Computational Methods and the Quantum Tunneling Effect

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I. ABSTRACT

This project consists of solving the Schrödinger equation in the case of a standard rectangular potential barrier being introduced. It begins with deriving the analytical solution to this particular problem to illustrate what the numerical solution is to be expected to look like in each specific region of the domain. This analytical solution will then be used to develop what will be referred to as the transmission coefficient to calculate tunneling probabilities. This equation will be used to illustrate how tunneling probability changes as the parameters of the system are altered (particle energy, barrier width). The main numerical method implemented in this project to solve Schrödinger's equation around the rectangular potential barrier was through the use of finite difference techniques to discretize the second derivative operator as well as to discretize the derivative operator with respect to time. The numerical integration technique used to evaluate and display the time evolution of the Schrödinger equation was a combination of the forward Euler method and the backward Euler method, known as the Cronk-Nicholson Method. For all relevant derivations to the equations mentioned in this project, see the appendix.

II. INTRODUCTION

In classical mechanics, if a particle with energy E approaches a potential barrier V_0 such that $E < V_0$, then that particle will reflect off the potential barrier and reverse course. In quantum mechanics, however, particles do not simply obey the laws of classical mechanics, they instead experience and obey what physicists call the wave-particle duality, which is a concept that in essence states that any particle or entity in quantum mechanics can be described as both a wave and a particle. Because of this duality, quantum particles are not restricted to the laws of classical mechanics but can also now act under the scope of wave mechanics. Now, because the laws of classical mechanics do not fully model the scope and movement of quantum particles, a new model, and hence, new equations are needed. The Schrödinger equation is the perfect expression for non relativistic quantum particles, similar to Newton's laws in classical mechanics, given a set of initial conditions, the Schrödinger Equation can make great predictions of the evolution of any quantum system. A very interesting and unique consequence of the wave-particle duality of quantum particles and the Schrödinger equation is the phenomena known as quantum tunneling. Quantum tunneling is when a quantum mechanical wavefunction successfully propagates through a given potential barrier despite having insufficient energy. As previously mentioned, this is not predicted and previously thought to be impossible in the field of classical mechanics.

This project will look to provide insights into this phenomenon known as Quantum tunneling by providing answers to the following questions:

- How does the tunneling effect change as a function of barrier width?

- How does the ratio of particle energy to barrier width effect the tunneling probability?

What you will see in this project is the results from the previously raised questions along with plots figures to display the movement of probability density curve of the wave packet through space.

The structure of the report will first consist of the analytical solution of the problem I will be modeling that will look to serve as a type of verification of the numerical solutions. Then afterward the numerical method will be lain out with all relevant formulations included in the methodology section and other side derivations/formulations can be found in the appendix. Following the methodology, the results and discussion can be found where all plots, figures, and tables can be found.

III. METHODOLOGY

III.1. Analytical Solution to the Square Box Potential

For the time-independent case, the Schrödinger Equation yields us that for some wavefunction $\psi(x)$ and potential $V(x)$, then the following relationship holds:

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

Where E, m is the is the energy eigenvalues of ψ. We can rearrange the expression and see that:

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

We want to establish what the potential is so we can set up some initial conditions and go ahead and solve the equation, so lets say that:

$$V(x) = \begin{cases} 0 & \text{if } x < 0 \\ V_0 & \text{if } 0 \leq x \leq a \\ 0 & \text{if } x > a \end{cases}$$

Where V_0 and a are arbitrary with $V_0 > E$. This is what is commonly reffered to as a rectangular potential barrier, an idealized problem with some real world applications. Now we can essentially look at this as solving three seperate ODEs, one where $x < 0$, one where $0 \leq x \leq a$, and one where $x > a$. We will denote the region where $x < a$ as region A, the region where $0 \leq x \leq a$ as region B, and the region $x > a$ as region C. Our boundary conditions that ψ must obey are that:

$$\begin{cases} \psi_A(0) = \psi_B(0) \\ \frac{d\psi_A}{dx}\Big|_{x=0} = \frac{d\psi_B}{dx}\Big|_{x=0} \\ \psi_B(a) = \psi_C(a) \\ \frac{d\psi_B}{dx}\Big|_{x=a} = \frac{d\psi_C}{dx}\Big|_{x=a} \end{cases}$$

Now that we have our boundary conditions, lets begin by looking at region A. In region A, $V(x) = 0$, so:

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

For simplicity, we can go ahead and make a substitution by setting $\frac{2mE}{\hbar^2} = k_A^2$, so in region A our equation becomes:

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

And this is just a simple second order ODE that we can find an analytical expression for by solving for the roots of the characteristic equation to find our general solution. Doing so we get:

$$\frac{d^2}{dx^2}\psi(x) = -k_A^2\psi(x) \to \frac{d^2}{dx^2}\psi(x) + k_A^2\psi(x) = 0$$

$$\lambda^2 + k_A^2 = 0$$

$$\lambda = \pm ik_A$$

So our eigenvalues for this second order ODE are $\pm ik_A$ where i is the imaginary unit. So our general solution then in region A is:

$$\psi_A(x) = A_1 e^{ik_A x} + A_2 e^{-ik_A x} = A_1 e^{i\frac{\sqrt{2mE}}{\hbar}x} + A_2 e^{-i\frac{\sqrt{2mE}}{\hbar}x}$$

