Time Dependent Schrödinger Equation

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April 13, 2015

Abstract

In this project, we have analyzed the solutions to the Time Dependent Schödinger Equation obtained through the finite difference scheme. Two different methods have been implemented and the results from each algorithm are compared. For simplicity, in this project we let $\hbar = m = \omega = 1$. This report contains heatmap plots of the amplitude vs time of the solutions to the TDSE, but we encourage the reader to run our code through the GUI to see the solutions animated.

1 Free Particle

1.1 Comparing Methods

In this project, we have implemented two different finite difference schemes. The first uses the "obvious" finite difference scheme below

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

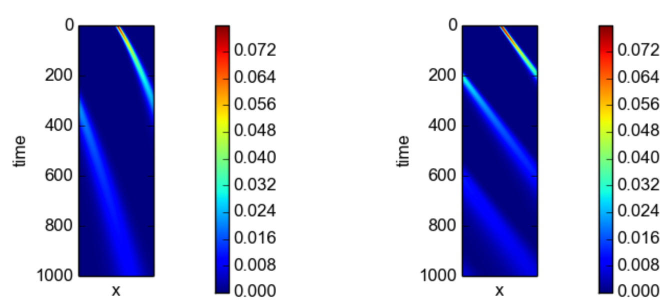
The second uses a slightly modified approach. This method is superior because it is stable and unitary. The algorithm for this method is

1.2 Periodic Boundary Conditions

By applying periodic boundary conditions, we see the particle exit the frame on the right and reappear on the left, as expected. The results from the two different algorithms are shown in Figure 1

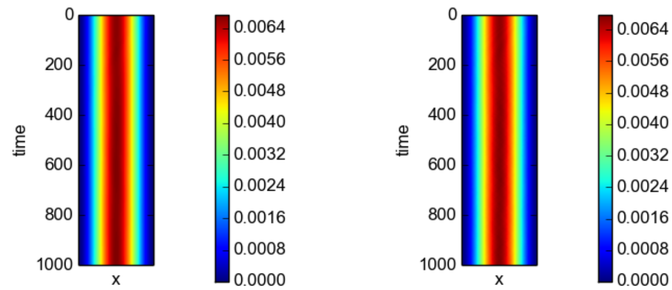
1.3 Zero Boundary Conditions

By applying zero boundary conditions, we effectively place the particle in the infinite square well. For an analysis of this scenario, please see the following section.



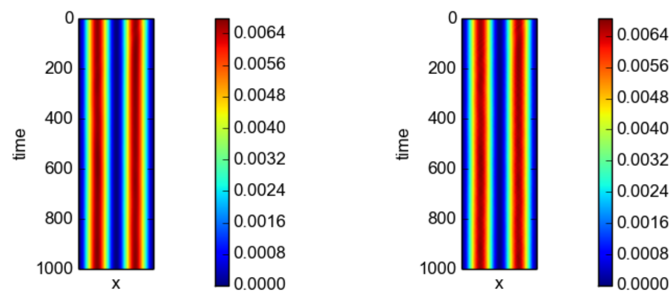
(a) Algorithm 1 (b) Algorithm 2

Figure 1: Free particle with periodic boundary conditions



(a) Algorithm 1 (b) Algorithm 2

Figure 2: Ground state of the infinite square well



(a) Algorithm 1 (b) Algorithm 2

Figure 3: First excited state of the infinite square well

2 Common Potentials

2.1 Infinite Square Well

We first look at the classic infinite square well potential. This potential is of the form,

$$V(x) = \begin{cases} 0 & : -\frac{a}{2} \leq x \leq \frac{a}{2} \\ \infty & : x < -L, x > L \end{cases}$$

The eigenvalues for a particle in the infinite square well are

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{n^2\pi^2}{2a^2} \tag{2}$$

with corresponding eigenfunctions

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi}{a}x\right) \tag{3}$$

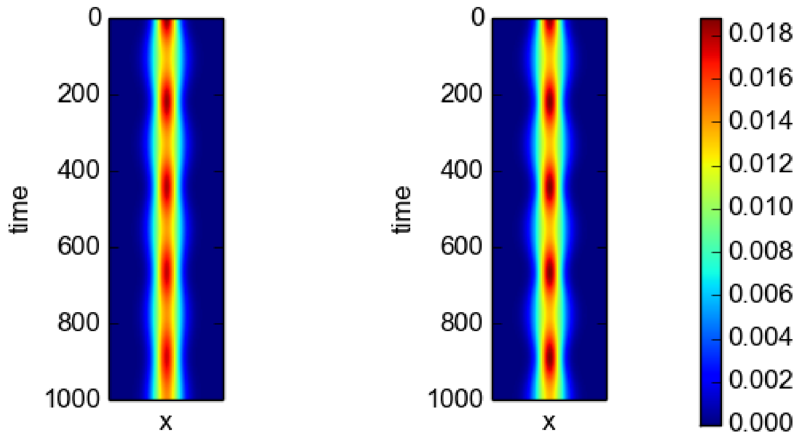
The first and second eigenstates for both algorihms are shown in Figures 2 and 3

