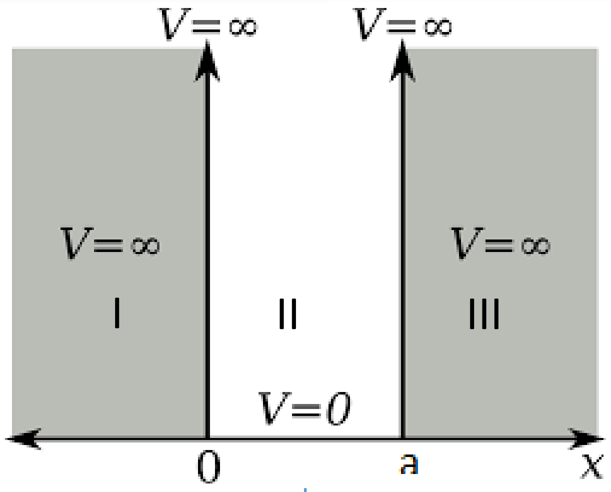
# Quantum Mechanics - Lecture 7

Brajesh Kumar Mani

## Infinite square well/Particle in a box

"bound states"

The particle is in the potential well, such that $V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$




Find:

(a) Wave function of the particle, $\psi(x)$

(b) Energy of the particle, $E$

(c) Time evolved wave function, $\Psi(x, t)$

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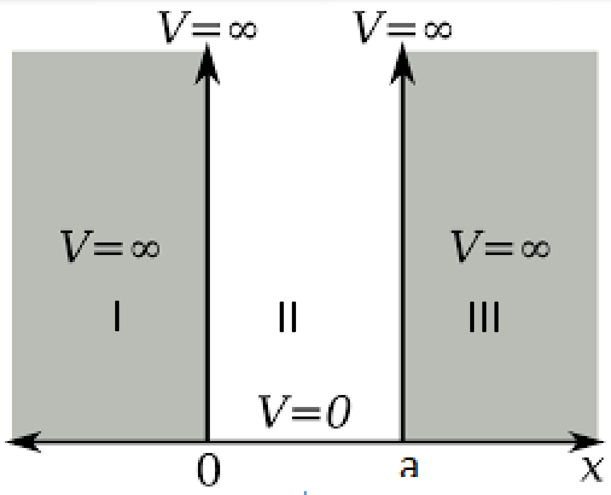


In region I and III wave function is zero because infinite potential

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- The time independent Schrodinger equation in region II is

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

$$\Rightarrow \frac{d^2\psi}{dx^2} = -k^2\psi \text{ , where } k = \frac{\sqrt{2mE}}{\hbar} \qquad \text{Eq.(1)}$$

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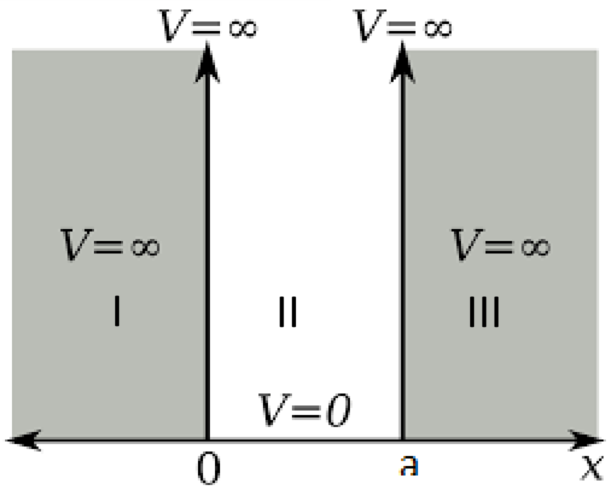


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- Let us assume the solution of this equation in the form

$\psi(x) = A\sin kx + B\cos kx$, where A and B are the constants

- At boundary, the wave function must vanish. That is, it should satisfies

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  Using BC(2) we get: $\psi(a) = A\sin ka = 0 \;\Rightarrow\; ka = \pm m\pi \;\Rightarrow k = \pm\frac{m\pi}{a}$, where m = 0, 1, 2, 3 …..

