Time Dependant Schrodinger Equation

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This project is concerned with modeling the Time Dependant Schrödinger equation. While the the case independent of time is immanently solvable, introducing the wave evolving over time makes it much more complex. We focus on two algorithms, the Crank-Nicholson and the Finite Difference Method, in attempt to simulate the wavefunction.

1. The Algorithms

The Crank-Nicholson Algorithm

The Crank-Nicolson algorithm is the more stable one of the two we implemented. This method is implicit, in that the value of a future function at some point depends on both the preceding and concurrent values. It is a combination of the forward and backward Euler methods. This means that the method requires that a minimum of three points be solved at at some future time, implying linear algebra is the perfect tool to solve for them. When implemented, it involves solving a system of tridiagonal matrices.

While this algorithm is impressively stable, it runs into odd behavior when the time step is too big and the space step is too small. This is illustrated in the following figures. Figure 2 is a working model of a free wave packet at some time. The left of Figure 1 is one whose time-step was multiplied by 10, and the right is one whose space-step was divided by 10.

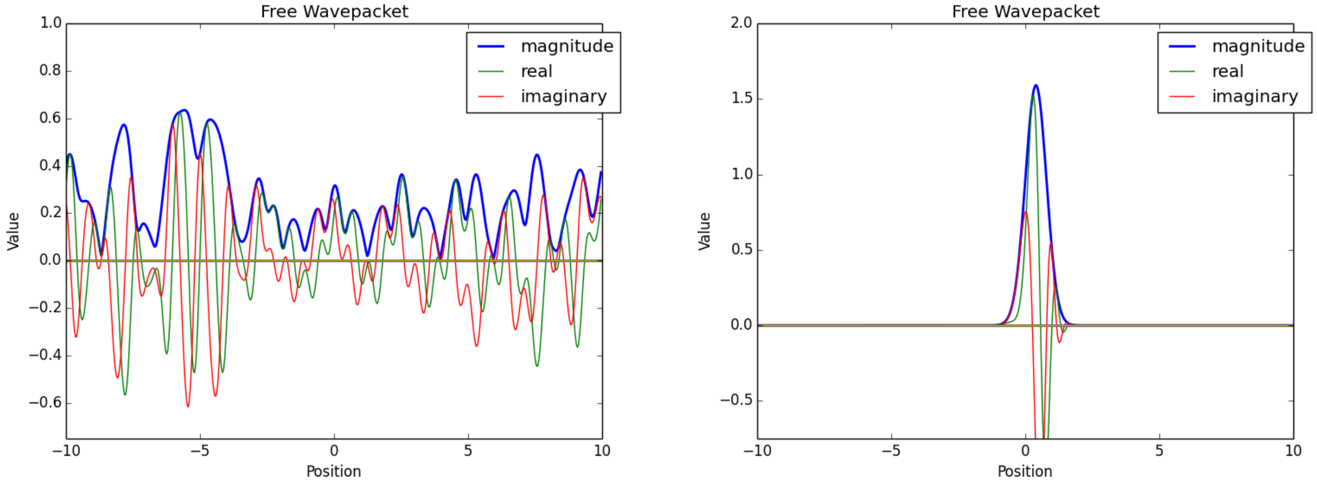

Figure 1: Altering Step Sizes by Factors of Ten

When the time-step is set too high, the wave packet takes on strange jumpy behavior. The same general behavior is observed when the space-step is set too high. When the space-step is set too low, however, barely any time evolution occurs. This makes sense, because the time-step and space step are linked in our algorithm.

For the time-dependent Schrödinger equation (TDSE), the Crank-Nicholson algorithm is implicit in time and second-order accurate. For our implementation, the evolution of the wave packet is discretized into a square matrix, with rows representing space and columns representing time. The wave is initialized according to a Gaussian distribution at t = 0. Then, the TDSE is used to generate the next row of the matrix, which is then linearly solved. For this, the matrix was originally inverted, which was costly in terms of time, making the total matrix operation clock in at upwards of $O(n^3)$. The simulation time was later decreased by using sparse matrices. It also means the number of time iterations must equal the number of spatial divisions into which the wave packet is discretized.

