A particle constrained in a box.

Let's imagine that we put a particle in a box, what then is its wave function?

We need to solve Schrödinger's equation,

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

but what is \( U(x) \)?

If it is held in the box, then it looks like

\[ U(x) = \begin{cases} 0, & \text{for } 0 < x < L \\ \infty, & \text{otherwise} \end{cases} \]

\[ \Rightarrow \text{free particle in jail} \]

This is often called an infinite square well potential. With this \( U(x) \), we can then proceed to solve the Schrödinger equation...
Well, the particle is in the box, so it is not outside the box.

\[ \Rightarrow \psi(x) = 0 \quad \text{for} \quad x \leq 0 \neq x \geq L \]

That is easy.

And, we've already solved the \( V(x)=0 \) case:

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi(x) \]

\[ \Rightarrow \psi(x) = A e^{ikx} \]

\[ \frac{d\psi}{dx} = iAk e^{ikx} \]

\[ \frac{d^2\psi}{dx^2} = i^2Ak^2 e^{ikx} = -k^2\psi(x) \]

\[ \Rightarrow \frac{\hbar^2}{2m} k^2 = E \quad \Rightarrow \]

Fine, but what are \( k \) and \( E \)? They are not so simply definite now, because of the boundary conditions.
The boundary conditions are that \( \psi(x) = 0 \) at \( x = 0 \) and \( x = L \). It must continuously match that inside... just as in classical physics.

(Note that normally \( \frac{d\psi(x)}{dx} \) should normally also be continuous just as velocity is except when acceleration \( \to \infty \) at an infinite

F, i.e., \( \frac{du}{dx} \to \infty \). Our walls do that.)

We can make \( \psi(x) = A e^{ikx} = 0 \) at \( x = 0 \) \& \( x = L \) only by making \( A = 0 \). \( \Rightarrow \) particle is nowhere.

As before, we can generalize the solution to

\[
\psi(x) = A_1 e^{ikx} + A_2 e^{-ikx}
\]

You should see that this still satisfies the Schrödinger equation with

\[
\frac{\hbar^2 k^2}{2m} = E
\]

it is just two waves in opposite directions.

Does it now satisfy the boundary conditions?
\[ \psi(x=0) = 0 = A_1 e^0 + A_2 e^0 \]

\[ \Rightarrow A_2 = -A_1 \]

\[ \psi(x=L) = 0 = A_1 e^{i k L} - A_1 e^{-i k L} \]

\[ \Rightarrow e^{i k L} = e^{-i k L} \]

\[ \cos(kL) + i \sin(kL) = \cos(kL) - i \sin(kL) \]

\[ \sin(kL) = -\sin(kL) \]

\[ \Rightarrow \sin(kL) = 0 \]

So, \[ kL = n \pi \quad n = 1, 2, 3, \ldots \]

\[ k = \frac{n \pi}{L} \]

\[ \frac{2\pi}{\lambda} = \frac{n \pi}{L} \quad \Rightarrow \quad \lambda = \frac{2L}{n} \]

This is just like standing waves on a string! Of course, because it is just two waves with the same \( \lambda \) moving in opposite directions.
Let's write out \( \psi \) fully now.

\[
\psi(x) = A_1 e^{ikx} - A_2 e^{-ikx}
\]

still use \( k \) for brevity.

\[
= A_1 \left[ \cos kx + i \sin kx - \cos kx + i \sin kx \right]
\]

\[
= 2iA_1 \sin kx = 2iA_1 \sin \left( \frac{n\pi x}{L} \right)
\]

\[
= C \sin \frac{n\pi x}{L}
\]

where we just replaced the constant \( 2A_1 i \) by \( C \). \( C \) is of course complex, but no prob we'll get used to them all being complex, \( A_1 \), too.

The probability density, though, is real.

Using the complex conjugate guarantees that.

So, we find \( C \) by normalization:

\[
1 = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = \int_{-\infty}^{\infty} \psi(x)^* \psi(x) \, dx
\]

\[
= \int_0^L |C|^2 \sin^2 \frac{n\pi x}{L} \, dx = \frac{|C|^2}{L} \int_0^L \left( 1 - \cos \frac{2n\pi x}{L} \right) \, dx
\]

\[
1 = \frac{1}{2} |C|^2 \left[ x + \sin \frac{2n\pi x}{L} \right]_0^L
\]

\[
2 = |C|^2 \left[ L + \sin \frac{2n\pi L}{L} \right]_0^0
\]
\[ |c|^2 = \frac{2}{L} \]

\[ C = \sqrt{\frac{2}{L}} \]

\[ \psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad n = 1, 2, 3, \ldots \quad 0 \leq x \leq L \]

\[ \psi_n = 0 \quad \text{for} \quad x < 0 \quad \text{or} \quad x > L \]

One more thing, \[ E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left( \frac{n\pi}{L} \right)^2 \]

\[ \Rightarrow E_n = \frac{n^2 \pi^2 \hbar^2}{2amL^2} \quad n = 1, 2, 3, \ldots \]

These are energy levels like we found in the hydrogen atom. They "fall out" of Schrödinger's equation because it has wave solutions and we get "harmonics" as in standing waves.
Note that the energy levels,

\[ E_n = \frac{n^2\pi^2\hbar^2}{2amL^2} = \frac{n^2\hbar^2}{8amL^2} \]

is somewhat reminiscent of the energy levels in a hydrogen atom, \( E = \frac{m^2a^4}{8\hbar^2 n^2a^2} \).

The form differs because the potential energy shape differs, but \((nh)^2 \Rightarrow quantized\) energy levels in both cases.

The energy levels arise from the wave nature of particles --- we are not surprised to find standing waves on a string --- same math.

Notice that \( E \neq 0 \). If \( n > 0 \), that is if the wave exists (the particle exists), then \( E > 0 \).

\( E_1 \) is called the "zero point energy," because it is the lowest possible energy. It is not zero!

That makes sense from the uncertainty principle because \( \Delta x = L \Rightarrow \Delta p = \frac{\hbar}{L} \) which is not zero.

If \( E = 0 \Rightarrow p = 0 \) then \( \Delta x \rightarrow \infty \) which is not possible in a box.
Now, let's think about the probability density. For \( n=1 \), what is the most likely position to find the particle? In the middle.

\[
P(x) = \left| \psi(x) \right|^2 = \frac{2}{L} \sin^2 \frac{n \pi x}{L}
\]

For \( n=2 \), what is the most likely position?

\[
\left| \psi \right|^2 = \begin{cases} 1 & 0 \leq x \leq \frac{L}{2} \\ 0 & \frac{L}{2} < x < L \end{cases}
\]

Equally likely on the two halves. Zero probability at exact center.

As \( n \to \infty \) the probability distribution goes to high frequency and \( \int \sin^2 \frac{n \pi x}{L} dx \to \frac{1}{2} \) for any non-zero range of integration.

\( n \to \infty \) corresponds to the classical limit, where we expect the particle to be found with uniform probability.

\[
\left| \psi \right|^2 = \frac{2}{L} \sin^2 \frac{n \pi x}{L} \to \frac{2}{L} \cdot \frac{1}{2} = \frac{1}{L} \text{ as } n \to \infty
\]