To:	Professor Grove
From:	Mason Averill
Subject:	PHYS-442: Computational Project
Date:	10/15/2021

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Purpose

The purpose of this memo is to communicate the results of the *Computational Project: Infinite Square Well* for PHYS-442: Quantum Mechanics, completed October 15th 2021. This project was individually completed.

Problem Statement

The purpose of this project was to numerically solve an infinite square well problem. More specifically, an animation showing the probability density function (representative of the probability of a particle assuming any position inside of the square well) versus time was requested. An initial condition for the wave function, bounds of the square well, and conditions for the potential energy inside and outside of the square well are shown by Equations 1-2.

$$\Psi(x,0) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \exp[ik_0 x - \alpha x^2] \qquad -\frac{a}{2} < x < \frac{a}{2} \qquad \alpha, k_0 \in \mathbb{R}$$ Equation 1

$$V = \begin{cases} 0, & \text{if } |x| < \frac{a}{2} \\ \infty, & \text{otherwise} \end{cases}$$ Equation 2

Analytical Solution

The partial differential equation that $\Psi(x,t)$ must satisfy is shown by Equation 3. This equation is referred to as the Schrodinger Equation.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$ Equation 3

$\Psi(x,t)$ must also satisfy the property shown in Equation 4 if it is to represent a probability density function. The physical interpretation of this equation is that if you were to look everywhere that the particle could be, then you will find the particle.

$$\int_{-\infty}^{\infty} \Psi^*\Psi \, \mathrm{dx} = \int_{-\frac{a}{2}}^{\frac{a}{2}} \Psi^*\Psi \, \mathrm{dx} = 1$$ Equation 4

By assuming that $\Psi(x,t) = \psi(x) * f(t)$, Equation 3 can be re-written as shown by Equation 5. It is important to note that the LHS of Equation 5 is only dependent upon x, and the RHS of Equation 5 is only dependent upon t. Realizing this, the only way that equality between the LHS and RHS of Equation 5 can hold is if both are equal to the same constant, which is denoted as E.

$$-\frac{\hbar^2}{2m} * \frac{1}{\psi} * \frac{d^2\psi}{dx^2} = \mathrm{i}\hbar\frac{df}{dt} = E \qquad \text{Equation 5}$$

Since the LHS of Equation 5 is independent from the RHS, $\psi(x)$ and $f(t)$ can be solved separately. The general solution for $f(t)$ is shown by Equation 6, where C_3 is some undetermined constant.

$$f(t) = C_3 * exp(\frac{-iE}{\hbar} * t) \qquad \text{Equation 6}$$

One can then verify that E must be greater than 0 to satisfy the boundary conditions shown in Equation 2 (it can also be shown that this constant E is proportional to energy, which also indicates that it must be greater than 0), this results in the general solution for $\psi(x)$ shown in Equation 7.

$$\psi(x) = C_1 * sin(\frac{\sqrt{2mE}}{\hbar} * x) + C_2 * cos(\frac{\sqrt{2mE}}{\hbar} * x) \qquad \text{Equation 7}$$

Using the results of Equation 6 and 7, the general solution for $\Psi(x,t)$ is shown by Equation 8.

$$\Psi(x,t) = \left[C_1 * sin(\frac{\sqrt{2mE}}{\hbar} * x) + C_2 * cos(\frac{\sqrt{2mE}}{\hbar} * x)\right] * \left[C_3 * exp(\frac{-iE}{\hbar} * t)\right] \qquad \text{Equation 8}$$

The next step in determining a specific solution for $\Psi(x,t)$ is to apply boundary conditions and an initial condition. The boundary conditions for this problem can be discovered by analyzing its physical interpretation. At x=$\pm\frac{a}{2}$, V (the potential energy) tends towards infinity. Since it is impossible for a particle to possess an infinite potential energy, this means that the probability of finding the particle at these bounds must be 0. That is, $\Psi^*\Psi$ at x=$\pm\frac{a}{2}$, must be 0. This implies that Ψ at x=$\pm\frac{a}{2}$, must be 0. This idea also further explains why the bounds in the integral shown in Equation 4 must be true. Equation 9 summarizes the boundary conditions and initial condition that must be applied to $\Psi(x,t)$ to determine a specific solution.

