Phys 410 Project 2 — The Time Dependent Schrodinger Equation

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1 Introduction

One of the most important differential equations in Physics is Schrodinger's Equation. Schrodinger's Equation was postulated by Erwin Schrodinger in 1925 and describes a mathematical prediction of a quantum particle's position given by the particle's wavefunction [1]. By applying computational methods to solving the time-dependent Schrodinger equation we can create meaningful simulation of systems such as a particle in a well or through a double slit.
This report will utilize the Crank-Nicolson ADI scheme to numerically compute the solution to the one and two dimensional Schrodinger Equation.

2 Mathematical and Computational Background

Crank–Nicolson Method
The Crank-Nicolson Method is a discrete computational method using finite difference method to solve systems of different equations [2]. The Crank-Nicolson method works based on the trapezoidal rule and is a combintion of the forward and backward Euler methods with form:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2}\left[F_i^{n+1}\left(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}\right) + F_i\left(u, x, t, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}\right)\right] \tag{1}$$

One Dimensional Schrodinger Equation
By setting appropriate constants and values such as $\hbar$ and mass to be 1, we can represent the One-Dimensional time dependent Schrodinger mathematically as:

$$i\frac{\partial}{\partial t}\psi(x,t) = \left[\frac{\partial^2}{\partial x^2} + V(x,t)\right]\psi(x,t) \tag{2}$$

Where ψ is complex in nature having real and imaginary components like:

$$\psi_{Re} = i\psi_{Im}$$

Also, we can restrict our domain to:

$$0 \leq x \leq 1, \quad 0 \leq y \leq 1, \quad 0 \leq t \leq t_{max}$$

with the initial and boundary conditions:

$$\psi(0,t) = \psi(1,t) = 0, \quad \psi(x,0) = \psi_0(x)$$

For $\psi_0(x)$ describes the initial wavefunction at $t = 0$ or:

$$\psi_0(x) = \sin(m\pi x)$$

for a stationary particle of 'exact family', and:

$$\psi_0(x) = e^{ipx} e^{-((x-x_0)/\sigma)^2}$$

for a boosted Gaussian particle, or a particle with a momentum.

Two Dimensional Schrodinger Equation
The 2-Dimensional Schrodinger is the similar to the 1-Dimensional case, except extended in the xy-plane instead just along the x-axis.
Specifically the Two-Dimensional time dependent Schrodinger equation can be represented mathematically as:

$$i\frac{\partial}{\partial t}\psi(x,y,t) = \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + V(x,y,t)\right]\psi(x,y,t) \tag{3}$$

Again, we can restrict our domain to:

$$0 \leq x \leq 1, \quad ,0 \leq y \leq 1, \quad 0 \leq t \leq t_{max}$$

with the initial and boundary conditions:

$$\psi(x,y,0) = \psi_0(x,y), \quad \psi(0,y,t) = \psi(1,y,t) = \psi(x,0,t) = \psi(x,1,t) = 0$$

Where ψ_0 denotes the initial wavefunction at t=0

3 Discretization of the 1D and 2D Schrodinger Equation

Discretization for 1D Shrodinger Equation
First we should discretize the temporal and spatial domain as well as define important variables:

$$\lambda = \frac{\Delta t}{\Delta x}, \quad n_x = 2^l + 1 \quad \Delta x = 2^{-1} \quad \Delta t = \lambda \Delta x \quad n_t = \text{round}(t_{max}/\Delta t) + 1$$

Now we can apply the discussed Crank-Nicolson discretization of (1) to (2) resulting in:

$$i\frac{\psi_j^{n+1}-\psi_j^n}{\Delta t} = -\frac{1}{2\Delta x^2}\left(\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1} + \psi_{j+1}^{n1} - 2\psi_j^{n1} + \psi_{j-1}^{n1}\right) + \frac{1}{2}V_{ij}^{n+\frac{1}{2}}\left(\psi_j^{n+1} + \psi_j^n\right) \tag{4}$$

