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Topic:

Elements of Modern Physics (1): One Dimensional Infinitely Rigid Box, Energy Eigenvalues and Eigen Functions, Normalization; Quantum Dot as example.

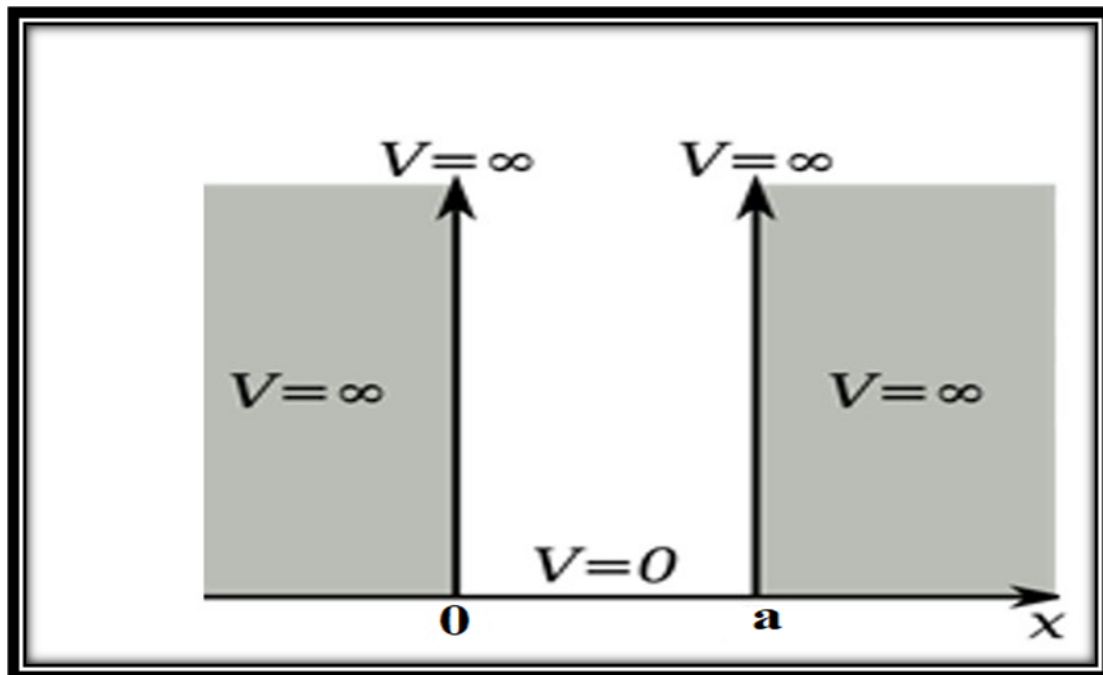
Elements of Modern Physics (1):

One Dimensional Infinitely Rigid Box:

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

i.e. $V(x) = 0, 0 \leq x \leq a$

and $V(x) = \infty, x < 0$ and $x > a$



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

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

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



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

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

Inside the box the Schrödinger's equation becomes-

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

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

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

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

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, $\Psi(x) = 0$ at $x = 0$ and $\Psi(x) = 0$ at $x = a$ (1)

Applying conditions (1) we get, $0 = A\sin 0 + B\cos 0$

$$\text{Or, } 0 = B$$

Therefore, $\Psi(x) = A\sin\alpha x$

Applying boundary condition (2),

We get, $0 = A\sin\alpha a$

Therefore, $\alpha a = n\pi$, where, $n = 1, 2, 3, \dots$ (Since, $A \neq 0$)

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

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

Energy Eigen Value:

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

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



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

$$E_n = n^2 E_1$$

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

Normalization of wave function:

$$\psi_n(x) = A \sin \frac{n\pi x}{a} \text{ for } 0 < x < a$$

And $\psi_n(x) = 0$ for $x < 0$ and $x > a$

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

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

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

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

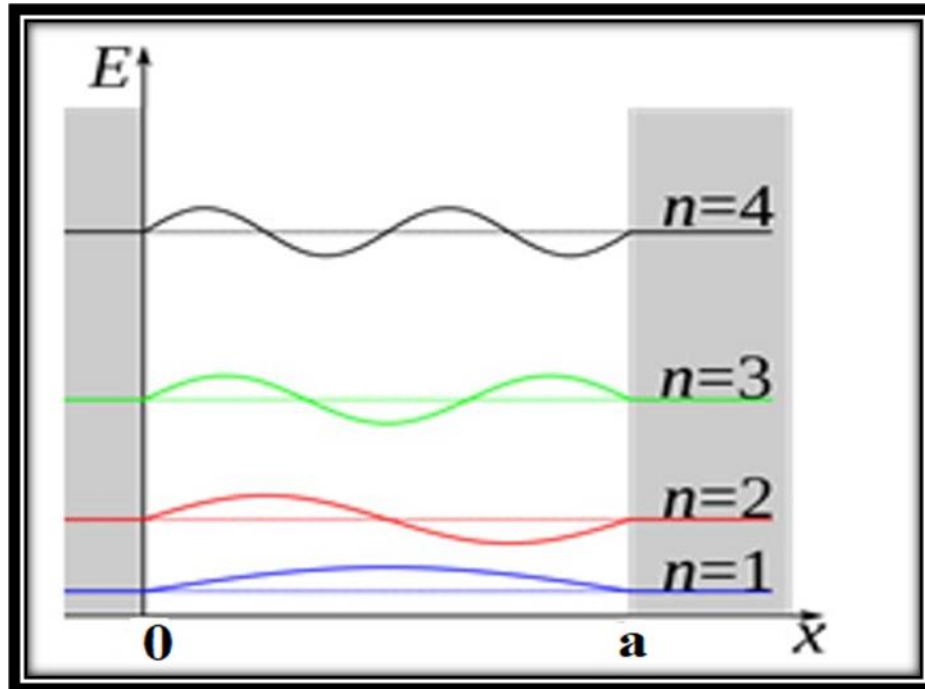
$$\text{Or, } A^2 \frac{a}{2} = 1 \text{ or, } A = \sqrt{2}/A$$

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



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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 nodes at $x = 0, \frac{a}{3}, \frac{2a}{3}, a$

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

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>



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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>