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- By dropping $k = 0$ (as it gives $\psi(x) = 0$ ) and all negative values (they give the same solutions as positive k values), the distinct solutions corresponds to

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$$k = +\frac{n\pi}{a}, \text{ where n = 1, 2, 3 .....}$$

- Then we can write the wave function and energy of the particle as

$$\psi_n(x) = A\sin kx = A\sin\left(\frac{n\pi x}{a}\right) \quad \text{and } \mathrm{E_n} = \frac{\mathrm{k}^2\hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

- We can calculate the normalization constant A as

$$\int_0^a \psi^*(x)\psi(x)dx = 1 \Rightarrow \int_0^a |A|^2 \sin^2 kx\, dx = 1 \Rightarrow |A|^2 \times \frac{a}{2} = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$$

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$$\psi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)\ ;\ E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

$$\psi_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)\ ;\ E_2 = \frac{4\pi^2\hbar^2}{2ma^2}$$

$$\psi_3(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi x}{a}\right)\ ;\ E_3 = \frac{9\pi^2\hbar^2}{2ma^2}$$ , and so on.

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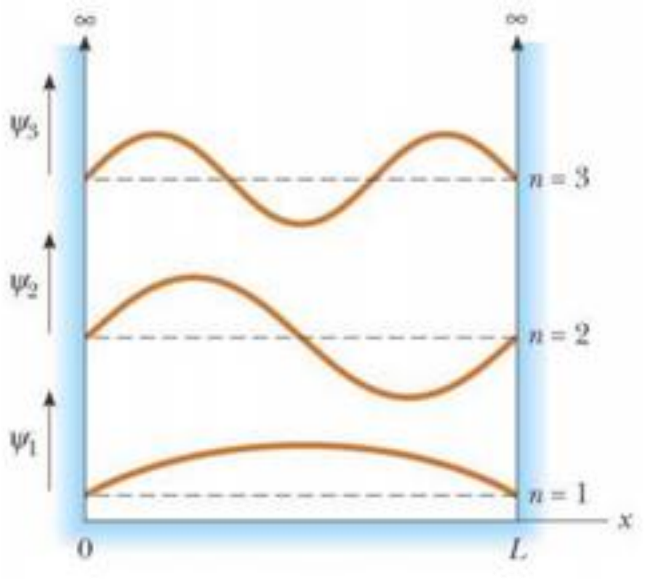
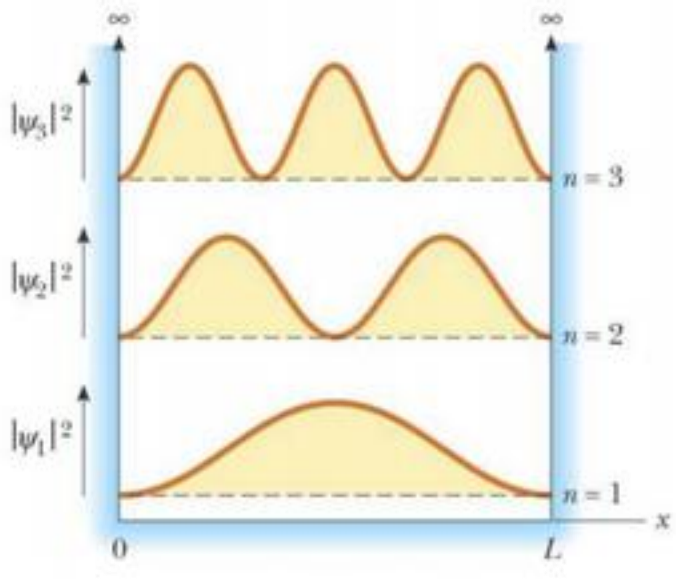
$$\text{"} \rightarrow \psi_1, \psi_2, \psi_3 \dots \text{. represent the ground state, first excited, second excited state, } \dots \dots \text{."}$$

