The ∞ square well

Austin Brandenberger

Introduction:

This project was meant to explore what happens to the probability function of a moving particle inside an infinite square well.

To do this, I had to make use of the concepts gone over in the first two months of a semester intro to quantum mechanics class. Since much of this report will not make sense without a foundational knowledge of the concepts involved, I will briefly outline them to explain what I'm doing. Note that the context given is meant to be a rough outline of the mathematics and background that went into my results, not a comprehensive explanation. To produce an explanation that would do these subjects justice would require a few chapters in a textbook. Once the background information is given, I will go into more detail to explain the mathematics and concepts that describe the infinite square well.

I bounced ideas off Zach Blogg, Kyle Laskowski, and Desmond Walker

Context:

De Broglie

Light has a sort of wave particle duality. In some experiments it is observed to act like a wave (ex: double slit experiment), and in others it acts like a particle (ex: photoelectric effect). In 1924 Louis de Broglie introduced the idea of matter having a wave-particle nature and this phenomenon was later observed in the Davisson-Germer experiment that identified wave-like properties in electrons.

Around the same time, the challenge, taken on by Erwin Schrödinger and Werner Heisenberg, became to quantitatively represent these "matter waves," and that is where the Schrödinger equation comes in.

Schrödinger's equation

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

Here, Schrödinger uses $\Psi(x,t)$ to represent the wave function that describes the wave-like properties of matter.

This is the time dependent Schrödinger equation. For my case $V = V(x)$ (The potential energy is only dependent upon position), which means we can use the time-independent Schrödinger equation.

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

Where:

$$\Psi(x,t) = \psi(x) * e^{\frac{-iE_n}{\hbar}t}$$

The infinite square well:

Now that I've briefly talked about the tools I'm using, it's time to talk about how I applied them to the physical situation. In this exploration, I am considering an infinite square well where the potential is 0 between two bounds and ∞ elsewhere. I have some given initial distribution and the goal is to find $\Psi(x,t)$ to see what happens to that distribution as time varies. To start, it will be important to find $\psi(x)$, the time independent solution, and then make our way to $\Psi(x,t)$, the time dependent solution. Note that this computational project considers a square well centered at 0 where $V(x) = 0 \; if \; -\frac{a}{2} \leq x \leq +\frac{a}{2}$. Since the location of the square well is essentially arbitrary, I will use x = 0 and x = a as the lower and upper bounds for the derivation of $\psi(x)$, and then introduce a shift in the end to rectify this.

$$V(x) = \; 0 \; if \; 0 \leq x \leq a \; \; and \; \infty \; otherwise$$

$$\Psi(x,0) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} e^{ik_0x-\alpha x^2}$$

(The initial distribution/wavefunction at t = 0)

where $\alpha \neq a$ and k_0, α are positive, real constants

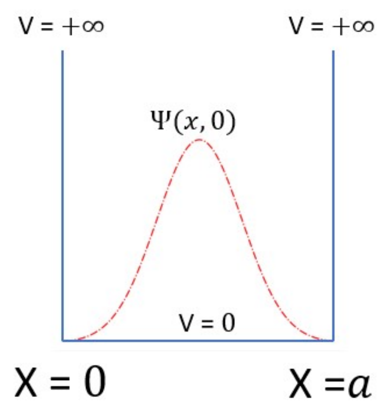

Figure 1: A visualization of the infinite square well

This situation requires that $\psi(x)$ is zero at the bounds (because there is no probability of finding a particle elsewhere) and that $\psi(x)$ is normalizable. The normalization condition comes from the Born interpretation of $\psi(x)$ where $\psi^*(x)\psi(x)$ (* denote a complex conjugate) is the probability of finding the particle at x, ranging in value from 0 to 1. If you look everywhere from $x \; = \; \pm \infty$, all the individual probabilities must add up to 1, because the particle necessarily must be somewhere if it is to exist.

Formalizing the normalization and boundary conditions:

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

$$\psi(x=a) = 0$$

$$1 = \int_{x=-\infty}^{x=+\infty} \psi^*(x)\psi(x)\ dx$$

From here, we make use of the time independent Schrödinger's equation to find a general solution for $\psi(x)$. Starting off, we recognize that the particle must be in the box because the potential is infinite everywhere else. Since a particle cannot have infinite energy, it will never be able to be in a region other than the box where $V(x) = 0$.

