# A Real-Time Numerical Integrator for the One-Dimensional Time-Dependent Schrödinger Equation

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**Abstract**

In this paper, I investigate a numerical method of integrating the One-Dimensional Time-Dependent Schrödinger Equation. A numerical method is derived using a method that is reminiscent of Runge Kutta, but implicit in the algorithm. This method is written into an integrator and tested for validity of results with respect to quantum constructs as well as accuracy with a quantum tunneling benchmark. A Java applet is used to show results of particle wave propagation in real time for various potential energy functions and initial conditions. The applet can be found at http://www.cs.hmc.edu/~ccecka/QuantumModel/ (Best viewed in Windows Explorer and tends to be moderately variable with respect to the speed of the machine. LAC computers are fantastic.)

## Introduction

At the beginning of the twentieth century, experimental evidence suggested that atomic particles were also wave-like in nature. For example, electrons were found to give diffraction patterns when passed through a double slit in a similar way to light waves. Therefore, it was reasonable to assume that a wave equation could explain the behavior of atomic particles.

Schrödinger was the first to write down such a wave equation. Much discussion then centered on what the equation meant. The eigenvalues of the wave equation were shown to be equal to the energy levels of the quantum mechanical system, and the best test of the equation was when it was used to solve for the energy levels of the Hydrogen atom, and the energy levels were found to be in accord with Rydberg's Law.

It was initially much less obvious what the wave function of the equation was. After much debate, the wave function is now accepted to be a probability distribution. The Schrodinger equation is used to find the allowed energy levels of quantum mechanical systems (such as atoms, or transistors). The associated wave function gives the probability of finding the particle at a certain position.

Many physicists spent years interpreting the Schrödinger equation, finding new ways to visualize particles, and generally attempting to reformulate the classic image of physics. An extreme difficulty is that the Schrödinger equation includes a function called the Potential Energy Function $V(x)$, which changes based on the system you are interested in. Thus, the Schrödinger equation cannot have a stand alone solution and many systems with rather simple Potential Functions also do not have closed form solutions. Numerical integration methods must then be used to find an approximation of the solution. This paper presents the quantum world as a tangible by providing a real time integration method that is coded into an applet so the user can interact with a particle and watch the quantum mechanical results.

Many computational physicists have tackled this problem to produce movies and examples of certain educationally interesting examples in order to provide a medium in which the effects of quantum mechanics can literally be seen. In my research I could not find a method that was applied to integrating the Time-Dependent Schrödinger Equation in real time nor could I find anyone who had implemented one. This project was inspired from quantum movies shown in class that were ancient and could be improved upon greatly. A tool that can utilize Schrödinger's proposition in real time can be very powerful to a student attempting to understanding some of the implications, as I have already found it to be very useful in my interpretation and visualization of quantum mechanics.

## Derivaion of Numerical Method

Feynman, in many of his computational methods, assumed all constants to be one for simplicity of calculations. In the numerical approach here, we will do the same. We define $\hbar = 1, m_e = 1, q_e = -1$. The time dependent Schrödinger Equation in one dimension then becomes

$$\imath \frac{\partial \Psi(x,t)}{\partial t} = -\frac{1}{2}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) \tag{1}$$

To integrate this numerically, we must of course work in a discrete world. Thus, $\Psi(x,t)$ must be reduced to a domain of equally spaced points: $x_j = x_0 + jdx$. At these points define $\Psi(x_j,t) = \Psi_j(t)$ and $V(x_j) = V_j$. The Schrödinger Equation then becomes

$$\imath\frac{\partial\Psi_j(t)}{\partial t} = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi_j(t) + V_j\Psi_j(t) \tag{2}$$

where we can approximate $\frac{\partial^2}{\partial x^2}\Psi_j(t)$ as $\frac{\Psi_{j+1}(t)-2\Psi_j(t)+\Psi_{j-1}(t)}{\partial x^2}$ (the simplicity of this approximation is intentional, we will see why in a moment)

$$\imath\frac{\partial\Psi_j(t)}{\partial t} = -\frac{\Psi_{j+1}(t) - 2\Psi_j(t) + \Psi_{j-1}(t)}{2\partial x^2} + V_j\Psi_j(t) \tag{3}$$