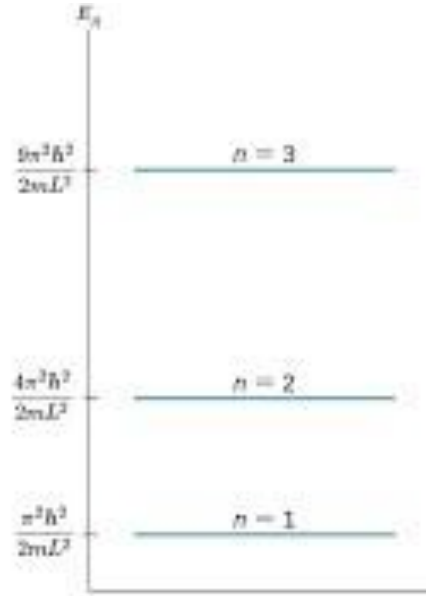
- Let us sketch the wave functions and corresponding energy




(wavefunction)




(probability)




(energy level)

→ Wave functions are continuous

→ Confined quantum mechanical systems have discrete energies

→ Represents an example of “bound” quantum system.

- We can write the initial wave function as a linear combination

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n\, \psi_n(x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

Where, $c_n = <\psi_n(x)|\Psi(x,0)> = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi x}{a}\right)\, \Psi(x,0)\, dx$

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- The stationary states are then written as

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-i\left(\frac{n^2\pi^2\hbar}{2ma^2}\right)t}$$

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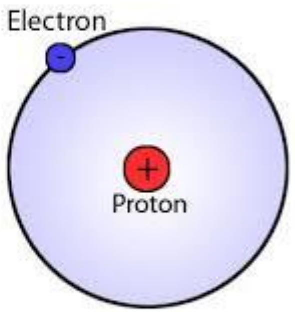
- The most general solution of the time-dependent Schrodinger equation is then

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) e^{-i\left(\frac{n^2\pi^2\hbar}{2ma^2}\right)t}$$