$$\Psi\left(\mathrm{x} = \pm\frac{a}{2}, t\right) = 0, \qquad \Psi(x,0) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \exp[ik_0x - \alpha x^2] \qquad \text{Equation 9}$$

By reviewing the boundary conditions shown in Equation 9, it is evident that a coordinate transformation will simplify the application of the boundary conditions. By shifting the domain from $-\frac{a}{2} < x < \frac{a}{2}$ to $0 < x < a$, the conditions shown in Equation 9 become those shown by Equation 10. Note that the results shown in Equation 8 are independent of this coordinate transformation.

$$\Psi(0,t) = 0, \Psi(\mathrm{a},t) = 0, \qquad \Psi(x,0) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \exp\left[ik_0(x-\frac{a}{2}) - \alpha(x-\frac{a}{2})^2\right] \quad \text{Equation 10}$$

Application of $\Psi(0,t) = 0$ is shown by Equation 11.

$$\begin{aligned}\Psi(0,t) &= \left[C_1 * sin(\frac{\sqrt{2mE}}{\hbar} * 0) + C_2 * cos(\frac{\sqrt{2mE}}{\hbar} * 0)\right] * \left[C_3 * exp(\frac{-iE}{\hbar} * t)\right] \\ &=> \Psi(0,t) = [0 + C_2] * \left[C_3 * exp(\frac{-iE}{\hbar} * t)\right] \\ &=> \Psi(0,t) = C_2 * C_3 * exp(\frac{-iE}{\hbar} * t) = 0\end{aligned} \quad \text{Equation 11}$$

If C_3=0, then $f(t)$ constantly equals 0, which causes $\Psi(x,t)$ to constantly be 0. This solution for $\Psi(x,t)$ cannot satisfy Equation 4 (the physical interpretation of this would be that the particle isn't anywhere in the box, which is clearly unacceptable), so C_2 must equal 0.

Application of $\Psi(\mathrm{a},t) = 0$ is shown by Equation 12.

$$\Psi(a,t) = \left[C_1 * sin(\frac{\sqrt{2mE}}{\hbar} * a)\right] * \left[C_3 * exp(\frac{-iE}{\hbar} * t)\right] = 0 \quad \text{Equation 12}$$

As was previously discussed, $C_3 \neq 0$, and if $C_1 = 0$, then the same issue as before arises, except now $\psi(x)$ constantly equaling 0 causes the issue. The only other way equality can be met for Equation 12 is if the argument of sin causes equality. This condition is shown by Equation 13.

$$\begin{aligned}&\Psi(a,t) = sin\left(\frac{\sqrt{2mE}}{\hbar} * a\right) = 0 \\ &=> \frac{\sqrt{2mE}}{\hbar} * a = n\pi \quad where\ n \in \mathbb{N}^+ \\ &=> \frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{a} \\ &=> E = \frac{n^2\pi^2\hbar^2}{2 * m * a^2}\end{aligned} \quad \text{Equation 13}$$

$\Psi(x,t)$ can now be written as shown by Equation 14.

$$\Psi(x,t)_n = C_n * sin(\frac{n\pi}{a} * x) * exp(\frac{-i * n^2\pi^2\hbar}{2 * m * a^2} * t) \quad \text{Equation 14}$$

Without applying the initial condition, we cannot determine each C_n. However, by using Equation 4 we can at least determine the magnitude of C_n (it is important to note that C_n may be a complex number). Equation 15 indicates the results of applying the conditions of Equation 4 (updated to the new translated coordinate system) to Equation 14.

$$\int_{-\infty}^{\infty} \Psi^*\Psi \, \mathrm{dx} = \int_0^a \Psi^*\Psi \, \mathrm{dx} = \int_0^a |C_n|^2 * sin^2(\frac{n\pi}{a} * x) \, \mathrm{dx} = 1$$

$$=> |C_n| = \sqrt{\frac{2}{a}} \quad \text{Equation 15}$$

The most general solution for $\Psi(x,t)$ satisfying the boundary conditions shown in Equation 10 and meeting the criteria of Equation 4 is shown by Equation 16 (the linear combination of all solutions possible).