Now, the Schrödinger equation is like a first order differential equation in time of a vector with a dimension $j$, where $j$ is the number of spatial points. Integrals involving $\Psi(x,t)$ can be approximated using the discretized approximation of $\Psi$. For example,

$$\int \Psi^*\Psi dx = \int \|\Psi(x,t)\|^2 dx = \sum_j \|\Psi_j(t)\|^2 \tag{4}$$

$$\langle x\rangle(t) = \int \Psi^* x\Psi dx = \sum_j x_j\|\Psi_j(t)\|^2 \tag{5}$$

There is a difficulty in solving the time dependent Schrödinger equation in that the differential equation is "stiff". Thus if you try the Euler approximation (despite its notorious inaccuracy) $\frac{\partial\Psi_j(t)}{\partial t} = \frac{\Psi_j(t+dt)-\Psi_j(t)}{\partial t}$ with the resulting equation

$$\Psi_j(t+dt) = \Psi_j(t) - \imath\partial t\left(\frac{-\Psi_{j+1}(t) - 2\Psi_j(t) + \Psi_{j-1}(t)}{2\partial x^2} + V_j\Psi_j(t)\right) \tag{6}$$

You will find that the eigenvalues of the Jacobean matrix for this equation differ greatly in magnitude, resulting in the norm of the wave function diverging fairly quickly. This is deemed a "stiff" system. One of the primary results of the "postulates" of Quantum Mechanics is the Principle of Conservation of Probability, which will clearly not occur if the norm of the wave function is changing. Thus, a more accurate approach is needed. A Runge Kutta method is not possible since we have no way of evaluating half time steps or half spatial steps arbitrarily. The resolution I found was to embed an approach reminiscent of Runge Kutta into equation. We can form a much better approximation when it is noted that $\partial\Psi_j(t+\frac{dt}{2}) = \frac{\Psi_j(t+dt)-\Psi_j(t)}{\partial t}$ and $\Psi_j(t+\frac{dt}{2}) = \frac{\Psi_j(t)+\Psi_j(t+dt)}{2}$. These equations can be combined with those in Equation (6) to yeild

$$\Psi_j(t+dt) + \imath\frac{\partial t}{2}\Big(-\frac{\Psi_{j+1}(t+dt) - 2\Psi_j(t+dt) + \Psi_{j-1}(t+dt)}{2\partial x^2} + V_j\Psi_j(t+dt)\Big) \tag{7}$$

$$= \Psi_j(t) - \imath\frac{\partial t}{2}\Big(-\frac{\Psi_{j+1}(t) - 2\Psi_j(t) + \Psi_{j-1}(t)}{2\partial x^2} + V_j\Psi_j(t)\Big) \tag{8}$$

The right hand side of this equation is something that you can calculate; I call it $\Phi_j$.

$$\Phi_j(t) = \Psi_j(t) - \imath\frac{\partial t}{2}\Big( - \frac{\Psi_{j+1}(t) - 2\Psi_j(t) + \Psi_{j-1}(t)}{2\partial x^2} + V_j\Psi_j(t)\Big) \tag{9}$$

The wave function at time $t + dt$ can then be obtained from

$$D_j\Psi_j(t + dt) + \mu\Psi_{j-1}(t + dt) + \mu\Psi_{j+1}(t + dt) = \Phi_j(t) \tag{10}$$

where $D_j = 1 + \Big(\imath\frac{\partial t}{2}\Big)\Big(V_j + \frac{1}{\partial x^2}\Big)$ and $\mu = -\imath\frac{\partial t}{4\partial x^2}$. This linear equation for $\Psi(t + dt)$ can be written as

$$\mu\Psi_2 + D_1\Psi_1 = \Phi_1 \tag{11}$$
$$\mu\Psi_3 + D_2\Psi_2 + \mu\Psi_1 = \Phi_2 \tag{12}$$
$$\mu\Psi_4 + D_3\Psi_3 + \mu\Psi_2 = \Phi_3 \tag{13}$$

etc.