## Other examples of bound system: Hydrogen atom




Hydrogen atom

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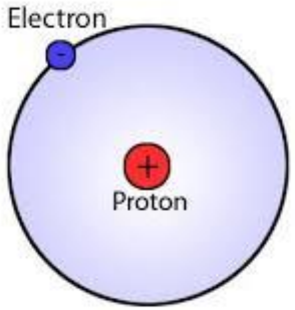
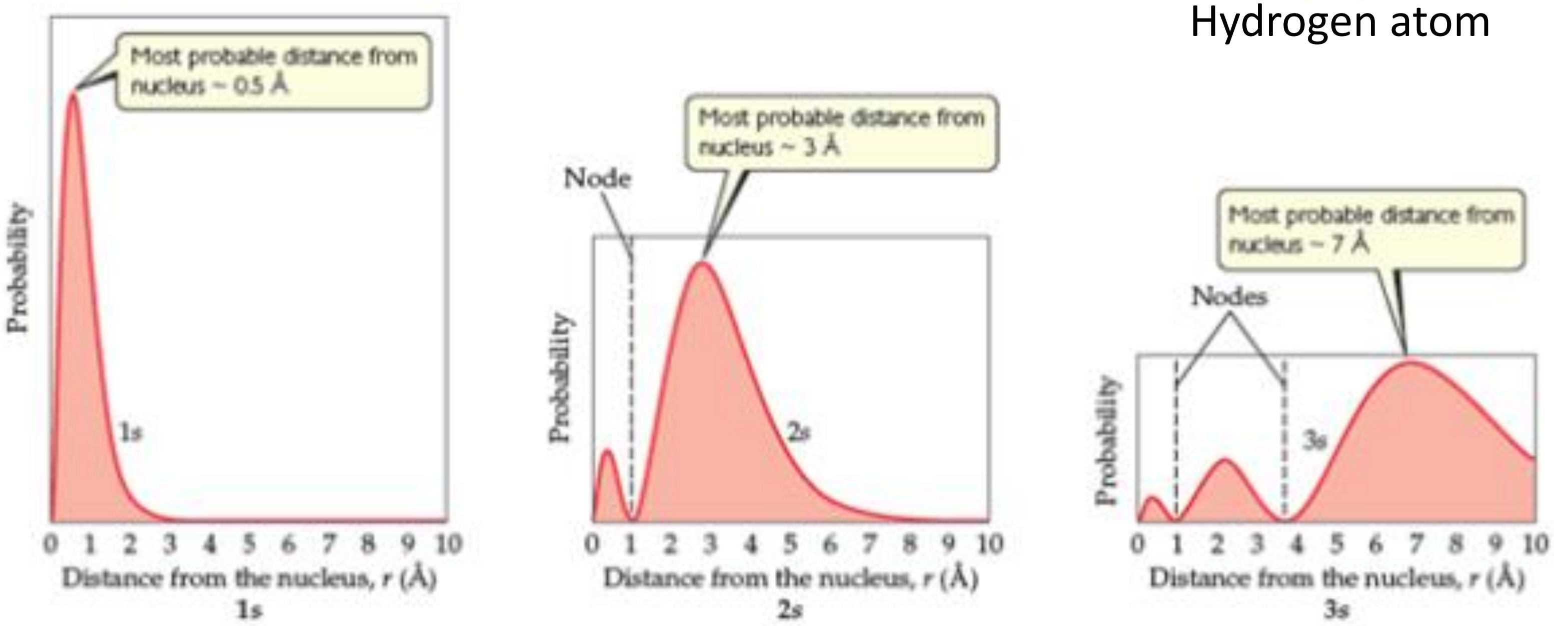
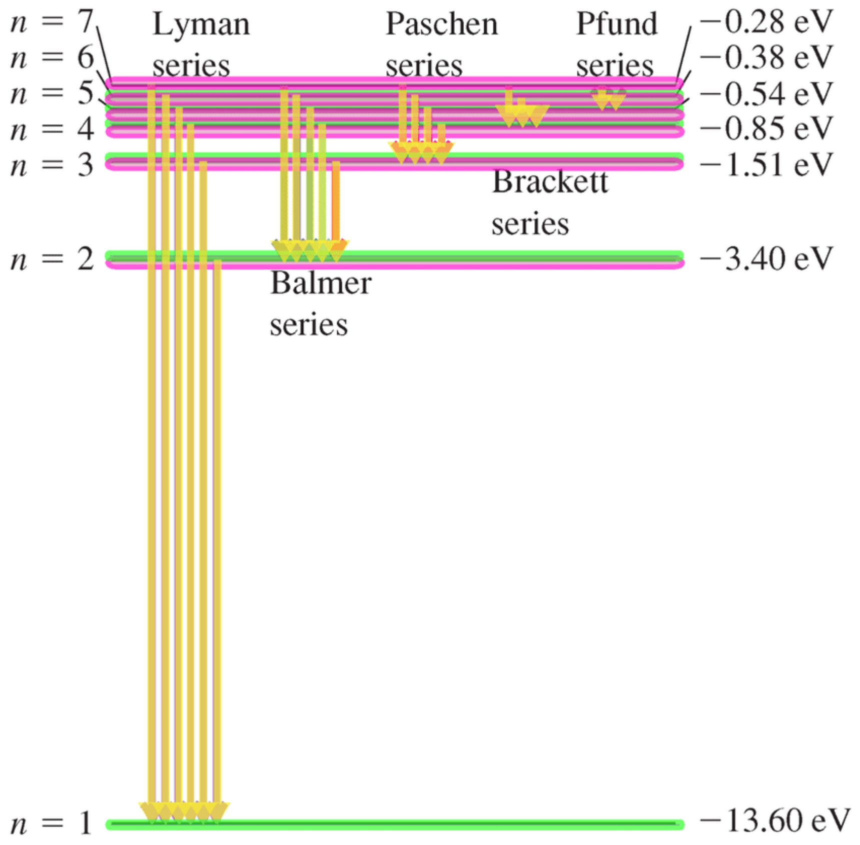



