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PHYS460 Project 4: Quantum Tunneling using Implicit Algorithm

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ABSTRACT

This experiment aims to simulate a quantum particle incident on a potential barrier. We use the implicit algorithm as an accurate solution of the time-dependent Schrödinger equation and alter it into a product of matrices. Then we examine quantum tunneling of a single and double barrier, and compute the transmission coefficient to further examine its properties.

Keywords: Quantum Mechanics — Computational Methods — Analytical Mathematics

1. INTRODUCTION

Classical physics holds an important benefit that it is deterministic, often being intuitive and can be simulated through tangible labs. A simple example is a one dimensional particle incident on a barrier, which will clearly reflect and then move away from the barrier (unless our particle is a cannonball and our barrier is a thin wall). However, if our particle is sufficiently small (e.g. subatomic particles) it will behave by quantum mechanics (or QM) instead. Then, we lose our intuition on the particle's motion, and we need to understand the properties of a quantum particle to understand how it behaves.

Unfortunately QM is not deterministic, so we cannot know the exact position or momentum of a particle. We can, however, determine the *probability* of the particle being within some space. To do this, QM particles are defined by their *wavefunctions* $\psi(x)$, which has a real and imaginary part. The complex conjugate is denoted $\psi^\dagger$ and their product is entirely real. Then, the probability of the particle's position across space is equal to $\psi^\dagger\psi$, which needs to be normalized so that the sum of all probabilities (or integral) is equal to 1 (see Figure 1). Then the evolution of ψ over time follows the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) \quad (1)$$
$$\frac{\partial}{\partial t}\psi(x,t) = \frac{i}{2}\frac{\partial^2}{\partial x^2}\psi(x,t) - iV(x)\psi(x,t) \quad (2)$$

where Eq.(2) is a normalized version of the Schrödinger equation, scaled to effectively (but not actually) set $\hbar = m = 1$, to simplify our calculations. These equations are not immediately insightful, and often are

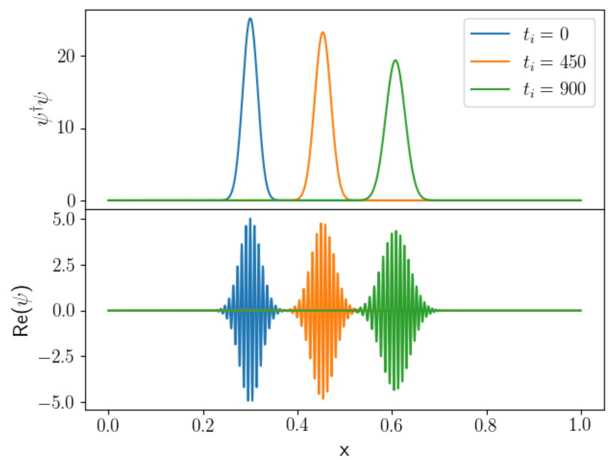

Figure 1. Initialized wave packet according to Eq.(3) and plotted at time steps $t_i = 0$, 450, and 900 with no potential barrier. Note the subtle decrease in amplitude and increase in spacial variance over time. **Top:** Probability density of wave packet $\psi^\dagger\psi$. **Bottom:** Real component of the wave function ψ.

not even analytically solvable. We explore a solution to this equation by implementing a numeric matrix using an implicit algorithm. Before we do this, however, we need to define the initial state of our particle. We use the following Guassian wave packet:

$$\psi(x, t=0) = \frac{1}{\sqrt[4]{2\pi\sigma^2}} e^{\frac{-(x-x_0)^2}{4\sigma^2}} e^{ik_0(x-x_0)} \quad (3)$$

where x_0 is the initial center of the wave packet, σ is the spacial width, and k_0 is the momentum. At first we use $x_0 = 0.3$, $k_0 = 700$, and $\sigma^2 = 2.5\cdot 10^{-4}$. We examine how this wave packet evolves over time with our implicit algorithm, ensuring it behaves as a QM wave function.

Then we add potential barriers to our spacial domain and examine quantum *tunneling*.