$$\Psi(x,t) = \sum_{n=1}^{\infty} C_n * \sqrt{\frac{2}{a}} * sin(\frac{n\pi}{a} * x) * exp(\frac{-i * n^2\pi^2\hbar}{2 * m * a^2} * t) \quad \text{Equation 16}$$

The only step remaining to gather the full solution and solve for C_n is to apply the initial condition, which is also shown in Equation 10. There are a few methods to determine C_n, but the most straightforward method is to realize that by translating the coordinate system as was performed between Equations 9 and 10, we have transformed this problem into a Dirichlet condition for the PDE shown in Equation 3. This guarantees that a Fourier Sine Expansion can be performed to determine C_n. Equation 17 shows the Fourier Sine Expansion for the translated initial condition.

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

$$=> C_n = \sqrt{\frac{2}{a}} * \int_0^a sin\left(\frac{n\pi}{a} * x\right) * \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} * \exp\left[ik_0(x - \frac{a}{2}) - \alpha(x - \frac{a}{2})^2\right] \; dx \quad \text{Equation 17}$$

The complete solution for $\Psi(x,t)$ is then shown by Equation 18.

$$\Psi(x,t) = \sum_{n=1}^{\infty}\left[\sqrt{\frac{2}{a}} * \int_0^a sin\left(\frac{n\pi}{a} * x\right) * \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} * \exp\left[ik_0(x - \frac{a}{2}) - \alpha(x - \frac{a}{2})^2\right] \; dx\right] * \sqrt{\frac{2}{a}} * sin(\frac{n\pi}{a} * x) * exp(\frac{-i * n^2\pi^2\hbar}{2 * m * a^2} * t) \quad \text{Equation 18}$$

The only step remaining is to translate the coordinate system back to what was requested in Equation 1. The final complete solution is shown by Equation 19.

$$\Psi(x,t)_{requested} = \Psi\left(x+\frac{a}{2},t\right) \qquad -\frac{a}{2}<x<\frac{a}{2} \qquad \text{Equation 19}$$

In summary, this solution process translated the coordinate system such that the PDE shown in Equation 3 had Dirichlet boundary conditions, allowing for a relatively easy application of boundary conditions and a Fourier Sine Expansion to account for the initial condition. There are multiple ways to solve this problem, but this method is, at least in my opinion, the most straightforward way.

A Fourier transform of the initial condition, along with an appropriate inverse Fourier Transform could also have been completed to solve this problem. The issue with this method is that information about the nature of the solution is lost (the discretized energy levels that the Separation of Variables method reveals is critical to a complete understanding) and the integration can be difficult to perform analytically.

This problem could also have been solved without translating the coordinate system and still employing the separation of variables method, but this results in a messier solution process that ultimately leads to the same solution.

Numerical Solution

This problem was solved computationally in MATLAB. The complete script to solve this problem can be viewed in the appendix, but the overall methodology is as follows:

1. The user can input desired values for $\alpha, k_0, a, and\ m$. They can also specify the maximum number of terms to consider for the solution (n), the maximum time to consider for the animation (max_time), and the resolution to consider for the domain in position (x) and time (t).
2. The only remaining constant, $\hbar$, is assigned it's appropriate value.
3. C_n is solved for up to the requested 'n' number of terms. Numerical integration of Equation 17 is performed to compute each C_n.
4. Equation 16 is utilized to compute the linear combination of the solution $\Psi(x,t)$ up to 'n' number of terms.
5. The normalization of $\Psi(x,t)$, as computed in step 4, is checked to ensure that the resolution specified in 'x' is adequate.
6. At this point, a matrix of $\Psi^*\Psi$ values has been computed for each index in position and time. Each row in this matrix represents $\Psi^*\Psi$ at a discrete point in time.
7. The animation works by first plotting $\Psi^*\Psi$ at time equal to 0 (the first row of the matrix mentioned above). The plot is then updated using the next row of the matrix for $\Psi^*\Psi$ (the next increment in time). This updating process continues until all information in the matrix for $\Psi^*\Psi$ has been read and plotted.

