PH 107 :Quantum Physics and Applications

Particle in a infinite box potential

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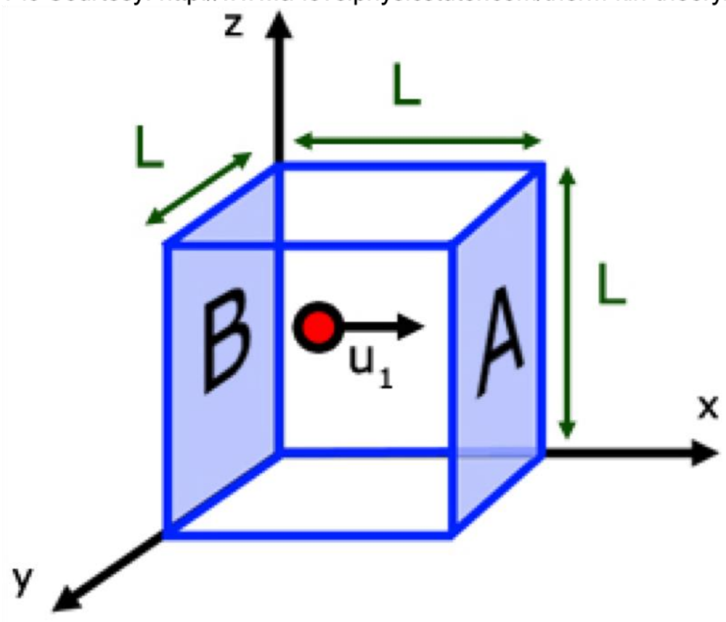
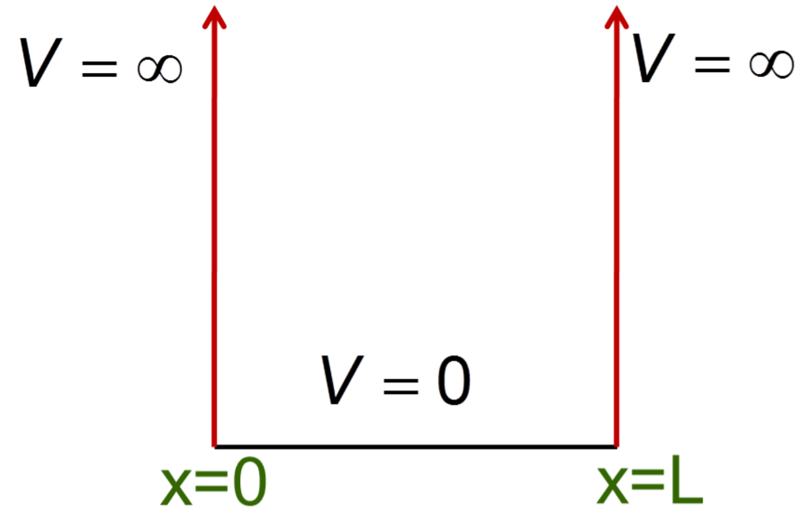
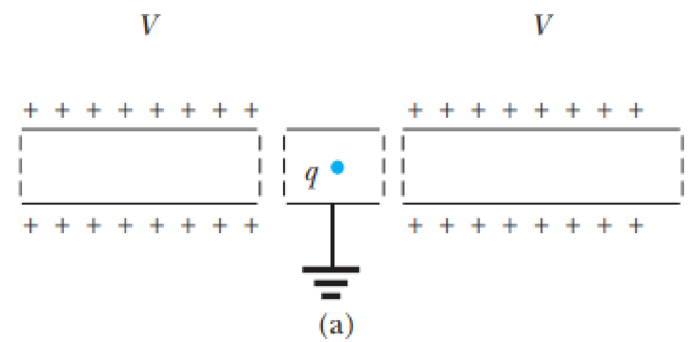
Particle in a Rigid Box (1D)

Pic Courtesy: http://www.a-levelphysicstutor.com/therm-kin-theory.php





Identifying box potential



$$V(x) = 0 \quad \text{for } 0 < x < L$$
$$= \infty \ \text{ for } x < 0 \text{ or } x > L$$

