

* The eigen functions of Hermitian operators are complete, i.e.

$$\psi(x) = \sum_{n=1}^{\infty} a_n u_n(x)$$

↓
normalizable

where $\boxed{a_n = \int u_n^* \psi dx}$

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Proof

$$\sum_{m=1}^{\infty} \int u_n^* a_m u_m dx = \sum_{m=1}^{\infty} a_m \delta_{mn} = a_n$$

Q Now total probability $\int_{-\infty}^{\infty} \psi^* \psi dx = 1$

Hence, $\int_{-\infty}^{\infty} \psi^* \psi dx = \sum_m \sum_n \int_{-\infty}^{\infty} a_m^* a_n u_m^* u_n dx$

$$= \sum_m \sum_n a_m^* a_n \delta_{mn} = \sum_{n=1}^{\infty} |a_n|^2$$

$$\therefore \sum_{n=1}^{\infty} |a_n|^2 = 1$$

↓
Probability of measuring the physical state associated with eigen function u_n .

Particle in an infinite potential Well

Suppose we have a single particle of mass m confined to within a region with the following specification,

$$\begin{aligned} V(x) &= 0 & \text{for } 0 < x < L \\ &= \infty & \text{for } x > L \text{ \& } x < 0 \end{aligned}$$

This simple model is useful to describe (in one dimension), the properties of the gas particles in a gas or the properties of a conduction electron within a metal.

Our goal is to learn about the properties of the particle on the basis of what we have learned so far.

The boundary conditions are the following $\psi(0, t) = \psi(L, t) = 0$

This is primarily because the particle can not be found in the regions $x > L$ or $x < 0$

Between the barriers, the energy of the particle is purely kinetic. Let's the total energy is E , therefore,

$$\boxed{\frac{p^2}{2m} = E}$$

The time independent Schroedinger equation becomes:

$$\boxed{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E \psi} \quad \text{--- (1)}$$

Eq. (1) can also be written as $\frac{d^2 \psi}{dx^2} + k^2 \psi = 0$, where $k = \sqrt{\frac{2mE}{\hbar^2}}$ --- (2)

The most general solution for eqn (2) is given by

$$\begin{aligned} \psi &= A' e^{ikx} + B' e^{-ikx} \\ &= A \cos kx + B \sin kx \end{aligned}$$

Now applying the boundary Condⁿ we will get

$$\psi(0) = A = 0 \quad \text{and} \quad \psi(L) = B \sin kL = 0$$

Since $B \neq 0 \quad \therefore \sin kL = 0 \quad \therefore kL = n\pi$
② $\therefore k_n = \frac{n\pi}{L} \quad n=1, 2, 3, \dots$

we exclude $n=0$, then the wave function will not exist.

$\therefore$ $E_n = \frac{k_n^2 \hbar^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2m L^2} \Rightarrow$ The energy is quantized.

Now $\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx = B^2 \int_0^L \sin^2 k_n x dx = B^2 \times \frac{L}{2} = 1$

$$\boxed{\therefore B = \sqrt{\frac{2}{L}}}$$

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad \text{for } 0 < x < L$$

$$= 0 \quad \text{for } x < 0, x > L$$

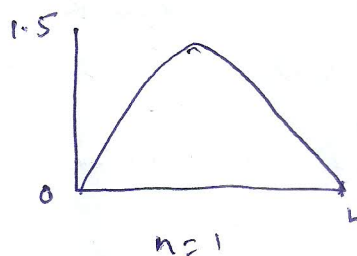
Also, note that the particle can only have energies E_n , and in particular, the lowest energy, E_1 , is greater than zero, as required by uncertainty principle.

Energy eigenvalues and eigenfunctions

The above wave functions can be written in the form

Energy eigen function $\leftarrow \Psi_n(x, t) = \Psi_n(x) e^{-\frac{iE_n t}{\hbar}}$

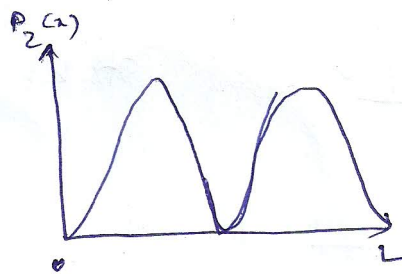
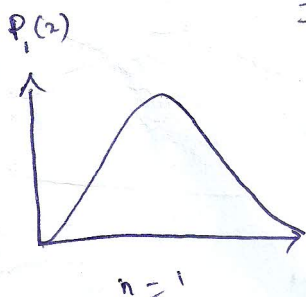
$\hookrightarrow$ The time dependence of the wave function for any system in a state of given energy is always of this form.



Probability distribution for Position

$$P_n(x) = |\Psi_n(x, t)|^2 = \frac{2}{L} \sin^2 \frac{n\pi x}{L} \quad 0 < x < L$$

$$= 0 \quad x < 0, x > L$$



For very large 'n' the probability oscillates very rapidly, averaging out to be $\frac{1}{L}$.

Particle is equally likely to be found anywhere in the well.

The expectation value of the Position

$$\langle x \rangle = \frac{2}{L} \int_0^L x \sin^2 \frac{n\pi x}{L} dx = \frac{L}{2}$$

It is in the middle of the well.

Probability distribution ~~is~~ is symmetric about $\frac{L}{2}$.

In fact, for, say $n \geq 2$, the particle is most likely to be found in the vicinity of $x = \frac{L}{4}$ and $x = \frac{3L}{4}$.

