Simulating the 1-D Time-Dependent Schrödinger Equation

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Honor Pledge: *On our honor, we have neither given nor received unauthorized aid on this examination.*

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Abstract

Ever since Schrödinger first formulated his revolutionary theory describing the behavior of non-relativistic subatomic particles in terms of the newly invented wavefunction, ψ, the implications for modern physics have been nearly endless. The time-dependent Schrödinger equation (TDSE) compactly describes the evolution of a particle's wavefunction, ψ, in the presence of a potential. While very powerful, Schrödinger's equation is only directly solvable in special cases. For this reason, accurate and efficient numerical methods are an active area of research. We implemented two methods to solve the TDSE: a Crank-Nicolson iterative method as described by MacDonald, and a Chebyshev-Fast Fourier Transform (Chebyshev-FFT) method [2]. We tested our implementations on several systems with varying initial conditions and potentials, including some with known analytic solutions for comparison. The Crank-Nicolson method accurately simulated the evolution of the wavefunction in a wide variety of potentials; the Chebyshev-FFT method produced similar results for a free particle and a particle in an infinite well, but constraints on stability criteria made more complex potentials unmanageable. The results of both methods were qualitatively consistent with analytical expectations, and the Crank-Nicolson solver proved especially powerful.

Background and Theory

The time-dependent Schrödinger equation (1) (TDSE) describes the evolution of a wavefunction in a potential V:

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle = H\left|\Psi(t)\right\rangle. \tag{1}$$

The Dirac notation of $|\Psi(t)\rangle$ is the most generalized, and reflects that the wavefunction is in some state (not necessarily given in position basis) at time t. The Hamiltonian operator H is classically analogous to the total energy of the wavefunction. It is given in the 1-D position basis (which we will be using for the remainder of this paper) by

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

and "operating" it on some wavefunction in the same basis $\psi(x,t)$ will result in observing the wavefunction's total energy E, given by the time independent Schrödinger equation, an eigenvalue equation for H of the form

$$H\psi = E\psi.$$

(The difference of notation between Ψ and ψ will be described in a moment).

In quantum mechanics, most of the analytically solvable situations are where the potential V does not change with time, so that (1) can be solved by assuming Ψ is composed of the product of two, separable equations dependent on only position or time, respectively. Switching to a V that *does* change with time greatly complicates things, so for this project, we will only be dealing with the time-independent potential case. If the potential is time independent, the wavefunction solution $\Psi(x,t)$ can be written as the multiplication of two separable functions

$$\Psi(x,t) = \psi(x,t)\phi(t). \tag{3}$$

By applying the method of separation of variables and plugging (3) into (1) and discretizing the time with step size Δt, we achieve the solutions

$$\phi(t) = e^{-iHt/\hbar} \qquad \Rightarrow \qquad \Psi(x, t_0 + \Delta t) = e^{-iH\Delta t/\hbar}\psi(x, t_0), \tag{4}$$

or

$$\psi(t_0 + \Delta t) = e^{-iH\Delta t/\hbar}\psi(t_0), \tag{5}$$

which describes the time evolution of some state $\psi(x,t)$ from some initial time t to $t + \Delta t$; this exponential is known as the time-evolution operator.

Methods

We decided to implement two different methods to solve the TDSE. The first, known as the MacDonald method, utilizes a finite differencing mesh to approximate the second derivative in the Hamiltonian operator, and computes the wavefunction at subsequent times using a Crank-Nicolson step (computed by averaging explicit and implicit Euler steps); the second, known as Chebyshev-Fast Fourier Tranformation (CFFT), uses Chebyshev polynomials to compute the time-evolution operator combined with fast Fourier transforms to propagate the wavefunction (as suggested by Tal-Ezer and Kosloff).

