Project 2

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Table of Contents

How to run Codes: In order to run the codes and reproduce the results, you can start with the main.m file. You can also reproduce the results for numerical experiments and convergence tests. You only need to run the appropriate file and then run the corresponding script that has “plot” in its name. For example for problem2, to run the bouncing experiment, you first need to run “Experiment3.m” and then run “Experiment3_plots.m” to generate the plots.

Problem 1:

1 Theory and Derivation

In this section I will describe the theory of the computational methods used to solve the problem of 1D schrodinger equation.

In this part, I have used finite difference approximation to solve the following differential equation.

$$i\psi = -\psi_{xx} + V(x,y)\psi$$

And the finite difference method I am going to use is Crank-Nicolson method as follows:

$$i(\psi_i^{n+1} - \psi_i^n) = -\frac{\Delta t}{2\Delta x^2}(\psi_{i-1}^n - 2\psi_i^n + \psi_{i-1}^n + \psi_{i-1}^{n+1} - 2\psi_i^{n+1} + \psi_{i-1}^{n+1}) + \frac{V_i^{n+1/2}}{2}(\psi_i^n + \psi_i^{n+1})$$

Now I define the operator δ^2 which acts on ψ_i^n as follows:

$$\delta^2\psi_i^n = \psi_{i-1}^n - 2\psi_i^n + \psi_{i+1}^n$$

And with defining the variable R as :

$$R = \frac{\Delta t}{\Delta x^2}$$

We can re write the FDA approximate of the schrodinger equation as:

$$(i - \Delta t/2V_i^{n+1/2} + R/2\delta^2)\psi_i^{n+1} = (i + \Delta t/2V_i^{n+1/2} - R/2\delta^2)\psi_i^n$$

And now with defining the following new variables:

$$\tilde{C}^{n+1/2} = i - \Delta t/2V_i^{n+1/2}$$
$$C^{n+1/2} = i + \Delta t/2V_i^{n+1/2}$$

We can write the original equation on more compact form of matrix equation:

$$(\tilde{C}^{n+1/2}I + R/2\Delta^2)\Psi^{n+1} = (\tilde{C}^{n+1/2}I - R/2\Delta^2)\Psi^n$$

In which I is the identity matrix and Δ^2 is the following tridiagonal matrix:

$$\Delta^2 = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{pmatrix}$$

And Ψ^n is a column vector containing ψ_i^n as its elements.

So in the nutshell we can Write:

$$\Psi^{n+1} = (\tilde{C}^{n+1/2}I + R/2\Delta^2)^{-1}(C^{n+1/2}I - R/2\Delta^2)\Psi^n$$

2 Code Exploration

sch_1d_cn.m: This file implements the Crank-Nicolson method used above.
main.m: This script is written for the user (in this case TA!) to easily call the sch_1d_cn.m function. This script also generate the appropriate outputs
Experiment1.m: This script performs the numerical experiment for particles and potential barriers.
Experiment1_plots.m: This script generates the appropriate plots using data generated in Experiment1.m script
Experiment2.m: This script performs the numerical experiment for particles and potential well.
Experiment2_plots.m: This script generates the appropriate plots using data generated in Experiment2.m script
ConrergenceTest1_1.m: This script performs the standard 4level convergence tests.
ConvergenceTest1_2.m: This script performs convergence tests using the exact solution
ConvergenceTest1_Xplots: Generates appropriate plots.
ConvergenceTest2.m: performs the second case of convergence test.
ConvergenceTest2_plots: Generates appropriate plots.
Exact_1d_sch.m: This script contains the exact solution of the 1D schrodinger equation.

3 Convergence Test

To perform the convergence test, I use the following approach. I define $d\psi^l$ as:

$$d\psi_l = \psi^{l+1} - \psi^l$$

In which l denotes the discretization level. Using the following formular for the second norm, we can calculate the norm of $d\psi^l$ as the function of time.

$$||v|| = \sqrt{\frac{\sum_{j=1}^{n} |v^j|^2}{n}}$$

3.1 Case 1:

3.1.1 Standard Convergence Test

In the following plot you can see the values of $||d\psi^6||$, $||d\psi^7||$, $||d\psi^8||$.

