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Topic:

Nanoscale System (1): Applications of Schrodinger equation- Infinite potential well, potential box.

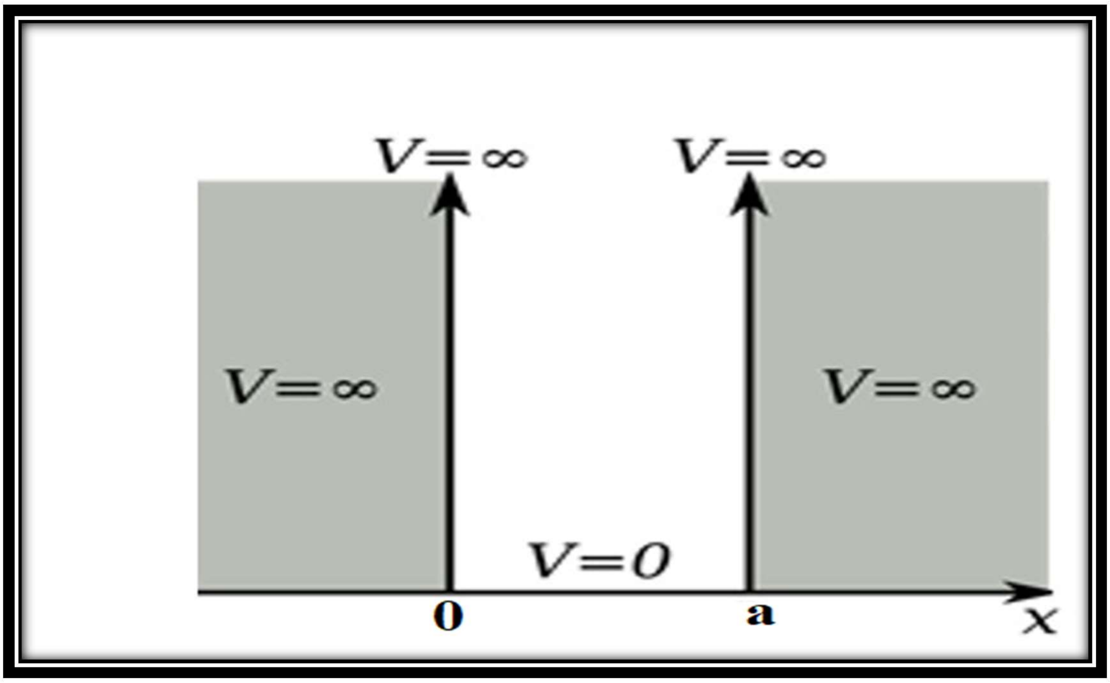
Nanoscale Physics (1):

One Dimensional Infinitely Rigid Box:

Let us take a particle of mass m and energy E moving in a region from $\boldsymbol{x = 0 \; to \; x = a}$ in a 1D infinitely rigid potential box. The potential inside the box is $V(\boldsymbol{x}) = \mathbf{0}$

i.e. $V(\boldsymbol{x}) = \mathbf{0}, \mathbf{0} \le \boldsymbol{x} \le \boldsymbol{a}$

and $V(\boldsymbol{x}) = \infty, \boldsymbol{x} < \mathbf{0} \; \boldsymbol{and} \; \boldsymbol{x} > \boldsymbol{a}$



The probability is given by $|\Psi|^2$, the wave function $\Psi\,(x)$ $\boldsymbol{at \; x = 0 \; and \; x = a}$ must vanish.

$\psi(x)|_{x=0} = \psi(x)|_{x=a} = 0$

The time independent Schrödinger's equation in the region $\boldsymbol{x < 0 \; and \; x > a}$ is given by,

$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E-\infty)\psi = -\infty\psi$

Therefore, $\psi(x) = \frac{1}{\infty}\frac{d^2\psi}{dx^2} = 0\,, for, \boldsymbol{x < 0\ and\ x > a}$

Inside the box the Schrödinger's equation becomes-

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

Or, $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$

Or, $\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0$…………………..(1)

Where, $\alpha = \sqrt{(\frac{2m}{\hbar^2}E)}$

The solution of equation (1) becomes- $\psi(x) = A\ Sin\alpha x + B\ Cos\alpha x$

Where A, B are constants of integration.