At every step, the wave should be normalized and its boundaries should be adjusted. These are simple procedures adapted to this model specifically. The potential used in the TDSE comes from one of several types defined elsewhere in the program.

The Obvious Discrete Algorithm

The Finite Difference Method replaces the derivatives from the Schrödinger equation with differences, per the name. Since we are solving a second order partial differential equation, each step requires three previous steps in order to be solved. We implemented the implicit method of the Finite Difference Method, which solves for Ψ_n from Ψ_{n+1}. The formula is defined as:

$$Psi_j^n = \frac{i}{2}\left((1 + 2\frac{\Delta t}{\Delta x^2})\Psi_j^{n+1} - \frac{\Delta t}{\Delta x^2}\Psi_{j-1}^{n+1} - \frac{\Delta t}{\Delta x^2}\Psi_{j+1}^{n+1}\right)$$

Like the Crank-Nicolson Method, the Finite Difference Method is numerically stable. It also involves solving a tridiagonal matrix and has second order accuracy. The data of psi is initialized and stored in the same manner as described above. Although marginal, as both share the same time complexity, we found that this method was slightly faster.

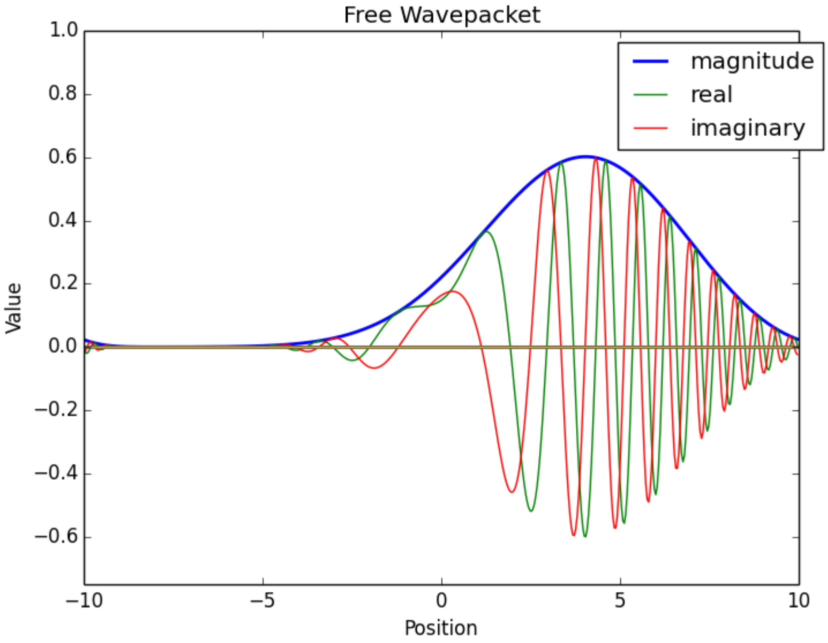

Figure 2: Free WavePacket

We found that our free wave packet behaved more or less as expected, giving the weird spacial constraints applied to our system. We found that increasing k caused the wave packet to become less spread out spatially, which agrees with what we know quantum mechanically.

2. A Few Simple Test cases

However, we want more comparison than just a free wave packet. Using a few simple test cases, we can get a better look at how accurately our simulators are working. In examining the free wave packet, we found the Crank-Nicolson algorithm to be the more reliable and usable algorithm, and we will move forward testing its behavior.