These equations can be solved in the following manner. Multiply Eq. (11) by $-\frac{\mu}{D_1}$ and add to Eq. (12) to get

$$\mu\Psi_2 + D_1\Psi_1 = \Phi_1 \tag{14}$$
$$\mu\Psi_3 + d_2\Psi_2 = f_2 \tag{15}$$
$$\mu\Psi_4 + D_3\Psi_3 + \mu\Psi_2 = \Phi_3 \tag{16}$$

etc.

where $f_2 = \Phi_2 - \mu\frac{\Phi_1}{D_1}$ and $d_2 = D_2 - \mu\frac{\mu}{D_1}$. Now multiply Eq. (15) by $-\frac{\mu}{d_2}$ and add to Eq. (16) to get

$$\mu\Psi_2 + D_1\Psi_1 = \Phi_1 \tag{17}$$
$$\mu\Psi_3 + d_2\Psi_2 = f_2 \tag{18}$$
$$\mu\Psi_4 + d_3\Psi_3 = f_3 \tag{19}$$

etc.

where $f_3 = \Phi_3 - \mu\frac{f_2}{d_2}$ and $d_3 = D_3 - \mu\frac{\mu}{d_2}$. This can be repeated for all points. The algorithm can be written as
(1) $d_1 = D_1$ and $f_1 = \Phi_1$
(2) For j greater than or equal to 2 and less then or equal the number of spatial points:

$$f_j = \Phi_j - \mu\frac{f_{j-1}}{d_{j-1}} \text{ and } d_j = D_j - \mu\frac{\mu}{d_{j-1}}.$$

This gives the equations

$$\Psi_n = f_n/d_n \tag{20}$$

$$\Psi_{n-1} = \frac{f_{n-1} - \mu\Psi_n}{d_{n-1}} \tag{21}$$

$$\Psi_{n-2} = \frac{f_{n-2} - \mu\Psi_{n-1}}{d_{n-2}} \tag{22}$$

etc.

Notice that if you evaluate the equations in the order given then the right hand side in each equation is already calculated by the time it is needed. This sequence of steps gives $\Psi_j(t + dt)$. An important property of this numerical propagator is that the norm of the wave function does not change with time, as we will show. An important point to remember with this propagator is that it used $\Psi_0 = 0$ and $\Psi_{n+1} = 0$. Thus, we have implicitly built in the stipulation that we are propagating Schrödinger's equation with the potential $V(x)$ with infinite walls at the points $x_0$ and $x_{n+1}$. This is reflected in the applet by the red potential lines at the edges of the box.

## Evaluation of the Algorithm

As claimed, this algorithm prevents deterioration or inflation of the norm and ensures that the Law of Conservation of Probability is upheld. This is accomplished by implicitly including an approximation algorithm much like that of Runge Kutta into the algorithm for time integration of the wave. I claim that this will compensate for the stiff character of the system and the failure of the naive Euler approximation approach.

To verify or deny this claim, I run the algorithm for some benchmark test. I choose the Barrier Potential with Peak Position = 75 and Peak Width = 5 with all other variables default. See Figure 1. This will serve as our test case to determine the variability of the norm, how fast it may be changing, whether it is diverging or converging, and if it matters.

```
public double integratePsiPsi(int a, int b)
     {
     double result = 0;
     for( int i = a; i < b - 1; ++i )
           result += (Complex.squareAbs(psi[i])+Complex.squareAbs(psi[i+1]))/2.0;
     return result;
     }
```

The small integrating function calculates the norm of the wave function. The algorithm is modified for this test so that the function is called each time the graph is printed to the screen (which is actually every 10 times steps of the integrator to save on rendering time). This will allow us to determine how the norm changes over time. The results are more than satisfactory. As we can see in Figure 2, the norm changes insignificantly over a period of interest. In the 35000