From here we can separate the ψ terms apart in time like:

$$\psi_j^{n+1}\left(\frac{i}{\Delta t} - \frac{1}{\Delta x^2} - \frac{1}{2}V_j^{n+\frac{1}{2}}\right) + \psi_{j-1}^{n+1}\frac{1}{2\Delta x^2} + \psi_{j+1}^{n+1}\frac{1}{2\Delta x^2} = \psi_j^n\left(\frac{i}{\Delta t} + \frac{1}{\Delta x^2} + \frac{1}{2}V_j^{n+\frac{1}{2}}\right) - \psi_{j-1}^n\frac{1}{2\Delta x^2} - \psi_{j+1}^n\frac{1}{2\Delta x^2} \tag{5}$$

Now we have a form where if ψ^n is known – or the wavefunction at a given time – then we can calculate ψ^{n+1} or the wavefucntion at the next time increment. To do this we can construct a $nx \times nx$ matrix, A, with diagonals corresponding to c_-, c_0, c_+ where:

$$c_- = c_+ = \frac{1}{2\Delta x^2}, \quad c_0 = \frac{i}{\Delta t} - \frac{1}{\Delta x^2} - \frac{1}{2}V_j^{n+\frac{1}{2}}$$

We can define a vector f to be the right hand side of (6) and by taking $A\backslash f$ in Matlab we can estimate psi_j^{n+1} at a given time step. Repeating this for all time steps, and we are able to solve all $\psi(x,t)$

Discretization for 2D Schrodinger Equation

Building the ADI discretization of the Schrodinger Equation in Two Dimensions we get:

$$\left(1 - i\frac{\Delta t}{2}\partial_{xx}^h\right)\psi_{i,j}^{n+\frac{1}{2}} = \left(1 + i\frac{\Delta t}{2}\partial_{xx}^h\right)\left(1 + i\frac{\Delta t}{2}\partial_{yy}^h - i\right) \tag{6}$$

$$\left(1 - i\frac{\Delta t}{2}\partial_{yy}^h + \frac{i\Delta t}{2}V_{i,j}\right)\psi_{i,j}^{n+1} = \psi_{i,j}^{n+\frac{1}{2}} \tag{7}$$

As in the 1-Dimensional case we can define c_-, c_0, c_+ to help us solve for the incremental time step (for 7):

$$c_- = c_+ = -\frac{i\Delta t}{2\Delta x^2}, \quad c_0 = 1 + \frac{i\Delta t}{\Delta x^2}$$

We can now Solve (7) By constructing a matrix A with diagonals (c_-, c_0, c_+) and performing matrix division to solve for a 2D matrix at every time step along the rows of the matrix we can get:

$$\psi_{ij}^{n+\frac{1}{2}} = A \backslash f$$

Finally we can construct a second matrix A2 for (8) c_-, c_0, c_+ resembling:

$$c_- = c_+ = -\frac{i\Delta t}{2\Delta y^2}, \quad c_0 = 1 + \frac{i\Delta t}{\Delta y^2} + \frac{i\Delta t}{2} V_{i,j}$$

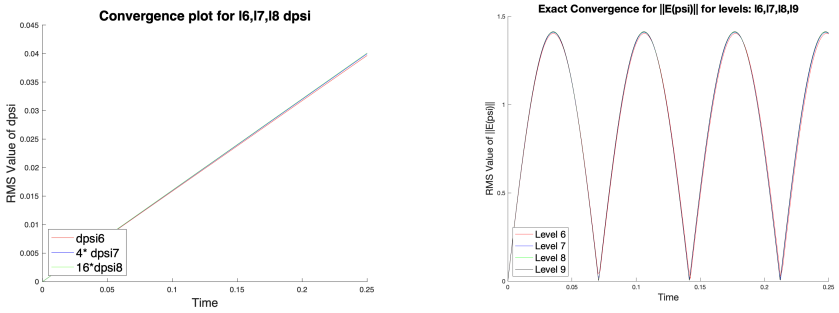
And solve this matrix along the columns we get the solution ψ_{ij}^{n+1}:

$$\psi_{i,j}^{n+1} = A_2 \backslash \psi_{ij}^{n+\frac{1}{2}}$$

4 One Dimensional Schrodinger Equation Results

We can summarize our 1-D Shrodinger findings in Covergence plots, Surveys and the analysis of those figures.