How Solution Was Verified

The computational solution was verified by viewing the solution when time equals 0 and confirming that the solution displayed matches that expected from the given initial condition shown by Equation 1. Figure 1, shown below, displays $\Psi^*(\mathrm{x},0)\Psi(\mathrm{x},0)$ obtained from the computational solution. The value shown by $\Psi(x,0)$ can be easily checked when x=0. At x=0, $\Psi(x,0)$ reduces to $\left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}}$ so $\Psi^*(\mathrm{x},0)\Psi(\mathrm{x},0) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}}$, the value of α shown in Figure one is 100 (this can be viewed in Figure 1 as well). With α=100, $\left(\frac{2\alpha}{\pi}\right)^{\frac{1}{2}} \cong 8$, which confirms the results displayed by Figure 1.

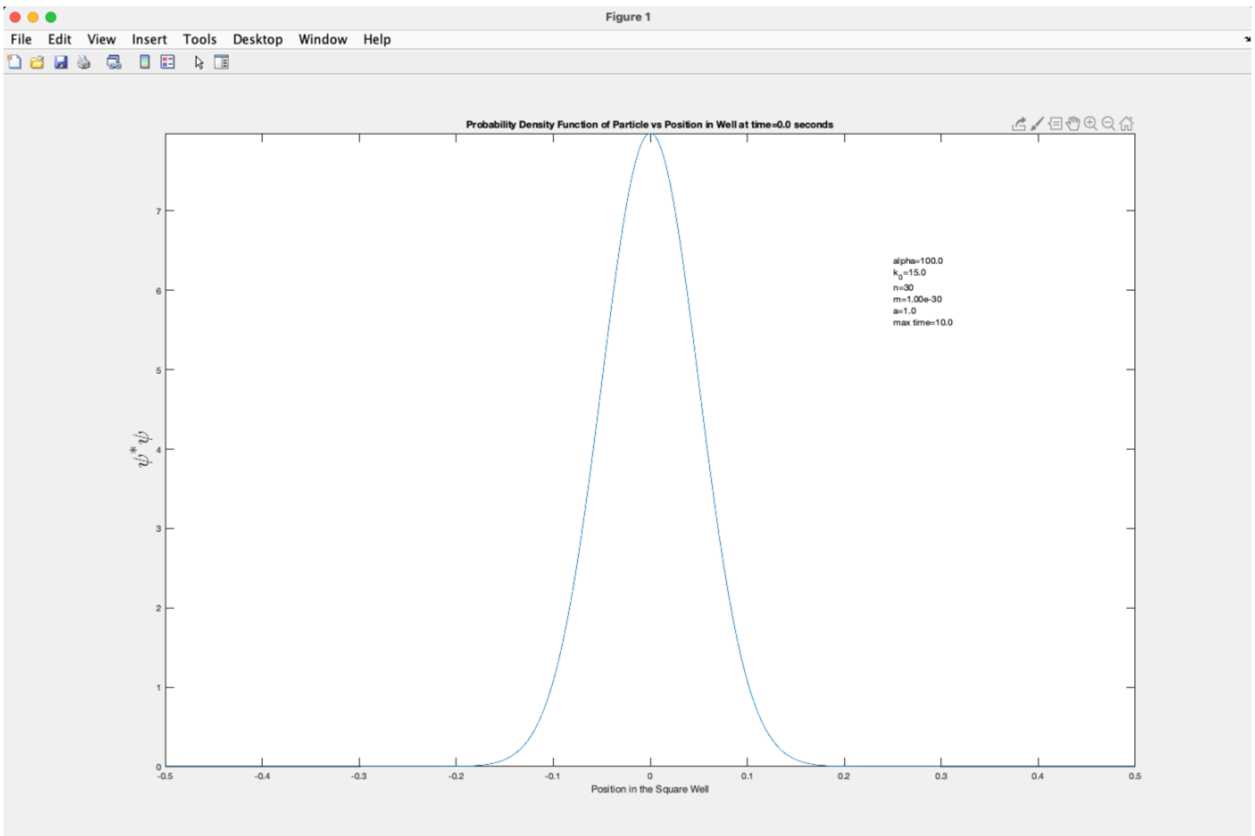


Figure 1: $\Psi(x,0)\ \Psi^*(x,0)$

In addition, the normalization of the solution was verified (i.e. confirming that the relationship shown in Equation 4 was true). Figure 2 indicates how this was computationally verified.