MacDonald Method

For this method, we begin with a simple forward Euler approximation of the TDSE:

$$\psi^{n+1} = \psi^n - \frac{i\Delta t}{\hbar} H\psi^n \tag{6}$$

with the "slope" term times Δt coming from a rearranging of terms in the TDSE. To approximate the $\partial^2/\partial x^2$ term that appears in the Hamiltonian operator, we use the central difference scheme to second order in x-spacing (FTCS Scheme):

$$\frac{\partial^2 \psi_k^n}{\partial x^2} = \frac{\psi_{k+1}^n - 2\psi_k^n + \psi_{k-1}^n}{\Delta x^2} + \mathcal{O}(\Delta x)^2$$

where n is the particular time at which we are evaluating the position of our particle, k is the x-location of the particle, and Δx is our chosen spacing between x-locations. Placing this into equation (6), with $V(x,t) = 0$ for a free particle, we get:

$$\psi_k^{n+1} = \psi_k^n + iQ(\psi_{k+1}^n - 2\psi_k^n + \psi_{k-1}^n), \qquad Q = \frac{\hbar \Delta t}{2m\Delta x^2}$$

To test the stability of this method, we apply Von Neumann analysis. Assuming our discretized wavefunction is of the form $\psi_k^n = \xi^n e^{i\kappa k \Delta x}$, where our spatial variable x is discretized into $k\Delta x$, we can substitute this into the FTCS scheme and derive that

$$\xi^{n+1} = \xi^n(1 - 2iQ[1 - cos(\kappa \Delta x)])$$

We see that each new ξ is the previous multiplied by an amplifying factor , we'll call it α, in Fourier space. Taking the modulus of α, we see that this method must be unstable because for some values of κ, our amplifying factor is > 1 and will cause our solution amplitude to grow without limit. This method clearly will not work, thus we need to set up a new method of approximating the second derivative term in our Euler step that limits the growth of the wavefunction and maintains the condition that the integral over all space $(-\infty, \infty)$ of the mod-squared wavefunction (the probability density) is equal to 1 (i.e. unitarity must be preserved; the wavefunction must stay normalized). To do this, we implement a method that averages explicit and implicit Euler methods called the Crank-Nicolson(CN) Method. Using the same process as described above now applied to the CN method, we get:

$$\psi_k^{n+1} = \psi_k^n + i\frac{Q}{2}(\psi_{k+1}^{n+1} - 2\psi_k^{n+1} + \psi_{k-1}^{n+1}) + i\frac{Q}{2}(\psi_{k+1}^n - 2\psi_k^n + \psi_{k-1}^n)$$

which produces an amplifying factor, α, when we perform Von Neumann analysis as before, that has magnitude equal to 1 over all possible values of Δx and Δt (this results from the new α being $\alpha_{explicit}/\alpha_{implicit}$, which is just 1 when we take its modulus because $\alpha_{explicit}$ and $\alpha_{implicit}$ are complex conjugates). Applying this approach, including an arbitrary potential function $V(x_k, t_n) = V_k^n$, and rearranging terms, we get:

$$\psi_k^{n+1} - i\frac{Q}{2}(\psi_{k+1}^{n+1} - 2\psi_k^{n+1} + \psi_{k-1}^{n+1}) + i\frac{\Delta t}{2\hbar}V_k\psi_k^{n+1} = \psi_k^n + i\frac{Q}{2}(\psi_{k+1}^n - 2\psi_k^n + \psi_{k-1}^n) - i\frac{\Delta t}{2\hbar}V_k\psi_k^n$$

Although this looks more like a jumbled mess of Greek and English letters than a solvable equation, we can easily solve this by converting the ψ^{n+1} values and their coefficients into two separate matrices (one

column and one tridiagonal) multiplied together, and the ψ^n values and their coefficients into a single column matrix (because all of these values are already known and can be determined definitively). Solving for the ψ^{n+1} matrix using simple matrix inversion (even though the tridiagonal coefficient matrix has complex values), we get our answer very easily. This process can be repeated for as many time steps as we would like for whatever time and x mesh sizes we choose, giving us the correct results we display later in this paper.