1D Convergence
As a diagnostic to inspect the convergence of our implementation of the 1D Schrodinger Equation, we can calculate the Root-Mean-Squared value of the difference between chosen levels – which represent the degree of how fine the x and t meshgrid are.



(a) Relative Convergence (b) Exact Convergence

Figure 1: Convergence Graphs for Exact Family

From Figure 1a we see that dpsi converges to a linear line for all three level differences. From this we can interpert that as time increases there is a greater difference in psi between consecutive levels and it follows a fourth-order FDA. Similarly for the convergence of exact families, we can see the RMS difference between the exact Psi and the Calculated Psi vary in sinusoidal squared fashion over time. We can also see that all four levels converge to this relation meaning the Schrodinger interpretation for the exact family converges to a fourth order FDA.

And the second Convergence plot for a Boosted Gaussian is:

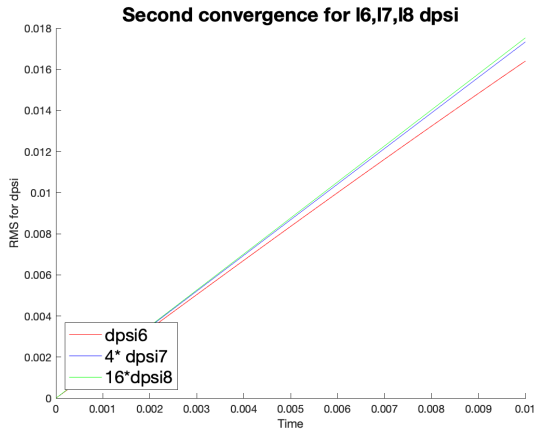


Figure 2: Boosted Gaussian Covergence

From figure 2 we see a larger deviation from the linear convergence line we saw in figure 1a. As a result, for a boosted Gaussian there is a greater discrepancy on the results based on the level order we choose. Namely, for boosted Gaussian systems we should simulate with at least level 7.

1D Barrier Survey

By running a simulation with a boosted Gaussian Initial $\Psi_0(x)$ for different potentials for a barrier existing from $x = [0.6, 0.8]$, we can model the fractional probability that particle will spend in a potential by the following graph:

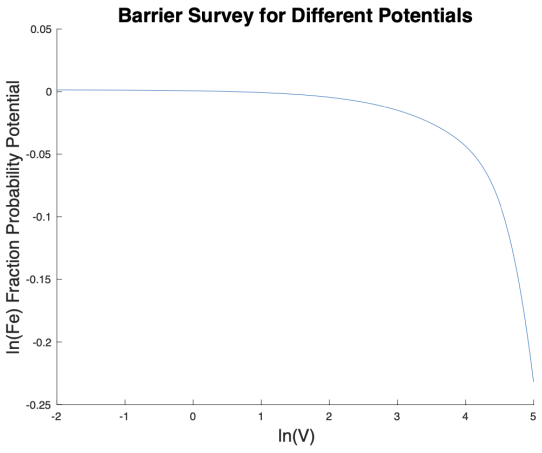


Figure 3: Barrier Survey for Different Potentials

To get this fractional probability we need to find the the probability a particle exists from $0 \rightarrow x$ can described as:

$$P(x,t) = \int \psi(\bar{x},t)\psi^*(\bar{x},t)d\bar{x} \tag{8}$$

or in discrete terms:

$$\bar{P}_j = \frac{\sum_{n=1}^{n_t} P_j^n}{n_t}$$

where $\bar{P}_j$ is normalized by:

$\bar{P}_j = \frac{\bar{P}_j}{\bar{P}_{n_x}}$

and to get the fractional probability:

$$\bar{F}_e(x_1,x_2) = \frac{\bar{P}_j(x_2) - \bar{P}_j(x_1)}{x_2 - x_1}$$

Now knowing the meaning of $ln(F_e)$, we can interpret Figure 3. Because $ln(F_e)$ falls off as Potential increases we can make the conclusion that the particle will be more likely to be found to the right of the barrier for a barrier with a smaller potential. We can also make the conclusion based on our normalized constants and domain that from $ln(V) = [1,4]$ the chance of the particle being to the right of the barrier is about the same, but beyond this the probability that the particle exists to the right of the potential drops off exponentially.