Hydrogen atom

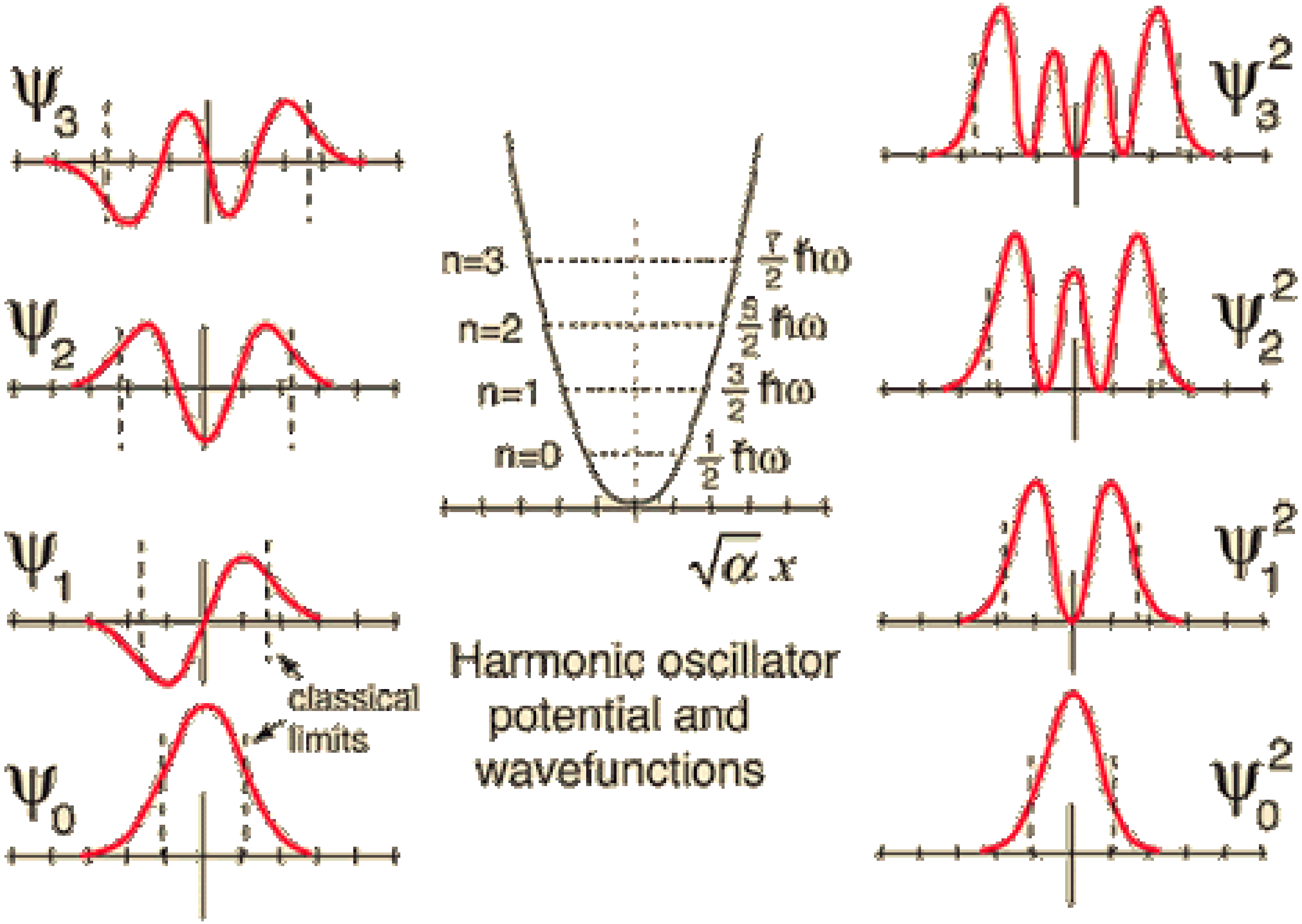



(Probability as function of distance from nucleus)




(Energy level diagram)

## Other examples of bound system: Harmonic oscillator



**Example Problem 4:** A particle of mass *m* moves freely inside an infinite potential well of length *a*. Initially (at *t=0*), the particle is in the state

$$\Psi(x,0) = \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \sqrt{\frac{1}{5a}}\sin\left(\frac{5\pi x}{a}\right)$$

Find $\Psi(x,t)$ at any later time *t*.

