Modern Physics

Lecture 17

Particle in a Box

Particle in a box

Step 1: Define the potential energy

Step 2: Solve the Schrodinger equation

Step 3: Define the wave function

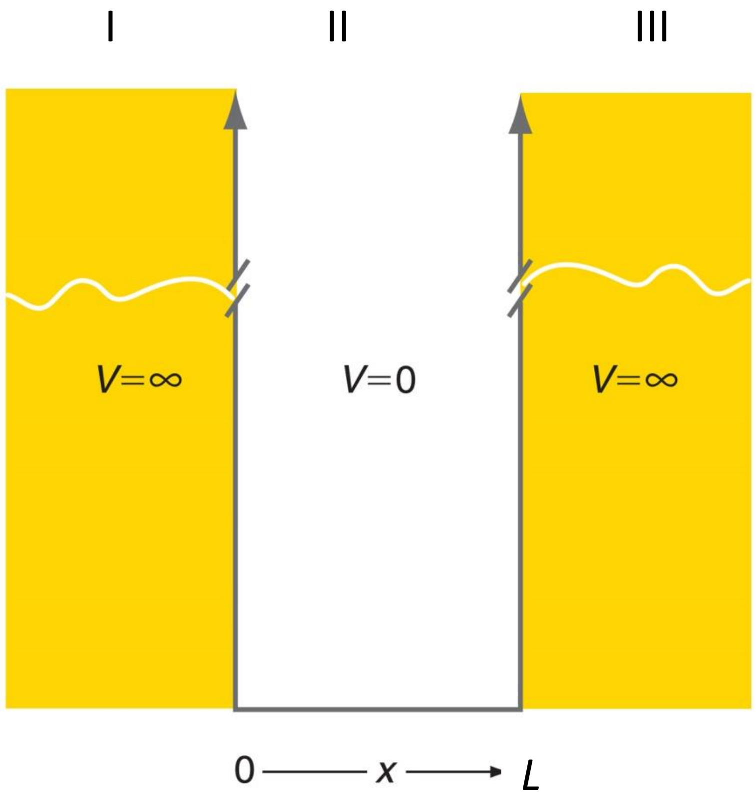
Step 4: Determine the allowed energies

Step 5: Interpret its meaning

Particle in 1-dimensional box

- Infinite walls

Regions



Potential *V* is function of *x*

Time Independent Schrödinger Equation

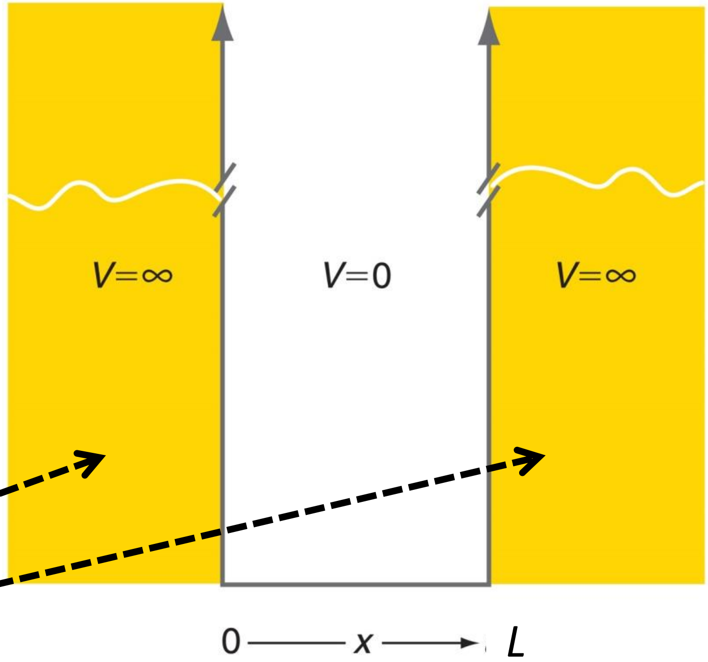
$$\underbrace{\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}}_{\text{KE}} + \underbrace{V(x)\psi}_{\text{PE}} = \underbrace{E\psi}_{\text{TE}}$$