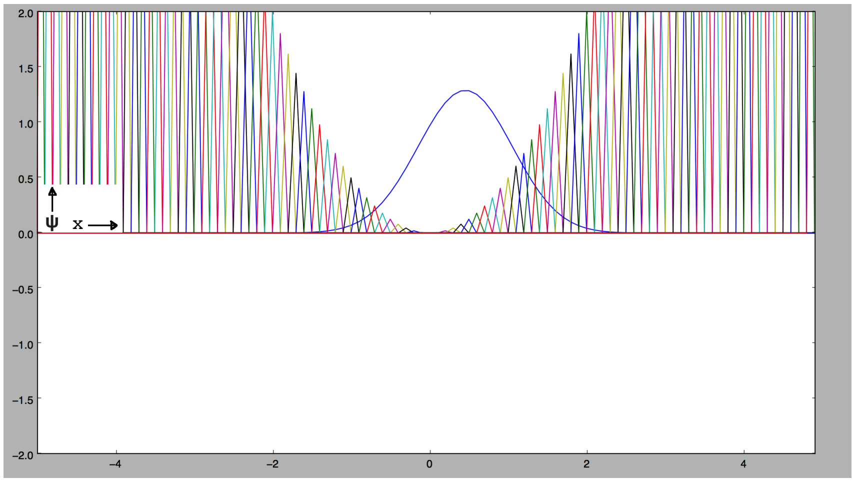

Figure 3: Harmonic Oscillator

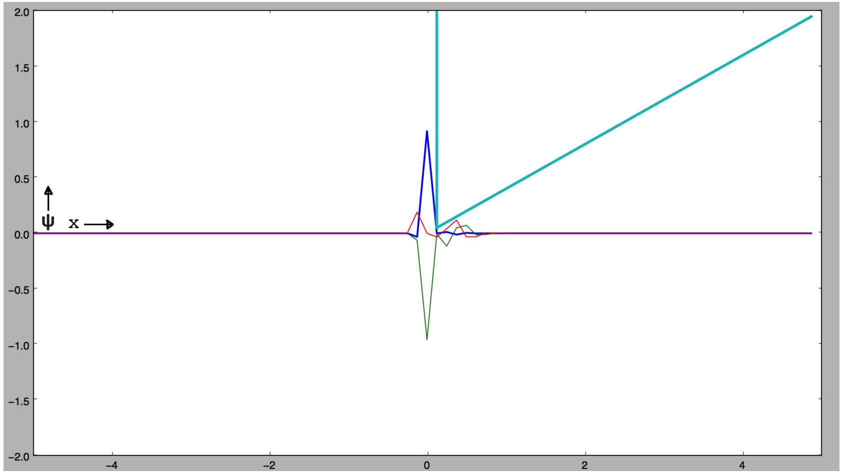

Figure 4: Triangular Well

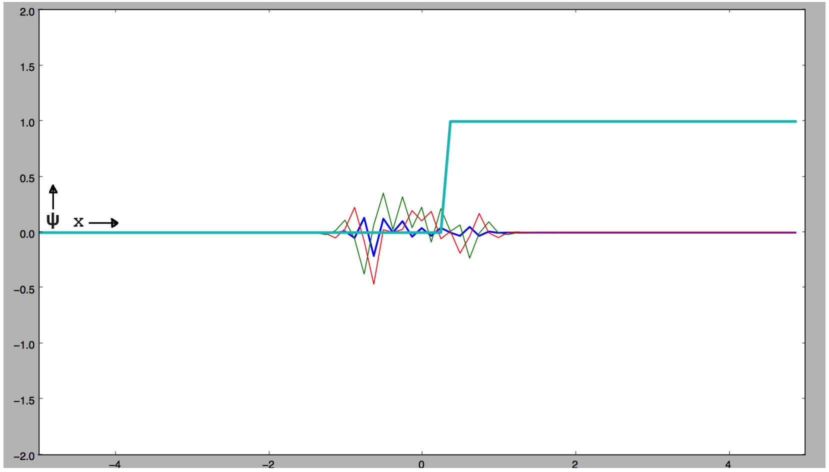

Figure 5: Potential Step

In Figure 3, the Harmonic Oscillator the well is made up of the crisscrossing colored lattice. The function behaves mostly as expected as it goes through the well.

