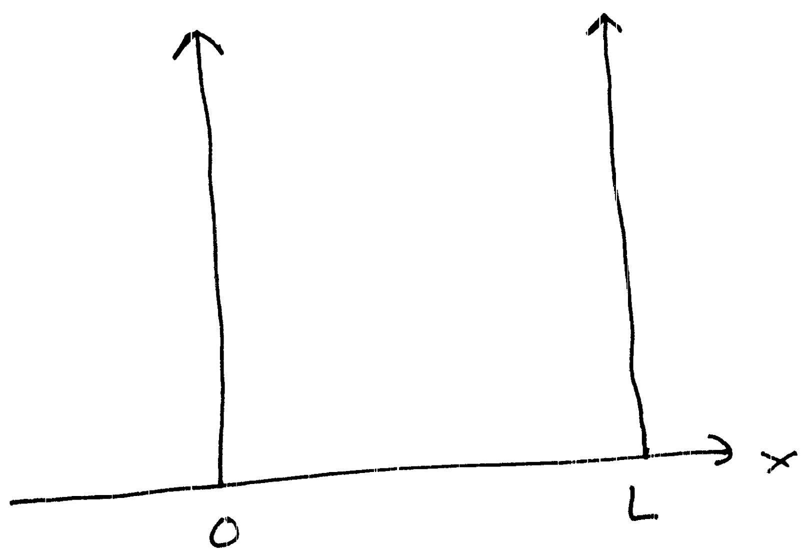
Infinite Square Well

Consider the potential

$$V = \begin{cases} \infty & x < 0 \\ 0 & 0 < x < L \\ \infty & x > L \end{cases}$$



$\Longrightarrow$ The wave function is continuous, period.

Since it requires infinite energy for the particle to enter the regions $x<0$ and $x>L$, there must be zero probability of finding the particle outside the well.

$$\psi(x) = 0 \qquad x < 0$$

$$\psi(x) = 0 \qquad x > L$$

Since the potential is continuous,

$$\psi(0) = 0$$

$$\psi(L) = 0$$

at all times.

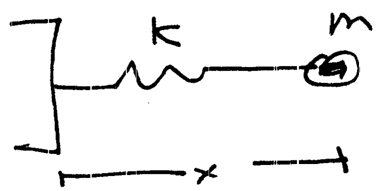
Solve the TISE inside the well

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

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

$\Rightarrow$ Simple Harmonic oscillator equation.

For a mass on a spring,



$$F = -kx = m\frac{d^2x}{dt^2}$$

$$\frac{dx^2}{dt^2} + \frac{k}{m}x = 0$$

$$\frac{dx^2}{dt^2} + \omega^2 x = 0$$

<u>Solutions</u> $A\sin\omega t$, $B\cos\omega t$

or

$$Ae^{i\omega t}, \quad Be^{-i\omega t}$$

with $\omega = \sqrt{\frac{k}{m}}$

Back to the infinite square well

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

$$\Downarrow$$

$$\frac{d^2\phi}{dx^2} + k^2\phi = 0$$

We use ω when the oscillations are in time;
k when the oscillations are in space.

<u>General Solution</u>

$$\phi = A\sin kx + B\cos kx$$

or

$$\phi = Ce^{ikx} + De^{-ikx}$$

Note,

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

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

Very suggestive if we compare with the DeBroglie relation

$$p = \hbar k$$

for a free particle.

