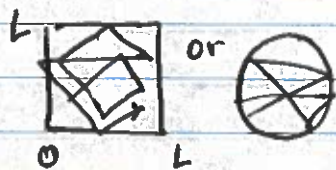


Infinite square well in the worlds of different dimensions

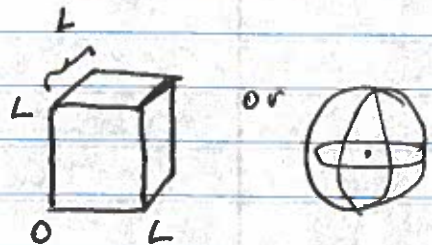
1D



2D



3D



In each case a particle moves freely inside the allowed region

$$\hat{H} = \frac{\hat{p}^2}{2m}; \text{ in Cartesian } \hat{H} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$$

in spherical coordinates $\hat{H} = -\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{\hat{L}^2}{2\mu r^2}$

Boundary conditions $x_i = 0 \ \& \ x_i = L \quad \psi(\vec{x}) = 0$

The geometry of a boundary determines the symmetry of the solution

Rectangular boundaries \rightarrow Cartesian coordinates
 Spherically sym boundaries \rightarrow spherical coordinates

Cartesian coordinates \rightarrow Schrodinger equation

$$1D: -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0$$

$$\psi(x) = A \cos kx + B \sin kx \quad k = \sqrt{\frac{2mE}{\hbar^2}} = p/\hbar$$

Boundary conditions $\psi(0) = \psi(L) = 0$

$$\psi_n(x) = B \sin \frac{\pi n x}{L} \Rightarrow \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L} \quad k_n = \frac{\pi n}{L}$$

$$2D: -\frac{\hbar^2}{2m} \left(\frac{d^2\psi(x,y)}{dx^2} + \frac{d^2\psi(x,y)}{dy^2} \right) = E\psi$$

Separation of variables (since x- and y- motions are independent)

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

$$-\frac{\hbar^2}{2m} \left(\frac{d^2X}{dx^2} \cdot Y + X \frac{d^2Y}{dy^2} \right) = E X \cdot Y \quad \cdot \frac{1}{X \cdot Y}$$

$$\frac{1}{X} \frac{d^2X}{dx^2} + \frac{1}{Y} \frac{d^2Y}{dy^2} + \frac{2mE}{\hbar^2} = 0$$

depends only on x depends only on y constant

$-C_1$ must be C_2

$$-\frac{2mE_x}{\hbar^2} = -\frac{p_x^2}{2m} \quad \text{constant} \quad -\frac{2mE_y}{\hbar^2} = -\frac{p_y^2}{2m}$$

$$\frac{1}{X} \frac{d^2X}{dx^2} + \frac{2mE_x}{\hbar^2} = 0$$

$$\frac{1}{Y} \frac{d^2Y}{dy^2} + \frac{2mE_y}{\hbar^2} = 0$$

$$X'' + k_x^2 X = 0$$

$$Y'' + k_y^2 Y = 0$$

Two independent

1D motions

$$X_n(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}$$

$$Y_s(y) = \sqrt{\frac{2}{L}} \sin \frac{\pi s y}{L}$$

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

$$E_{ys} = \frac{\pi^2 \hbar^2 s^2}{2mL^2}$$

$n, s = 1, 2, \dots$

Total (kinetic) energy $E_{n,s} = E_{x,n} + E_{y,s}$

$$E_{n,s} = \frac{\pi^2 \hbar^2}{2mL^2} (n^2 + s^2)$$

If the well is rectangular $L_x \times L_y$

$$E_{n,s} = \frac{\pi^2 \hbar^2}{2mL^2} \left(\frac{n^2}{L_x^2} + \frac{s^2}{L_y^2} \right)$$

Energy spectrum for 3D case (cube)

$$E_{n,s,t} = \frac{\pi^2 \hbar^2}{2mL^2} (n^2 + s^2 + t^2)$$

| | 1D | 2D | 3D |
|-------------------------------|--|------------------------------------|---|
| Ground state energy | $n=1$ $\frac{\pi^2 \hbar^2}{2mL^2} = E_1$ | $n=s=1$ $2E_1$ | $n=s=t=1$ $3E_1$ |
| 1 st excited state | $n=2$ $4E_1$ | $n=1, s=2$ $n=2, s=1$ $5E_1$ | $n=3, s=1, t=2$ and $n=2, s=2, t=1$ $6E_1$ |
| 2 nd excited state | $n=3$ $9E_1$ | $n=s=2$ $8E_1$ | $n=1, s=t=2$ and $n=2, s=2, t=2$ $9E_1$ |

Note: Red arrows in the original image indicate energy differences of $+3E_1$ between adjacent levels in each column.

While the energy levels are different in these three cases even for the ground state, we are only able to measure the difference between energy levels via induced transitions

$$\hbar \omega_{ij} = E_i - E_j$$

and there is more similarities b/w the three ~~spectra~~ absorption spectra, especially for low-energy states