The Chebyshev-FFT Method

The Time-Dependence of the Wavefunction

The following method is from van Dijk et al. [2]. First, we discretize x and t with the standard approach $x_j = x_0 + j\Delta x$ and $t_n = t_0 + n\Delta t$, with $j \in \{0, 1, \cdots J\}$ and $n \in \{0, 1, 2 \cdots\}$. Next, note that equation (5) describes the basic prescription for the "stepping" of the wavefunction through time. There are multiple ways to compute the time-evolution operator; for example, Tal-Ezer and Kosloff describe in [2] writing the operator as an expansion of Chebyshev polynomials $T_n(x)$, which are orthogonal and defined over the interval [-1, 1].

$$\langle T_n(x)|T_m(x)\rangle = \int_{-1}^{1} \frac{T_n(x)T_m(x)}{\sqrt{1-x^2}}\,\mathrm{d}x = C_n\delta_{nm} \qquad C_n = \begin{cases} \pi & n = 0 \\ \pi/2 & n = 1, 2, 3\cdots \end{cases}.$$

Because the time evolution operator $e^{-iH\Delta t/\hbar}$ has a complex argument, we need to use the generalized complex Chebyshev polynomials, $\phi_n(y) = i^n T_m(-iy)$, in the expansion of the operator. The orthogonality statement of these polynomials (with weight function $-i/\sqrt{1-|y|^2}$) is given by

$$\langle \phi_n(y)|\phi_m(y)\rangle = -i\int_{-i}^{i} \frac{\phi_n(y)\phi_m^*(y)}{\sqrt{1-|y|^2}}\,\mathrm{d}y = (-1)^n C_n\delta_{nm},$$

where $\phi_m^*(y)$ is the complex conjugate of $\phi_m(y)$. These polynomials can be found by the recursion relationship

$$\phi_n(y) = 2y\phi_{n-1}(y) + \phi_{n-2}(y) \qquad \begin{cases} \phi_0(y) = 1 \\ \phi_1(y) = y \end{cases} \tag{7}$$

Tal-Ezer and Kosloff [2] use an interesting approach of scaling the Hamiltonian (2) such that it's energy eigenvalues all lie within $[-1, 1]$ (so that the Chebyshev polynomials can be correctly applied). If the eigenvalues, E, of H satisfy

$$E \in [E_{\min}, E_{\max}] \qquad \begin{cases} E_{\min} \equiv V_{\min} \\ E_{\max} \equiv \hbar^2\pi^2/2m(\Delta x)^2 + V_{\max} \end{cases}$$

where $V_{\min}$ and $V_{\max}$ are the minimum and maximum values that the potential V reaches in the domain of interest, then the scaled Hamiltonian can be found with

$$H_{\text{scaled}} = \frac{H}{\Delta E} - \left(1 + \frac{E_{\min}}{\Delta E}\right),$$

where $\Delta E \equiv (E_{\max} - E_{\min})/2$. We then define $y \in [-i, i]$ as

$$y \equiv -iH_{\text{scaled}} = \frac{z}{\Delta E\Delta t/\hbar} + i\left(1 + \frac{E_{\min}}{\Delta E}\right), \qquad z \equiv -iH\Delta t/\hbar.$$

From this, as z can be expressed in terms of y, and because the Chebyshev polynomials (including their complex variants) are complete and orthogonal, they can be expanded:

$$e^z = \sum_{n=0}^{\infty} a_n\phi_n(y),$$

where the coefficients a_n can be found with

$$a_n \equiv -ie^{-i(\Delta E + E_{\min})\Delta t/\hbar} \int_{-i}^{i} \frac{e^{\Delta E \Delta t y/\hbar}\phi_n^*(y)}{\sqrt{1-|y|^2}}\,\mathrm{d}y$$

$$a_n \equiv e^{-i(\Delta E + E_{\min})\Delta t/\hbar} D_n J_n(\Delta E \Delta t/\hbar), \qquad D_n = \begin{cases} 1 & n = 0 \\ 2 & n \geq 1 \end{cases},$$

where J_n is the Bessel function of the first kind of order n (which can be implemented into Python with `scipy.special.jv()`). Equation (6) says that the time evolution of the wavefunction from some time t to $t + \Delta t$ is described by

$$\psi(t+\Delta t) = e^{-iH\Delta t/\hbar}\psi(t) \equiv e^z \psi(t) \equiv \sum_{n=0}^{\infty} a_n \phi_n(y)\psi(t).$$