Thus region A is solved for, now lets move on to region B, here $V(x) \neq 0$ so we will get a different form of a solution than we did for region A. In region B, $V(x) = V_0$ so our ODE is:

$$\frac{d^2}{dx^2}\psi(x) = \frac{2m}{\hbar^2}(V(x) - E)\psi(x) = \frac{2m}{\hbar^2}(V_0 - E)\psi(x)$$

For simplicity, we'll call $k_B^2 = \frac{2m(V_0-E)}{\hbar^2}$ so we can substitute that into our expression and carry out the same process as we did in A to find the eigenvalues and the general solution in region B.

$$\frac{d^2}{dx^2}\psi(x) = k_B^2\psi(x) \rightarrow \lambda^2 - k_B^2 = 0$$

$$\lambda = \pm k_B$$

So now we can use the eigenvalues and get an expression for our general solution.

$$\psi_B(x) = B_1 e^{k_B x} + B_2 e^{-k_B x} = B_1 e^{\sqrt{\frac{2m(V_0-E)}{\hbar^2}}x} + B_2 e^{-\sqrt{\frac{2m(V_0-E)}{\hbar^2}}x}$$

Region C will have exactly the same general solution as we had in region A only with different coefficients.

$$\psi_C(x) = C_1 e^{i\frac{\sqrt{2mE}}{\hbar}x} + C_2 e^{-i\frac{\sqrt{2mE}}{\hbar}x}$$

So all together we have:

$$\psi(x) = \begin{cases} A_1 e^{i\frac{\sqrt{2mE}}{\hbar}x} + A_2 e^{-i\frac{\sqrt{2mE}}{\hbar}x} & \text{for } x < 0 \\ B_1 e^{\sqrt{\frac{2m(V_0-E)}{\hbar^2}}x} + B_2 e^{-\sqrt{\frac{2m(V_0-E)}{\hbar^2}}x} & \text{for } 0 \leq x \leq a \\ C_1 e^{i\frac{\sqrt{2mE}}{\hbar}x} + C_2 e^{-i\frac{\sqrt{2mE}}{\hbar}x} & \text{for } x > a \end{cases}$$

These are reasonable expressions, since there is no potential barrier in regions A and C we would expect (I use this term loosely when dealing with quantum mechanics) for the particle to be able to move freely in oscillatory fashion and when the particle hits the barrier there is to be a type of decay going on where the expectation of finding the particle in that region of space declines exponentially.

Now since we are only dealing with one particle and we are also assuming that the particle is moving along in the positive x direction, we don't expect there to be another particle let alone one to be coming in the reverse direction in region C, so we can go ahead set $C_2 = 0$. And looking at our piecewise equations for $\psi(x)$, A_1 represents the initial movement of the particle, A_2 represents the reflected coefficient ie. if the particle hits the barrier V_0 and reflects backward, and the coefficient C_1 represents the tunneling coefficient, which is the main coefficient and topic of interest in this project.

Using the coefficients, we can develop an expression that will give us the tunneling probability (for the derivation see appendix). Where we get:

$$T = \frac{|C_1|^2}{|A_1|^2} = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)}\sinh^2(\frac{a}{\hbar}\sqrt{2m(V_0 - E)})} \tag{1}$$

Here we can see that the tunneling probability is dependent on both the particles energy as well as the barrier width. This analytical expression will be used to guide and help verify the results from the numerical method and model.

III.2. Numerical Approach to the Square Box Potential Problem

Now, numerically we can save ourselves a lot of the trouble by discretizing our derivative operators through the use of finite-difference methods (which appeared on a homework in this class however I don't think was every formally introduced as such) as well as using linear algebra methods to find the eigenvalues of our hamiltonian matrix.

Firstly, when we see the expression, $\frac{\partial^2\psi}{\partial x^2}$, we can use what is called a finite difference method to approximate our second derivative for ψ, in this project I will use the second-order accurate central difference method (Derivation can be found in the appendix) where:

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{h^2}$$

So using this fact, we can construct a square matrix ($n \times n$) operator that will act on our column vector ψ that will have the form:

$$\frac{\partial^2}{\partial x^2} = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & \ddots & & & 0 \\ 1 & -2 & 1 & 0 & \ddots & & 0 \\ 0 & 1 & -2 & 1 & 0 & \ddots & \vdots \\ \vdots & 0 & \ddots & & \ddots & \ddots & \\ & & \ddots & & & & \\ 0 & \dots & & 0 & 1 & -2 & 1 \\ 0 & \dots & & & 0 & 1 & -2 \end{bmatrix}$$

And then our potential $V(x)$ can just be written as a square $(n \times n)$diaganol matrix operating on our wavefunction ψ as well. And it will have the form:

$$V(x) = \begin{bmatrix} V_1 & 0 & 0 & \ddots & & & 0 \\ 0 & V_2 & 0 & 0 & \ddots & & 0 \\ 0 & 0 & V_3 & 0 & 0 & \ddots & \vdots \\ \vdots & 0 & \ddots & & \ddots & \ddots & \\ & & \ddots & & & & \\ 0 & \dots & & 0 & 0 & V_{n-1} & 0 \\ 0 & \dots & & & 0 & 0 & V_n \end{bmatrix}$$

