



ENGINEERING PHYSICS

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ENGINEERING PHYSICS

Unit II : Quantum Mechanics of simple systems



Class #17

- Bound particle system
- 1D infinite potential well
- Solution of the Schrodinger's wave equation
- Characteristics of the wave function

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Unit II : Quantum Mechanics of simple systems



➤ *Suggested Reading*

1. *Concepts of Modern Physics, Arthur Beiser, Chapter 5*
2. *Learning Material prepared by the Department of Physics*

➤ *Reference Videos*

1. *Video lectures : MIT 8.04 Quantum Physics I*
2. *Engineering Physics Class #12-14*

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Particle in an 1D infinite potential well

A particle restricted to move in a small region of space with zero potential – a bound particle system

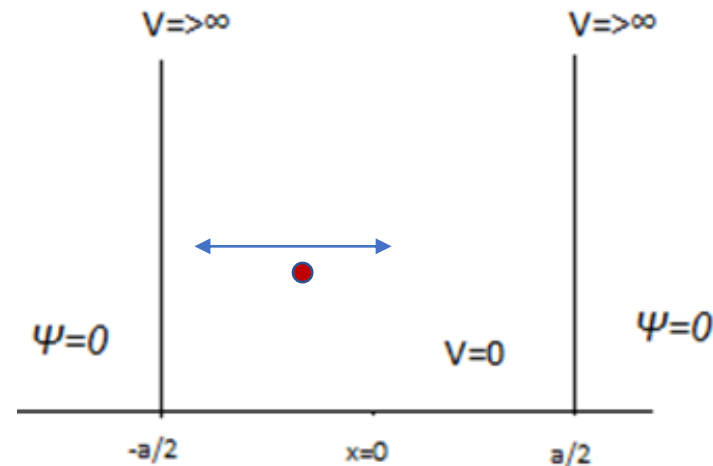
The binding comes from an infinite potential (wall) existing at the boundaries at $x = \pm \frac{a}{2}$

The particle of mass m and energy E is in a state of motion between $-\frac{a}{2}$ and $+\frac{a}{2}$

$$V = 0 \text{ for } -\frac{a}{2} < x < +\frac{a}{2}$$

$$V = \infty \text{ at } x = \pm \frac{a}{2}$$

Particle has zero probability of being outside the bound region



1D infinite potential Schrodinger's wave equation

- *The Schrodinger's wave equation*

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi(x) = 0$$

- *Reduces to the free particle wave equation for the region between $-\frac{a}{2}$ and $+\frac{a}{2}$ with $V = 0$*

- *The general solution could be written as*

$$\psi(x) = A \sin(kx) + B \cos(kx)$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$ which gives the energy of the particle

$$E = \frac{\hbar^2 k^2}{2m}$$

$$e^{i\theta} = \cos\theta + i\sin\theta$$

1D infinite potential Schrodinger's wave equation

the boundary conditions for the problem

$$\psi = 0 \text{ and } d\psi = 0 \text{ at } x = -\frac{a}{2} \text{ and } x = \frac{a}{2}$$

Additionally the wave function has to be normalizable

At $x = -\frac{a}{2}$

$$\psi\left(x = -\frac{a}{2}\right) = A\sin\left(-k\frac{a}{2}\right) + B\cos\left(k\frac{a}{2}\right) = 0$$

results in $-A\sin\left(k\frac{a}{2}\right) + B\cos\left(k\frac{a}{2}\right) = 0$ [1]

At $x = \frac{a}{2}$

$$\psi\left(x = \frac{a}{2}\right) = A\sin\left(k\frac{a}{2}\right) + B\cos\left(k\frac{a}{2}\right) = 0$$

results in $A\sin\left(k\frac{a}{2}\right) + B\cos\left(k\frac{a}{2}\right) = 0$ [2]

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1D infinite potential Schrodinger's wave equation



[1] and [2] indicate the two distinct possibilities

either $A = 0$ if $B \neq 0$ or $B = 0$ if $A \neq 0$

if $A = 0$ then $B \neq 0$

[1] leads to $\cos\left(k\frac{a}{2}\right) = 0$ $k\frac{a}{2} = n\frac{\pi}{2}$

where n is an odd number $n=1,3,5,7,\dots$

$$k = n_{\text{odd}} \frac{\pi}{a}$$

if $A \neq 0$ then $B = 0$

[2] leads to $\sin\left(k\frac{a}{2}\right) = 0$ $k\frac{a}{2} = n\pi$

where n is an integer

$$k = n_{\text{even}} \frac{\pi}{a}$$

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1D infinite potential Schrodinger's wave equation

The general solution ...

$$\psi_n(x) = B \cos(kx) = B \cos\left(n \frac{\pi}{a} x\right) \quad \text{for } n \text{ odd}$$

and

$$\psi_n(x) = A \sin(kx) = A \sin\left(n \frac{\pi}{a} x\right) \quad \text{for } n \text{ even}$$

n = 1, 2, 3, 4, 5... correspond to the allowed wave functions of the particle

n describes the state of the system

1D infinite potential Schrodinger's wave equation

The constant A and B can be evaluated by normalizing the wave function i.e.,

integrating the wave function between limits of $-\frac{a}{2}$ and $\frac{a}{2}$

$$\int \psi^* \psi dx = 1$$

$$\int_{-a/2}^{a/2} \left[A \sin\left(\frac{n\pi}{a} x\right) \right]^2 dx = \frac{A^2}{2} \int_{-a/2}^{a/2} \left[1 - \cos\left(\frac{2n\pi}{a} x\right) \right] dx$$

$$\frac{A^2}{2} \left[x - \frac{L}{2n\pi} \sin\left(\frac{2n\pi}{a} x\right) \right]_{-a/2}^{a/2} = \frac{A^2}{2} [a - 0] = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

In a very similar way the second wave function can be

normalized to get $B = \sqrt{\frac{2}{a}}$

1D infinite potential Schrodinger's wave equation

The eigen wave function becomes

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi}{a}x\right) \quad \text{for } n \text{ odd} \quad (\text{even parity})$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad \text{for } n \text{ even} \quad (\text{odd parity})$$

The propagation constant $k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{a}$ is quantized and hence the momentum and energy of the particle are also quantized.

The energy of the allowed states

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2ma^2} = \frac{h^2 n^2}{8ma^2}$$

$$p_n = \hbar k = \hbar \frac{n\pi}{a}$$
$$\lambda_n = \frac{h}{p}$$

These are the eigen energy values of the bound particle.

The concepts which are true of a particle in a box...

1. Particle in a box is an example of a bound particle system
2. The eigen function of the particle in the second state is an even parity function
3. The propagation constant is determined by the width of the box.
4. The energy of the particle in the ground state is non zero
5. Particle can have any momentum inside the box
6. The de Broglie wavelength depends on the size of the box



THANK YOU

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