From here, define $\Phi_n \equiv \phi_n(y)\psi(t)$ such that

$$\psi(t+\Delta t) = \sum_{n=0}^{\infty} a_n(\Delta t)\Phi_n(x), \tag{8}$$

and apply the recurrence relationship (7) to obtain

$$\begin{aligned} \Phi_0 &= \psi(t) \\ \Phi_1 &= y\psi(t) = y\Phi_0 = -\frac{i}{\Delta E}H\Phi_0 + i\left(1 + \frac{E_{\min}}{\Delta E}\right)\Phi_0 \\ \Phi_n &= -\frac{2i}{\Delta E}H\Phi_{n-1} + 2i\left(1 + \frac{E_{\min}}{\Delta E}\right)\Phi_{n-1} + \Phi_{n-2}. \end{aligned} \tag{9}$$

Equation (8) can be used to compute the wavefunction at some time t from some initial wavefunction at an earlier time, presumably with the infinite series truncated at some point. The coefficients a_n can be obtained in advance of the process, although because (8) needs to be completed for each new step in the iterations, it will be computationally intensive to do so.

Applying Position-Dependence of the Wavefunction

Consider that for our numerical purposes, the grid of position steps (domain of x) will be equally spaced with mesh size h. From (2), for some function $\chi(x)$, the hamiltonian acting on $\chi(x)$ will give

$$H\chi(x) = -\frac{\hbar^2}{2m}\chi''(x) + V(x)\chi(x), \tag{10}$$

where $\chi''(x)$ denotes $\partial^2\chi/\partial x^2$. Now, we can apply our discretization of x by $x = x_0, x_1, \cdots, x_j, \cdots, x_J$ with

$$(H\chi)_j = -\frac{\hbar^2}{2m}\chi_j'' + V_j\chi_j \qquad (V_j \equiv V(x_j)).$$

From here, there are multiple methods to the obtain the χ'' of equation (10). The most elegant (and fastest, according to [2]), is the so-called fast-Fourier-transform (FFT) method.

Recall that the Fourier transform and the inverse Fourier transform of some $\chi(x)$ are defined as

$$X(\xi) = \int_{-\infty}^{\infty} \chi(x)e^{2\pi i\xi x}\,\mathrm{d}x \quad \text{and} \quad \chi(x) = \int_{-\infty}^{\infty} X(\xi)e^{-2\pi i\xi x}\,\mathrm{d}\xi.$$

Due to a useful differentiation property of Fourier transforms, differentiating $\chi(x)$ twice gives

$$\chi''(x) = -4\pi^2 \int_{-\infty}^{\infty} \xi^2 X(\xi) e^{-2\pi i \xi x} \, \mathrm{d}\xi.$$

Thus, $\chi''(x)$ can therefore be found be taking the (fast) Fourier transform of $\chi(x)$, multiplying that by $-4\pi^2\xi^2$, and then taking the inverse Fourier transform of the result. So, the $H\chi(x)$ of (10) can be found in a fairly straight-forward manner in this way. This can then be used to compute the $H\Phi_{n-1}$ term of (9) for the expansion of the time-evolution operator, thus giving us a way to numerically solve for the wavefunction at that point.

This method is fairly computationally intensive, it seems, and we will thus need to find ways to reduce our computing time when implementing and running this method.

Testing

The TDSE is a very important equation describing non-relativistic quantum mechanics, and its simulation is both intriguing and widely applicable. While our implementations were restricted to the somewhat limiting case of systems with constant potential functions, we collected several common and informative examples with known analytical or qualitatively expected solutions. We tested the effectiveness of each method by comparing our numerical solutions to their known counterparts.

Free Particle

One of the simplest potentials is that of a free particle, which is simply $V(x) = 0$. Plugging this into the time-dependent Schrödinger equation gives a second order ODE, which can be solved for the time-independent wavefunction, after which the time dependence can easily be found by attaching the time evolution operator. The solution for the wavefunction is simply that of a traveling plane wave,

$$\psi(x,t) = Ae^{i(kx-\omega t)}.$$

While a numerical solution can be achieved using much simpler methods than our TDSE solvers, testing our methods against this edge case first provides a good test before more complicated systems are analyzed.

