The Schrödinger Equation (Part 1)

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

Kinetic Energy + Potential Energy = Total Energy

Wave Function

Postulate: Particles are described by a complex-valued wave function $\Psi(x,t)$. Properties of the wave determine the physical properties of the particle.

Wavelength of the wave function determines the particle's momentum:

$$p = \frac{h}{\lambda} \qquad p = \hbar k$$

Frequency of the wave function determines the particle's energy:

$$E = hf \qquad E = \hbar\omega$$

Q: How do you “do physics” with a wave function?

A: You need a wave equation that tells the wave how to behave.

Math Interlude: Partial Derivative

A partial derivative considers changes in one variable at a time. All variables not in the derivative are treated as constants.

Example: $$\frac{\partial}{\partial x}(ax^2t^3) = at^3\frac{\partial}{\partial x}(x^2) = 2axt^3$$

$$\frac{\partial}{\partial t}(ax^2t^3) = ax^2\frac{\partial}{\partial t}(t^3) = 3ax^2t^2$$

$$\frac{\partial}{\partial y}(ax^2t^3) = 0$$

Example

Determine if traveling waves of the form $\psi(x,t) = Ae^{i(kx-\omega t)}$ are solutions to the following wave equation:

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v_p^2}\frac{\partial^2 \psi}{\partial t^2}$$

Schrödinger's equation

(Conservation of energy for wave functions)

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

$m =$ particle mass

$\Psi(x,t) =$ wave function

$U(x) =$ potential energy defining the system

Traveling Wave Solution to Schrödinger's Equation with Constant Potential U_0

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar\frac{\partial\Psi}{\partial t} \qquad\qquad U(x) = U_0$$

Show that the complex, traveling wave $\psi(x,t) = Ae^{i(kx-\omega t)}$ is a solution to the Schrödinger equation (with constant potential U_0).

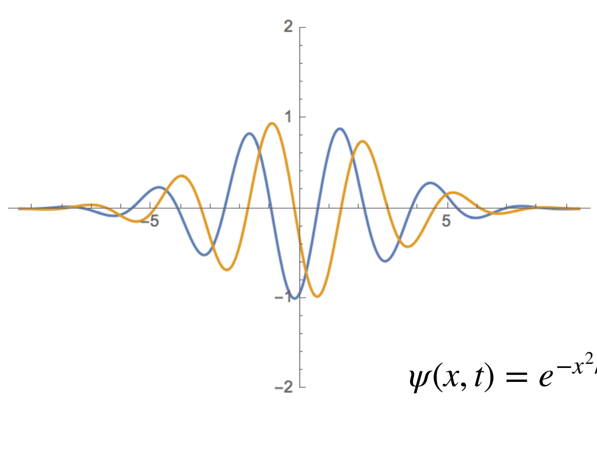
After plugging in the traveling wave, you should find:

$$\frac{\hbar^2 k^2}{2m} + U_0 = \hbar\omega \quad \Rightarrow \quad \frac{p^2}{2m} + U_0 = E$$

This is just a statement of energy conservation!

Properties of Time-Dependent Wave Functions $\psi(x,t)$

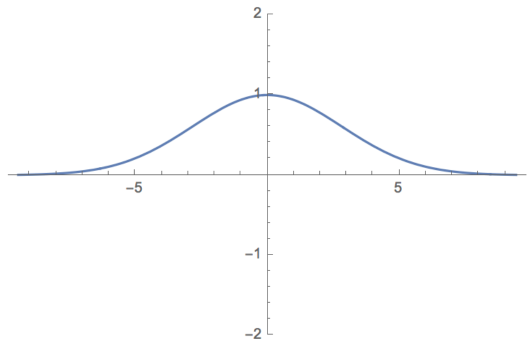
$\psi(x,t) =$ wave function (complex-valued). Also called the "probability amplitude"



$$\psi(x,t) = e^{-x^2/4^2}e^{i(2x-3t)}$$

Properties of Time-dependent Wave Functions $\psi(x,t)$

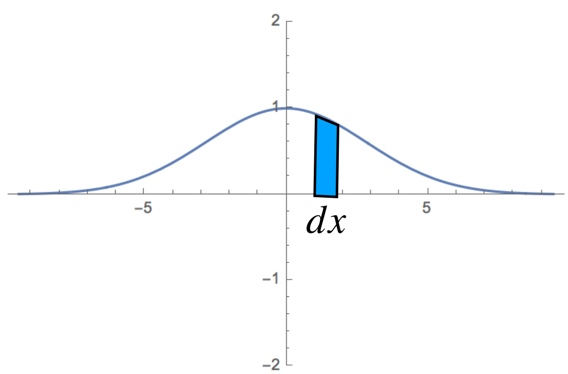
$|\psi(x,t)|^2 = \psi^*(x,t)\,\psi(x,t) =$ probability density (real-valued).