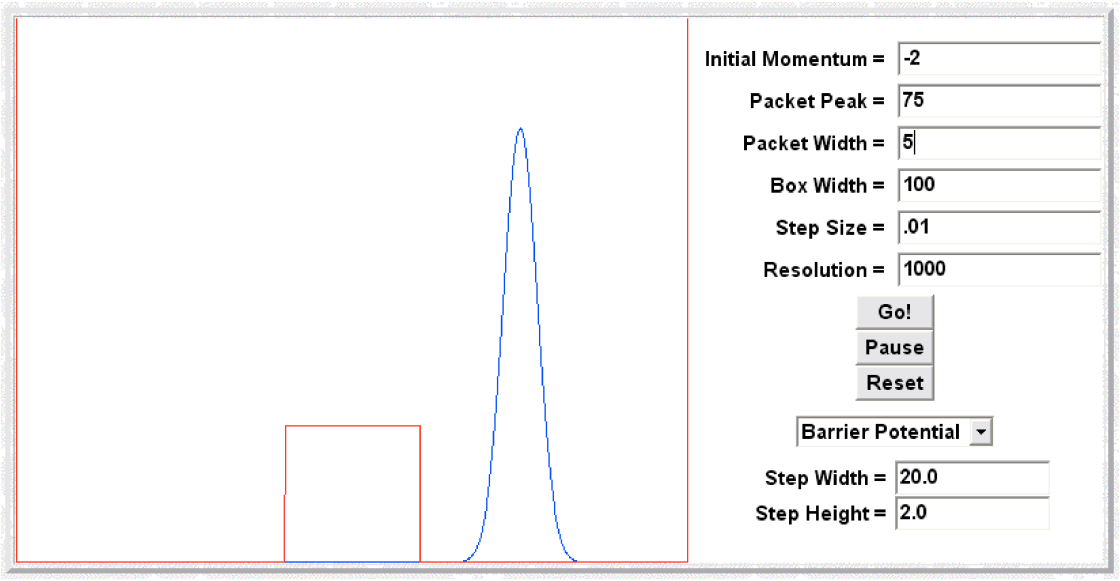


Figure 1: Initial Conditions of the Integrator

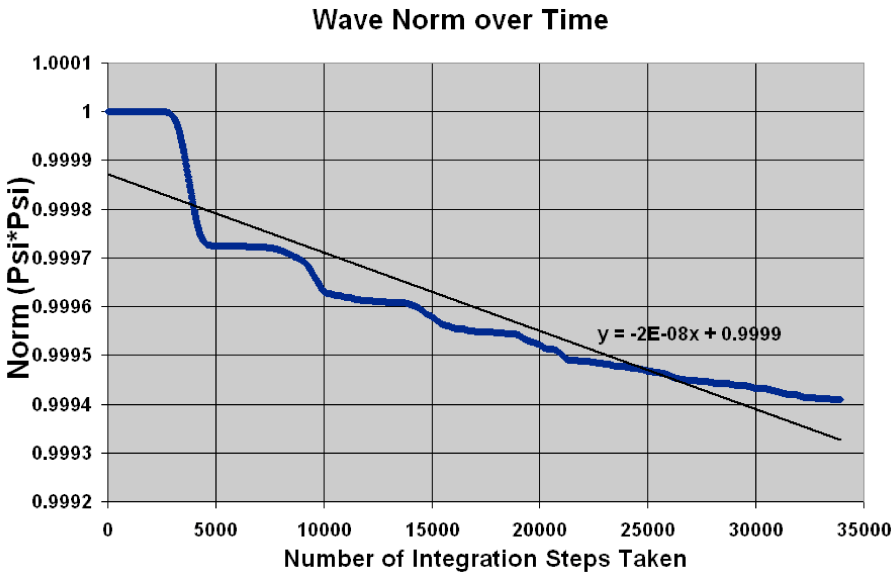


Figure 2: The evolution of the norm of the wave over the number of integration steps is extremely slow. Here, over the course of 35000 time steps, the norm has decreased by less than .06%.