For the MacDonald method, we achieved the plot to the right in Fig. 1 using 100 spatial support points, a time step of 1.0, and a spatial step of 0.01. We used these values for all MacDonald plots for the remainder of this paper. From this plot, we can already see that our MacDonald integrator accurately produces the expected result. The initial wavefunction was a Gaussian wavepacket centered at x = 0. As the wavepacket evolves over time, the packet diffuses outward as expected until its value is nearly 0 everywhere. This is because the initial packet is a combination of many plane waves whose likelihood to remain in one central location decrease drastically with time as shown in the plot. Thus, our MacDonald method seems to be a good fit for the free particle case.

For the Chebyshev-FFT Method, we achieved the same expected diffusing Gaussian result as we did for the MacDonald method, although it is much less smooth and took slightly longer to run. To the right in Figure 2, we can see the very choppy and imprecise nature of our CFFT result. Although it does exhibit the same large-scale behavior as the analytical solution, it does not do so nearly as well as the MacDonald Method. Additionally, CFFT was highly unstable for more than 30 spatial support points (keeping the other parameters the same as for MacDonald), so we were forced to use a very coarse mesh. The maximum number of support points allowed without causing instability was determined by repeated trial and error tests rather than a thorough stability criteria derivation, and in future work we would hope to discover why this smaller amount of spatial points was necessary.

Infinite Well

We consider a particle confined in an infinite square well of length a and centered at $x = \frac{a}{2}$. The potential, $V(x)$, can be expressed by the following piece-wise function:

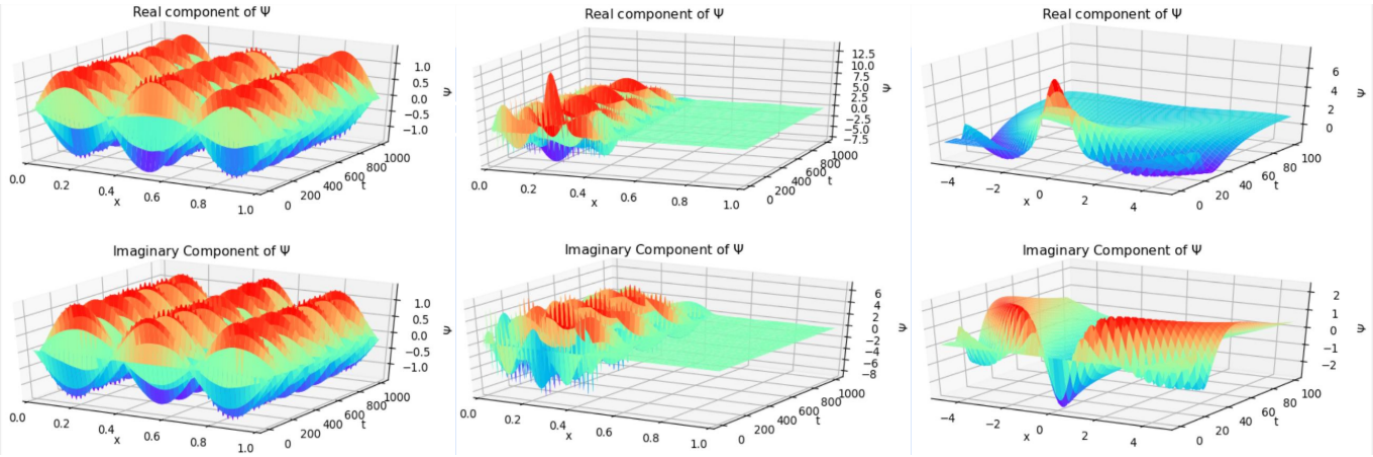

Figure 1: Wavefunctions integrated via the MacDonald (Crank-Nicolson) Method for (from left to right) the infinite well potential, potential with a barrier in the middle, and the free particle potential, with initial wavefunctions of the 2^{nd} excited eigenstate, a Gaussian wavepacket between the finite and infintie barriers, and a centered Gaussian wavepacket, respectively.