Now we have transformed the operators in the Schrödinger equation into matrices, so our transformed expression will have the form:

$$\frac{-\hbar^2}{2m}\frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & \ddots & & & 0 \\ 1 & -2 & 1 & 0 & \ddots & & 0 \\ 0 & 1 & -2 & 1 & 0 & \ddots & \vdots \\ \vdots & 0 & \ddots & & \ddots & \ddots & \\ & & \ddots & & & & \\ 0 & \dots & & 0 & 1 & -2 & 1 \\ 0 & \dots & & & 0 & 1 & -2 \end{bmatrix}\psi(x) + \begin{bmatrix} V_1 & 0 & 0 & \ddots & & & 0 \\ 0 & V_2 & 0 & 0 & \ddots & & 0 \\ 0 & 0 & V_3 & 0 & 0 & \ddots & \vdots \\ \vdots & 0 & \ddots & & \ddots & \ddots & \\ & & \ddots & & & & \\ 0 & \dots & & 0 & 0 & V_{n-1} & 0 \\ 0 & \dots & & & 0 & 0 & V_n \end{bmatrix}\psi(x) = E\psi(x)$$

Where ψ is a column vector. Now E is also a matrix since it is the eigenvalues of the Hamiltonian. Our Hamiltonian Matrix in this case is the sum of our Kinetic Energy and Potential Energy Matrices, which are the discretized second derivative matrix and diaganol potential matrix resprectively, ie.

$$\hat{H} = \begin{bmatrix} \frac{2\hbar^2}{2mh^2}+V_1 & \frac{-\hbar^2}{2mh^2} & 0 & \ddots & & & 0 \\ \frac{-\hbar^2}{2mh^2} & \frac{2\hbar^2}{2mh^2}+V_2 & \frac{-\hbar^2}{2mh^2} & 0 & \ddots & & 0 \\ 0 & \frac{-\hbar^2}{2mh^2} & \frac{2\hbar^2}{2mh^2}+V_3 & \frac{-\hbar^2}{2mh^2} & 0 & \ddots & \vdots \\ \vdots & 0 & \ddots & & \ddots & \ddots & \\ & & \ddots & & & & \\ 0 & \dots & & 0 & \frac{-\hbar^2}{2mh^2} & \frac{2\hbar^2}{2mh^2}+V_{n-1} & \frac{-\hbar^2}{2mh^2} \\ 0 & \dots & & & 0 & \frac{-\hbar^2}{2mh^2} & \frac{2\hbar^2}{2mh^2}+V_n \end{bmatrix}$$

Now that we have our Hamiltonian we will want to then implement it so we can solve for the time-dependent case of the Schrödinger equation, namely:

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi(x,t)$$

Similar to how we went ahead and discretized our second derivative operator, we will go ahead and do the same with our first derivative operator with respect to time. Where we approximate:

$$\frac{\partial\psi}{\partial t} \approx \frac{\psi(x,t+\Delta t)-\psi(x,t)}{\Delta t}$$

Substituting this back into the Schrödinger equation will give us:

$$i\hbar\frac{\psi(x,t+\Delta t)-\psi(x,t)}{\Delta t} \approx \hat{H}\psi(x,t) \tag{2}$$

But since Δt is infinitesimally small, we can also go ahead and say that:

$$i\hbar\frac{\psi(x,t+\Delta t)-\psi(x,t)}{\Delta t} \approx \hat{H}\psi(x,t+\Delta t) \tag{3}$$

By combining (1) and (2) we get:

$$2i\hbar\frac{\psi(x,t+\Delta t)-\psi(x,t)}{\Delta t} \approx \hat{H}\psi(x,t+\Delta t)+\hat{H}\psi(x,t) \tag{4}$$

Now we can go ahead and solve for $\psi(x,t+\Delta t)$ in (3) by the following:

$$2i\hbar(\psi(x,t+\Delta t)-\psi(x,t)) = \Delta t(\hat{H}\psi(x,t+\Delta t)+\hat{H}\psi(x,t))$$

$$\psi(x,t+\Delta t)-\psi(x,t) = -\frac{i\Delta t}{2\hbar}(\hat{H}\psi(x,t+\Delta t)+\hat{H}\psi(x,t))$$

$$\psi(x,t+\Delta t)+\frac{i\Delta t}{2\hbar}\hat{H}\psi(x,t+\Delta t) = \psi(x,t)-\frac{i\Delta t}{2\hbar}\hat{H}\psi(x,t)$$

$$(\hat{I}+\frac{i\Delta t}{2\hbar}\hat{H})\psi(x,t+\Delta t) = (\hat{I}-\frac{i\Delta t}{2\hbar}\hat{H})\psi(x,t)$$

Where $\hat{I}$ is the identity matrix. Now by construction, the quantity $\hat{I}+\frac{i\Delta t}{2\hbar}\hat{H}$ is an $n\times n$ matrix and so we can go ahead and take the inverse of it so we can get $\psi(x,t+\Delta t)$ on one side of the equality, which gives:

$$\psi(x,t+\Delta t) = (\hat{I}+\frac{i\Delta t}{2\hbar}\hat{H})^{-1}(\hat{I}-\frac{i\Delta t}{2\hbar}\hat{H})\psi(x,t) \tag{5}$$