2. METHODS

2.1. *Implicit Algorithm*

To simulate $\psi(x,t)$ numerically we implement it as a two-dimensional array, where the outer array holds each $\psi(x)$ at different time steps Δt, and the inner array holds the values of the wavefunction at different spacial steps Δx. It is important these steps are sufficiently small to resolve the wave, so $\Delta x << \sigma$ and $\Delta t << k_0$. We use $\Delta x = 5 \cdot 10^{-4}$ across a spacial domain from 0 to 1, and $\Delta t = 5 \cdot 10^{-7}$ for about 1000 time steps. Furthermore, we represent the spacial index with n and time index with i, such that $\psi(x + \Delta x, t + \Delta t) = \psi(x_{n+1}, t_{i+1})$. We initialize our array at $t = 0$ by stepping through the spacial domain and storing the values according to Eq.(3). To evolve our system we need to compute each value of the spacial domain at the following time step.

Then the solution we seek is determining the spacial array/vector $\psi(x_n, t_{i+1})$, depending on $\psi(x_n, t_i)$ one time step backward. The solution we use is derived from the linear expansion and the Cayley form, which takes the following form:

$$\left[1 + i\frac{\Delta t \hat{H}}{2}\right]\psi(x, t_{i+1}) = \left[1 - i\frac{\Delta t \hat{H}}{2}\right]\psi(x, t_i) \tag{4}$$

where $\hat{H}$ is the Hamiltonian operator. We define $q = \frac{1}{4}\Delta t \Delta x^{-2}$, $Q_n = 1 + 2iq + \frac{i}{2}V(x_n)\Delta t$, and $D_n = 1 - 2iq + \frac{i}{2}V(x_n)\Delta t$. For now we set $V = 0$, but we use it to insert a potential barrier in Section 3.1. Putting all of this together we write our solution as:

$$\left[1 + i\frac{\Delta t \hat{H}}{2}\right]\psi(x, t_{i+1}) = \\ -iq\psi(x_{n+1}, t_{i+1}) + Q_n\psi(x_n, t_{i+1}) - iq\psi(x_{n-1}, t_{i+1}) \tag{5}$$

$$\left[1 - i\frac{\Delta t \hat{H}}{2}\right]\psi(x, t_i) = \\ iq\psi(x_{n+1}, t_i) + D_n\psi(x_n, t_i) + iq\psi(x_{n-1}, t_i) \tag{6}$$

A clever implementation of this solution is to note that both equations 5 and 6 are products of matrices. Eq.(5) is the same as the entire vector $\psi(x, t_{i+1})$ multiplied by a tridiagonal matrix with elements $-iq$ and Q_n. We then rewrite Eq.(4) as simply $A\psi(x, t_{i+1}) = B\psi(x, t_i)$, with the following matrices:

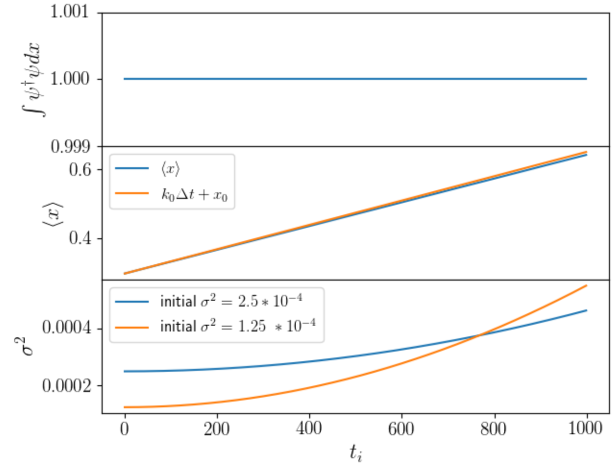

Figure 2. Top: The total probability of ψ across the entire spacial domain, which over time varies so little from 1 it is not visible on this scale. **Middle:** The expectation value of the particle's position over time, which almost exactly shares the slope of our expected momentum k_0. **Bottom:** The spacial variance of the particle over time expands. The second wave packet, initialized to be more narrow, expands faster than the first.

$$A = \begin{pmatrix} Q_0 & -iq & 0 & \cdots & & & 0 \\ -iq & Q_1 & -iq & 0 & \cdots & & 0 \\ 0 & -iq & Q_2 & -iq & 0 & \cdots & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & \cdots & & & & & -iq \\ 0 & \cdots & & & & -iq & Q_n \end{pmatrix}$$

$$B = \begin{pmatrix} D_0 & iq & 0 & \cdots & & & 0 \\ iq & D_1 & iq & 0 & \cdots & & 0 \\ 0 & iq & D_2 & iq & 0 & \cdots & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & \cdots & & & & & iq \\ 0 & \cdots & & & & iq & D_n \end{pmatrix}$$

Then to determine $\psi(x, t_{i+1})$ we just need to multiply both sides of our equation with inverse A, and we get:

$$\psi(x, t_{i+1}) = A^{-1}B\psi(x, t_i) \tag{7}$$

Given that we have properly initialized our wave function at $t = 0$ we now use Eq.(7) to iterate our wave function a small time step, and repeating this several times we get a simulation of the QM particle over time.