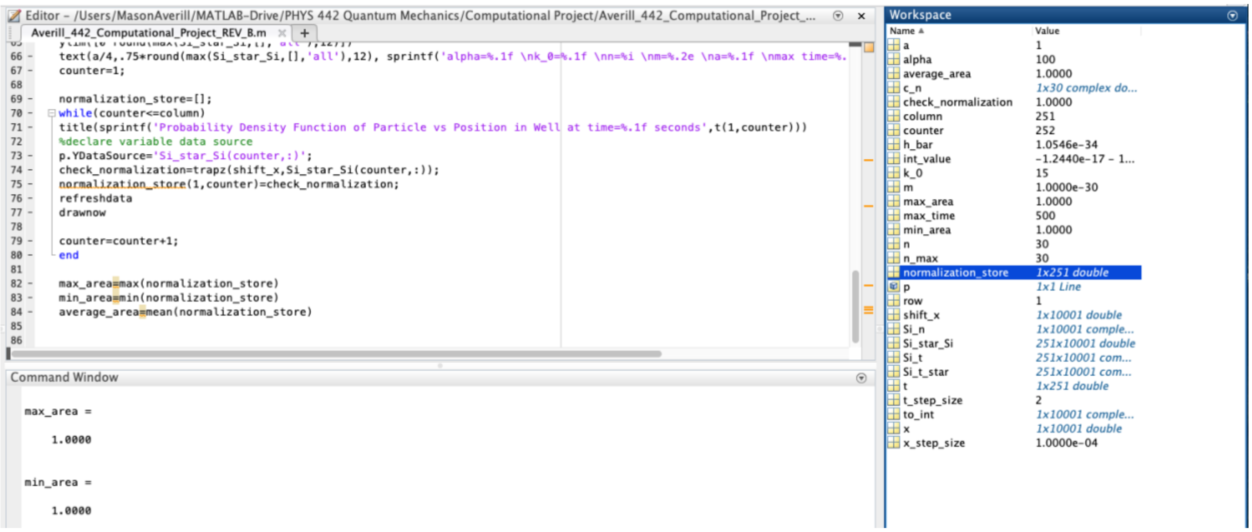


Figure 2: Normalization Checking

There are a few critical things to note about Figure 2. The first being that Figure 2 is the computational solution when $0 \leq t \leq 500$ and that the "steps" in t=2 seconds, i.e. the solution is found at t=0, 2, 4, 6, …, 500. This means that 251 different values of time were considered when computing $\Psi^*\Psi$. The normalization of $\Psi^*\Psi$ was checked for each increment in time considered by numerically integrating $\Psi^*\Psi$ over $-\frac{a}{2} < x < \frac{a}{2}$, this numerical integration can be seen in line 74 of the code displayed in Figure 2. Each normalization value was then stored in a row vector named 'normalization_store'. This means that the row vector 'normalization_store' contains the results of numerically integrating $\Psi^*\Psi$ over $-\frac{a}{2} < x < \frac{a}{2}$ for 251 different values in time. By reviewing the output shown in the command window in Figure 2, the maximum and minimum values stored in 'normalization_store' were 1.0000. This means that all values within the vector had to obtain a value of 1.0000, indicating that $\Psi^*\Psi$ was correctly normalized for each value of time considered.

With the initial condition matching the computational solution and the normalization of $\Psi^*\Psi$ checked, one can confidently conclude that the computational solution is accurate.

Video Analysis

The video shown consists of the following parameters: $\alpha = 100\,, k_0 = 15, n = 30, m = 10^{-30}, and\ a = 1$. Initially, as must be the case, $\Psi^*\Psi$ appears exactly as the initial condition dictates as a normal distribution centered at x=0. With a positive value for k_0 one would anticipate the "wave" shown in the video to initially be moving to the right, which is what occurs. As the "wave" approaches the right side of the infinite square well, one would anticipate that it would "reflect" off of the right side since the potential energy there is infinity (the particle cannot cross this barrier since it cannot posses infinite energy). Again, this is in fact what the video displays. The "wave" then travels towards the left side of the well where this same phenomena occurs, except this time it is reflected to the right. It is also important to note that by the time the "wave" begins to approach the left hand side, it is no longer as tightly-packed as it initially was when it approached the right hand side. Due to this, the reflection off the left hand side is not as evident as it was initially off the right hand side. This behavior continues in a manner analogous to a standing wave on a string with endpoints pinned at 0.