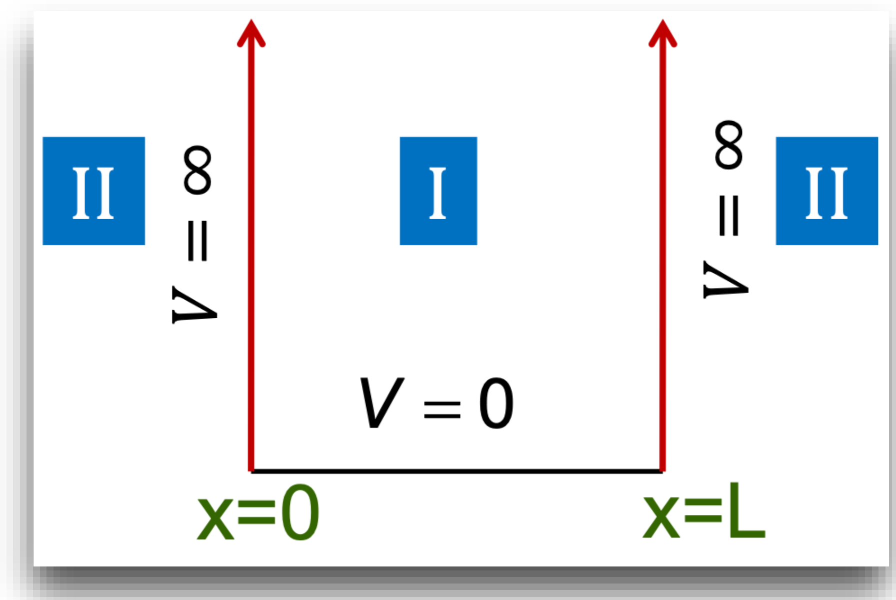
Particle is free to move inside the box; however at the boundary, it experiences a strong force.

Particle in a Rigid Box (1D)

For Region II

$$x < 0 \; and > L$$

$$\phi(x) = 0$$

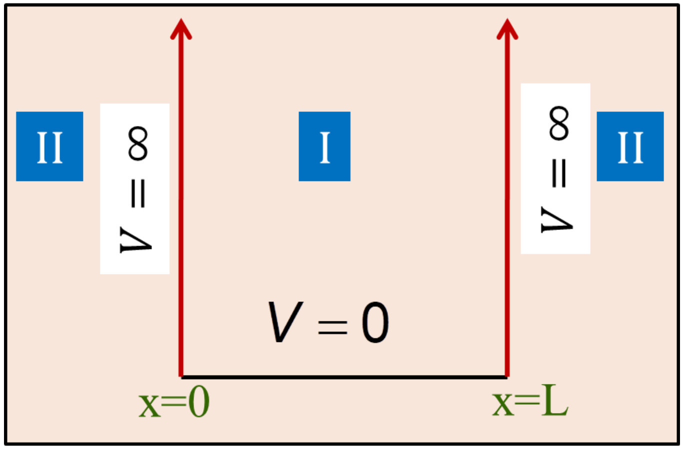


For Region I $\quad i.e. \, 0 \le x \le L$

$$-\frac{\hbar^2}{2m}\frac{d^2\phi(x)}{dx^2} = E\phi(x) \;\; or \;\; \frac{d^2\phi(x)}{dx^2} + \frac{2mE}{\hbar^2}\phi(x) = 0$$

Particle in a rigid (1-D) box

For Region $\boxed{\mathrm{I}}$ $i.e.\, 0 \leq x \leq L$



$$\frac{d^2\phi(x)}{dx^2} + \frac{2mE}{\hbar^2}\phi(x) = 0$$

The general solution of this equation is

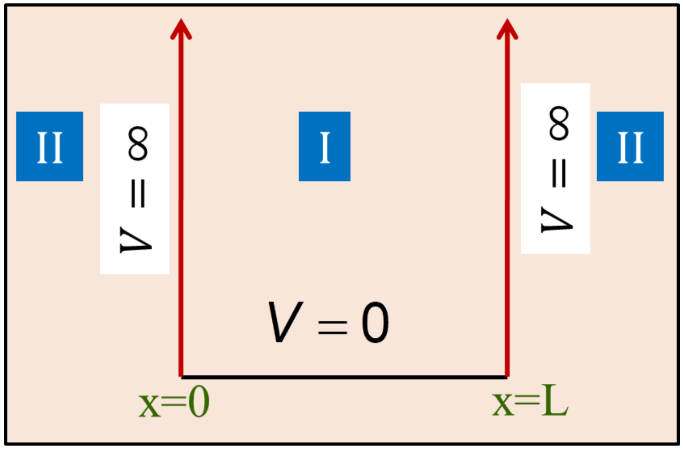
$$\phi(x) = A \sin kx + B \cos kx$$

where $\boldsymbol{k = \frac{\sqrt{2mE}}{\hbar}}$

How do we find the constants A and B ?