For this potential, the two algorithms gave the same output. This is due to the fact that these are *stationary states*, so the method used to evolve the wavefunction through time did not matter

2.2 Harmonic Oscillator

The eigenvalues for a particle in this potential are

$$E_n \left(n + \frac{1}{2}\right) \hbar\omega = \left(n + \frac{1}{2}\right) \tag{4}$$



(a) Algorithm 1 (b) Algorithm 2

Figure 4: Ground state of the harmonic oscillator

with corresponding eigenfunctions

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(x) e^{-x^2/2} \tag{5}$$

where $H_n(x)$ is the n$^{\text{th}}$ Hermite Polynomial. The plots of the first two eigenstates form both algorithms are shown in Figure 4 Note that the oscillations are periodic, as expected. Also notice how the maximum amplitude of the oscillations decreases throughout time in the first algortihm, and stays constant in the second.

3 Barrier Potential

We now look at a potential barrier. In order to examine how a particle will interact with a barrier, we must multiply our initial gaussian wavepacket by e^{ikx} which results in a gaussian wave packet moving to the right. In this section and those that follow, we will restrict our analysis to the superior finite difference scheme. Figure 5 shows a wavepacket colliding with barriers of different energies. Notice how when $E = V/2$, some of the wavepacket is still transmitted. Classically, this scenario is forbidden. In quantum mechanics, however, this process is allowed and is known as *tunneling*.

3.1 Transmition and Reflection Coefficients

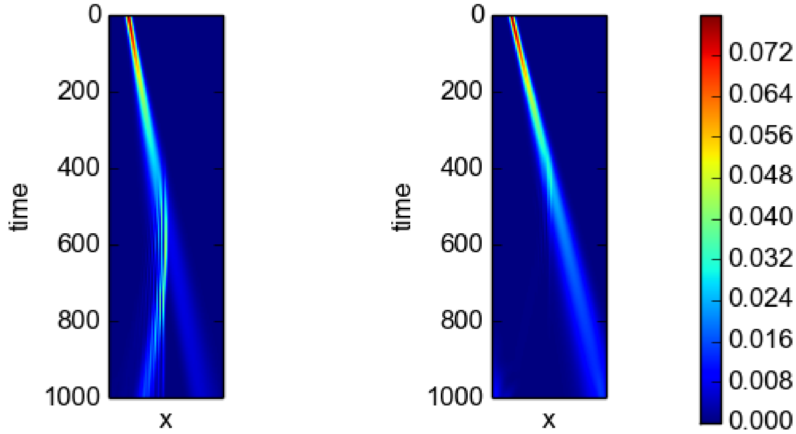
Analytically, we expect the reflection and transmission coefficients to be of the form

$$T = \frac{4k_0 k_1 e^{-ia(k_0-k_1)}}{(k_0+k_1)^2 - e^{2iak_1}(k_0-k1)^2} \qquad R = \frac{(k_0^2-k_1^2)\sin(ak_1)}{2ik_0k_1\cos(ak_1) + (k_0^2+k_1^2)\sin(ak_1)} \tag{6}$$

where $k_0 = \sqrt{2mE/\hbar^2} = \sqrt{2E}$ and $k_1 = \sqrt{2m(E-V)/\hbar^2} = \sqrt{2(E-V)}$. Letting $E = 100$ and $V = 200$, we calculate that $R = .99588$ and $T = .00412$. However, from the formula above we expect T to be on the order of 10^{-12}

3.2 Incident Energy Equal to the Barrier Height

We now look at the situation in which the incident energy E equals the height of the potential barrier V. In this situation, we have that $k_1 = 0$



(a) E = V/2 (b) E = 2V

Figure 5: Barrier Potential

4 Kronig-Penney Crystal

The next potential that we looked at was a periodic array of potential wells, i.e. a Kronig-Penny crystal.

5 Non-Hermition Hamiltonian

We now look at the potential

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

Although this potential yields a Hamiltonian that is non-Hermitian, it does have real eigenvalues