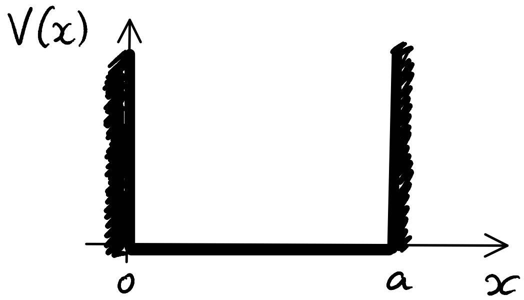
Lecture 4

The infinite square well



$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$

A particle in this potential is completely free, except at the two ends, where an infinite force prevents it from escaping.

Let's solve the Schrödinger equation!

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

First, we seek stationary states

$$\Psi(x,t) = \psi(x) e^{-iEt/\hbar}$$

We need to solve the time-independent Schrödinger equation

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

to find $\psi(x)$.

Outside of the well $\psi(x) = 0$.

Inside the well, where V= 0, the time-independent Schrödinger equation becomes:

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

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

We introduce $k = \frac{\sqrt{2mE}}{\hbar}$ and write

$$\boxed{\frac{d^2\psi}{dx^2} = -k^2\psi} \qquad (E \geq 0)$$

Simple harmonic oscillator equation; its general solution is

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

where A and B are arbitrary constants that are generally obtained from boundary conditions.

What are the boundary conditions for $\psi(x)$?

Usually, both $\psi(x)$ and $\frac{d\psi}{dx}$ are continuous, but where $V \to \infty$ only the first applies.

Continuity of $\psi(x)$ requires that

$$\boxed{\psi(0) = \psi(a) = 0} \leftarrow \text{Boundary conditions}$$

Now we can find out something about A and B

$$\psi(0) = A\sin 0 + B\cos 0 = B \Rightarrow \boxed{B = 0}$$

$$\psi(a) = A\sin ka \Rightarrow \text{either } A = 0$$

(trivial solution, discard)

or $\sin ka = 0 \Rightarrow$

$$ka = 0, \pm\pi, \pm 2\pi, \pm 3\pi \ldots$$

$k=0$ also gives $\psi(x) = 0 \Rightarrow$ discard

Negative solutions give nothing new, since $\sin(-\theta) = -\sin(\theta)$ and sign can be absorbed into A.

Therefore, the distinct solutions are

$$\boxed{k_n = \frac{n\pi}{a}, \text{ with } n = 1, 2, 3\ldots}$$

and

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

and quantum particle in the infinite square well can not have just any energy. It has to be one of these special allowed values.

Now, we find A by normalizing $\psi(x)$:

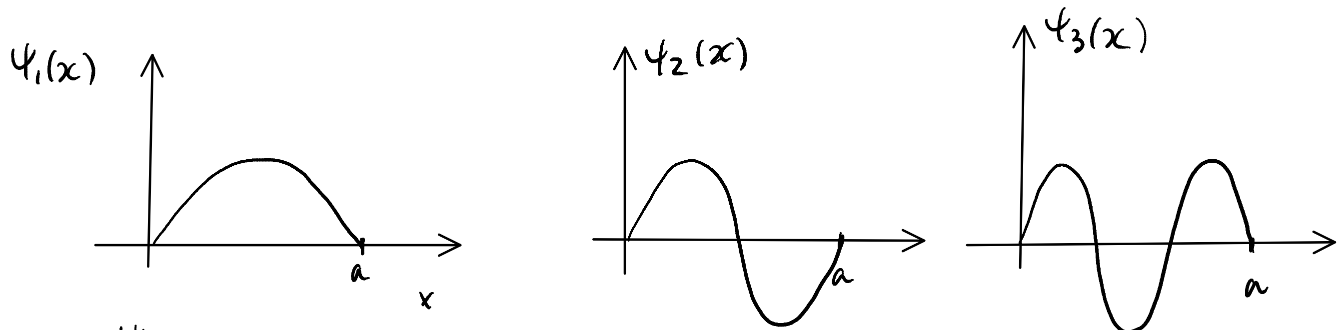
$$\int_a^b |A|^2 \sin^2 kx \, dx = |A|^2 \frac{a}{2} = 1 \Rightarrow |A|^2 = \frac{2}{a}$$

Global phase carries no significance in quantum mechanics, and we can pick positive root.

$$A = \sqrt{\frac{2}{a}}.$$

Therefore, $$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)}$$

These solutions look like:



ψ_1
carries
lowest energy
<u>It is called ground state.</u>

<u>Excited states</u>

The set of functions $\psi_n(x)$ has the following properties:

1. They are alternatively even and odd.

2. As you go up in energy, each successive state has one more node (zero-crossing).

3. They are mutually orthogonal, i.e.

$$\int \psi_m^*(x)\ \psi_n(x)\ dx = 0 \quad \text{if} \quad m \neq n$$

Also, if m = n $\quad \int \psi_m^*(x)\ \psi_m(x)\, dx = 1$ (normalization)

We can combine orthogonality and normalization into single statement

$$\boxed{\int \psi_m^*(x)\ \psi_n(x)\, dx = \delta_{mn}}$$

Kronecker delta

$$\boxed{\delta_{mn} = \begin{cases} 0, & \text{if } m \neq n \\ 1, & \text{if } m = n \end{cases}}$$

We say that functions $\psi_n(x)$ are orthonormal.

4. They are complete, in the sense that any other function $f(x)$ can be expressed as a linear combination of them.

$$(1) \qquad f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a} x\right).$$

Note: the coefficients c_n may be evaluated using Fourier's trick:

multiply both sides of Eq. (1) by $\psi_m^*(x)$ and integrate

$$\int \psi_m^*(x) f(x)\, dx = \sum_{n=1}^{\infty} c_n \int \psi_m^*(x) \psi_n(x)\, dx = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m$$

$$\boxed{c_n = \int_{-\infty}^{\infty} \psi_n^*(x)\, f(x)\, dx}$$

Summary:

Stationary states for an infinite square well are:

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

The most general solution is

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

How to find c_n for a given initial function $\Psi(x,0)$?

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

using $c_n = \int \psi_n^*(x) f(x)\, dx.$

$|c_n|^2$ tells you the probability that a measurement of the energy would yield the value E_n.

$$\sum_{n=1}^{\infty} |c_n|^2 = 1.$$