$|\psi(x,t)|^2 = e^{-2x^2/4^2}$

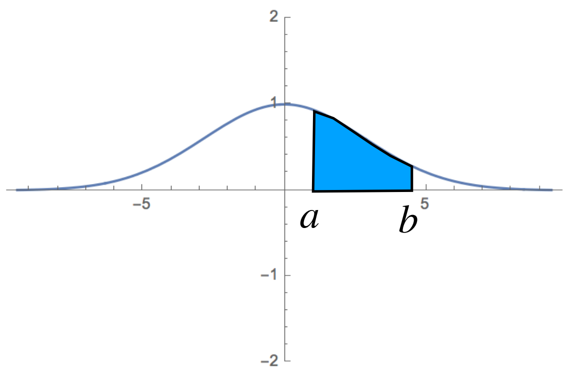
Properties of Time-dependent Wave Functions $\psi(x,t)$

$|\psi(x,t)|^2\,dx =$ probability of finding the particle on the interval $(x, x+dx)$



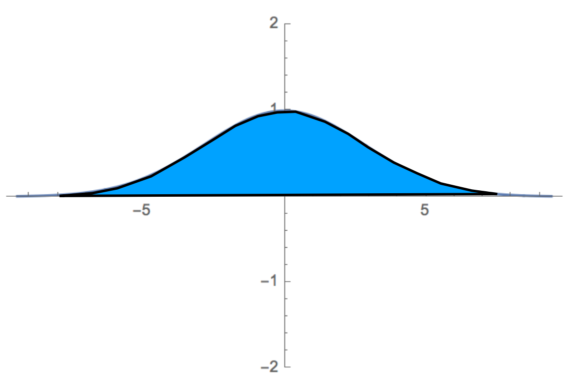
Properties of Time-dependent Wave Functions $\psi(x,t)$

$$\int_a^b |\psi(x,t)|^2 dx =$$ probability of finding the particle on the interval $a < x < b$



Properties of Time-dependent Wave Functions $\psi(x,t)$

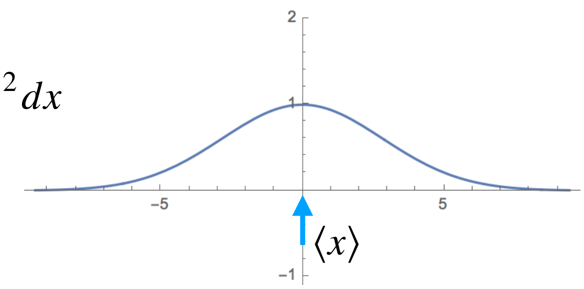
$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$$ Normalization condition: probability that the particle is found somewhere = 1



Expectation Value

The expectation value of the particle's position given a wave function $\psi(x,t)$ is the average position that results from many measurements.

$$\langle x \rangle = \int_{-\infty}^{\infty} x\,|\psi(x,t)|^2\,dx$$

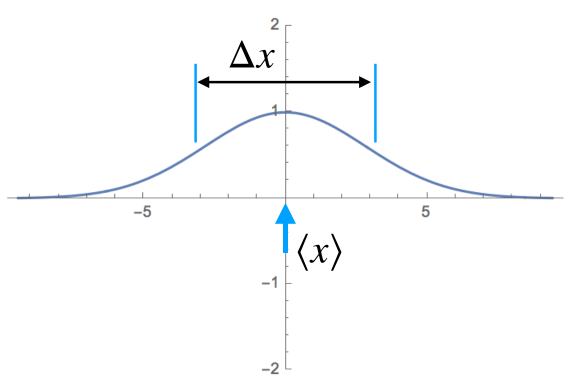


In general, the expectation of a function of any function *f(x)* is:

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)\,|\psi(x,t)|^2\,dx$$

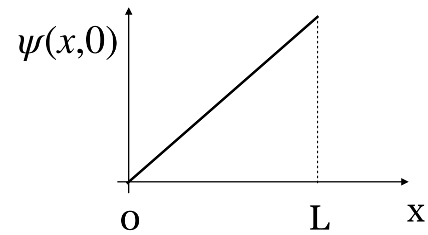
Uncertainty

The measurement uncertainty in the position x of a particle is given by $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$



Example

(a) Use the normalization condition to solve for the constant A in the following wave function



$$\psi(x,t) = Axe^{-i\omega t} \quad \text{for} \quad 0 < x < L$$

(b) Find the expectation value $\langle x \rangle = \int_{-\infty}^{\infty} x\,|\psi(x,t)|^2\,dx$

(c) What is the probability of finding the particle on $0 < x < L/2$?