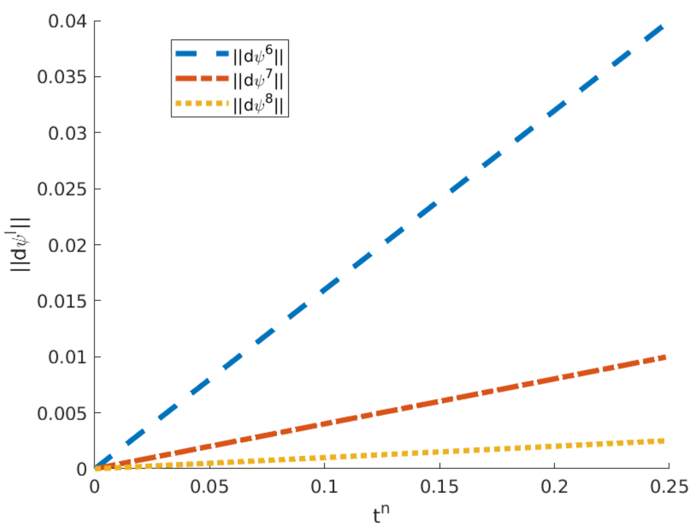

Fig. 1. Values of $||d\psi^l||$ showed on a single scale

As you can see the error rate is decreasing as desired. But we don’t know yet if the error is decreasing with the power of 4. To test that I simply multiply each error at the coefficient that I expect the errors scale according to that.

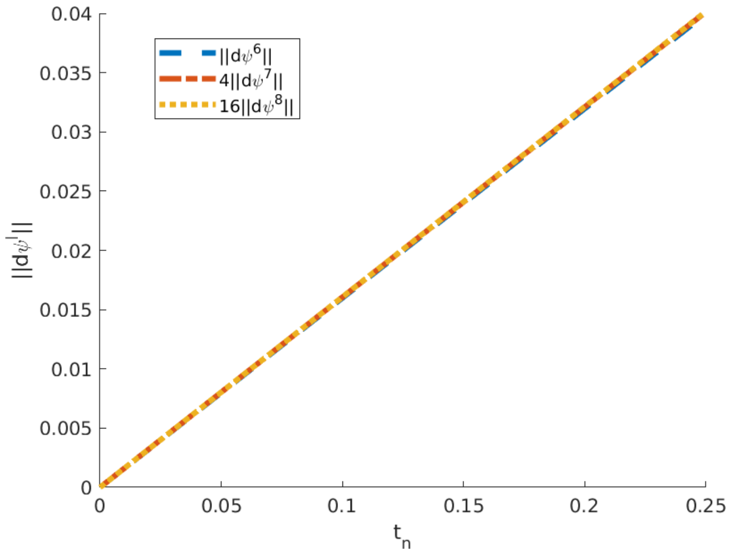

Fig. 2. Scaled errors plotted on the same plot

As we can observe in the plot above, the scaled error rates coincide perfectly. So it means that our solver converges properly.

3.1.2 Comparison with the exact solution

In this case we know the exact solution. Along with the standard convergence test, I am also going to compare the result of simulation with the exact solution:

$$||E(\psi^l)||(t^n) = ||\psi_{exact} - \psi^l||(t_n)$$

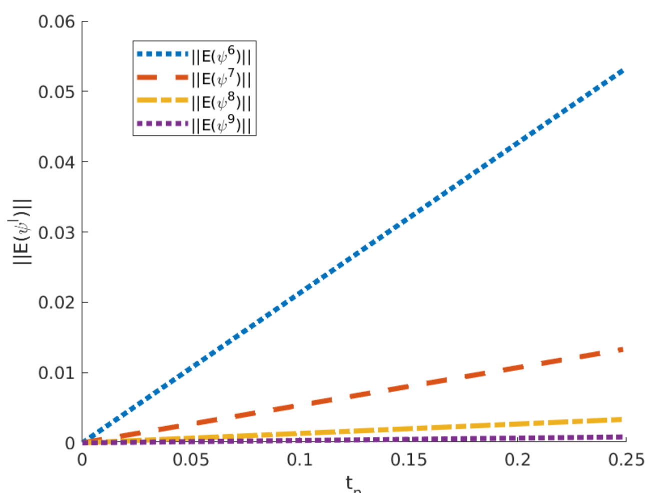

Fig. 3. Comparing the numerical solution with exact solution

As you can see in Fig. 3, we clearly see that the error goes down as we increase the discretization level. To better see this convergence, I will plot the scaled errors:

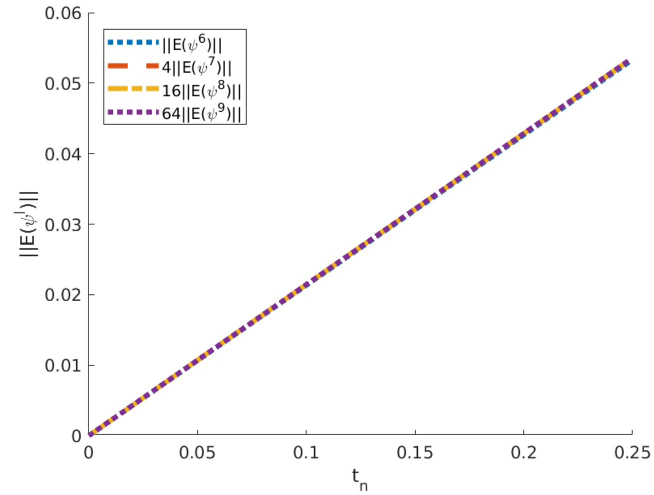

Fig. 4. Scaled error of numerical solutions with respect to the exact solution

3.2 Case 2:

In this case, we perform the convergence test on a particle with boosted gaussian as its initial value. To do that, as I did previously, I wil plot the values of $||d\psi^6||$, $||d\psi^7||$, $||d\psi^8||$.

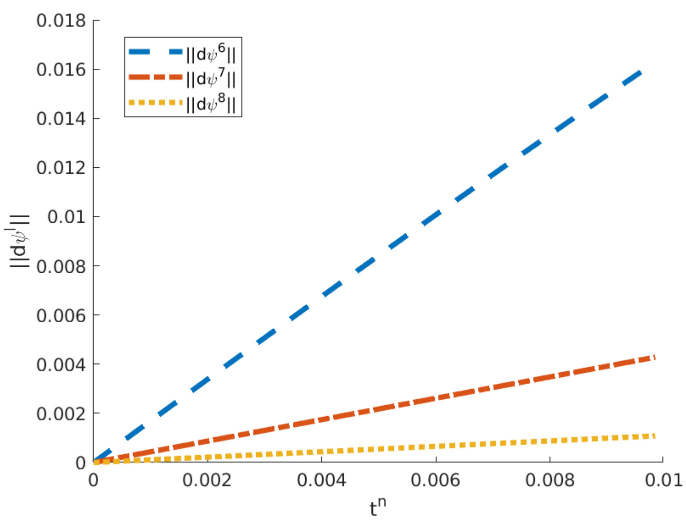

Fig. 5. Values of $||d\psi^l||$ showed on a single scale

As you can see the error goes down with increasing the discretization level. But to better see by how much the error rate goes down, I will also plot the scaled error values in the following picture.

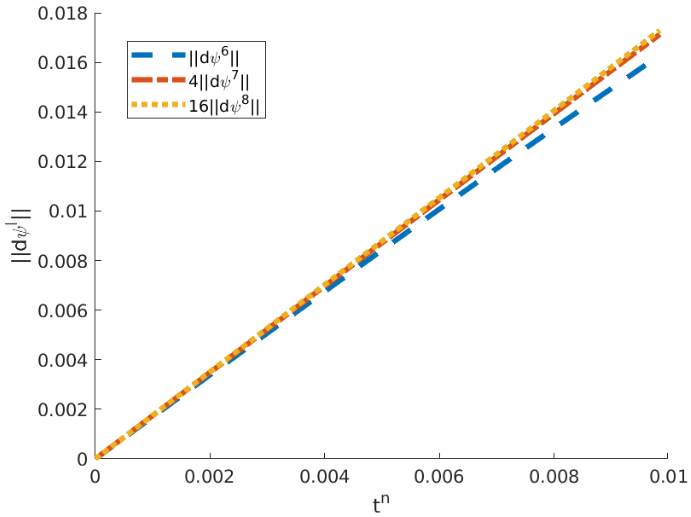

Fig. 6. Scaled errors plotted on the same plot

3 Numerical Experiments

3.1 Potential Barrier:

In this section we put a potential barrier in front of the particle and then measure the mean time that particle spends in an interval.

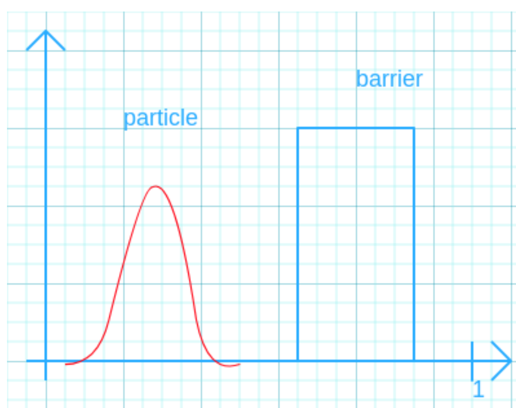

Fig. 7. Initial configuration of the system.