Boundary Conditions

The wavefunction must be continuous.



$$\phi(x=0)=0$$

$$\Rightarrow \quad A\sin k(0) + B\cos kx = 0$$

$$\Rightarrow \quad B = 0$$

$$\text{and } \phi(x=L)=0$$

$$\Rightarrow \quad A\sin k(L) = 0$$

$$\Rightarrow \quad kL = n\pi, \qquad n = 1,2,3 \ldots$$

$$\Rightarrow k = \frac{\sqrt{2mE}}{\hbar} = n\pi/L \text{ or } \boldsymbol{E = \frac{\pi^2\hbar^2 n^2}{2mL^2}} \; n \geq 1$$

Energy is quantized !

Derivative continuity is not required since potential is infinite.

Normalization of wave function

How about $\phi(x)$?

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

since

$$kL = n\pi, \qquad n = 1,2,3 \ldots$$

To find A, we normalize $\phi(x)$,

$$\int_0^L |\phi(x)|^2 dx = A^2 \int_0^L \sin^2\left(\frac{n\pi}{L} x\right) dx = 1$$

$$\Rightarrow \quad |A|^2 = \frac{2}{L} \quad \Rightarrow \quad A = \sqrt{\frac{2}{L}} e^{i\theta}$$

Wave function of the stationary states

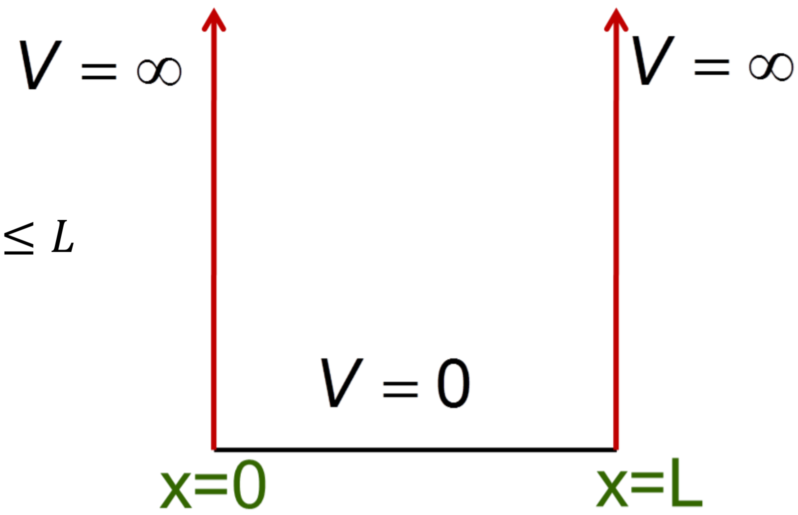
Simplest is to pick a positive real root: $A = \sqrt{\frac{2}{L}}$

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \text{ with } n = 1,2,3 \ldots$$

$$\phi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L} x\right); E = \frac{\pi^2 \hbar^2}{2mL^2}$$

$$\phi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi}{L} x\right); E = \frac{4\pi^2 \hbar^2}{2mL^2}$$

Solutions of SE for particle in an infinite box potential



$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right)$ with $n = 1,2,3 \ldots$ for $0 \leq x \leq L$