The energy is then $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

Boundary Conditions

$$\phi(0) = 0 \qquad \phi(L) = 0$$

Substitute general solution

$$\phi(0) = A \sin k \cdot 0 + B \cos k \cdot 0$$

$$= B = 0$$

$$\phi(L) = 0 = A \sin kL$$

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

$$k_n = \frac{n\pi}{L}$$

$n \neq 0$, because not normalizable

$\Rightarrow$ Energy is quantized

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

Full Solution

$$\psi_n(x,t) = A \sin k_n x \, e^{-iE_n t/\hbar}$$

$$= A \sin k_n x \, e^{-i\omega_n t}$$

$$\omega_n = \frac{E_n}{\hbar} = \frac{\hbar}{2m}\left(\frac{n\pi}{L}\right)^2$$

Normalize

$$\psi_E^* \psi_E = \phi_E^* \phi$$ since exponentials cancel

$$1 = A_n A_n^* \int_0^L \sin^2 k_n x \, dx$$

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

Let $u = \dfrac{n\pi x}{L}$ $\quad du = k_n dx$

$$1 = \frac{A_n A_n^*}{k_n} \int_0^{n\pi} \sin^2 u \, du$$

$$\int_0^{n\pi} \sin^2 u \, du = \int_0^{n\pi} \cos^2 u \, du = \frac{1}{2} \int_0^{n\pi} \sin^2 u + \cos^2 u \, du$$

$$= \frac{1}{2} \int_0^{n\pi} du = \frac{n\pi}{2}$$

$$1 = \frac{A_n A_n^*}{k_n} \cdot \frac{n\pi}{2} = A_n A_n^* \left(\frac{L}{n\pi}\right)\left(\frac{n\pi}{2}\right) = A_n A_n^* \frac{L}{2}$$

$$A_n A_n^* = \frac{2}{L}$$

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

$$\phi_n = \sqrt{\frac{2}{L}} \sin k_n x$$

$$\psi_n = \phi_n e^{-i\omega_n t}$$

- The only energies we can measure are E_i.
- Upon measurement of E_i the wave function immediately becomes ϕ_i

Properties of ϕ_i

1. Orthogonality

$$\int_0^L \phi_n^* \phi_m \, dx = \delta_{nm}$$

Kronecker Delta

$$\delta_{nm} = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases}$$

2. **Completeness** Any solution $f(x)$ of the TISE can be written as a combination of ϕ_i

$$f(x) = \sum c_n \phi_n(x)$$

Fourier's Trick Multiply by ϕ_m^*

and integrate

$$\int_0^L \phi_m^* f(x)\,dx = \int_0^L \phi_m^* \sum c_n \phi_n \,dx$$

$$= \sum_n \int_0^L \phi_m^* c_n \phi_n \,dx$$

$$= \sum_n c_n \delta_{nm} = c_m$$

$$\Longrightarrow \quad c_m = \int_0^L \phi_m^* f(x)\,dx$$

Time Evolution - We can predict the time evolution of a number of quantities

(1) $\rho(x,t) = \psi^* \psi$

(2) $\rho(p,t) = \Psi^* \Psi$

(3) $\langle Q(x,p)\rangle(t)$ - Time evolution of averages.

(4) $\mathcal{P}_i(t)$ - Time evolution of the probability to observe E_i as a function of time

Time evolution of the wave function - Given $\psi(x,0)$ how do we predict $\psi(x,t)$?

By completeness,

$$\psi(x,0) = \sum c_i \phi_i(x)$$

then we know how each energy states evolves in time.

$$\psi(x,t) = \sum c_i \phi_i(x) e^{-i\omega_i t}$$

$$\omega_i = E_i/\hbar$$

Are there other ways to get this? <u>NO</u>

(2) $\mathcal{P}(p,t) = \Psi^*(p,t)\,\Psi(p,t)$

$$\Psi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x,t)\, e^{-ipx/\hbar}\, dx$$

integration is over x, so time evolution is no problem.

(3) $\langle Q(x,p)\rangle(t) = \int \psi^*(x,t)\, Q(x,\hat{p})\, \psi(x,t)\, dx$

Is there other ways to get this? <u>YES</u>

(4) $\mathcal{P}_i(t)$ = Probability to observe E_i

$$\mathcal{P}_i(0) = c_i^* c_i$$

$$c_m(t) = \int \phi_m^*(x)\, \psi(x,t)\, dx$$

$$= \sum_n \int c_n(0)\, \phi_m^*(x)\, \phi_n(x)\, e^{-i\omega_n t}\, dx$$

$$= c_m(0)\, e^{-i\omega_m t}$$

$$\mathcal{P}_i(t) = \left(c_i e^{-i\omega_i t}\right)^* \left(c_i e^{-i\omega_i t}\right) = c_i^* c_i = \text{constant}$$