Properties of Time-dependent Wave Functions $\psi(x,t)$

$\Psi(x,t)$ must be single-valued and continuous

$\Psi(x,t)$ must be smooth (i.e. $\frac{d\Psi(x,t)}{dx}$ must be continuous) if the potential energy curve U(x) has no spikes,

$\Psi(x,t) \to 0$ when $x \to \pm\infty$

$\Psi(x,t) \to 0$ when $U \to \infty$

Time-Independent Schrödinger Equation

In many physics applications, we are interested in standing wave solutions to the Schrödinger equation.

We look for solutions of the form: $\Psi(x,t) = \psi(x)e^{-i\omega t}$

Plug this expression for $\Psi(x,t)$ into the full time-dependent Schrödinger equation to derive the Time-Independent Schrodinger Equation:

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

Method for Solving Time-Independent Schrödinger Equation (SE)

Step 1. Define potential U(x), draw a picture and plug into SE

Step 2. Solve SE or guess general solutions to the SE.

Step 3. Write down boundary conditions.

Step 4. Use boundary conditions to place constraints on unknown constants and coefficients.

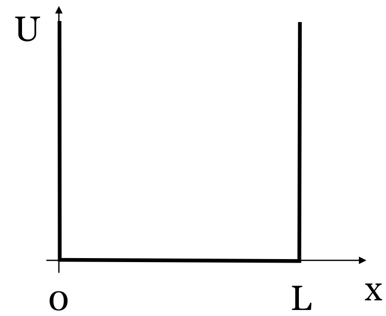
Step 5. Use boundary constraints to solve for energy levels E_n

Step 6. Use normalization to solve for remaining unknown constants and write down final wave functions $\psi_n(x)$ associated with each energy level E_n

Infinite Potential Well: Particle in a Box

step 1 Define the potential

$$U(x) = \begin{cases} +\infty & \text{for } x \le 0 \\ 0 & \text{for } 0 < x < L \\ +\infty & \text{for } x \ge L \end{cases}$$



Inside the well, $U(x) = 0$

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

Infinite Potential Well: Particle in a Box

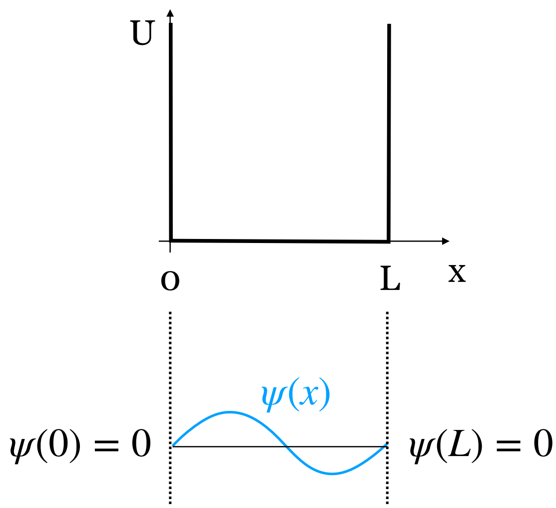
step 2 Solve Schrödinger equation $\frac{d^2\psi(x)}{dx^2} = -\frac{2m}{\hbar^2}E\psi(x)$

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

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

Infinite Potential Well: Particle in a Box

step 3 Write down boundary conditions



Infinite Potential Well: Particle in a Box

step 4 Use B.C. to constrain unknown constants

General Solution: $\psi(x) = A\sin(kx) + B\cos(kx)$ $\quad k = \dfrac{\sqrt{2mE}}{\hbar}$

Boundary Conditions:

$$\psi(0) = 0 \quad \Rightarrow \quad B = 0 \quad \Rightarrow \quad \psi(x) = A\sin(kx)$$

$$\psi(L) = 0 \quad \Rightarrow \quad A\sin(kL) = 0 \quad \Rightarrow \quad kL = n\pi$$

Infinite Potential Well: Particle in a Box

step 5 Use B.C. to solve for quantized energies

$\psi(L) = 0 \Rightarrow kL = n\pi$ where $k = \frac{\sqrt{2mE}}{\hbar}$

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

Tidy up solution: $\psi(x) = A\sin(kx)$ where $kL = n\pi$

$$\Rightarrow \psi_n(x) = A\sin\left(\frac{n\pi x}{L}\right)$$

Infinite Potential Well: Particle in a Box

step 6 Use normalization to solve for constant A

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

Integrate over domain from 0 to L and solve for A:

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

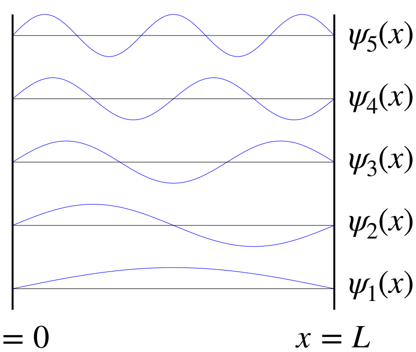
Use $\int \sin^2 ax dx = \frac{x}{2} - \frac{\sin(2ax)}{4a}$ to find $A = \sqrt{\frac{2}{L}}$

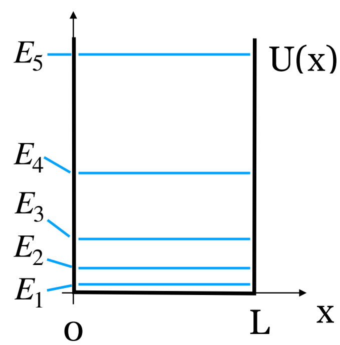
Infinite Potential Well: Particle in a Box

step 6   Combine final results

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

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





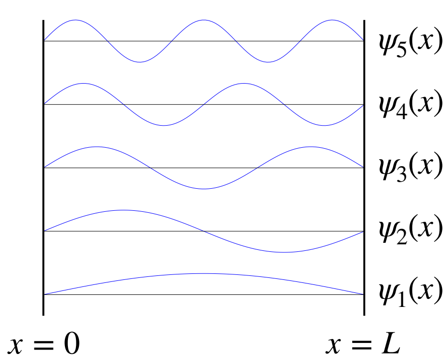
Infinite Potential Well: Particle in a Box

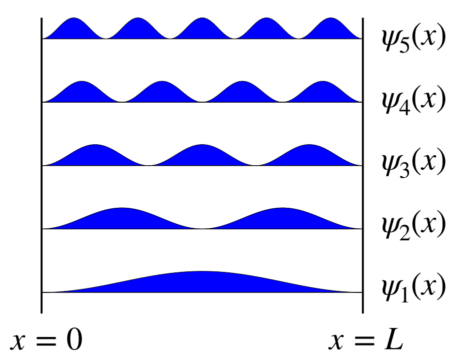
Wave Function

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

Probability Density

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



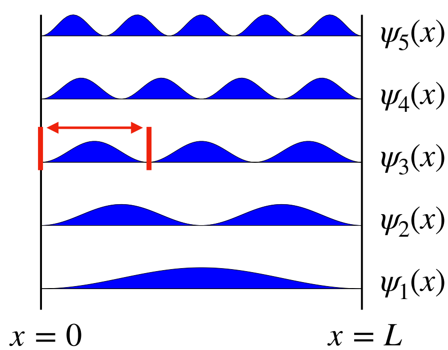


Problem

Calculate the probability of finding the particle between $0 < x < L/3$ for the n = 3 state.

$$P = \int_0^{L/3} |\psi_n(x)|^2 = \int_0^{L/3} \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right) dx$$

$$P = \frac{1}{3}$$

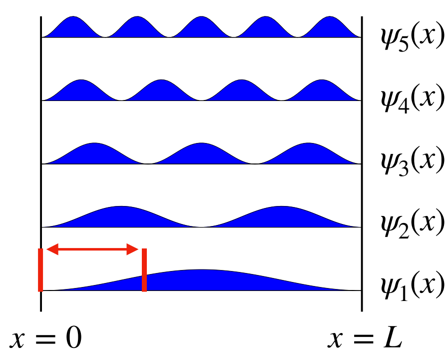


Problem

Calculate the probability of finding the particle between $0 < x < L/3$ for the n = 1 state.

$$P = \int_0^{L/3} |\psi_n(x)|^2 = \int_0^{L/3} \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right) dx$$

$$P = ?$$



Summary

We have solved the time-independent Schrödinger equation for the infinite potential well. Here are some key points:

- The solution is an infinite sequence of standing waves $\psi_n(x)$, each with energy E_n
- These solutions are called the quantum states of the infinite potential well.
- The integer n is the quantum number that labels the states.
- The quantum number n equals the number of half wavelengths present in the standing wave function. As n increases, one must “squeeze in” more wavelengths, thus increasing the particle energy.