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**Solution:** For a particle in an infinite box of length *a*

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \text{ where: } \mathrm{n} = 1, 2, 3, 4, \dots.$$

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Using this wave function we can write

$$\Psi(x,0) = \sqrt{\frac{3}{5a}}\sin\left(\frac{3\pi x}{a}\right) + \sqrt{\frac{1}{5a}}\sin\left(\frac{5\pi x}{a}\right) = \sqrt{\frac{3}{10}}\,\psi_3(x) + \sqrt{\frac{1}{10}}\,\psi_5(x)$$

We can write the time-dependent wavefunction as $\Psi(x,t) = \sum \quad \Psi_n(x,0)\, e^{-\frac{iE_n t}{\hbar}}$

$$\Psi(x,t) = \sqrt{\frac{3}{10}}\,\psi_3(x)e^{-\frac{iE_3 t}{\hbar}} + \sqrt{\frac{1}{10}}\,\psi_5(x)\,e^{-\frac{iE_5 t}{\hbar}}$$

Where, $\mathrm{E}_3 = \dfrac{9\pi^2\hbar^2}{2ma^2}$

$$\mathrm{E}_5 = \frac{25\pi^2\hbar^2}{2ma^2}$$

Example Problem 5: A particle which is confined to move in an one-dimensional region $0 \le x \le a$ is represented by the wavefunction $\Psi(x,t) = \sin\left(\frac{\pi x}{a}\right)\exp(-i\omega t)$. Then

(a) Find the potential V(x)

(b) Calculate the probability of finding the particle in the interval $\frac{\mathrm{a}}{4} \le x \le \frac{3a}{4}$

Solution:

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(a) Find the potential V(x)

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Solution: (a) We know that the time-dependent Schrodinger equation is

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(\mathrm{x},\mathrm{t})$$

From the given wavefunction, we can calculate: $\frac{\partial\Psi(x,t)}{\partial t} = -i\omega\sin\frac{\pi x}{a}\exp -i\omega t = -i\omega\,\Psi(x,t),$

and $\frac{\partial^2\Psi(x,t)}{\partial x^2} = -\left(\frac{\pi}{a}\right)^2\,\Psi(x,t)$

We can now write

$$i\hbar\,(-i\omega)\Psi(x,t) = -\frac{\hbar^2}{2m}\left(-\frac{\pi^2}{a^2}\right)\Psi(x,t) + V(x)\Psi(\mathrm{x},\mathrm{t})$$

$$\Rightarrow\ V(x) = h\omega - \frac{\hbar^2\pi^2}{2ma^2}$$

(b) We can write the probability as

$$P = \frac{\int_{\frac{a}{4}}^{\frac{3a}{4}} \Psi^*(x,t)\Psi(x,t)\,dx}{\int_0^a \Psi^*(x,t)\Psi(x,t)\,dx} = \frac{\int_{\frac{a}{4}}^{\frac{3a}{4}} \psi^*(x)\psi(x)\,dx}{\int_0^a \psi^*(x)\psi(x)\,dx}$$

$$\Rightarrow \qquad \frac{\int_{\frac{a}{4}}^{\frac{3a}{4}} \sin^2\left(\frac{\pi x}{a}\right)\,dx}{\int_0^a \sin^2\left(\frac{\pi x}{a}\right)\,dx} = \frac{(\pi + 2)}{2\pi} = 0.82$$

## Home work problem:

A particle in the infinite square well has the initial wave function

$$\Psi(x,0) = Ax(a-x);\ 0 \leq x \leq a.$$

The constant $A$ is a normalization constant. Calculate the wave function $\Psi(x,t)$.