Figure 4 shows the waves in a triangular well, creating an interesting effect with the real and non-real elements.

Figure 5 depicts how the wave reacts to a potential step.

3. Introducing a Potential Barrier

The potential barrier problem provides the opportunity to compare results to analytical values. In theory, increasing the k (momentum) of a wave packet approaching a potential barrier would increase the amount of tunneling. This was examined for a narrow, tall potential barrier for k's varied from 1 to 6. Results are shown in Figure 6:

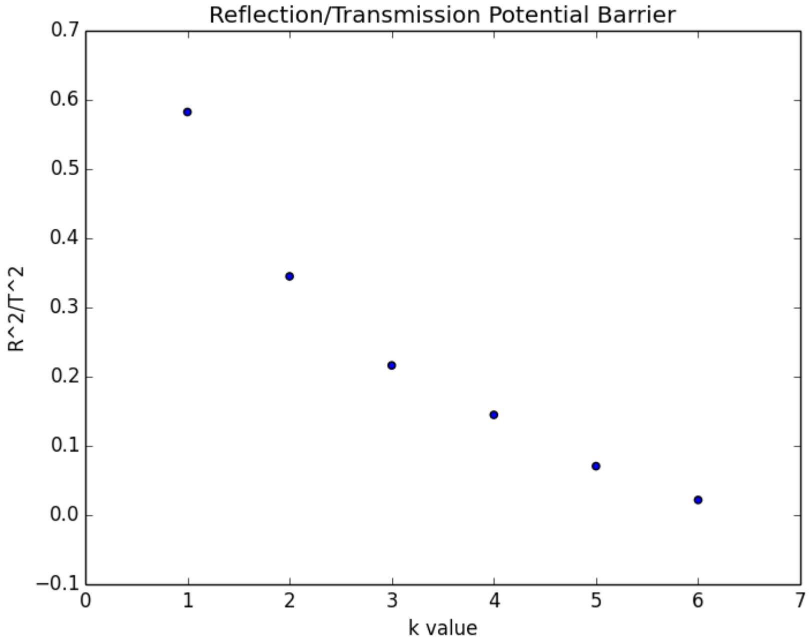

Figure 6: Reflection and Transmission Coefficients

This graph shows the amount of reflected wave packet squared divided by the amount of transmitted wave packet squared. It shows that the higher the incident energy, the less of the wave packet gets through the barrier.

Additionally, barriers of different heights at constant k values were examined to see the effect the potential would have. For a small potential barrier of 1 shown below, it was observed that a large amount of the wave packet passes through.

For a larger V, significantly less of the wave packet gets past the potential barrier. This is shown in Figure 7:

4. Equal Energy Potential Barrier

The energy of the incoming wave packet can be approximated from the relation

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

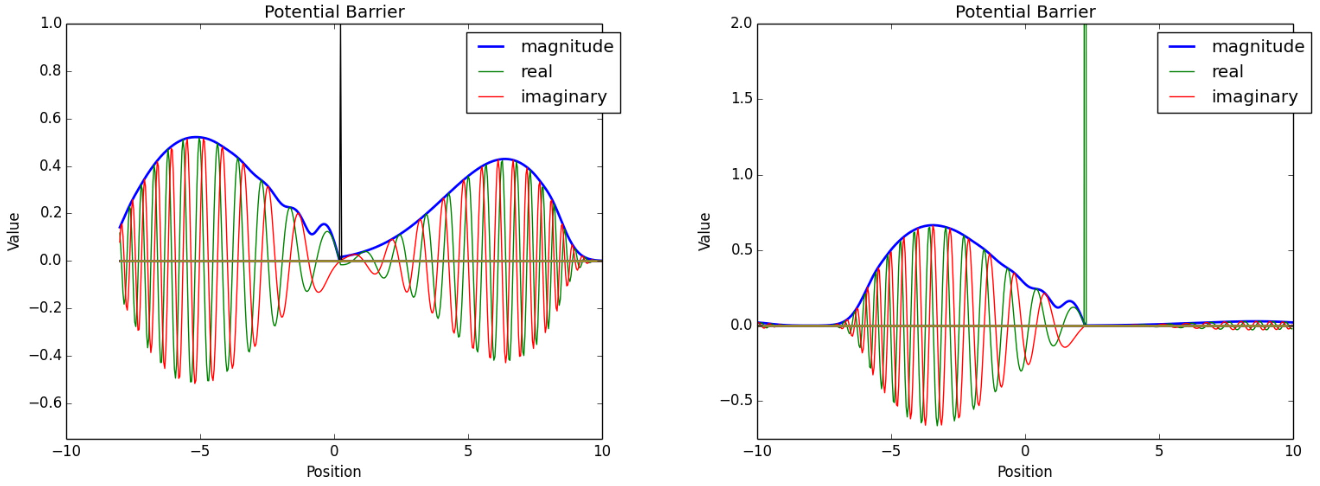

Figure 7: Varying Potential Barriers

where k comes from the wave packet, and is essentially the initial momentum of the packet. From this we can find that:

$$E = k^2/2$$

Setting the potential barrier height equal to this height yields interesting results.

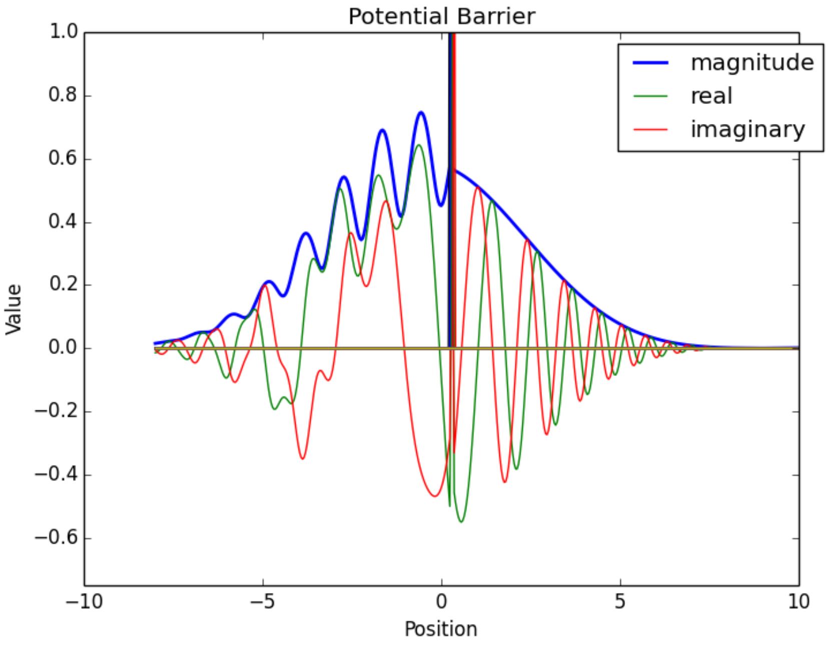

Figure 8: Potential Barrier

Figure 8 is a snapshot of the first quarter of the time evolution. If allowed to run longer, the wave packet evolves into Figure 9.