Using a variety of default parameters, we can begin to implement equation (4) to help us solve/model the Schrödinger Equation. To do this, we will first initialize a Gaussian wave packet that will be moving in free space that will have the form:

$$\psi(x, t=0) = \frac{1}{\sqrt{2\sigma\sqrt{\pi}}} e^{-\frac{(x-x_0)^2}{4\sigma^2}} e^{ip_0 x}$$

Where σ is the width of the wave packet, x_0 is the initial position of the wave packet, and p_0 is the initial momentum of the wave packet which is calculated from the expression:

$$E = \frac{p_0^2}{2m} \rightarrow p_0 = \sqrt{2mE}$$

In this project, $\sigma = 0.2$, $x_0 = -4$, and V was held at a constant 100 eV and placed at the origin (x=0) and only E (and hence p_0) and the barrier width, a, were altered to exhibit different tunneling behaviors. The width of the barrier a is in units of Å and the x scale of each plot is in nm. E was varied as a fraction of the potential energy of the barrier V (e.g. $E = 0.25V$, $E = 0.5V$, etc.). Each calculation for the position of the wave packet was done at steps of $\Delta t = 0.001$. The Hamiltonian matrix $\hat{H}$ was constructed to be size $n \times n$ where $n = 250$.

All calculations were carried out in the Julia programming language to utilize its main purpose of working in a linear algebra environment. However all of the code was translated over into python so there are two notebook files to this project, if you do not have a Julia kernel installed into your jupyter notebook or set up in Colab then the python notebook will contain all of the exact same material.

IV. RESULTS AND DISCUSSION

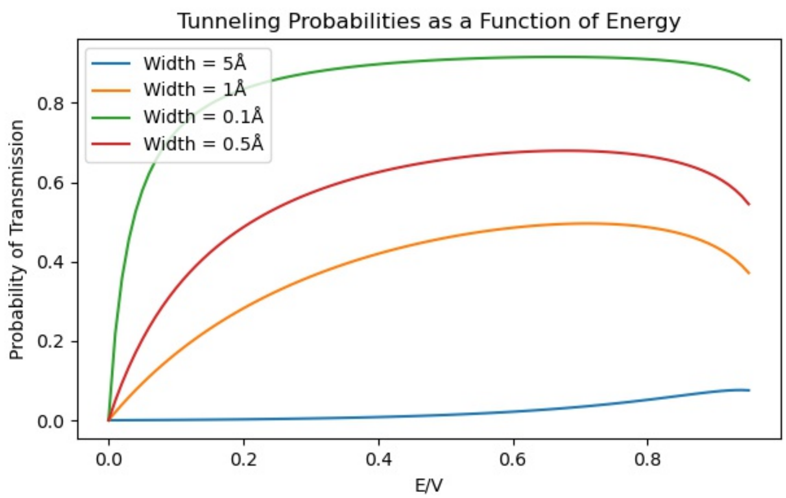

FIG. 1. The tunneling probabilities of a Gaussian wave-packet as a function of Energy relative to the barrier potential. Barrier widths vary from 1Å, 5Å, 0.1Å, and 0.5Å

Figure 1 was calculated using the equation derived for the tunneling probability. Here it can be seen that when the wave packet has no energy, regardless of the barrier width, the tunneling probability is always 0. This intuitively makes sense, if a particle has no energy it cannot have any momentum and therefore will have no chance at penetrating through a barrier. At very small barrier widths, particularly when the barrier width is 0.1Å, the transmission probability rises dramatically, a very interesting result from this curve is that when the energy of the particle is around 25% of the that of the potential, the transmission probability is almost 90%.

Another interesting consequence from Figure 1 is how the rise in transmission probability is drastically different in the 5Å case as opposed to the rise in every other case. When the barrier width is 5Å, the transmission probability does not begin to rise until the energy of the particle is around 50% of that of the potential barrier, for all energies preceding this, the transmission probability is essentially 0.

Figures 2 through 4 display the evolution of the square of the modulus of the wave packet as it moves through space toward the potential barrier. The energy of the wave packet is 0.25V and the barrier width is 1Å. As the

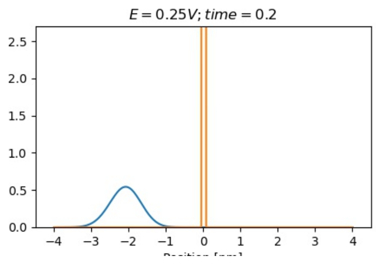

FIG. 2. Initial Wave-Packet @ t = 0.2 seconds (barrier width: 1Å)

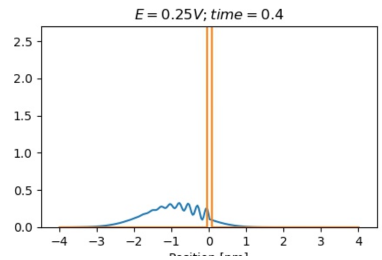

FIG. 3. Evolved Wave-Packet @ t = 0.4 seconds (barrier width: 1Å)