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & x < 0,\ x > a. \end{cases}$$

The analytical solution for the evolution of the wavefunction over time is [1]

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \text{ For } n \equiv 1, 2, 3....$$

We used this analytical solution to check the accuracy of our solvers against how the particle should behave in this potential.

In the diagram to the left of Figure 1, we clearly see this desired result. Using the same number of spatial support points, time step value, and spatial step value for MacDonald as we used previously, we produced the third harmonic ($n = 3$, or the second excited energy eigenstate) of the given analytic solution. Instead of passing our solver the same initial Gaussian as we did for the free particle (which would yield a very jumbled combination of different harmonics that would not be useful to analyze), we passed it an initial wavefunction that already was the third harmonic to see if it would be preserved. Looking at the given figure, it clearly does oscillate as expected and gets adequately preserved. In our code, we also allow the user to specify which harmonic they would like to see, and any value they choose (within reason) produces the same respective result under the MacDonald method, with the probability amplitude $|\Psi(x,t)|$ mostly constant over time, (as it should be exactly constant analytically, since it's a stationary state, and the oscillatory behavior is only visible in the wavefunction itself).

We achieved decent results with the CFFT method, but again fell short of the precision acquired by the MacDonald Method. To maintain stability, we were limited by a maximum 20 spatial support points, hence the rigidity of the plot. In the leftmost diagram of Figure 2, we see that the original wavefunction is well preserved, but propagates much slower and with less accuracy than the MacDonald plot. Overall, however, we can confirm that our methods do work for this potential function quite well.

Large Potential Barrier

For the final test discussed in this paper (we also provided implementations for the potential due to a finite well, harmonic oscillator, and Hydrogen atom), we examined a situation without a true analytic solution but with an interesting expected result. Consider a particle confined by an infinite potential on its left and a large (but finite) potential barrier on its right. Although we don't have an exact analytic solution

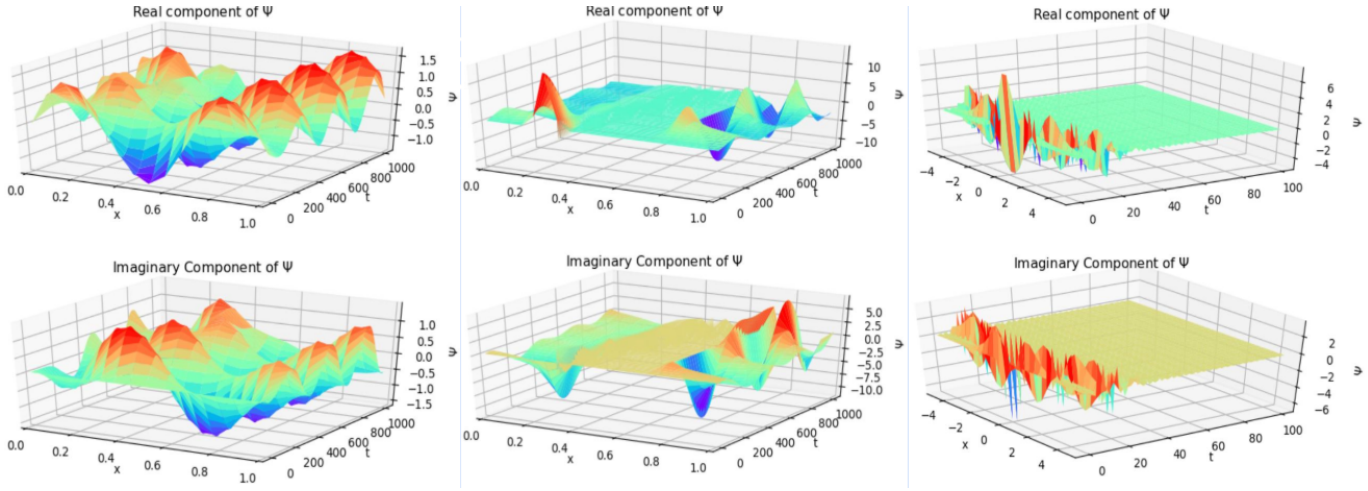

Figure 2: Wavefunctions integrated via the Chebyshev-FFT Method for (from left to right) the infinite well potential, potential with a barrier in the middle, and the free particle potential, with initial wavefunctions of the 2^{nd} excited eigenstate, a Gaussian wavepacket between the finitie and infintie barriers, and a centered Gaussian wavepacket, respectively.