Figure 9 indicates that the periodic boundary conditions may be interfering with the solution. Theoretically, a way to fix this would be to increase the range of values that the wavepacket is defined on, but, as shown in exploring

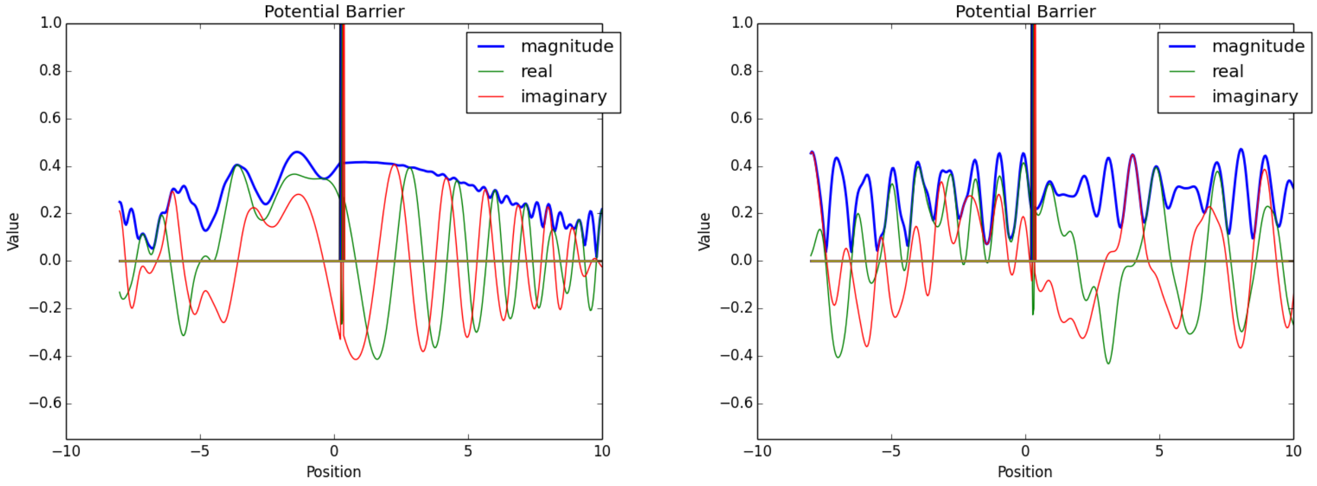

Figure 9: Potential Barriers

the Crank-Nicolson algorithm, changing the discretization leads to strange behavior. To change the x-range, the time-step must be varied correspondingly. More robust computation would improve the success of these changes.

Considering the first, most informational plot, the wave packet probably was supposed go right through the potential barrier. This is completely unintuitive and reveals that quantum mechanics is amazing.

5. Kronig-Penney

The Kronig-Penney potential traditionally illustrates the band structure of solids. The periodic potential is supposed to mimic that of a crystal, so the analytical solution to the TDSE shows the movement of electrons in a crystal. The solutions reveal that only certain energies are allowed, and that there are bands of allowed energies separated by bands of nonexistent ones. From this comes the understanding of the difference between insulators, semiconductors, and conductors. Insulators have bands that are completely filled, so the electrons are not free to move between them. If the electric field is very strong, however, there is a chance that they may jump into another band. A semiconductor is like an insulator with a narrow band gap, so it lets electrons move into conducting bands. Therefore, it sometimes conducts.