$\phi_n(x) = \; 0 \; elsewhere$

$$E_n = \frac{\boldsymbol{\pi^2 \hbar^2 n^2}}{\boldsymbol{2mL^2}}$$

$$H \; \phi_n(x) = E_n \; \phi_n(x)$$

E_n *are the eigen values corresponding to* $\phi_n(x)$

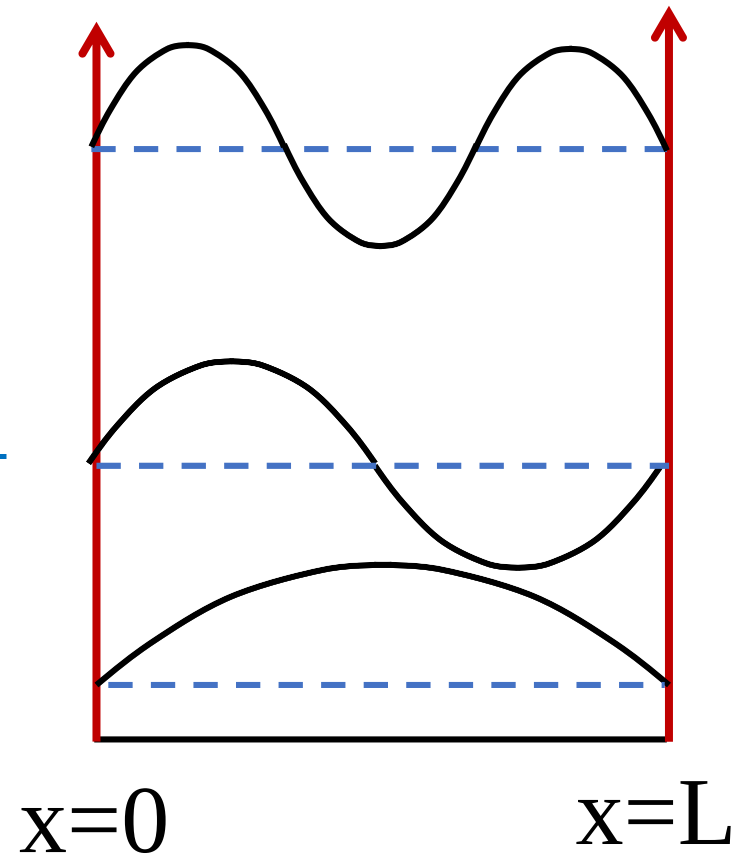
Plotting the stationary states

How do the plots of the stationary state wave functions look like?

$$\phi_3(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{3\pi}{L}x\right); E = \frac{9\pi^2\hbar^2}{2mL^2}$$

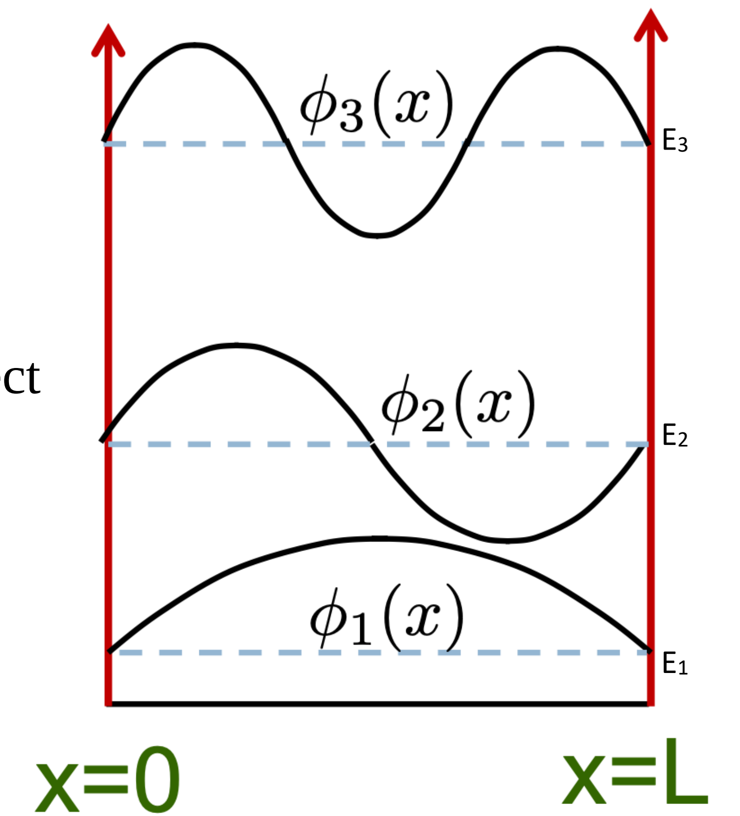
$$\phi_2(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi}{L}x\right); E = \frac{4\pi^2\hbar^2}{2mL^2}$$

$$\phi_1(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right); E = \frac{\pi^2\hbar^2}{2mL^2}$$



Properties of the stationary state solutions

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right); E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$



1. $E \propto n^2$

2. $\phi_n(x)$ are alternatively odd or even with respect to the centre of the box.