Putting the boundary conditions, $\Psi\ (\boldsymbol{x}) = \boldsymbol{0\ at\ x} = 0\ \boldsymbol{and}\ \Psi\ (\boldsymbol{x}) = \boldsymbol{0\ x = a}$ (1)

Applying conditions (1) we get, $0 = A\ Sin0 + B\ Cos0$

Or, $0 = B$

Therefore, $\Psi\ (\boldsymbol{x}) = A\ Sin\alpha x$

Applying boundary condition (2),

We get, $\mathbf{0} = A\ Sin\ \alpha a$

Therefore, $= \boldsymbol{n\pi}$, where, n= 1,2,3,… (Since, A ≠ 0)

Therefore, $\alpha = \frac{\boldsymbol{n\pi}}{a}$

Hence, $\Psi_n(\boldsymbol{x}) = A\ Sin\frac{\boldsymbol{n\pi x}}{a}$

Energy Eigen Value:

Here, $\sqrt{(\frac{2m}{\hbar^2}E)} = \frac{\boldsymbol{n\pi}}{a}$

Therefore, $E = \frac{n^2\boldsymbol{\pi}^2\hbar^2}{2ma^2} = E_n$ (where n is called the quantum number)

$$E_1 = \frac{\boldsymbol{\pi}^2 \hbar^2}{2ma^2}$$

$$E_n = \boldsymbol{n}^2 E_1$$

Where, E_1 is the energy at lowest energy state i.e. ground state.

Normalization of wave function:

$\psi_n\,(x) = A\,Sin\frac{n\pi x}{a}$ for , $\boldsymbol{x < 0\ < a}$

And $\psi_n\,(x) = 0$ for , $\boldsymbol{x < 0\ and\ x > a}$

$\int_0^a \psi_n\,(x)\,\psi_n^*(x)\,dx = 1$

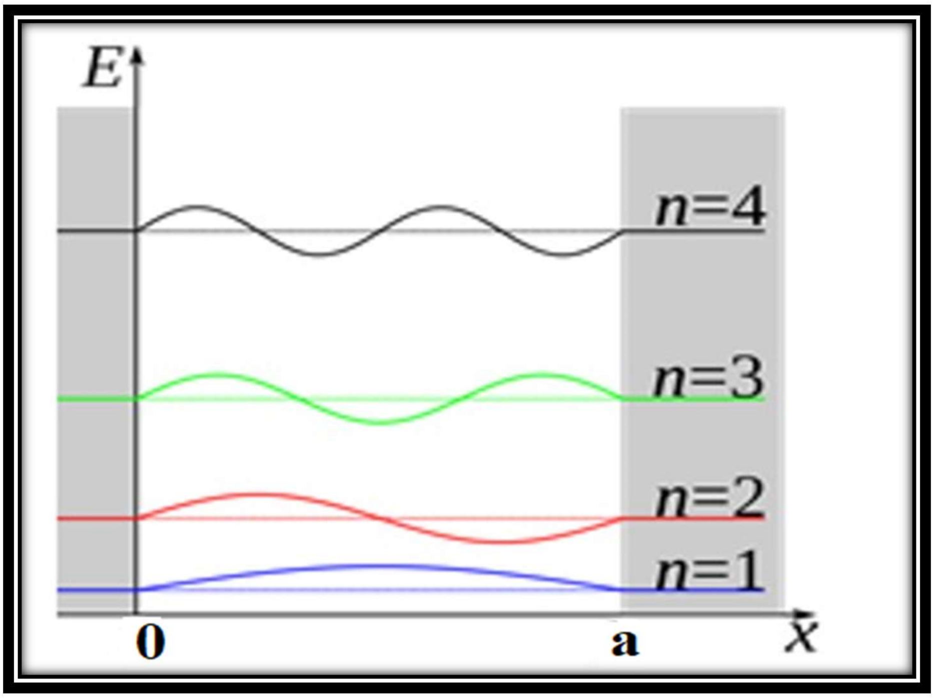
Or, $\int_0^a |\psi_n\,(x)|^2\,dx = 1$

Or, $A^2 \int_0^a Sin^2\,\frac{n\pi x}{a}\,dx = 1$

Or, $A^2 \int_0^a \frac{1}{2}[1 - Cos\frac{2n\pi x}{a}]\,dx = 1$

Or, $A^2\frac{a}{2} = 1$ or, $A = \sqrt{2}/A$

Therefore, $\psi_n\,(x) = \sqrt{\frac{2}{A}}\,Sin\frac{n\pi x}{a}$



Energy Eigen Function:

(i) For, $n = 1$ at $x = 0$ and $x = a, \psi_1(x) = 0$. Therefore, $\psi_1(x)$ has two nodes at $x = 0$ and $x = a$