The time independent Schrödinger's equation becomes:

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

Solving for $\frac{d^2}{dx^2}\psi(x)$

$$\frac{d^2}{dx^2}\psi(x) = -\ k^2\psi$$

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

From here, this is a 2nd order differential equation whose solution is of the form:

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

Now that we have a general solution for $\psi(x)$, we can apply our initial conditions to gain insight into the three unknown constants: A, B and E where $E = \frac{k^2\hbar^2}{2m}\left(recall\ k = \frac{\sqrt{2mE}}{\hbar}\right)$

If $\psi(x\ =\ 0)\ =\ 0$, then:

$$\psi(0) = 0 =\ A + B$$

$$A =\ -B$$

Applying $A =\ -B$ to our general solution:

$$\psi(x) = A(e^{ikx} - e^{-ik}\ )$$

From here we can use Euler's relationship to expand $\psi(x)$:

$$Eulers \rightarrow e^{i\theta} = cos\ cos\ (\theta)\ + isin(\theta)$$

$$\psi(x) = A[cos\ (kx)\ + isin(kx) - (cos\ (kx)\ - isin(kx)]$$

Then $\psi(x)$ becomes:

$$\psi(x) = 2iAsin(kx)$$

This form reduces our unknowns from 3 to 2, leaving only A and E. From here we can use this form and apply our second boundary condition.

If $\psi(x = a) = 0$, then:

$$\psi(a) = 0 = 2iAsin(ka)$$

$$2iAsin(ka) = 0$$

Here, we know $A \neq 0$ otherwise $\psi(x) = 0$ and that solution does not help us any. Therefore $sin\ (kx)\ = 0$.

$sin\ (ka)\ = 0$ if and only if $ka = n\pi$, where $n = 0, 1, 2, \ldots$

From $ka = n\pi$ we get the following:

$$k = \frac{n\pi}{a}$$

$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{a}$$

Solving for E:

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

We see here that the energy of this particle can't be just any energy, it is specified by certain values of n, or energy levels. In other words, the energy of a particle in a box is quantized and so is the wave function [$\psi(x) = \ \psi_n(x)$]

From here, we can apply the normalization condition to $\psi_n(x)$ to find A

$$1 = \int_{x=-\infty}^{x=+\infty} \psi_n^*(x)\psi_n(x)\ dx$$

Expanding this, it becomes:

$$1 = \int_{x=-\infty}^{x=0} \psi_n^*(x)\psi_n(x)\ dx\ + \int_{x=0}^{x=a} \psi_n^*(x)\psi_n(x)\ dx\ + \int_{x=a}^{x=+\infty} \psi_n^*(x)\psi_n(x)\ dx$$

Since a particle cannot be outside of the box, the integrals from -∞ to 0 and from a to +∞ are equal to zero (there is no chance of finding one there). So this integral becomes:

$$1 = \int_{x=0}^{x=a} \psi_n^*(x)\psi_n(x)\ dx$$

Let's quickly look at $\psi^*(x)\psi(x)$:

$$\psi_n(x) = 2iAsin(kx)$$

$$\psi_n^*(x) = \ -2iA^*sin(kx)$$

So $\psi_n^*(x)\psi_n(x) = 4A^*Asin(kx)$

It is interesting to note that $\psi_n^*(x)\psi_n(x)$ is real and positive. That will come into play later.

Throwing that into our normalization condition:

$$1 = 4A^*A\int_{x\,=\,0}^{x\,=\,a} \sin^2(kx)\ dx$$

To perform this integration, it is helpful to make use of the trigonometric identity $sin^2(\theta) = \frac{1}{2} - cos\,(2\theta)$

This will result in:

$$1 = (2a)A^*A$$

So $A = \sqrt{\frac{1}{2a}} * e^{i\phi}$ where $\phi = \frac{3\pi}{2}$ and $e^{i\phi} = -i$

Note that when calculating $\psi_n^*(x)\psi_n(x)$ the complex part goes away (that is, it doesn't matter), so I have chosen $e^{i\phi}$ to do that for me when applying A to $\psi(x)$.

$$A = -i * \sqrt{\frac{1}{2a}}$$

From here we can substitute A into $\psi(x)$ and we have our time independent solution for the infinite square well:

$$\psi_n(x) = \sqrt{\frac{2}{a}} sin\ (kx)\ where\ k = \frac{n\pi}{a}$$

<u>Finding</u> $\Psi\ (x,t)$**:**

The above, $\psi_n(x)$, will give me the time independent solution for a particle in the infinite square well, but what I am after is something with time dependence,$\Psi_n(x,t)$. From earlier, $\Psi_n(x,t\ ) = \psi_n(x)e^{-\frac{iE_n}{\hbar}t}$:

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} sin\ (kx)\ e^{-\frac{iE_n}{\hbar}t}$$

Looking at $\Psi_n^*(x,t)\Psi_n(x,t)$:

$$\Psi_n^*(x,t)\Psi_n(x,t) = \frac{2}{a}\sin^2(kx)$$

From this, we can see that our time dependence dropped out which is an issue.