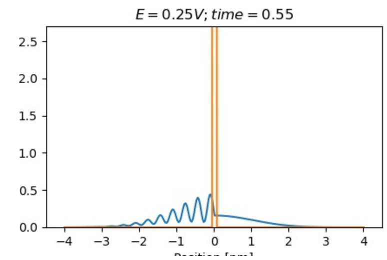

FIG. 4. Evolved Wave-Packet @ t = 0.55 seconds (barrier width: 1Å)

particle approaches the potential barrier and ultimately hits it, there is a spike in the probability distribution around the barrier on the incident side while the distribution is much smaller on the transmitted side. Notice that the transmission probability is nonzero, Figure 4 shows that there is some probability of finding the particle in that particular region of space. Using the plot from Figure 1 and the data in Table 1, we can calculate the transmission probability of this particular case which turns out to be 32.54%

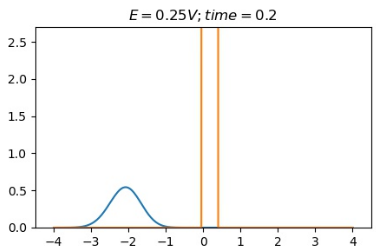

FIG. 5. Initial Wave-Packet @ t = 0.2 seconds (barrier width: 5Å)

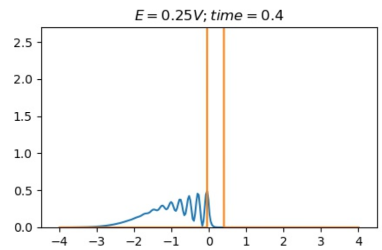

FIG. 6. Evolved Wave-Packet @ t = 0.4 seconds (barrier width: 5Å)

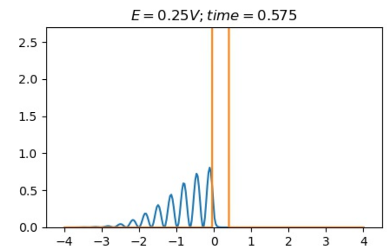

FIG. 7. Evolved Wave-Packet @ t = 0.575 seconds (barrier width: 5Å)

Figures 5 through 7 demonstrate what happens to the tunneling probability as well as where the particle is most likely to be found when the particle energy is left constant and the barrier width is increased. Comparing Figure 7 with Figure 4, the tunneling probability from figure 7 is 0. Nowhere beyond the barrier is the square of the modulus of the wavefunction nonzero, hence resulting in there being 0 probability of the particle tunneling through the barrier when the width is increased from 1Å to 5Å. The curve in Figure 1 as well as the entries in Table 1 indicate that when the energy of the particle is 0.25V and the barrier width is 5Å, that the transmission probability is 0.3%, which is nonzero but still very small, in essence verifying the distribution in Figure 7.

The tunneling probabilities and the motion of each wave-packet matches up quite well with reality. It has been experimentally verified that the probability of a particle tunneling through a potential barrier decays exponentially as barrier width increases (assuming every else in the system is held constant). The duality that exists on both sides of the barrier in the simulations is also an expected result. If only a percentage of particles are going to tunnel completely through the barrier and come out on the other side then it is to be expected that another percentage of particles will be reflected back in the direction in which they came from when making contact with the potential barrier. It is worth noting that, due to Heisenberg's uncertainty principle, there never can exist probabilities 1 or 0 that particles will tunnel through a barrier. This is particularly relevant with respect to Figure 7, where, upon visual inspection, there is no probability of the particle tunneling through the barrier under these conditions. This discrepancy with the uncertainty principle can be attributed to two possible explanations: 1) There actually is tunneling occurring in the figure, it is just too small to be quantified visually. And 2) If the numerical solution does result in 0 tunneling probability this could be due to the numerical resolution of the problem.

In Figures 8 through 10 display the wave packet when the barrier is shrunk further to 0.5Å. The result is largely what is expected, if the wave packet was able to tunnel through the 1Å barrier it is reasonable and an intuitive prediction to think that it should also be able to tunnel through the 0.5Å barrier. Upon visual inspection it looks like the final plot in Figure 10 matches very well with the probability calculated from the plot in Figure 1 and the value in Table 1. It looks like the barrier divides the wave packet in half, indicating that the tunneling probability should be somewhere around 50% and from Table 1 we see that the tunneling probability is 53.5%. Based upon the results from each plot and the analytical expression for transmission probability, it looks like the numerical method does a good job of making accurate and reasonable simulations for the motion of the wave packet.