1D Well Survey

Using the same notation for the fractional probability of a particle existing inside a well $x = [0.6, 0.8]$ for different negative potentials we produced the following relationship:

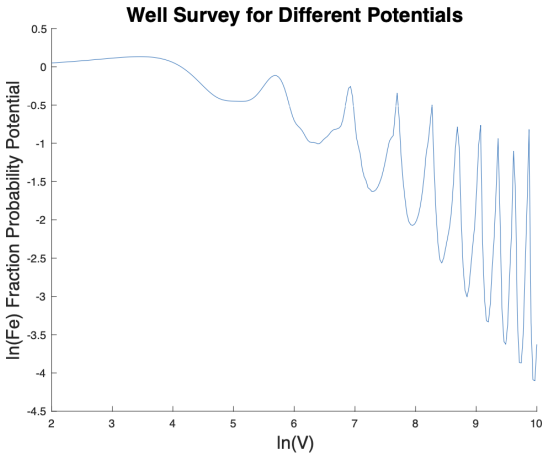


Figure 4: Well Survey for Different Potentials

From the results of the well survey we can make two conclusions. One – the fractional probability spent in the well is roughly constant for low potentials. And Two - As potential increases there are clear eigenstates that the particle's wavefunction exists in for those potential. The fractional probability troughs in Figure 4 represent these eigenstates which decrease in magnitude and width as potential increases.

5 Two Dimensional Schrodinger Equation Results

We can perform a convergence test just as done in [Figure 1(a)] except in two dimensions:

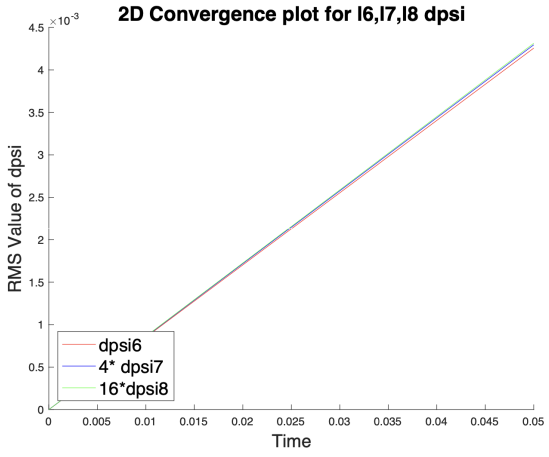


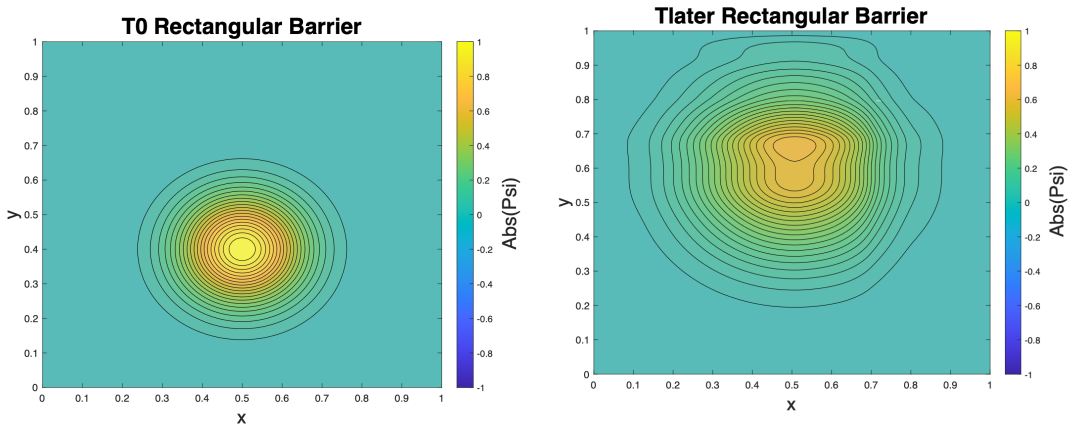
Figure 5: 2D convergence

Figure 5 shows a strongly correlated convergence plot for all three difference in levels for an exact family of 2D Schrodinger particle. We can make the same interpretation as we did in Figure 1a and conclude that the 2D particle converges to a fourth-order FDA approximation for all three difference in levels.

Simulating Finite Potential Barrier

Using our two-dimensional computational solution to the Schrodinger we can create meaningful simulations. One such simulation of importance is the finite rectangular potential barrier. For our potential barrier we can define it to be between $x = [0, 1], y = [0.7, 0.8]$ with an initial potential value of 400. We can initialize the particle's position to be $x = 0.5, y = 0.5, p_x = 0, p_y = -15$. This produces a contour map at time t=0 displayed by [Figure 6 (a)]. Because we set $p_x = -15$ the wavefunction will move upwards until it encounters the barrier as shown in [Figure 6(b)]. The wavefunction will mostly bounce off

the potential barrier with some of the wavefunction tunneling through. A full simulation is available either by running barrier2d.m or playing the animation barrier2dAnimation.avi.



(a) Contour plot at t=0

(b) Contour plot at tlater

Figure 6: Contour plot of Abs(Psi) at initial time and tlater when the wavefunction meets the finite potential barrier.

Simulating Finite Potential Barrier

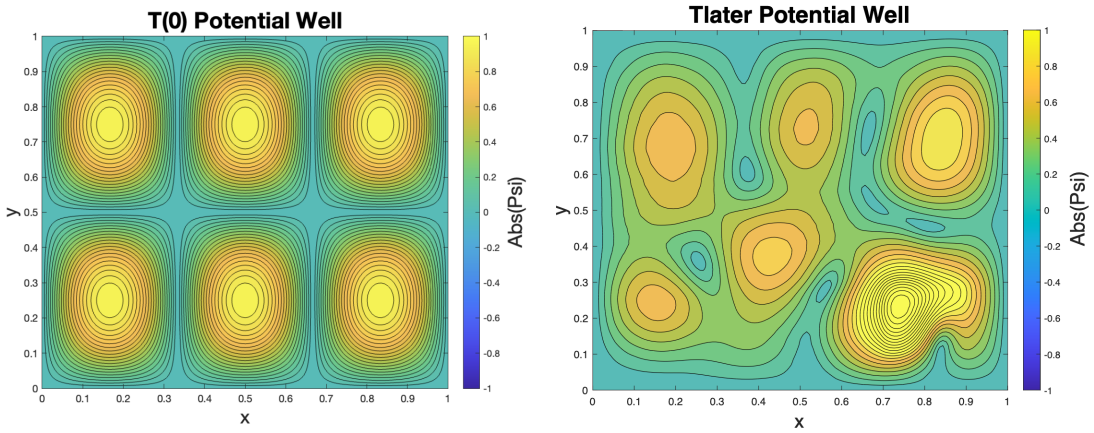
We can also simulate a finite potential well by creating a region that has a negative potential in area defined

$$V_x = [x_1, x_2], \quad V_y = [y_1, y_2]$$

. For my simulation I chose to create a square well at the lower right corner of the xy plane or:

$$x_1 = 0.7, x_9 = 0.8; \quad y = [0.1, .3]$$

with $V = -400$. I also chose the wavefunction to be defined by the exact Gaussian family discussed earlier, meaning the wavefuntcions would stay stationary if there was a constant potential. However the initial stagnant wavefunction shown in [Figure 6a] decays into a congregation of the wavefunction in the finite potential well at the lower right hand corner for [Figure 6b] at the final time. A full simulation is available either by running well2d.m or playing the animation well2dAnimation.avi.