for this situation, our intuition tells us that the wavefunction should behave very similarly to the one shown in the infinite well case within the two potential barriers. However, we also expected to observe quantum tunneling, the process allowing some of the wavefunction to "tunnel" through the finite potential barrier even though it would be impossible in classical mechanics. This means that the particle will have some very small, but nonzero, probability of existing to the right of the potential barrier. The underlying reason for this is that by the Schrödinger equation, the wavefunction should only be zero if the potential is infinite; the wavefunction should have a nonzero value over any finite potential.

At a first glance of the middle diagram in Figure 1, it appears that we only satisfied the first of these expected behaviors with our MacDonald Method as the wavefunction's values appear to be 0 everywhere to the right of where we defined our barrier (at x = 0.5). However, if we could zoom in on this seemingly uninteresting area, we would observe that the wavefunction value in this region is nonzero nearly everywhere with very small values over the whole region (this effect is much more visible within the animations that we created for our presentation). This is because the wavefunction almost entirely remains within the domain of the large potential barriers (and behaves as we would expect), but a very small portion "leaks" beyond the finite barrier producing the desired quantum tunneling effect. Thus, we can confirm our MacDonald Method accurately represents the quantum behavior of this situation.

Unfortunately, we were unable to get the CFFT Method to work for this potential for any appreciable number of spatial support points. In the given figure (middle diagram of Figure 2), we show the poor results for a mesh size of 20 spatial support points. Clearly, this result does not match what we would expect to happen at all, thus our implementation of this method is slightly flawed.

Conclusion

From a comparison of the results achieved using our two methods versus their analytic counterparts, we can clearly see that our implementation of the MacDonald Method outperforms the Chebyshev-FFT Method in terms of both accuracy and speed. The MacDonald method yielded accurate results for a wide variety of potentials and can be deemed a successful implementation. The CFFT method, however, was not as successful as was hoped.

The superior performance of the MacDonald Method arises from the simplicity of implementing its algorithm. Because the entire program consisted of writing a Crank-Nicolson approximation for the second derivative in the TDSE combined with an Euler stepper to approximate each successive iteration, we were easily able to comprehend how to write such a script using methods recently covered in class. This ensured

that we applied this method in a fairly rigorous manner that allowed for the higher precision of its results. Additionally, in our derivation of this method, we proved that unitarity is unconditionally preserved, and we encountered no issues with stability. This allowed us more freedom to make our plots as precise as we'd like while still faithfully executing the algorithm.

The downfall of the Chebyshev-FFT Method was its difficulty to comprehend and implement. Although this method is usually referred to as an industry standard, for us it was very ineffective [2]. The difficult implementation was daunting, and we initially doubted that we would get it to run at all. After extensive debugging, we were able to achieve some meaningful results, but these results were consistently inferior to those from the MacDonald method. The reason why CFFT doesn't work as intended is unknown to us, but we believe it could be due to translating the mathematical theory of the algorithm to computer code incorrectly, using parameters outside of the method's convergence criteria, or something else entirely.

Although our plans for implementing a numerical approach to solving the TDSE are limited to basic quantum mechanical situations, they can be extended to real-world applications through application of more rigorous methods and potential functions fairly easily. For example, if we had wished to represent the behavior of qubits in a quantum computer, all we would need to do is modify our potential well function such that we can easily change the conditions within the well to allow the system to exist at many different harmonics as they would in a quantum computing situation.

Additionally, as mentioned above, we can use this tool to simulate the actual behavior of a Hydrogen atom numerically. This peek into the quantum world is a fascinating way to understand the basics of how the fundamental components of matter work. It should also be possible to implement our TDSE solver to approximate the behavior of other atoms that lack analytical solutions. The drawback to doing this is that the potential functions and computing power needed to model these situations are far beyond the scope of our current knowledge and technological resources, which is why we tested with only a basic Hydrogen atom simulation.

References

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