2.2. *Verification*

Before we add any constraints to our system, we need to ensure that it behaves like a QM particle. We use the following calculations to verify some of wave function's properties:

$$1 = \int \psi^\dagger \psi \, dx \tag{8}$$

$$\langle x \rangle = \int \psi^\dagger x \psi \, dx \tag{9}$$

$$\langle x^2 \rangle = \int \psi^\dagger x^2 \psi \, dx \tag{10}$$

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 \tag{11}$$

The results of these calculations are all seen in Figure 2. Eq.(8) tells us the sum of all the probabilities must equal 1 (like any probability distribution). It is important that we also check this remains true while we evolve ψ over time using our algorithm. We find that the total probability does decrease over time, but only by about $1 \cdot 10^{-13}$ after 1000 time steps! It is sufficient to say our algorithm holds this property with impressive accuracy.

Eq.(9) shows us the position of the center of ψ, and we find that $\langle x \rangle$ increases over time. This indicates that our algorithm does propagate ψ across x as time passes. Recall in Section 1 that the momentum of our particle is equal to k_0. Then a more useful result is to check the slope of $\langle x \rangle$ to see if it equals k_0. By plotting $\langle x \rangle$ along with $y(t) = k_0 \Delta t + x_0$, we find that the slopes are not exactly equal, but again our algorithm is only off by an extremely small amount.

Lastly, Eq.(11) allows us to compute the spacial variance of ψ. As suggested in Figure 1, we expect σ^2 to increase over time (i.e. the wave function expands over time). Plotting σ^2 over time we do find that it increases. Another important property of wave functions is that narrow wave packets expand faster than wide ones. To ensure our algorithm holds this property, we initialized a new narrow wave packet at $\sigma^2 = 1.25 \cdot 10^{-4}$ (half of the wave packet described in Section 1), and plotted σ^2 over time against our original wave packet. We find that after about 800 time steps our initially narrow wave packet has a larger σ^2 value, and thus must be expanding at a faster rate.

Therefore, by the previous 3 results, we find that without any constraints our algorithm's evolution of ψ very accurately matches our expectations. Then we further examine the behaviour of the QM particle by adding constraints to our system.

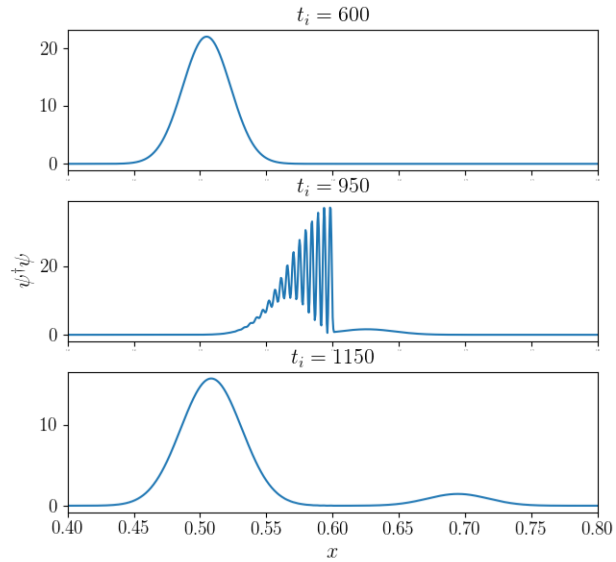

Figure 3. Probability density $\psi^\dagger \psi$ of a wave function incident on a potential barrier at $x = 0.6$ with width $d = 0.001$. The wave function is shown before, during, and after the collision of the barrier, from top to bottom. Note in the bottom picture there is a probability that the particle *tunneled* through the barrier.