(ii) For, $n = 2, , \psi_2(x) = 0$ at $x = 0, \frac{a}{2}, a$

(iii) For, $n = 3, , \psi_3(x) = 0$ at $x = 0, \frac{a}{3}, \frac{2a}{3}, a$

Hence, $, \psi_3(x)$ has four node at $x = 0, \frac{a}{3}, \frac{2a}{3}, a$

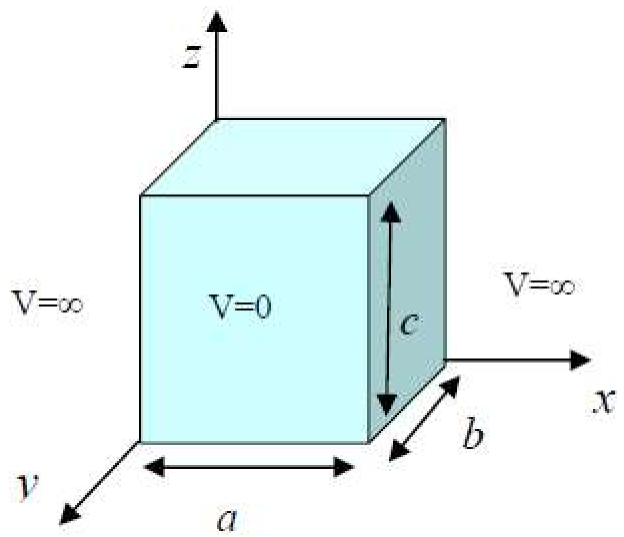
In this way $, \psi_n(x)\ has\ (n+1)\ nodes.$

For 3D case

If we consider a 3d rectangular "infinite square well" with the dimensions (a, b, c) and the potential boundary conditions:

$$V(x, y, z) = \{0, 0 < x < a, 0 < y < b, 0 < z < c$$

$$\{V(x, y, z) = \infty, otherwise$$



The Schrödinger equation becomes-

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

Taking separation of variable-

$$\frac{d^2X(x)}{dx^2} + k_x^2 X(x) = 0, \quad k_x^2 = \frac{2mE_x}{\hbar^2},$$

$$\frac{d^2Y(y)}{dy^2} + k_y^2 Y(y) = 0, \quad k_y^2 = \frac{2mE_y}{\hbar^2},$$

$$\frac{d^2Z(z)}{dz^2} + k_z^2 Z(z) = 0, \quad k_z^2 = \frac{2mE_z}{\hbar^2}.$$

Therefore the solution becomes-

$$\psi_n(x) = \sqrt{\frac{2}{a}}\, Sin\frac{n_x\boldsymbol{\pi x}}{a}$$

$$\psi_n(y) = \sqrt{\frac{2}{b}}\, Sin\frac{n_y\boldsymbol{\pi y}}{b}$$

$$\psi_n(z) = \sqrt{\frac{2}{c}}\, Sin\frac{n_z\boldsymbol{\pi z}}{c}$$

Therefore,

$$\psi_n(x)\psi_n(y)\psi_n(z) = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{b}}\sqrt{\frac{2}{c}}\, Sin\frac{n_x\boldsymbol{\pi x}}{a}\, Sin\frac{n_y\boldsymbol{\pi y}}{b}\, Sin\frac{n_z\boldsymbol{\pi z}}{c}$$

$$= \sqrt{\frac{8}{abc}}\, Sin\frac{n_x\boldsymbol{\pi x}}{a}\, Sin\frac{n_y\boldsymbol{\pi y}}{b}\, Sin\frac{n_z\boldsymbol{\pi z}}{c}$$

$$= \sqrt{\frac{8}{V}}\, Sin\frac{n_x\boldsymbol{\pi x}}{a}\, Sin\frac{n_y\boldsymbol{\pi y}}{b}\, Sin\frac{n_z\boldsymbol{\pi z}}{c}$$

$$\psi_n(x,y,z) = \sqrt{\frac{8}{V}}\, Sin\frac{n_x\boldsymbol{\pi x}}{a}\, Sin\frac{n_y\boldsymbol{\pi y}}{b}\, Sin\frac{n_z\boldsymbol{\pi z}}{c}$$

$$E = E_x + E_y + E_z$$

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

$$If\ a = b = c\ (for\ cubic)$$

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

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Frequently Asked Questions/Numerical:

For theoretical questions and problems in this section of 1D Potential Well, students can solve the problems of Concept of Atomic Physics, Author- S. P. Kuila, Published by NCBA (2018 Ed.) and Quantum Mechanics by Jyotirmoy Guha, Published by Books & Allied Pvt. Ltd. (2018 Ed.).

References:

(i) *Concept of Atomic Physics, Author- S. P. Kuila, Published by NCBA (2018 Ed.).*

(ii) *Refresher Course in Physics, Author- C. L. Arora, Published by S. Chand (2018 Ed.).*

(iii) *Quantum Mechanics- Author- Jyotirmoy Guha, Published by Books & Allied Pvt. Ltd. (2018 Ed.).*

(iv) *https://dradchem.files.wordpress.com/2015/09/particle-in-box.png*

Link to Audio visual Lectures (e-Lectures) on this topic given by Distinguish Professors of Indian & Foreign Universities:

(1) *https://www.youtube.com/watch?v=xaH0aQmNy-E*

(2) *https://av.tib.eu/media/18883*