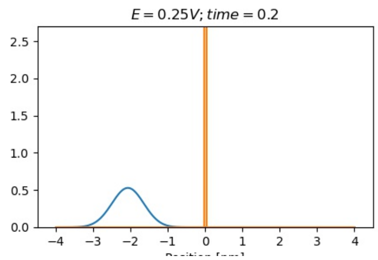

FIG. 8. Initial Wave-Packet @ t = 0.2 seconds (barrier width: 0.5Å)

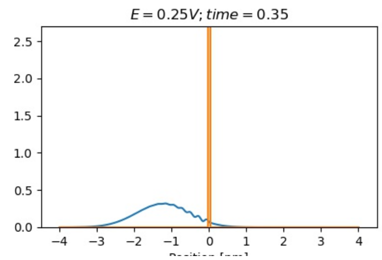

FIG. 9. Evolved Wave-Packet @ t = 0.35 seconds (barrier width: 0.5Å)

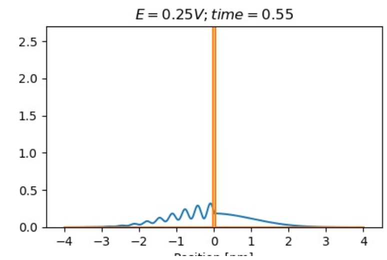

FIG. 10. Evolved Wave-Packet @ t = 0.55 seconds (barrier width: 0.5Å)

Tunneling Probability	Barrier Width	Relative Particle Energy
0.3%	5Å	$0.25V_0$
1.33%	5Å	$0.5V_0$
4.19%	5Å	$0.75V_0$
7.5%	5Å	$0.95V_0$
32.5%	1Å	$0.25V_0$
45.97%	1Å	$0.5V_0$
49.4%	1Å	$0.75V_0$
37.1%	1Å	$0.95V_0$
53.5%	0.5Å	$0.25V_0$
65.7%	0.5Å	$0.5V_0$
67.5%	0.5Å	$0.75V_0$
54.5%	0.5Å	$0.95V_0$

TABLE I. Table of Tunneling Probabilities calculated using equation 1 when the parameters of barrier width and relative particle energy are altered

V. CONCLUSIONS AND PERSPECTIVES

This method/model seems to do a good job at modeling the behavior of a Gaussian wave-packet around the rectangular potential barrier. Each of the figures provides intuitive illustrations of the tunneling probability based upon the results calculated using equation (4). The results can show that when the width of the potential barrier is increased, the tunneling probability decays accordingly. Similarly, as particle energy (relative to the barrier energy) goes up, so does the tunneling probability.

A notable pro to this model is its ability to provide accurate results with relatively large time step intervals. Each simulation in this model was carried out with time steps of size $\Delta t = 0.001$. This larger step size allows for faster run times and less computational costs but still provides reasonable accuracy for this particular problem. In reference 3. the step size used in that model was on the order of 10^{-5}, that small of a step size begins to add up quickly and can lead to very long run times, giving this model a slight edge in that regard. Some notable cons to this model is that this numerical method chosen becomes much more convoluted and complicated when the dimension increases from one to two, meaning it may be more beneficial or easier to carry out the simulation with a different method in multiple dimensions. Another con is that the numerical resolution is dependent on the size of each matrix, the larger the matrix the larger the resolution, but with large matrices the number of computations carried out goes up and run times follow.

Further applications for this model would be to carry out the calculation in more than one dimension, most realistically in 2D as opposed to this 1D example. This concept of tunneling and this model in particular can also be altered around different potential energies. The diagonal matrix of the potential energy listed in the methods can be altered to that of the Woods-Saxon potential, for example, to model quantum tunneling that can occur in nuclear fusion. Another possible avenue this model can be used to investigate is particle diffraction similar to the double-slit experiment. This can, presumably, provide an accurate and reliable model to recreate the findings that took place in the double-slit experiment.

VI. REFERENCES

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VII. APPENDICES

VII.1. Derivation of the Transmission Probability

Here we will still have our three separate solutions for each specified region around the potential, namely:

$$\psi(x) = \begin{cases} A_1 e^{i\frac{\sqrt{2mE}}{\hbar}x} + A_2 e^{-i\frac{\sqrt{2mE}}{\hbar}x} & \text{for } x < 0 \\ B_1 e^{\sqrt{\frac{2m(V_0-E)}{\hbar^2}}x} + B_2 e^{-\sqrt{\frac{2m(V_0-E)}{\hbar^2}}x} & \text{for } 0 \le x \le a \\ C_1 e^{i\frac{\sqrt{2mE}}{\hbar}x} & \text{for } x > a \end{cases}$$

We have gone ahead and set $C_2 = 0$ since we are dealing with one and only one particle and are therefore not expecting any to be coming from the positive direction moving towards the negative direction.

We know that at $x = 0$, ψ has to be continuous from region A to region B and also its derivative must be continuous at $x = 0$, the same goes for when $x = a$, evaluating ψ at these boundary conditions gives:

$$\psi(0) : A_1 e^0 + A_2 e^0 = A_1 + A_2 = B_1 e^0 + B_2 e^0 = B_1 + B_2 \tag{6}$$

$$\left.\frac{d\psi}{dx}\right|_{x=0} : i\frac{\sqrt{2mE}}{\hbar}A_1 e^0 - i\frac{\sqrt{2mE}}{\hbar}A_2 e^0 = \sqrt{\frac{2m(V0-E)}{\hbar^2}}B_1 e^0 - \sqrt{\frac{2m(V0-E)}{\hbar^2}}B_2 e^0 \tag{7}$$

$$\psi(a) : B_1 e^{\sqrt{\frac{2m(V0-E)}{\hbar^2}}a} + B_2 e^{-\sqrt{\frac{2m(V0-E)}{\hbar^2}}a} = C_1 e^{i\frac{\sqrt{2mE}}{\hbar}a} \tag{8}$$

$$\left.\frac{d\psi}{dx}\right|_{x=a} : \sqrt{\frac{2m(V0-E)}{\hbar^2}}B_1 e^{\sqrt{\frac{2m(V0-E)}{\hbar^2}}a} - \sqrt{\frac{2m(V0-E)}{\hbar^2}}B_2 e^{-\sqrt{\frac{2m(V0-E)}{\hbar^2}}a} = i\frac{\sqrt{2mE}}{\hbar}C_1 e^{i\frac{\sqrt{2mE}}{\hbar}a} \tag{9}$$