If you try to find the expectation value for the average position:

$$\langle x\rangle = \int_{x\,=\,0}^{x\,=\,a} \Psi_n^*(x,t)x\Psi_n(x,t)\ dx$$

$$\langle x\rangle = \frac{2}{a}\int_{x\,=\,0}^{x\,=\,a} \mathrm{x}\sin^2(kx)\ dx$$

Performing these integral yields:

$$\langle x \rangle = \frac{a}{2}$$

This is significant because there does not seem to be any time dependence on $\langle x \rangle$. Furthermore $\langle p \rangle = \frac{md\langle x \rangle}{dv} = 0$

This is a problem because for the particle in the well, it has a set energy where $E = K + V$

If $\langle p \rangle = 0$ then $\langle K \rangle = 0$. Since V is also equal to 0 inside the well, that means the particle has no energy, even if $E_n \neq 0$. Considering this, it is clear that $\Psi_n(x,t)$ is not quite what we're looking for, and to get a true time dependent solution, we will have to go further.

Perhaps the wave function should not be limited to one energy. Let's try adding together wave functions with energy where n = 1 and n =2→ $\Psi(x,t) = A[\Psi_1(x,t) + \Psi_2(x,t)]$. Does a linear combination of multiple $\Psi_n(x,t)$ terms result in a time dependent solution?

Let's look at this:

From earlier $\Psi_n(x,t) = \psi_n(x)e^{-\frac{iE_n}{\hbar}t} = \sqrt{\frac{2}{a}} sin\ (kx)\ e^{-\frac{iE_n}{\hbar}t}$

So $\Psi(x,t) = A[\Psi_1(x,t) + \Psi_2(x,t)]$ becomes:

$$\Psi(x,t) = A\sqrt{\frac{2}{a}}\left(sin\ \left(\frac{1\pi}{a}x\right)\ e^{-i1w_0t} + sin\left(\frac{2\pi}{a}x\right)e^{-i4w_0t}\right)$$

Where $w_0 = \frac{\pi^2\hbar}{2ma^2}$

Taking its complex conjugate:

$$\Psi^*(x,t) = A^*\sqrt{\frac{2}{a}}\left(sin\ \left(\frac{1\pi}{a}x\right)\ e^{i1w_0t} + sin\left(\frac{2\pi}{a}x\right)e^{i4w_0t}\right)$$

And then $\Psi^*(x,t)\Psi(x,t) = A^*A\left(\frac{2}{a}\right)\{\left(\frac{1\pi}{a}x\right) + \left(\frac{2\pi}{a}x\right) +$

$$sin\ \left(\frac{1\pi}{a}x\right)\ sin\ \left(\frac{2\pi}{a}x\right)\ [e^{-i3w_0t} + e^{i3w_0t}]\}$$

If you normalize this and find A, you will find $A = \frac{1}{\sqrt{2}}$ and that $\Psi(x,t)$ is a superposition of the two different states.

Through all that, notice that this time $\Psi^*(x,t)\Psi(x,t)$ has retained its time dependence. Perhaps $\Psi(x,t)$ is the sum of <u>every</u> $\Psi_n(x,t)$? With this in mind, we can move forward.

Since $\Psi(x,t)$ was found to be the sum of different $\Psi_n(x,t)$'s:

Let: $\Psi(x,t) = C_n\Psi_n(x,t)$ where $\Psi_n(x,t) = \psi_n(x)e^{-\frac{iE_n}{\hbar}t}$

So:

$$\Psi(x,t) = \sum_{n=1}^{\infty} C_n \psi_n(x) e^{-\frac{iE_n}{\hbar}t}$$

To find our solution for $\Psi(x,t)$ we will need to find our coefficients, C_n. To do this we will first set t equal to 0

$$\Psi(x,0) = \sum_{n=1}^{\infty} C_n \psi_n(x)$$

Then, multiply both sides by $\psi_j^*(x)$where $j = 1, 2, 3, \ldots$.

$$\psi_j^*(x)\Psi(x,0) = \sum_{n=1}^{\infty} C_n \psi_n(x)\psi_j^*(x)$$

From there, integrate both sides with respect to x from x = 0 to x = a

$$\int_{x=0}^{x=a} \psi_j^*(x)\Psi(x,0)\, dx = \int_{x=0}^{x=a} \sum_{n=1}^{\infty} C_n \psi_n(x)\psi_j^*(x) dx$$