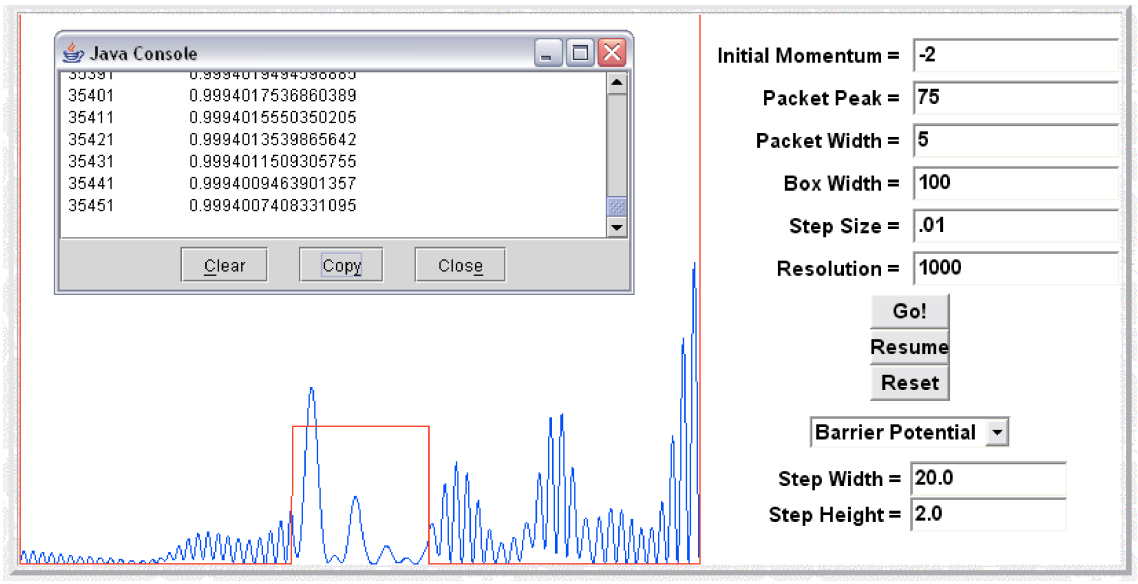


Figure 3: The Final Conditions of the Integrator.

time iterations it was run, the norm decreased by less 0.06%. This corresponds to approximately 2 minutes of actual runtime. I estimate that a system would have to be run for approximately 2-3 hours to give a "non-negligible" total change of 1%. The system would be of no qualitative or quantitative value at that point. Thus, for any reasonable use of this algorithm, Conservation of Probability holds.

The final state of the integrator is shown in Figure 3. It is tempting to try to explain the sudden drops in the norm. One promising theory was that the large drops are concurrent with larger interactions with the infinite potential walls. Perhaps the walls were acting as a tiny probability sink. After testing and watching many of these evolutions, this is not the case. At this point, I have no explanation for the sudden drops in norms, but fall back on the fact that regardless of their origin, the overall change will be negligible for any reasonable period of evolution.

Another qualitative check that should be performed is a check with theory. The algorithm should predict with some accuracy the predictions of quantum mechanics. The Barrier Potential is an interesting example. From theory, we know the transmission coefficients when $E < V_0$ and $E > V_0$

$$T_{E<V_0} = \left(1 + \frac{\sinh^2 k_1 a}{4\frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)}\right)^{-1} \qquad T_{E>V_0} = \left(1 + \frac{\sin^2 k_2 a}{4\frac{E}{V_0}\left(\frac{E}{V_0} - 1\right)}\right)^{-1} \tag{23}$$

for $k_1 = \sqrt{\frac{2mV_0a^2}{\hbar^2}\left(1 - \frac{E}{V_0}\right)}$ and $k_2 = \sqrt{\frac{2mV_0a^2}{\hbar^2}\left(\frac{E}{V_0} - 1\right)}$. Finally, we know that $E = \frac{p_0^2}{2m}$. Converting these to atomic units and setting $a = 1$ yields