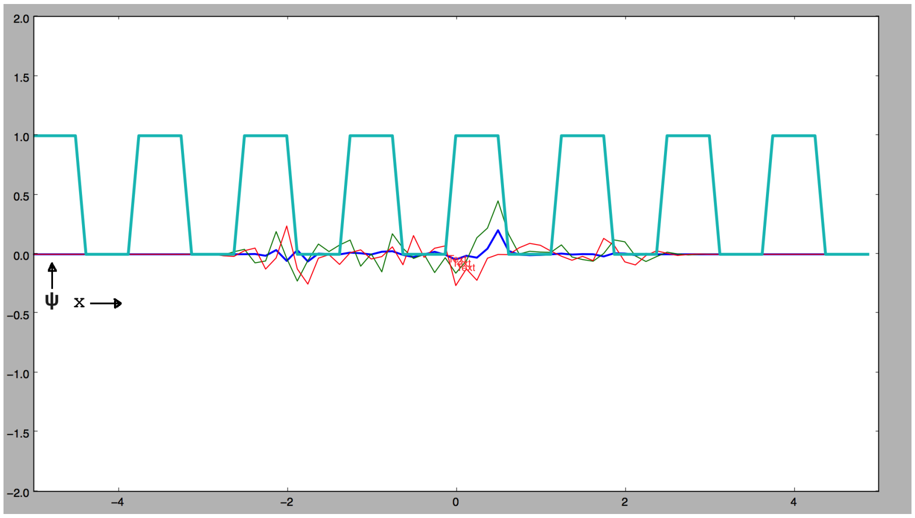

Figure 10: Kronig Penny Crystal

As is, our function is non-hermitian, and has non-real eigenvalues. However, by resetting the potential barriers, such that:

$$V(x) = \begin{cases} ix & : -L < x < L \\ \infty & : x \leq -L, x \geq L \end{cases}$$

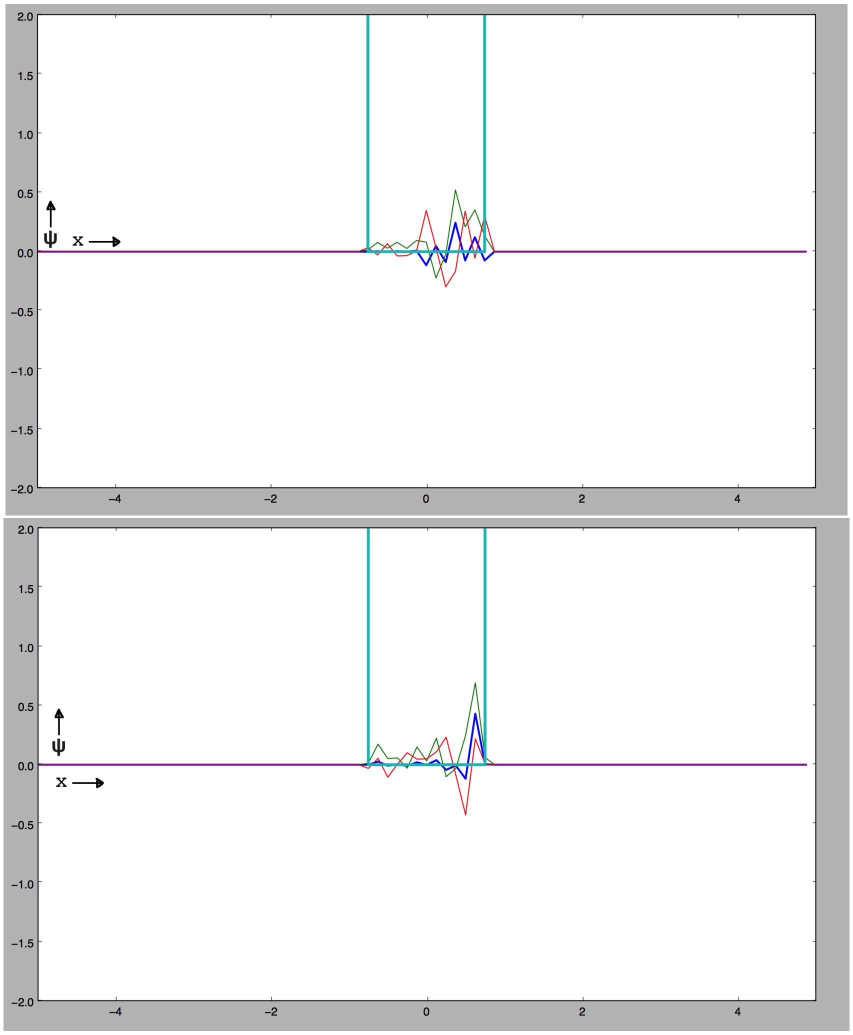

Figure 11: Non-Hermitian Edge States

We can create a condition in which we will have real eigenvalues at these boundary conditions. This creates Parity-Time (or PT) Symmetry, allowing us to have a normalizable wave function.

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