It is at this point that I want to make a diversion into something called the Kronecker delta. This comes up where we consider $\int_{x=0}^{x=a} \psi_j^*(x)\psi_n(x)\, dx$ and investigate the case where $j = n$ and $j \neq n$. With $\psi_n(x) = \sqrt{\frac{2}{a}} sin\,(\frac{n\pi}{a}x)$ we can perform the integral described above for the two different situations and we find that $j = n$ produces a value of 1, which is not entirely surprising because that matches our normalization condition, and $j \neq n$ equals zero. From here, we can conclude that $\int_{x=0}^{x=a} \psi_j^*(x)\psi_n(x)\, dx = \delta_{n,j} = \begin{cases} 0 \; if \; j \neq n \\ 1 \; if \; j = n \end{cases}$

Applying this to our stopping place from earlier produces the following:

$$\int_{x=0}^{x=a} \psi_j^*(x)\Psi(x,0)\, dx = \sum_{n=1}^{\infty} C_n \int_{x=0}^{x=a} \psi_j^*(x)\psi_n(x)\, dx$$

$$\int_{x=0}^{x=a} \psi_j^*(x)\Psi(x,0)\, dx = \sum_{n=1}^{\infty} C_n \delta_{n,j}$$

Going through the sum, the only term that is not zero is the case where $n = j$ so:

$$\int_{x=0}^{x=a} \psi_j^*(x)\Psi(x,0)\, dx = C_j$$

This is the integral that allows us to find the coefficient for some particular $\Psi_n(x,t)$ and it has no analytical solution. Subbing our solution for C_j $(where\ j = n)$ into our initial expression we get:

$$\Psi(x,t) = \sum_{n=1}^{\infty} \int_{x=0}^{x=a} \psi_n^*(x)\Psi(x,0)\, dx \psi_n(x) e^{-\frac{iE_n}{\hbar}t}$$

Recall $\Psi(x,0) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} e^{ik_0x-\alpha x^2}$ and $\psi(x) = \sqrt{\frac{2}{a}}\, sin\left(\frac{n\pi}{a}x\right)$

So $\Psi(x,t)$ becomes:

$$\Psi(x,t) = \left(\frac{2}{a}\right)\left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \sum_{n=1}^{\infty} \int_{x=0}^{x=a} sin\left(\frac{n\pi}{a}x\right)\, e^{ik_0x-\alpha x^2}\, dx\;\, sin\left(\frac{n\pi}{a}x\right)\, e^{-\frac{iE_n}{\hbar}t}$$

Earlier I stated that the location of the infinite square well was arbitrary and made my bounds x = 0 and x = a, but the computational project specifically denotes a well centered at 0. To fix this issue I am going to shift all the x values in $\psi_n(x)$ by $\frac{a}{2}$ to match the new bounds

Our new expression becomes:

$$\Psi(x,t) = \left(\frac{2}{a}\right)\left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \sum_{n=1}^{\infty} \int_{x=-\frac{a}{2}}^{x=\frac{a}{2}} sin\left(\frac{n\pi}{a}\left(x+\frac{a}{2}\right)\right)\, e^{ik_0x-\alpha x^2}\, dx\;\, sin\left(\frac{n\pi}{a}\left(x+\frac{a}{2}\right)\right)\, e^{-\frac{iE_n}{\hbar}t}$$

This is the time dependent solution to the infinite square well. To obtain something meaningful, I utilized python to calculate the solution for further analysis.

The code has the following structure:

1. Calculate the coefficients using numerical integration (Simpson's rule).
2. Calculate each $\Psi_n(x,t)$
3. Sum up each $\Psi_n(x,t)$ to find $\Psi(x,t)$ for some given time
4. Change the time and repeat the process

Analysis:

So, beyond the pure mathematics of it all, what does this solution look like, how can I know it is correct, and what meaning can be gathered from it?

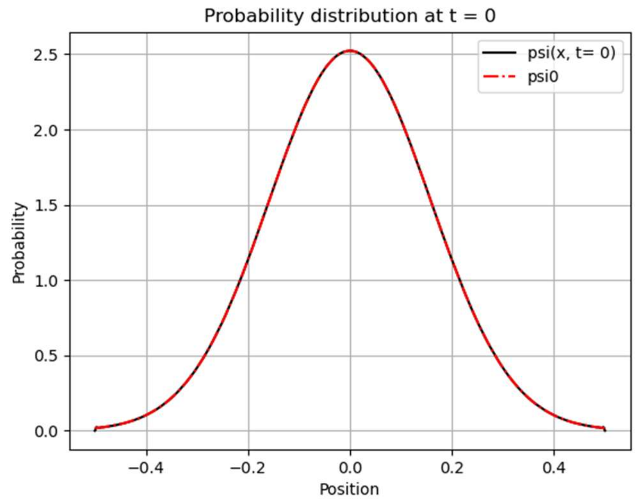

Figure 2: probability of $\Psi(x, t = 0)$ vs $\Psi(x, 0)$

To see if my solution for $\Psi(x, t)$ was correct and to ensure that my program was functioning as intended, I compared my given initial distribution to solved distribution at t = 0 on the same plot. We can see here that they are identical, and I can be confident that my computational method for finding $\Psi(x, t)$ is valid.