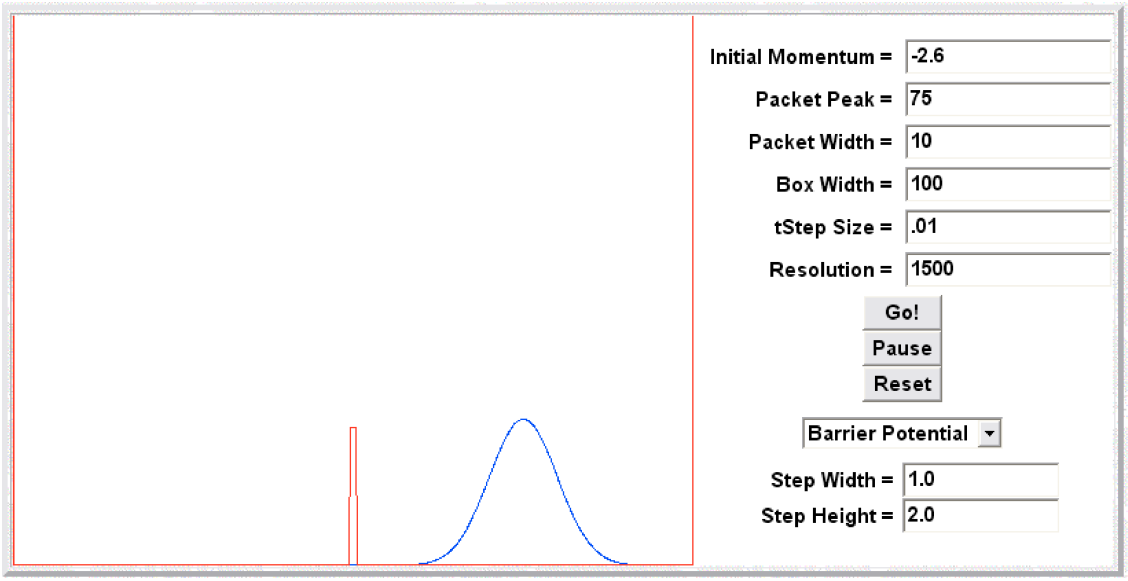


Figure 4: The Initial Conditions for Testing the Transmission Coefficient.

$$T_{E<V_0} = \left(1 + \frac{\sinh^2 k_1}{4\frac{p_0^2/2}{V_0}\left(1 - \frac{p_0^2/2}{V_0}\right)}\right)^{-1} \qquad T_{E>V_0} = \left(1 + \frac{\sin^2 k_2}{4\frac{p_0^2/2}{V_0}\left(\frac{p^2/2}{V_0} - 1\right)}\right)^{-1} \tag{24}$$

for $k_1 = \sqrt{2V_0\left(1 - \frac{p_0^2/2}{V_0}\right)} = \sqrt{2V_0 - p_0^2}$ and $k_2 = \sqrt{2V_0\left(\frac{p_0^2/2}{V_0} - 1\right)} = \sqrt{p_0^2 - 2V_0}$ . We can now test the theoretical results against the modeled results. We use the initial conditions shown in Figure 4 where the initial momentum $p_0$ will be variable and $V_0 = 2$.

Data was taken by using the same function as above to determine the ratio of the probability distribution that tunneled through the barrier to that which was reflected. An instance of the system would be run for some initial momentum and would be allowed to scatter. Visually, when the two peaks seemed separated enough (that is, they had no significant portion of their distribution over the center of the graph) I would pause the simulation and integrate each peak separately. The peak on the left would have a total probability equal to that of the transmission coefficient. It was easily shown that exactly when and where the peaks were stopped and integrated did not have a significant effect on the results as long as they were completely separated at the time of the integration. Figure 5 shows the typical final outcome of a run.

The data collected is shown in Figure 6.

Figure 6 shows an exceptional correlation between the theoretically expected values of the transmission coefficient and those collected from the simulation. In fact, the largest discrepancy in the data is only 1.25%, all others have a discrepancy less than 1%. Although there are no real uncertainties for these values, any uncertainty that can be bounded by 1% of the value is a precise one. From this data, we can maintain that the Laws of Probability Flux are maintained and that collisions in the simulation are faithful to those of theory.