From here we will go ahead and make two substitutions by letting: $k = \frac{\sqrt{2mE}}{\hbar}$ and $q = \sqrt{\frac{2m(V0-E)}{\hbar^2}}$ So from here we know our boundary conditions are:

$$A_1 + A_2 = B_1 + B_2 \tag{10}$$

$$ikA_1 - ikA_2 = qB_1 - qB_2 \tag{11}$$

$$B_1 e^{qa} + B_2 e^{-qa} = C_1 e^{ika} \tag{12}$$

$$qB_1 e^{qa} - qB_2 e^{-qa} = ikC_1 e^{ika} \tag{13}$$

Using (10), we can see that:

$$A_2 = B_1 + B_2 - A_1 \tag{14}$$

And then looking at (13) by dividing both sides of the equality by q renders:

$$B_1 e^{aq} - B_2 e^{-aq} = \frac{ik}{q} C_1 e^{ika} \tag{15}$$

By adding (13) and (15) together and subtracting (15) from (13), the expression is respectively:

$$2B_1 e^{aq} = \frac{ik}{q} C_1 e^{ika} + C_1 e^{ika} \tag{16}$$

$$2B_2 e^{-aq} = C_1 e^{ika} - \frac{ik}{q} C_1 e^{ika} \tag{17}$$

Simplifying (16) and (17) further gives expressions for B_1 and B_2

$$B_1 = \frac{ik+q}{2} C_1 e^{(ik-q)a} \tag{18}$$

$$B_2 = -\frac{ik-q}{2} C_1 e^{(ik+q)a} \tag{19}$$

Using equations (14), (18), and (19) into equation (11) can allow us to relate C_1 with A_1. Doing so gives us:

$$ikA_1 - ik(B_1 + B_2 - A_1) = qB_1 - qB_2 \tag{20}$$

$$2ikA_1 = ikB_1 + qB_1 + ikB_2 - qB_2 \tag{21}$$

$$2ikA_1 = (ik+q)B_1 + (ik-q)B_2 \tag{22}$$

$$2ikA_1 = \frac{(ik+q)^2}{2q} C_1 e^{(ik-q)a} - \frac{(ik-q)^2}{2q} C_1 e^{(ik+q)a} \tag{23}$$

Multiplying both sides of equation (23) by 2q

$$4ikqA_1 = (ik+q)^2 C_1 e^{(ik-q)a} - (ik-q)^2 C_1 e^{(ik+q)a} \tag{24}$$

$$4ikqA_1 = C_1 e^{ika} \left[(ik+q)^2 e^{-aq} - (ik-q)^2 e^{aq}\right] \tag{25}$$

$$4ikqA_1 e^{-ika} = C_1 \left[(ik+q)^2 e^{-aq} - (ik-q)^2 e^{aq}\right] \tag{26}$$

$$4ikqA_1 e^{-ika} = C_1 \left[(-k^2 + 2ikq + q^2) e^{-aq} - (-k^2 - 2ikq + q^2) e^{aq}\right] \tag{27}$$

$$4ikqA_1 e^{-ika} = C_1 \left[k^2 (e^{aq} - e^{-aq}) + 2ikq(e^{aq} + e^{-aq}) + q^2 (e^{-aq} - e^{aq})\right] \tag{28}$$

$$4ikqA_1 e^{-ika} = C_1 \left[(k^2 - q^2)(e^{aq} - e^{-aq}) + 2ikq(e^{-aq} + e^{aq})\right] \tag{29}$$

$$4ikqA_1 e^{-ika} = C_1 \left[2(k^2 - q^2)\sinh(aq) + 4ikq\cosh(aq)\right] \tag{30}$$

Now we have explicitly an equation relating A_1 with C_1 and so now we can solve for $\frac{C_1}{A_1}$:

$$\frac{C_1}{A_1} = \frac{4ikqA_1 e^{-ika}}{2(k^2 - q^2)\sinh(aq) + 4ikq\cosh(aq)} \tag{31}$$

$$\frac{C_1}{A_1} = \frac{2ikqA_1 e^{-ika}}{(k^2 - q^2)\sinh(aq) + 2ikq\cosh(aq)} \tag{32}$$