Region I and III:

$$V(x) = \infty$$

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

$$=> \psi = 0$$

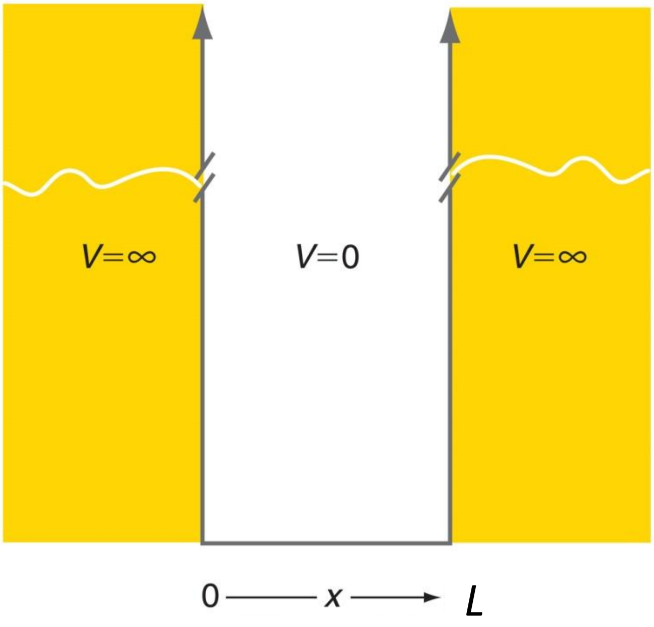


Wave function does not exist inside the wall

Region II:

Again we start from TISE

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



In region II $\quad V(x)=0$

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

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

This is similar to the general differential equation:

$$-\frac{d^2\psi(x)}{dx^2} = k^2\psi$$

where $k^2 = \dfrac{2\mathrm{m}E}{\hbar^2}$

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0$$

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

What are constants A and B ??

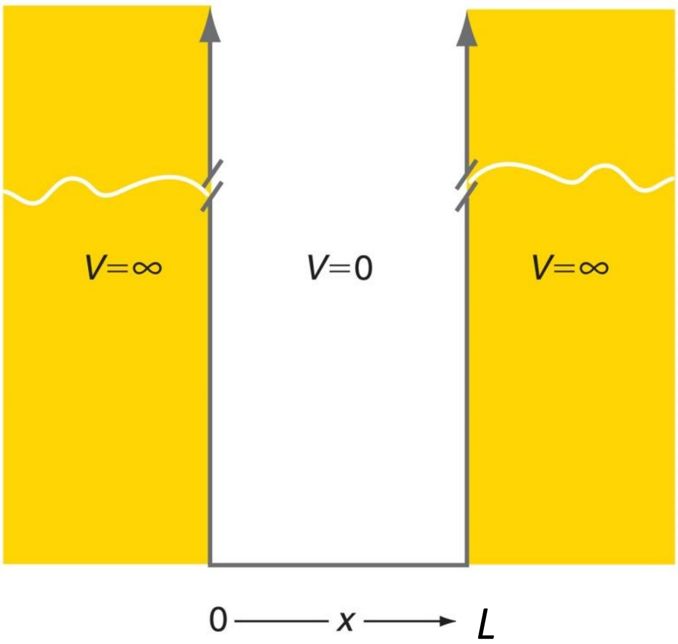
Applying boundary conditions:

