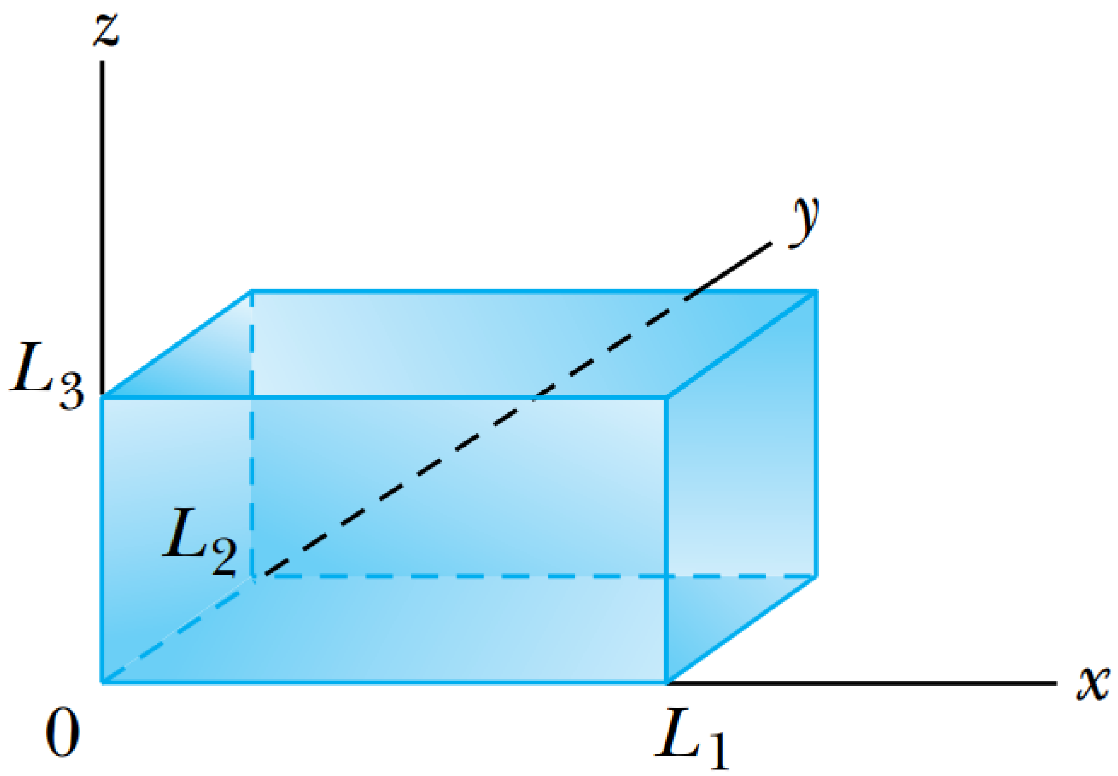
Schrödinger Equation in 3D

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

$$\nabla^2=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi+V\psi=E\psi$$

3D Infinite-Potential Well



Inside the box $V = 0$

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$

3D Infinite-Potential Well

The solution of the Schrödinger equation as in 2D

$$\psi(x, y, z) = A \sin(k_1 x)\sin(k_2 y)\sin(k_3 z)$$

$$k_1 = \frac{n_1 \pi}{L_1} \qquad k_2 = \frac{n_2 \pi}{L_2} \qquad k_3 = \frac{n_3 \pi}{L_3}$$

3D Infinite-Potential Well

In order to find the energies, we first need to take the appropriate derivatives of the wave function. We do this first for the variable *x*.

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial}{\partial x}\left[k_1 A \cos(k_1 x) \sin(k_2 y) \sin(k_3 z) \right]$$

$$= -(k_1)^2 A \sin(k_1 x) \sin(k_2 y) \sin(k_3 z)$$

$$= -k_1^2 \psi$$

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The derivatives for *y* and *z* are similar. With these derivatives we have

$$\frac{\hbar^2}{2m}(k_1^2 + k_2^2 + k_3^2)\psi = E\psi$$

$$E = \frac{\hbar^2}{2m}(k_1^2 + k_2^2 + k_3^2)$$

3D Infinite-Potential Well

$$E = \frac{\pi^2 \hbar^2}{2m}\left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2}\right)$$

The allowed energy values depend on the values of the three quantum numbers n_1, n_2, and n_3.

3D Infinite-Potential Well

The normalized wave function

$$\psi(x,y,z)=\left(\frac{8}{L_1L_2L_3}\right)^{1/2}\sin\left(\frac{n_1\pi x}{L_1}\right)\sin\left(\frac{n_2\pi y}{L_2}\right)\sin\left(\frac{n_3\pi z}{L_3}\right)$$

3D Infinite-Potential Well

For the *cubical* box, with $L_1 = L_2 = L_3 = L$.

$$E = \frac{\pi^2 \hbar^2}{2mL^2}(n_1^2 + n_2^2 + n_3^2)$$

3D Infinite-Potential Well

For the ground state $n_1 = n_2 = n_3 = 1$

$$E_{gs} = \frac{3\pi^2\hbar^2}{2mL^2}$$

$$\psi_{gs} = \sqrt{\frac{8}{L^3}}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)\sin\left(\frac{\pi z}{L}\right)$$

3D Infinite-Potential Well

What is the energy of the first excited state?

$$E = \frac{\pi^2 \hbar^2}{2mL^2}(n_1^2 + n_2^2 + n_3^2)$$

$$E_{1st} = \frac{\pi^2 \hbar^2}{2mL^2}(2^2 + 1^2 + 1^2) = \frac{3\pi^2 \hbar^2}{mL^2}$$

3D Infinite-Potential Well

n_1	n_2	n_3	E
1	1	1	E_{gs}
2	1	1	$2E_{\text{gs}}$
1	2	1	$2E_{\text{gs}}$
1	1	2	$2E_{\text{gs}}$
2	2	1	$3E_{\text{gs}}$
2	2	2	$4E_{\text{gs}}$

$$E = \frac{\pi^2\hbar^2}{2mL^2}(n_1^2 + n_2^2 + n_3^2)$$

$$E_{\text{gs}} = \frac{3\pi^2\hbar^2}{2mL^2}$$

Degenerate State

In physics we say that a given state is degenerate when there is more than one wave function for a given energy.

In our case all three possible wave functions for the first excited state have the same energy. The degeneracy in this case is a result of the symmetry of the cube.

If the box had sides of three different lengths, we say the degeneracy is removed, because the three quantum numbers in different orders (211, 121, 112) would result in three different energies.

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