Conclusion

Overall, this was a very interesting project. The mathematical behavior of the wave function versus time is what I found to be the most interesting component. By observing the animation for various input variable values I found that a cyclic behavior was exhibited. After looking into this, I found this cyclic behavior is referred to as a fractional revival. While I didn't research this behavior in depth, I found the overall idea to be very interesting.

Another aspect of this project that I found was very interesting is how the math indicated only discrete values of energy were obtainable. This is especially interesting considering that this is also what has been physically determined by measurements of quantum mechanical systems.

Appendix

Analytical Solution Hand Calculations:

given BC's and IC

$$\Psi(x,0) = \left(\frac{2\alpha}{\pi}\right)^{1/4} \cdot e^{-\alpha \cdot x^2 + i k_o \cdot x}$$

$\alpha, k_o \in \mathbb{R}$ $\quad -\frac{a}{2} < x < \frac{a}{2}$

$$V = \begin{cases} 0 & \text{if } |x| < \frac{a}{2} \\ \infty & \text{else} \end{cases}$$

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

SE

$$1 = \int_{-\infty}^{\infty} \Psi^* \Psi \, dx$$

normalization

$V = V(x)$

Assume $\Psi(x,t) = \psi(x) \cdot f(t)$

$$\frac{\partial \Psi}{\partial x} = \frac{d\psi}{dx} \cdot f(t)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2\psi}{dx^2} \cdot f(t)$$

$$\frac{\partial \Psi}{\partial t} = \psi(x) \cdot \frac{df}{dt}$$

$$\frac{-\hbar^2}{2m} \cdot \frac{d^2\psi}{dx^2} \cdot f(t) = i\hbar \cdot \psi(x) \cdot \frac{df}{dt}$$

$$\frac{-\hbar^2}{2m} \cdot \frac{1}{\psi(x)} \frac{d^2\psi}{dx^2} = i\hbar \cdot \frac{1}{f(t)} \frac{df}{dt} = E$$

Time ind. SE

$$\frac{-\hbar^2}{2m} \cdot \frac{1}{\psi} \cdot \frac{d^2\psi}{dx^2} = E$$

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

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

$$r^2 + \frac{2mE}{\hbar^2} = 0 \implies r^2 = \frac{-2mE}{\hbar^2}$$

$$r = \pm\sqrt{\frac{-2mE}{\hbar^2}} \quad \text{assume } E > 0$$

$$\implies \psi(x) = c_1 \cdot \sin\left(\frac{\sqrt{2mE}}{\hbar} \cdot x\right) + c_2 \cdot \cos\left(\frac{\sqrt{2mE}}{\hbar} \cdot x\right)$$

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

$$\psi(x) = c_1 \cdot \sin(kx) + c_2 \cdot \cos(kx)$$

Time dep. SE

$$i\hbar \cdot \frac{1}{f(t)} \cdot \frac{df}{dt} = E$$

$$\frac{df}{f} = \frac{-iE}{\hbar}$$

$$\ln(f) = \frac{-iE}{\hbar} t + C$$

$$f(t) = c_3 \cdot e^{\frac{-iE}{\hbar} \cdot t}$$

$$\Psi(x,t) = \psi(x) \cdot f(t) = \left[c_1 \cdot \sin(kx) + c_2 \cdot \cos(kx)\right] \cdot \left[c_3 \cdot e^{\frac{-iE}{\hbar} \cdot t}\right]$$

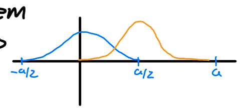
w/ $k \equiv \frac{\sqrt{2mE}}{\hbar}$ DE

general solution w/ $V(x) = 0$

BC'S: $\Psi(-\frac{a}{2}, t) = 0$

$\Psi(\frac{a}{2}, t) = 0$

This coordinate system is not ideal for BC's, so let's translate:



$\Psi(0,t) = 0$

$\Psi(a,t) = 0$

$$\Psi(x,0) = \left(\frac{2\alpha}{\pi}\right)^{1/4} \cdot e^{-\alpha \cdot (x - \frac{a}{2})^2 + i \cdot k_o \cdot (x - \frac{a}{2})}$$

IC:

$$\Psi(x,0) = \left(\frac{2\alpha}{\pi}\right)^{1/4} \cdot e^{-\alpha \cdot x^2 + i k_o \cdot x}$$

$\alpha, k_o \in \mathbb{R}$

Apply BC's:

$$\Psi(0,t) = [C_1 \cdot \sin(0) + C_2 \cdot \cos(0)] \cdot [C_3 \cdot e^{\frac{-iE}{\hbar} t}] = 0$$

$$\Rightarrow C_2 = 0$$

$$\Psi(x,t) = \psi(x) \cdot f(t) = C_1 \cdot \sin(kx) \cdot C_3 \cdot e^{\frac{-iE}{\hbar} \cdot t}$$

$$\Psi(x,t) = C_4 \cdot \sin(kx) \cdot e^{\frac{-iE}{\hbar} \cdot t}$$

$$\Psi(a,t) = C_4 \cdot \sin(k \cdot a) \cdot e^{\frac{-iE}{\hbar} \cdot t} = 0$$

$$\Rightarrow \sin(ka) = 0$$

$$\Rightarrow ka = n\pi \qquad n = 1, 2, \ldots$$

$$\Rightarrow \boxed{k = \frac{n\pi}{a} \quad n \in \mathbb{Z}}$$

recall $k \equiv \frac{\sqrt{2mE}}{\hbar}$

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

$$\Rightarrow \boxed{E = \frac{\pi^2 \hbar^2 \cdot n^2}{a^2 2m}}$$

$$\Psi(x,t) = C_4 \cdot \sin(kx) \cdot e^{-\frac{iE}{\hbar} \cdot t}$$

how to determine $|C_4|$?

Normalization

$$1 = \int_{-\infty}^{\infty} \Psi^* \Psi \, dx = \int_0^a |C_4|^2 \cdot \sin^2(kx) \, dx$$

$$\Rightarrow |C_4| = \sqrt{\frac{2}{a}}$$

so $\Psi(x,t) = \sqrt{\frac{2}{a}} \cdot \sin(k_n a) \cdot e^{\frac{-iE}{\hbar} \cdot t}$

or

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

=

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

now, to determine C_n must use IC:

$$\Psi(x,0) = \left(\frac{2\alpha}{\pi}\right)^{1/4} \cdot e^{-\alpha\cdot(x-\frac{a}{2})^2 + i\cdot K_0\cdot(x-\frac{a}{2})} = \sum_{n=1}^{\infty} C_n \cdot \sqrt{\frac{2}{a}} \cdot \sin\left(\frac{n\pi}{a}\cdot x\right)$$

Exploit this property

$$\int_0^L \sin\left(\frac{n\pi}{L}x\right)\sin\left(\frac{m\pi}{L}x\right)dx = 0, \quad m \neq n$$
$$= L/2, \quad m = n$$

Choose m=n

$$\int_0^a \left(\frac{2\alpha}{\pi}\right)^{1/4} \cdot \sin\left(\frac{n\pi}{a}\cdot x\right) \cdot e^{-\alpha\cdot(x-\frac{a}{2})^2 + i\cdot K_0\cdot(x-\frac{a}{2})} dx = \sum_{n=1}^{\infty} \int_0^a C_n \cdot \sqrt{\frac{2}{a}} \cdot \sin\left(\frac{n\pi}{a}\cdot x\right) \cdot \sin\left(\frac{m\pi}{a}\cdot x\right) dx$$

$$\int_0^a \left(\frac{2\alpha}{\pi}\right)^{1/4} \cdot \sin\left(\frac{n\pi}{a}\cdot x\right) \cdot e^{-\alpha\cdot(x-\frac{a}{2})^2 + i\cdot K_0\cdot(x-\frac{a}{2})} dx = \sqrt{\frac{2}{a}} \cdot \sum_{n=1}^{\infty} C_n \cdot \frac{a}{2}$$