Now we can calculate

$$\langle x^2 \rangle = \frac{2}{L} \int_0^L x^2 \sin^2 \frac{n\pi x}{L} dx = L^2 \frac{2n^2\pi^2 - 3}{6n^2\pi^2}$$

$\therefore$ The uncertainty in position is

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

orthonormality

$$\int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) dx = \frac{2}{L} \int_0^L \sin \frac{m\pi x}{L} \sin \frac{n\pi x}{L} dx = \delta_{mn}$$

$$\begin{aligned} \delta_{mn} &= 1 \quad \text{if } \underline{m=n} \Rightarrow \text{normalization cond}^n \\ &= 0 \quad \text{if } m \neq n \Rightarrow \text{orthogonal cond}^n \end{aligned}$$

Linear Superpositions

Let us consider the superposition of two such wave functions representing the particle having energies E_1 and E_2 .

$$\psi(x, t) = \frac{1}{\sqrt{2}} [\psi_1(x, t) + \psi_2(x, t)]$$

$\checkmark$
Normalized to unity.

$$= \frac{1}{\sqrt{2}} \left[\sin \frac{\pi x}{L} e^{-iE_1 t} e^{-i\omega_1 t} + \sin \frac{2\pi x}{L} e^{-iE_2 t} e^{-i\omega_2 t} \right] \quad 0 < x < L$$

$$= 0 \quad x < 0 \text{ and } x > L$$

The probability distribution is

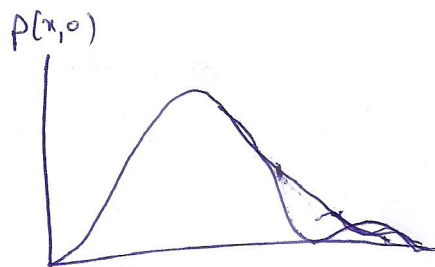
$$P(x, t) = |\psi(x, t)|^2 = \frac{1}{2} \left[\sin^2 \frac{\pi x}{L} + \sin^2 \frac{2\pi x}{L} + 2 \sin \frac{\pi x}{L} \sin \frac{2\pi x}{L} \cos(\Delta\omega t) \right]$$

Where $\Delta\omega = \frac{E_2 - E_1}{\hbar}$

$\rightarrow$ Time dependent
Probability distribution.

At $t=0$

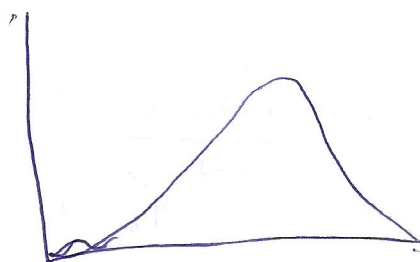
$$P(x,0) = \frac{1}{L} \left(\sin \frac{\pi x}{L} + \sin \frac{2\pi x}{L} \right)^2$$



$$P(x, \frac{\pi}{2\Delta\omega}) = \frac{1}{L} \left(\sin^2 \frac{\pi x}{L} + \sin^2 \frac{2\pi x}{L} \right)$$



$$P(x, \frac{\pi}{\Delta\omega}) = \frac{1}{L} \left(\sin \frac{\pi x}{L} - \sin \frac{2\pi x}{L} \right)^2$$



The maximum probability swings from left to the right hand side of the well but without the max^m moving through the centre of the well
 (11)

Classical analogue behaviour of the particle bouncing back and forth between the walls.

The total probability of finding the particle on the left hand half of the well,

$$P_L = \int_0^{\frac{L}{2}} P(x,t) dx = \frac{1}{2} + \frac{\sin(2\pi\Delta\omega t)}{\pi}$$

$$\therefore P_R = \int \frac{1}{2} - \frac{\sin(2\pi\Delta\omega t)}{\pi}$$

which illustrates the 'See-sawing' of the probability from one side to the other side, with frequency $(2\pi\Delta\omega)$.



Particle momentum

We can write down $\psi_n(x, t) = \sqrt{\frac{2}{L}} \frac{e^{i(k_n x - \omega_n t)} - e^{-i(k_n x - \omega_n t)}}{2i}$

$\therefore$ It is associated with particle having momentum $p_n = \hbar k_n$, the other with the particle having momentum $p_n = -\hbar k_n$. Both of them have equal weight.

Here, momentum has a probability distribution which is peaked at the values $p_n = \pm \hbar k_n$

$$\langle P \rangle = \frac{1}{2} \hbar k_n + \frac{1}{2} (-\hbar k_n) = 0$$

$$\langle P^2 \rangle = \frac{1}{2} (\hbar k_n)^2 + \frac{1}{2} (-\hbar k_n)^2 = \hbar^2 k_n^2$$

$$\therefore (\Delta P)^2 = \langle P^2 \rangle - \langle P \rangle^2 = \hbar^2 k_n^2 = \hbar^2 \left(\frac{n\pi}{L} \right)^2$$

$$\therefore (\Delta x)^2 (\Delta P)^2 = L^2 \frac{n^2 \pi^2 - 6}{12 n^2 \pi^2} \hbar^2 \left(\frac{n\pi}{L} \right)^2 = \frac{\hbar^2}{4} \left(\frac{n^2 \pi^2 - 6}{3} \right) \geq \frac{\hbar^2}{4}$$

$$\Delta x \Delta P \geq \frac{\hbar}{2}$$