3. ANALYSIS

3.1. *Single Barrier Tunneling*

In our classical reference we used a particle simply reflecting off of a barrier, here we add a barrier to our QM system and find that a QM particle does not behave as intuitively. To do this, we must recall in Section 2.1 that both Q_n and D_n include a term for $V(x_n)$, which we had set equal to 0 to test the algorithm. To insert a potential barrier we then just need to recompute the Q_n and D_n at the location of the barrier to include this extra term. However, first we must define 3 major properties of our barrier: The height of the barrier $V_0 = 9.8 \cdot 10^5$ (which is also equal to $4E_0$ of the wave packet), the width of the barrier $d = 0.001$, and the position of the barrier at $x = 0.6$. Then we insert the new Q_n and D_n values into their matrices and repeat the process of evolving ψ over time.

Before the collision we know our wave function simply propagates toward the barrier (as it did with no barrier), and similar to the classical case we expect the wave function to reflect off the barrier, so during the collision the wave function has complicated interference as the right half of the wave function reflects toward the left half. Then after the collision the wavefunction should resolve to its original shape but propagate backwards. In Figure 3 we see all 3 stages of this collision, but we find the

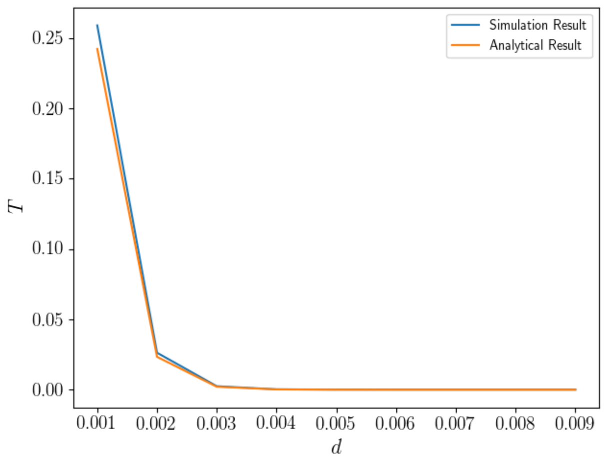

Figure 4. Transmission coefficient plotted against increasing barrier widths. Unsurprisingly, a thick enough barrier has about 0 probability of a particle tunneling through. Computed T values approximately match analytical result from Eq.(12).

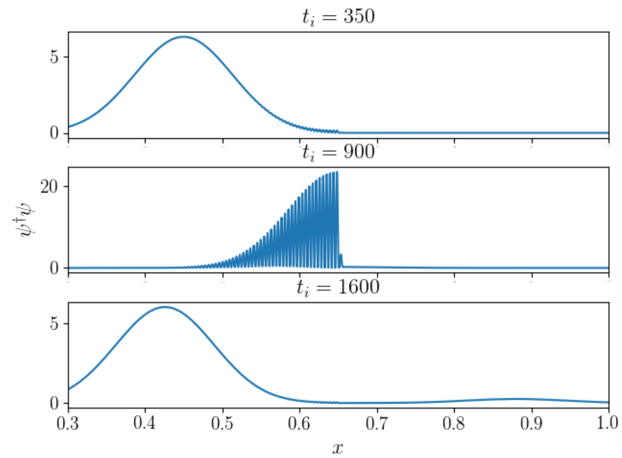

Figure 5. Similar to Figure 3 this shows $\psi^\dagger\psi$ before during and after the barrier collision. However, with barrier position at $x = 0.65$ and a second barrier of equal width at $x = 0.655$. For this case (where $k_0 = 700$) the results seem almost identical to the single barrier.

wave function after the collision opposes our expectation from a classical particle. After the collision with the barrier the wave function splits into two smaller waves, the larger one following the expected reflection off the barrier, and the smaller wave beyond the barrier. That is, the probability of the particle's position is likely to have reflected off the barrier, but it is also probable that the particle *tunnelled* through the barrier.