$$\int_0^a \left(\frac{2\alpha}{\pi}\right)^{1/4} \cdot \sin\left(\frac{n\pi}{a}\cdot x\right) \cdot e^{-\alpha\cdot(x-\frac{a}{2})^2 + i\cdot K_0\cdot(x-\frac{a}{2})} dx = \sqrt{\frac{a}{2}} \cdot \sum_{n=1}^{\infty} C_n$$

$$\sum_{n=1}^{\infty} C_n = \sqrt{\frac{2}{a}} \cdot \int_0^a \left(\frac{2\alpha}{\pi}\right)^{1/4} \cdot \sin\left(\frac{n\pi}{a}\cdot x\right) \cdot e^{-\alpha\cdot(x-\frac{a}{2})^2 + i\cdot K_0\cdot(x-\frac{a}{2})} dx$$

$$\sum_{n=1}^{\infty} C_n = \sqrt{\frac{2}{a}} \cdot \left(\frac{2\alpha}{\pi}\right)^{1/4} \cdot \int_0^a \sin\left(\frac{n\pi}{a}\cdot x\right) \cdot e^{-\alpha\cdot(x-\frac{a}{2})^2 + i\cdot K_0\cdot(x-\frac{a}{2})} dx$$

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

MATLAB Script:

```
%Mason Averill
%PHYS-442: Quantum Mechanics
%Fall 2021
%Computational Project

clear;
clc;

%Input Desired Constants
alpha=100;%changes initial wave function
k_0=15; %changes initial wave function
a=1; %dictates the size of the square well
m=10^-30;%mass of particle
n_max=30; %Number of terms to consider for solution
x_step_size=0.0001; %Specify resolution in x steps
t_step_size=5; %Specify resolution in time steps (seconds)
max_time=500; %Maximum time for animation (seconds)

%Other Physical Constants
h_bar=6.62607015*10^-34/(2*pi);

%Initialize x and t vector
x=0:x_step_size:a;
t=0:t_step_size:max_time;

%Solve for c_n up to specified number of terms
c_n=[];
for n=1:n_max
%Compute c_n

to_int=sin((n*pi/a).*x).*exp(-alpha.*(x-a/2).^2+1i*k_0.*(x-a/2));
int_value=trapz(x,to_int);

c_n(1,n)=sqrt(2/a)*(2*alpha/pi)^(1/4)*int_value;

end

%Compute the linear combination of the wave function

Si_t=[];
counter=1;
[row,column]=size(t);
while(counter<=column)
n=1;
Si_n=0;
for n=1:n_max
Si_n=Si_n+c_n(1,n)*sqrt(2/a)*sin(((n*pi)/a).*x).*exp(-
1i*((pi^2*h_bar*n^2)/(2*m*a^2))*t(1,counter));
end
Si_t=[Si_t;Si_n];
counter=counter+1;
end
```

```
%Si_n is si(x) for a specific value in time
%Si_t stores all Si_n, so each row in Si_t is for a new value in time
Si_t_star=conj(Si_t);
Si_star_Si=Si_t_star.*Si_t;
shift_x=x-a/2;
check_normalization=trapz(shift_x,Si_star_Si(1,:));

%Begin Animation
p=plot(shift_x,Si_star_Si(1,:));
xlabel('Position in the Square Well')
ylabel('\psi^\ast\psi','FontSize',24)
xlim([-a/2 a/2])
ylim([0 round(max(Si_star_Si,[],'all'),12)])
text(a/4,.75*round(max(Si_star_Si,[],'all'),12), sprintf('alpha=%.1f
\nk_0=%.1f \nn=%i \nm=%.2e \nmax time=%.1f',[alpha, k_0,n,m,max_time]))
counter=1;
while(counter<=column)
title(sprintf('Probability Density Function of Particle vs Position in Well
at time=%.1f seconds',t(1,counter)))

%declare variable data source
p.YDataSource='Si_star_Si(counter,:)';
check_normalization=trapz(shift_x,Si_star_Si(counter,:));
refreshdata
drawnow

counter=counter+1;
end
```