a) At x=0 ψ=0

$$0 = A\sin 0k + B\cos 0k$$

$$0 = 0 + B*1$$

$$B = 0$$



Therefore $$\psi_{II}(x) = A\sin kx$$

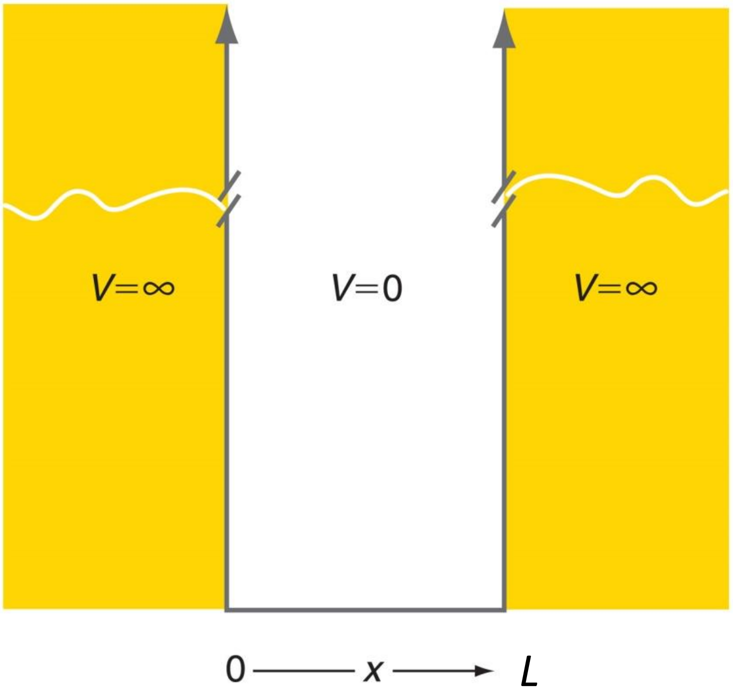
$$\psi_{II}(x) = A \sin kx$$

b) At x=L ψ=0

$$0 = A \sin kL$$

$$But\ A \neq 0$$

Therefore $$kL = n\pi$$



Thus, wave function in region II will be:

$$\psi_{II}(x) = A \sin \frac{n\pi x}{L}$$

But what is 'A'?

How can you find A

Normalizing wave function to find constant A:

$$\int_0^L (\psi(x))^2\,dx = 1$$

$$\int_0^L (A\sin kx)^2\,dx = 1$$

$$A^2\,\frac{1}{2}\int_0^L (2\sin^2 kx)\,dx = 1$$

$$\frac{A^2}{2}\int_0^L (1-\cos 2kx)\,dx = 1$$

$$A^2\left[\frac{x}{2}-\frac{\sin 2kx}{4k}\right]_0^L = 1$$

$$A^2\left[\frac{L}{2}-\cancel{\frac{\sin 2\frac{n\pi}{L}L}{4\frac{n\pi}{L}}}\right]_0^L = 1$$

$$A^2\left(\frac{L}{2}\right)=1$$

$$A=\sqrt{\frac{2}{L}}$$

Therefore the normalized (final) wave function is:

$$\boxed{\psi_{II}=\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}}$$

Calculating Energy Levels:

$$k^2=\frac{2mE}{\hbar^2}$$

We know previously

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

Substituting for $(\hbar = \frac{h}{2\pi})$

$$E = \frac{k^2 h^2}{2m4\pi^2}$$

$$E = \frac{n^2 \cancel{\pi^2}}{L^2} \frac{h^2}{2m4\cancel{\pi^2}}$$

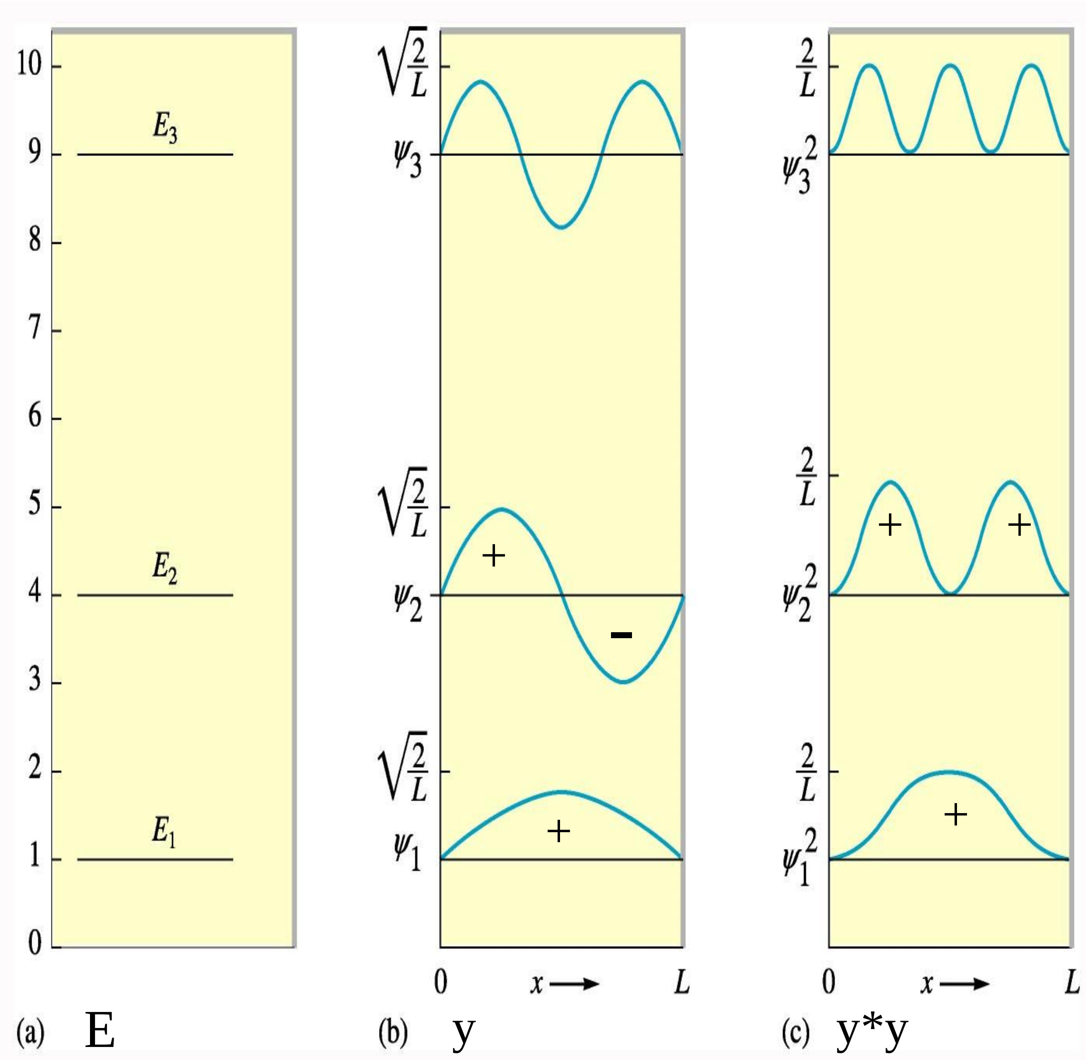
Substituting value of $k = \frac{n\pi}{L}$

Thus Energy expression of the system is:

$$E = \frac{n^2 h^2}{8mL^2}$$

Particle in a 1-Dimensional Box

$$\psi_{II} = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \qquad |\psi_{II}|^2 = \frac{2}{L}\left(\sin \frac{n\pi x}{L}\right)^2$$



1) Difference b/w adjacent energy levels:

$$\Delta E = E_{n+1} - E_n$$
$$= (2n + 1)\, E_1$$

2) Non-zero lowest level energy

3) Probability density is structured with regions of space demon- -strating enhanced probability.