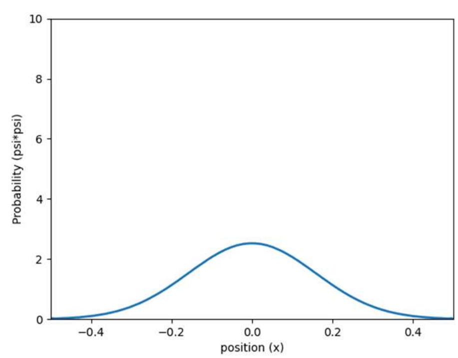

Figure 3: A GIF of $\Psi(x, t)$ as time progresses. The x axis is position, and the y axis is probability ($\Psi^*\Psi$). $a = 1, \alpha = 10$, and $k_0 = 100, t0 = 0, tf = 1500$

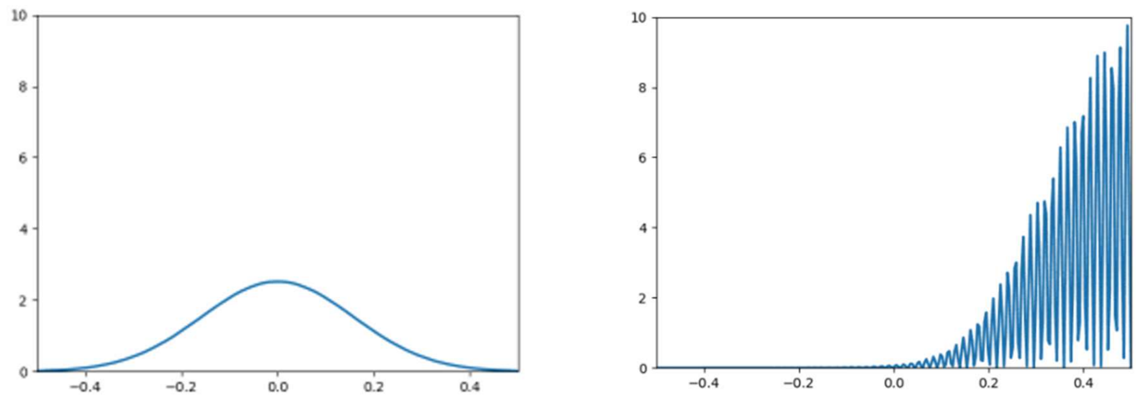

Figure 4: A side by side view of the initial probability distribution and the distribution as it interacts with the bounds.

The above is an animation of $\Psi(x,t)$ and a few snapshots to show the spatial distribution and the temporal changes of the probability function.

$\Psi(x,0)$ describes the initial conditions/distribution of atoms. At t = 0, the particle in its different states is most likely to be found in the middle and is moving towards the right wall. When the concept of the wave function was first introduced it was born out of the wave-particle duality of matter. This duality was later verified when electrons were shot through a slit and the pattern they made on a screen was one that mimicked the interference pattern of light. Matter can't really interfere with itself though as it can't construct or destruct in the same way a conventional wave can, so the wave function began to be understood as something that described the probability of a particle to be in a certain location. When we look at the animation above, we can see a clear distribution at t = 0. It appears that the particle has a range of possible places it can be, all localized within this condensed distribution. When the wavefunction starts moving, this distribution begins to change, and by the time it gets to the wall, it looks vastly different from the initial distribution. At t =0 there is a chance of finding a particle everywhere inside the square well but once the distribution reaches the wall, there are places where there is no chance of finding the particle. These places where the probability goes to zero represent interference patterns of matter. As time goes on further still, it eventually reaches a state where the probability function appears to be a wave instead of the starting gaussian. Using quantum mechanics, we have described the matter interference phenomenon that was observed experimentally.

Conclusion:

When interference patterns were observed with electrons it was confounding because matter can't interfere with itself. With quantum mechanics we see these interference patterns manifest through a probability distribution and have described the mechanism that causes said patterns. This is the main insight of the particle in a box problem and the computational program that provided a visualization of this process was the most valuable aspect of this exploration.