$$\phi_n(x) = \phi_n(-x) \quad n = 1.3.5...$$

$$\phi_n(x) = -\phi_n(-x) \quad n = 2, 4, 6...$$

3. As *n* increases, the number of nodes of (zero crossing) $\phi_n(x)$ increases.

Properties of the stationary state solutions

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

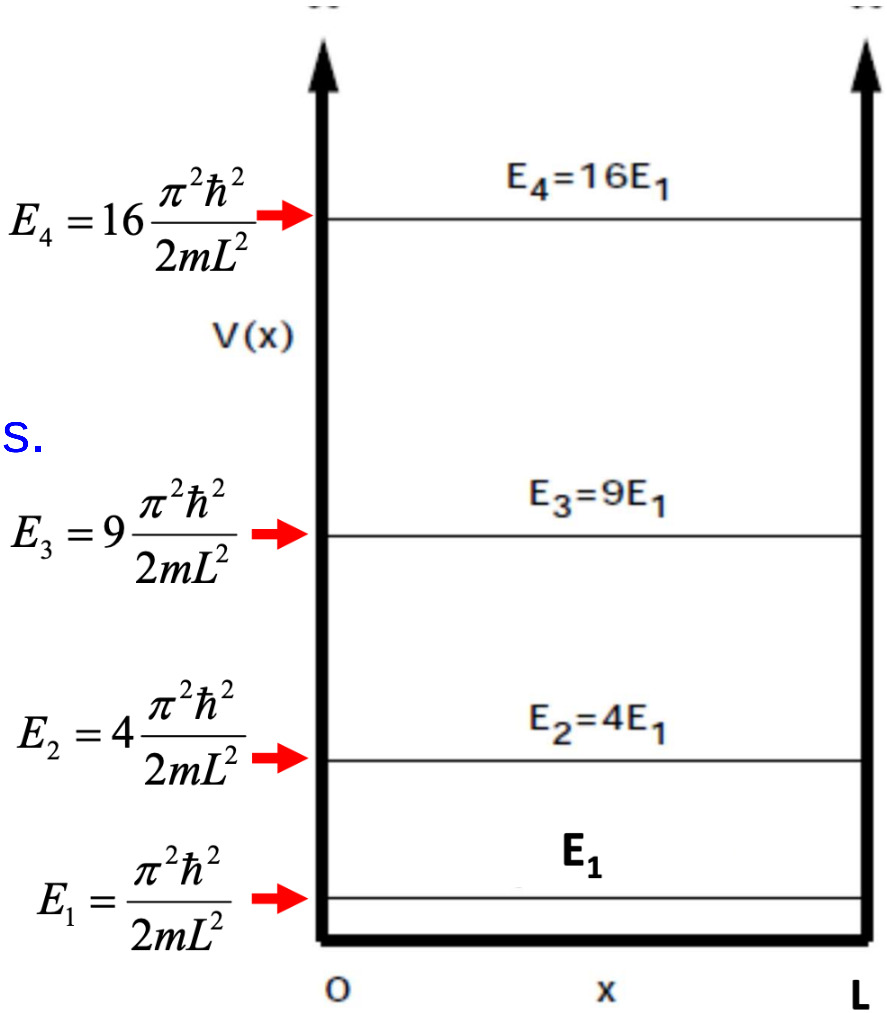
with $n = 1, 2, 3\ldots$

Occurrence of quantized energy levels.