Recall that the transmission coefficient (tunneling probability) is defined as: $T = \frac{|C_1|^2}{|A_1|^2}$. Using this we can see:

$$\frac{|C_1|^2}{|A_1|^2} = \frac{(2ikqA_1e^{-ika})(-2ikqA_1e^{ika})}{((k^2-q^2)\sinh{(aq)}+2ikq\cosh{(aq)})((k^2-q^2)\sinh{(aq)}-2ikq\cosh{(aq)})} \tag{33}$$

$$T = \frac{4k^2q^2}{(k^2-q^2)\sinh^2{(aq)}+4k^2q^2\cosh^2{(aq)}} \tag{34}$$

$$T = \frac{4k^2q^2}{(k^4-2k^2q^2+q^4)\sinh^2{(aq)}+4k^2q^2\cosh^2{(aq)}} \tag{35}$$

$$T = \frac{4k^2q^2}{(k^4+q^4)\sinh^2{(aq)}+4k^2q^2\cosh^2{(aq)}-2k^2q^2\sinh^2{(aq)}} \tag{36}$$

$$T = \frac{4k^2q^2}{(k^4+q^4)\sinh^2{(aq)}+2k^2q^2(2\cosh^2{(aq)}-\sinh^2{(aq)})} \tag{37}$$

Using the identity of hyperbolic trigonometry functions that $\cosh^2{(aq)} = 1+\sinh^2{(aq)}$ our equation becomes:

$$T = \frac{4k^2q^2}{(k^4+q^4)\sinh^2{(aq)}+2k^2q^2(2+\sinh^2{(aq)})} \tag{38}$$

$$T = \frac{4k^2q^2}{(k^4+q^4)\sinh^2{(aq)}+2k^2q^2\sinh^2{(aq)}+4k^2q^2} \tag{39}$$

$$T = \frac{4k^2q^2}{(k^2+q^2)^2\sinh^2{(aq)}+4k^2q^2} \tag{40}$$

This next step may seem somewhat pointless at first but turns out to helpful in getting to our final expression. We will flip the numerator and denominator in our fraction and raise it all to the -1 power

$$T = \left[\frac{(k^2+q^2)^2\sinh^2{(aq)}+4k^2q^2}{4k^2q^2}\right]^{-1} \tag{41}$$

$$T = \left[\frac{(k^2+q^2)^2\sinh^2{(aq)}2}{4k^2q^2}+1\right]^{-1} \tag{42}$$

$$T = \frac{1}{1+\frac{(k^2+q^2)^2}{4k^2q^2}\sinh^2{(aq)}} \tag{43}$$

And now, finally substituting back into the expression our previously defined constants of k and q we have:

$$T = \frac{1}{1+\frac{(\frac{2mE}{\hbar^2}+\frac{2m(V_0-E)}{\hbar^2})^2}{4(\frac{2mE}{\hbar^2})(\frac{2m(V_0-E)}{\hbar^2})}\sinh^2{(\frac{a}{\hbar}\sqrt{2m(V_0-E)})}} \tag{44}$$

$$T = \frac{1}{1+\frac{\frac{4m^2V_0^2}{\hbar^4}}{4\frac{4m^2E(V_0-E)}{\hbar^4}}\sinh^2{\frac{a}{\hbar}\sqrt{2m(V_0-E)}}} \tag{45}$$

Finally provides the expression for the transmission probability:

$$T = \frac{1}{1+\frac{V_0^2}{4E(V_0-E)}\sinh^2{(\frac{a}{\hbar}\sqrt{2m(V_0-E)})}} \tag{46}$$

VII.2. Derivation of the Second Order Central Finite Difference Formula

Consider the two expressions $f(x+\Delta x)$ and $f(x-\Delta x)$. By Taylor's Theorem, approximations can be made for each:

$$f(x+\Delta x) \approx f(x)+\Delta xf'(x)+\Delta x^2\frac{f''(x)}{2}+\Delta x^3\frac{f'''(x)}{6}+\Delta x^4\frac{f^{(4)}(\zeta)}{24}+... \tag{47}$$

$$f(x-\Delta x) \approx f(x)-\Delta xf'(x)+\Delta x^2\frac{f''(x)}{2}-\Delta x^3\frac{f'''(x)}{6}+\Delta x^4\frac{f^{(4)}(\zeta)}{24}+... \tag{48}$$

By adding equations (47) and (48) all of the odd ordered terms in the summation will cancel one another and the expression becomes:

$$f(x+\Delta x)+f(x-\Delta x)=2f(x)+\Delta x^2 f''(x)+\Delta x^4\frac{f^{(4)}(\zeta)}{12}+... \tag{49}$$

$$\Delta x^2 f''(x)=f(x+\Delta x)+f(x-\Delta x)-2f(x)-\Delta x^4\frac{f^{(4)}(\zeta)}{12}-... \tag{50}$$

All other terms of order 4 and higher are going to be very small, so the approximation can be made that:

$$\Delta x^2 f''(x)\approx\Delta x^2 f''(x)=f(x+\Delta x)+f(x-\Delta x)-2f(x) \tag{51}$$

And so,

$$f''(x)\approx\frac{f(x+\Delta x)+f(x-\Delta x)-2f(x)}{\Delta x^2} \tag{52}$$

When dealing with a set of points with the distance between each point being Δx, then the expression is:

$$f_i''\approx\frac{f_{i+1}+f_{i-1}-2f_i}{\Delta x^2} \tag{53}$$