Particle in a 3-D box

$$H(x,y,z)\Psi(x,y,z) = E\Psi(x,y,z)$$

$$H_x(x)\Psi_x(x) = E_x\Psi_x(x)$$
$$H_y(y)\Psi_y(y) = E_y\Psi_y(y)$$
$$H_z(z)\Psi_z(z) = E_z\Psi_z(z)$$

$$H(x,y,z) = H_x(x) + H_y(y) + H_z(z)$$

$$E = E_x + E_y + E_z$$

$$\Psi(x,y,z) = \Psi_x(x)\Psi_y(y)\Psi_z(z)$$

$$\Psi_{n_x n_y n_z}(x,y,z) = \sqrt{\frac{2^3}{abc}}\sin\left(\frac{n_x \pi x}{a}\right)\sin\left(\frac{n_y \pi y}{b}\right)\sin\left(\frac{n_z \pi z}{c}\right)$$

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

Question: An electron is in 1D box of 1nm length. What is the probability of locating the electron between x=0 and x=0.2nm in its lowest energy state?

Solution:

$$P(x_1, x_2) = \int_{x_1}^{x_2} |\psi(x)|^2 dx$$

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

Lowest energy state means *n = 1*

$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$$

$$P(0,0.2) = \frac{2}{L} \int_0^{0.2} \left[\sin \frac{\pi x}{L} \right]^2 dx$$

$$P(0,0.2) = \frac{2}{1} \int_0^{0.2} \sin^2 \frac{\pi x}{1} dx$$

$$P(0,0.2) = \frac{2}{1}\int_0^{0.2} \sin^2 \frac{\pi x}{1}\, dx$$

$$\int_0^{0.2} \sin^2 \pi x\, dx = \left[\frac{x}{2} - \frac{\sin(2\pi x)}{4\pi} \right]_0^{0.2}$$

Therefore, $$P(0,0.2) = \frac{2}{1}\left(\frac{0.2}{2} - \frac{\sin(2\pi \times 0.2)}{4\pi}\right)$$

$$= 0.05$$

This is the probability of finding the electron in between 0 and 0.2

Expectation value of position and its uncertainty

Expectation value for 2nd level

Position

$$\langle x \rangle = \int_0^L x \frac{2}{L} \sin^2\left(\frac{2\pi x}{L}\right) dx$$

$$= \frac{2}{L}\int_0^L x\left(\frac{1}{2} - \frac{1}{2}\cos\frac{4\pi x}{L}\right) dx$$

$$= \frac{1}{L}\frac{x^2}{2}\bigg|_0^L - \frac{1}{L}\frac{L^2}{16\pi^2}\left[\frac{4\pi x}{L}\sin\frac{4\pi x}{L} + \cos\frac{4\pi x}{L}\right]_0^L$$

$$= \boxed{\frac{L}{2}}$$

$$\langle x^2 \rangle = \frac{2}{L}\int_0^L x^2 \sin^2(n\pi x/L)\, dx \; = L^2 \frac{2n^2\pi^2 - 3}{6n^2\pi^2}.$$

Uncertainity $(\Delta x)^2 = L^2 \dfrac{n^2\pi^2 - 3}{n^2\pi^2} - \dfrac{L^2}{4} = L^2 \dfrac{n^2\pi^2 - 6}{12n^2\pi^2}.$

Example: What are the most likely locations of a particle in a box of length L in the state n=3

$$\psi_3 = \sqrt{\frac{2}{L}}\sin\left(\frac{3\pi x}{L}\right)$$

$$P(x) \propto \psi_3 \psi_3 \propto \sin^2\left(\frac{3\pi x}{L}\right)$$

The maxima and minima in P(x) corresponds to $\frac{dP(x)}{dx} = 0$

$$\frac{dP(x)}{dx} \propto \sin\left(\frac{3\pi x}{L}\right)\cos\left(\frac{3\pi x}{L}\right) \propto \sin\left(\frac{6\pi x}{L}\right)$$

$$\sin\theta = 0 \text{ when } \theta = \left(\frac{6\pi x}{L}\right) = n'\pi,\ n = 0,1,2.....$$

which corresponds to $x = \frac{n' L}{6},\ n' < 6.$

$n' = 0, 2, 4,$ and 6 corresponds to minima in

$n' = 1, 3,$ and 5 to maxima