Lowest energy

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2} > 0$$

Classically, $E_1 = 0$

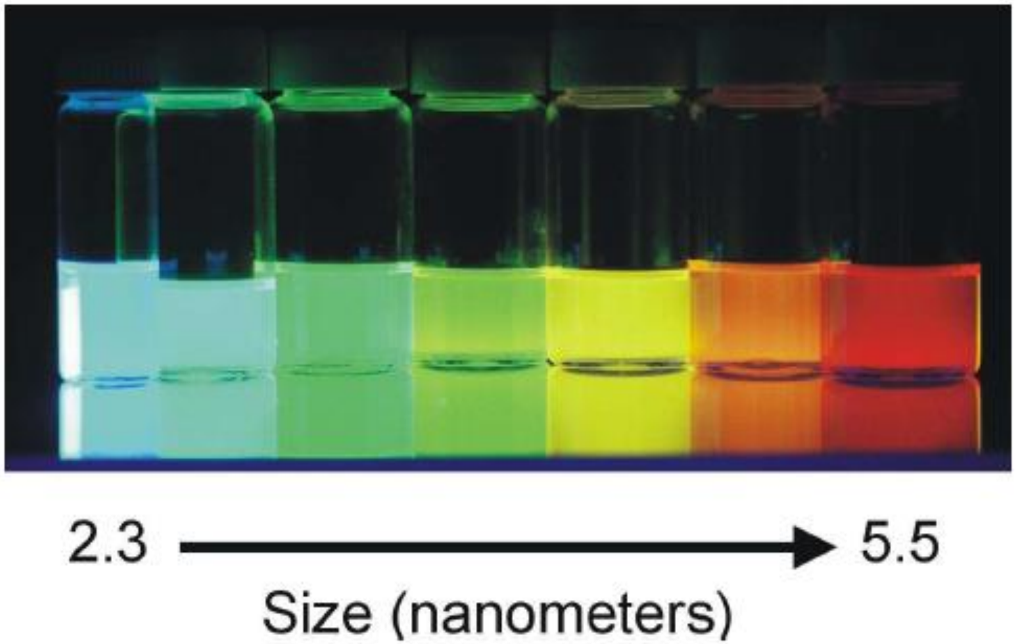


A classical particle can assume any value of Energy starting from zero

Quantum particle possesses "zero point energy"

Application: Quantum dots

A nanoscale semiconductor arrangement is called a quantum dot. They exhibit size dependent colours.



$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

L = size of the quantum dot

$$E_2 - E_1 = \frac{3\pi^2\hbar^2}{2m}\frac{1}{L^2}$$

Size increases, emission shifts to red side.

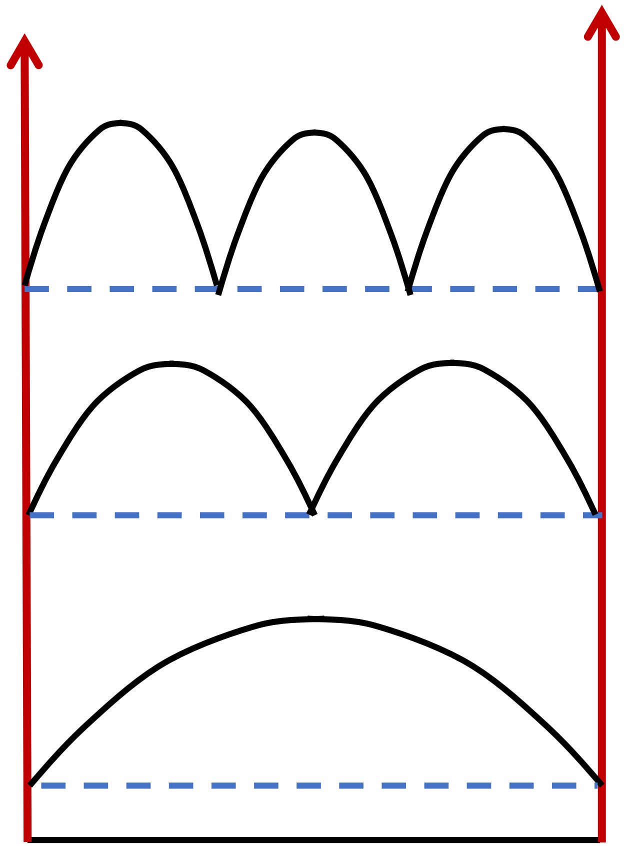
Probability density of the stationary states

How do the probability densities look like?

$$|\phi_3(x)|^2 = \frac{2}{L}\sin^2\left(\frac{3\pi}{L}x\right)$$

$$|\phi_2(x)|^2 = \frac{2}{L}\sin^2\left(\frac{2\pi}{L}x\right)$$

$$|\phi_1(x)|^2 = \frac{2}{L}\sin^2\left(\frac{\pi}{L}x\right)$$



Orthonormality of stationary state *wf*s

4. The stationary states are mutually orthonormal, i.e.

$$\int \phi_m(x)^* \phi_n(x) dx = \delta_{m,n}$$

Here,

$$\delta_{m,n} = \begin{cases} 0 \; \forall \; m \neq n \\ 1 \; \forall \; m = n \end{cases}$$