This is one of many bizarre properties of QM known as quantum tunneling. If there is a QM particle incident on a barrier there is a chance it tunnels through it (without destroying it). To get a handle on this, we define a *transmission coefficient* T as the probability that a QM particle tunnels through a potential barrier. We compute T for our wavefunction by using $\int \psi^\dagger \psi dx$ some time after the collision, but only for the spacial domain after the barrier (we also compute this for the domain before the barrier to ensure the total probability is still 1). We find for the above case that $T \approx 0.25$. We contrast this with the following analytical solution of the transmission coefficient (in our normalized units):

$$T = \left(1 + \frac{4}{3}\sinh^2\left(d\sqrt{2V_0 - k_0^2}\right)\right)^{-1} \tag{12}$$

Using this solution we find $T \approx 0.24$ for the above case, which shows our algorithm is still accurate. We further test this tunneling behavior by slowly increasing d to see how it affects T, and using Eq.(12) we verify that our algorithm is still functioning. In Figure 4 we find that increasing d decreases T, and for any $d \geq 0.003$ there is 0 probability for a particle to tunnel through the

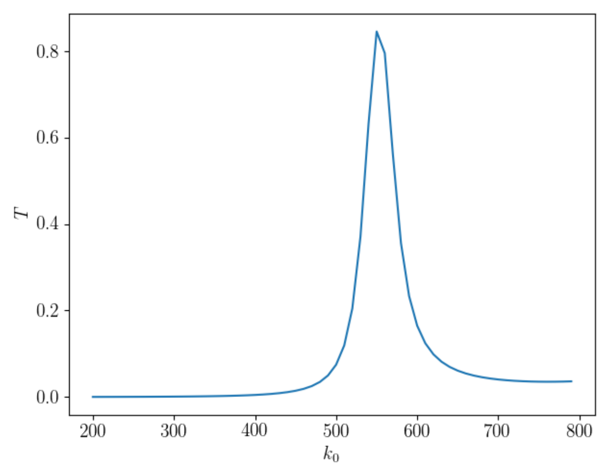

Figure 6. Transmission coefficient plotted against increasing momentum values k_0. We find that around $k_0 = 550$ there is a *resonance* such that the probability of the particle tunneling is approaching 1.

barrier. Plotting Eq.(12) for the same d values, we find our calculation is about the same.

3.2. *Double Barrier Tunneling*

We further explore this behavior by adding a second barrier to our system, keeping both barriers at width $d = 0.001$. Following the exact same process as Section 3.1 we insert the first barrier and the second barrier at a position $L = 0.004$ after the first. For the results of this experiment we need our initial wave packet to act as a plane wave (i.e. it needs to be wider), so we change the following parameters: Spacial width $\sigma^2 = 4 \cdot 10^{-3}$, spacial domain $x_{max} = 1.3$, initial position $x_0 = .33$, and barrier position $x = 0.65$. This ensures the wider wave packet fits within the domain and that we can examine the wave function after the collision without it interacting with the edges of the spacial domain.

We find in Figure 5 that this extra barrier does not immediately make any exciting changes, as the behavior is almost identical to Section 3.1. However, we find new results by varying the momentum of our particle k_0. We find that for certain k_0 the probability density $\psi^\dagger\psi$ after the barrier is much larger, and for some it is even larger than the reflected probability. Thus, there is some resonance behaviour with k_0 where at some values the particle almost always tunnels through the barriers.

To better show this, we use our definition of the transmission coefficient again but adjust to integrate over the new spacial domain after both barriers. Then we slowly increase k_0 from 200 to 800, and we find that T sharply increases and peaks at around $k_0 = 550$, as seen in Figure 6. We find its maximum is around $T = 0.8$, which in contrast to T for the single barrier, we find this particle is more likely to tunnel through the double barrier than the first particle was to reflect off the single barrier! Furthermore, this is not the only resonance value of k_0, but if we were to continue our plot beyond $k_0 = 800$ we would eventually find another peak, and another after that one, and so forth.

4. CONCLUSION

We simulated a quantum particle incident onto a potential barrier by using the implicit algorithm and Cayley form to write our solution of the time-dependent Schrödinger equation as a product of matrices. We verified that the solution followed QM properties of an evolving wave function, and found it to very accurately match expectations. Then we inserted a potential barrier and found that our wave function did follow quantum tunneling and the resulting transmission coefficient closely matched the analytical solution. Increasing the width of the single barrier resulted in a sharp decrease in transmission coefficient. Finally, inserting a second barrier, we found by varying the momentum of the initial wave packet that there was a resonance, where at certain momentum values the transmission coefficient approached 1. This algorithm was fairly easy to implement and resulted in extremely accurate representations of real observations made on quantum mechanics, and thus it is a very strong tool for these introductory simulations.