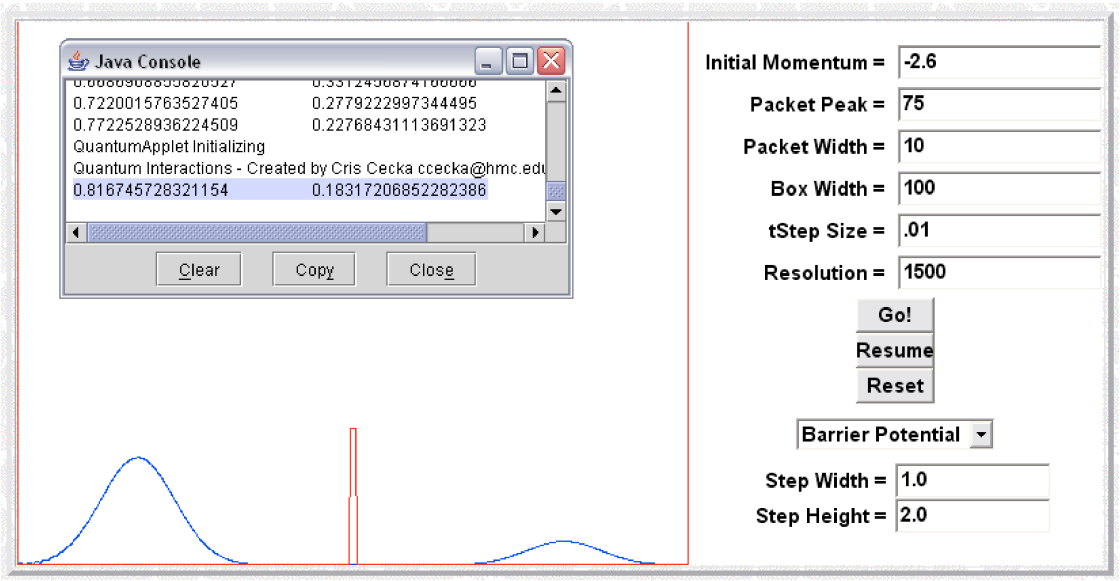


Figure 5: This shows a typical point at which the graph would be stopped and integrated.