is known as the Kronecker-delta

Proof: Orthonormality

$$\int_0^L \phi_m(x)^* \phi_n(x) dx$$

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

$$= \frac{1}{L} \int_0^L \left[\cos\left(\frac{(m-n)\pi}{L} x\right) - \cos\left(\frac{(m+n)\pi}{L} x\right)\right] dx$$

$$= 0 \ \forall\ m \neq n$$
$$= 1 \ \forall\ m = n$$

Operating $\hat{H}$ on the stationary states

$$\hat{H}\phi_n(x) = \hat{H}\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)$$

$$\hat{H} = \left(\frac{\hat{p}^2}{2m} + \hat{V}\right)$$

$$= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)$$

But inside the box *V(x)* = 0, so

$$\hat{H}\phi_n(x) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)$$

$$= \left(\frac{n^2\pi^2\hbar^2}{2mL^2}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) = E_n\phi_n(x)$$

Stationary states $\phi_n(x)$ are states of definite energy.

Operating $\hat{H}$ on the stationary states

$$\hat{H}\phi_n(x) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)$$

$$= \left(\frac{n^2\pi^2\hbar^2}{2mL^2}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right) = E_n\phi_n(x)$$

Stationary states $\phi_n(x)$ are states of definite energy.

These states are also known as the **eigen-states** of the operator $\hat{H}$.

E_n are known as the **eigen-values**.

Operating $\widehat{P}$ on the stationary states

$$\hat{P}\phi_n(x) = \left(-i\hbar\frac{d}{dx}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)$$

$$= \left(-i\hbar\frac{n\pi}{L}\right)\sqrt{\frac{2}{L}}\cos\left(\frac{n\pi}{L}x\right)$$

$$\neq p_n\phi_n(x)$$

Thus, the stationary states $\phi_n(x)$are not eigenstates of the momentum operator $\hat{P}$. In other words, $\phi_n(x)$ are not states of definite momentum.

What is the momentum of the particle is the stationary state $\phi_n(x)$?

Momentum of the particle in the stationary states

We can only talk about an average or expectation value of the momentum

$$\langle \hat{P} \rangle = \int_0^L \phi_n(x)^* \hat{P} \phi_n(x) dx$$

$$= \int_0^L \phi_n^*(x) \left(-i\hbar \frac{d}{dx} \right) \phi_n(x) \, dx$$

$$= \frac{2}{L} \int_0^L \sin\left(\frac{n\pi}{L} x \right) \left(-i\hbar \frac{d}{dx} \right) \sin\left(\frac{n\pi}{L} x \right) \, dx$$

$$= -i\hbar \frac{2n\pi}{L^2} \int_0^L \sin\left(\frac{n\pi}{L} x \right) \cos\left(\frac{n\pi}{L} x \right) \, dx = 0$$

Constancy of momentum (and energy)

The state of the particle at time t,

$$\phi_n(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)e^{-\frac{iE_nt}{\hbar}}$$

Therefore,

$$\langle\hat{P}\rangle = \int_0^L \phi_n(x,t)^*\hat{P}\phi_n(x,t)dx = \int_0^L \phi_n(x)^*\hat{P}\phi_n(x)dx = 0$$

As we saw before, it is true for any operator $\hat{O}$ that

$\langle\hat{O}\rangle(t) = \langle\hat{O}\rangle(0)$ in the stationary states

This is also true for $\langle\hat{H}\rangle$ and the value is E_n (check).

Stationary states of the 1-D infinite potential box

But here we additionally see that,

$$\Delta H = \left\langle \hat{H}^2 \right\rangle - \left\langle \hat{H} \right\rangle^2 = E_n^2 - \left(E_n \right)^2 = 0$$

which reveals that the stationary states have definite energies E_n.

Thus the stationary states of the 1-Dimensional box can be written as,

$$\phi_n(x,t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) e^{-i\frac{t}{\hbar}\left(\frac{\pi^2 \hbar^2 n^2}{2mL^2}\right)}$$

General solutions TISE

TISE

So, if we are given any $\Psi(x,0)$ we can write it in terms of the $\phi_n(x)$

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

TDSE

$$\Psi_n(x,t) = \sum_{n=1}^{\infty} c_n \; \phi_n(x) \; e^{-i\frac{E_n}{\hbar}t}$$

How to we calculate the coefficients c_n?

See in next class