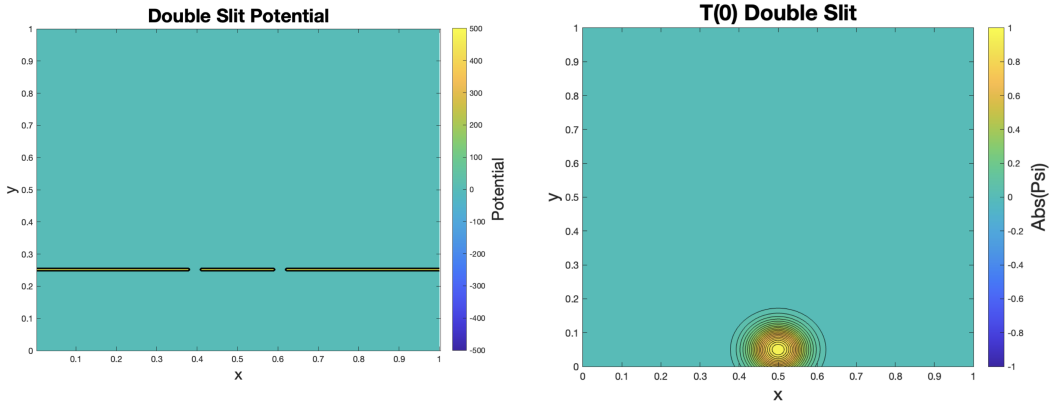
(a) Contour plot at t(0)

(b) Contour plot at t(final)

Figure 7: Contour plot of Abs(Psi) at initial time and final time for a stationary gaussian wavefunction subject to a finite potential well

Simulating Finite Double Slit Experiment

Finally we can simulate a double slit experiment by defining a finite potential barriers along a values ($y = 0.25$) as shown in [figure 8]. A particle is then generated at $x = 0.5, y = 0.05$ with an initial p_y upwards towards the double slit. The expected result is a diffraction pattern, however the actual result is a wave interference best described in the animation 'doubleSlit2dAnimation.avi' which is produced by, 'doubleSlit2d.m'.



(a) Contour plot of Potential

(b) Contour plot at t(final)

Figure 8: Contour plot of Abs(Psi) at initial time and final time for a stationary Gaussian wavefunction subject to a finite potential well

6 Conclusion

Using the Crank-Nicolson Method applied to the Schrodinger Equation, we were able to model and simulate the Shrodinger Eqution in one and two dimesions. In 1-dimensions we tested for accurate convergence in both exact and boosted gaussian family of initial conditions for the wavefunction. We were also able to simulate a 1-Dimensional barrier and well by modelling the fractional probability of the particle existing in different potentials. Then we applied the Crank-Nicolson method to a two scheme ADI solution of the Schrodinger equation in two dimensions. We simulated a moving 2-dimensional particle encountering a barrier and double slit as well as a stationary particle being interacting with a finite potential well.
Improvements could be made in confining the spatial locality of the boosted Gaussian particle in two-dimensions as well as a more exhaustive analysis in effects of double-slits and barrier with different starting potentials. The double slit results in particular were unexpected and could be an indicator of flawed implementation of incorporating the potential into the two stage ADI. Meaningful future extensions on this project including modelling a three-dimensional Schrodinger Equation, or simulating multiple boosted Gaussian wave functions interacting with each other.

References

References

[1] Schrödinger equation Wikipedia Page. Last Accessed December 5, 2022, from `https://en.wikipedia.org/wiki/Schr%C3%B6dinger_equation`

[2] Crank–Nicolson method Wikipedia Page. Last Accessed December 5, 2022, from `https://en.wikipedia.org/wiki/Crank%E2%80%93Nicolson_method`

[3] Phys 410 Project 2 Description `http://laplace.physics.ubc.ca/410/homework/pr2.pdf`