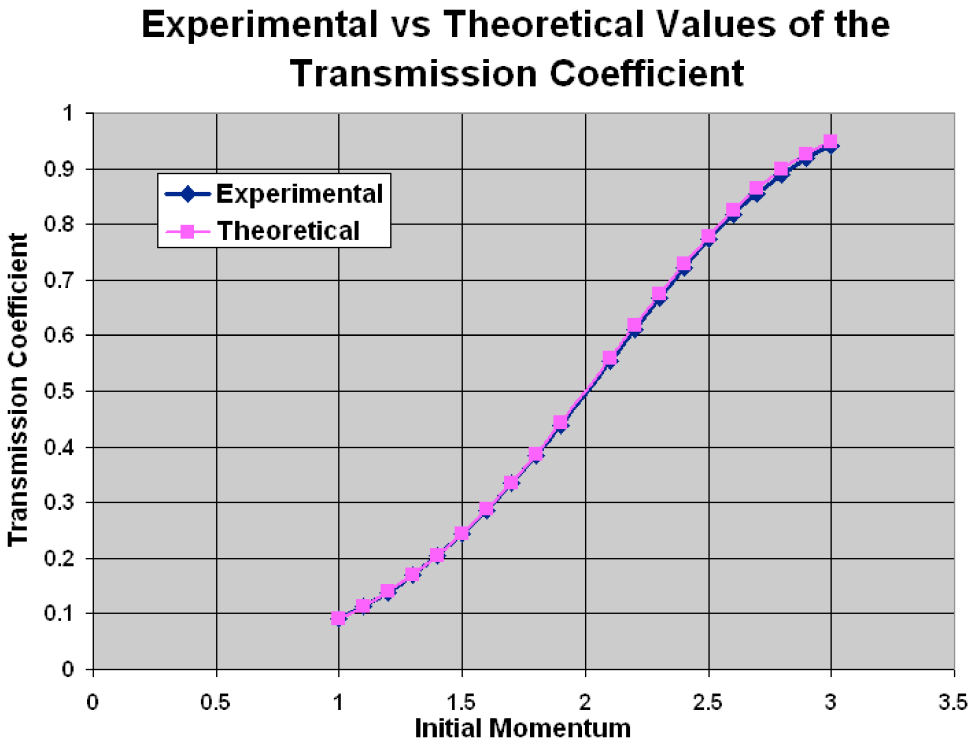


Figure 6: The data collected for the transmission coefficient test. The near perfect correlation shows that the simulation is faithful to the Laws of Probability Flux and quantum tunneling.

## Conclusion

We have derived a numerical method for solving the One-Dimensional Time-Dependent Schrödinger Equation and have shown that it functions faithfully in real time. In context, faithfully means that in the short term and in specific cases the outcomes are close/comparable to theory and experiment. Here we have shown that the method preserves the norm of a wave function to a valid degree in the short term, allowing it to uphold an accurate Law of Conservation of Probability. We have also shown that the method upholds a Law of Probability Flux and Quantum Tunneling by showing the strong correlation between the predicted transmission coefficients and the theoretical values as they depend on energy and momentum. The strength of this algorithm is present in its clarity, speed, and overall accuracy of the results. Being able to watch the real time evolution of a wave function over some potential gives an insight into the working of quantum mechanics and the flow of waves and probability that theory simply cannot.

## Future Plans and Development

In working on this algorithm further, I plan to allow for a "User Defined Potential" in which the user may draw their own potential energy function on the screen and run an instance of the integrator on it. Also, with the current set-up, there is nothing keeping me from evaluating time dependent potential energy functions, which could yield interesting results. For example, we could "smash" the particle with two encroaching Dirac Potentials to determine where and when the spatial approximation breaks. Although not physically significant, the mathematical implications of a complex-valued potential function would also be an interesting modification. Determining the momentum space of the particle would also benefit the viewer in visualizing and understanding the events.

Recently while playing with the applet, I started the particle in the center of a free potential with no initial momentum and a packet width of 2 to watch the scattering and particle in a box effect. What I found was promising. Naturally, the particle will scatter and interfere with itself, causing a sequence of interference peaks. The number of peaks I observed over time formed a pattern, which I recognized at resembling the Towers of Hanoi and Gray's Binary sequence. I promptly realized that these sequences also had a relation to the GCD interference sequence, which is the model for this instance of the system when eigenfunction phasors are used with varying angular velocities, as is expected from Physics. Two interesting results: (1) The fact that these eigenfunctions and their phasors are preserved and act according to theory (I waited until they formed a single peak, which I found to be qualitatively perfect) without having any active knowledge of them is a statement for the accuracy of this model. (2) The eigenfunction expansion of this packet should be derivable by determining the angular velocity of each eigenfunction's phasor that is required to achieve the interference patterns observed at their relative times. I find that this model has a great ability to function as a tool for further research and realizations into the workings of Quantum Physics.

## References


[1] A. Askar and A.S. Cakmak, Explicit Integration Method for the Time-Dependent Schrödinger Equation for Collision Problems, J. Chem. Phys. (1978).

I used this source in conjunction with Visscher to formulate my version of the numerical integrator shown above. Although the math presented here was of a level high enough to be out of my scope, I was still able to use concepts from special cases in writing the applet and integrator.

[2] Visscher, P. B. A fast explicit algorithm for the time-dependent Schrodinger equation.

I used this source in conjunction with Askar and Cakmak to formulate my version of the numerical integrator shown above. This article gives an algorithm to calculate the time-dependent Scrödinger equation. I made some modifications and assumptions in deriving my version so as to make it run faster and be able to function in real time.

[3] Robert Eisberg and Robert Resnick, Quantum Physics (John Wiley & Sons, Inc., New York, 1974)

Class Text.

[4] L. G. de Pillis, *private communcation*, 2004.

In Scientific Computing Math 164, we learned about stiff systems and solvers. I was able to recognize the system was stiff and work around it from de Pillis.