As you can see in the following plot, in the case of a barrier particle gets confined behind the potential wall.

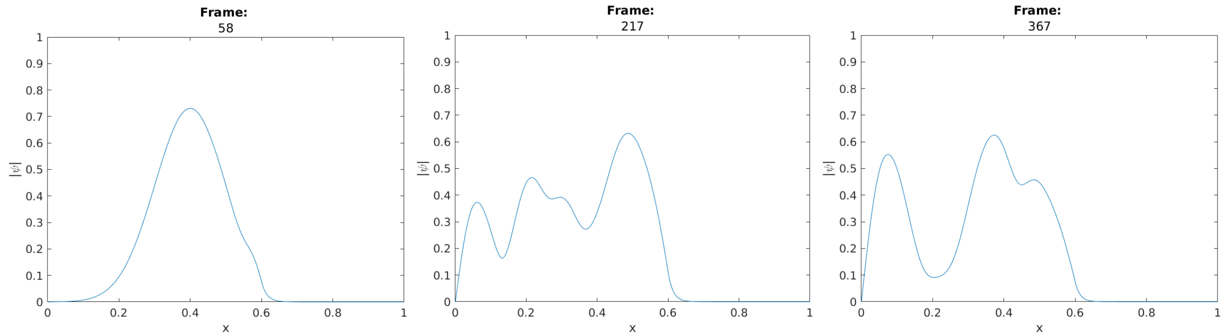

Fig. 8. Configuration of quantum system in the presence of potential barrier

You can find the animation of the above plots in the animations folder (“PotentialBarrier.avi”).

In the following plots you can see the plot of excess fraction vs. the height of potential barrier.

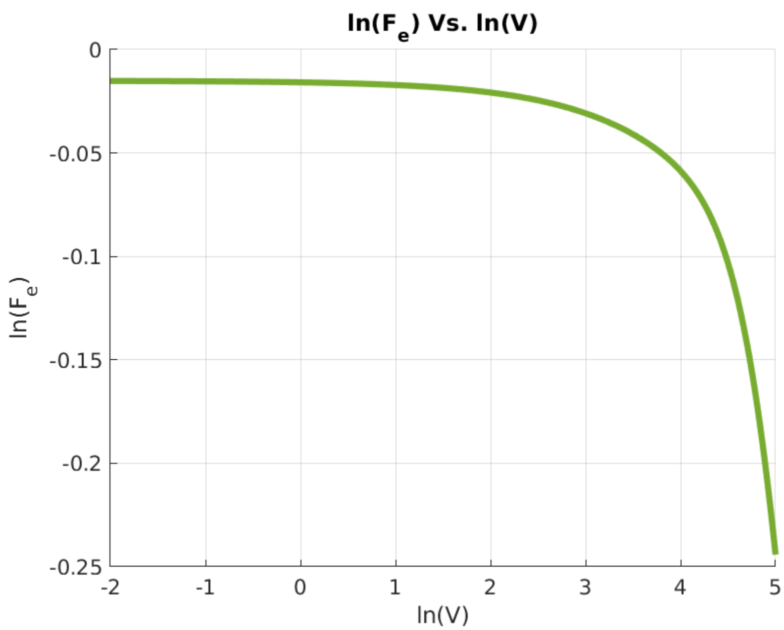

Fig. 9. Plot of excess fraction Vs. strength of potential barrier

My interpretation of this plot is that as we increase the strength of the potential wall, it becomes harder for the particle to penetrate the potential wall. So with increasing the strength of potential, the average time that particle spends in the “post wall” region decreases (in comparison with a free particle).

3.2 Potential Well:

In this configuration, we put a potential well in front of the particle (see the picture below)

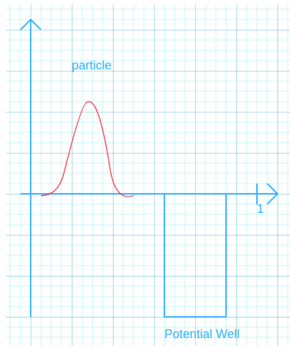

Fig. 10. Potential Well configuration of numerical experiment

As you can see in the following plot, a portion of particle wave function gets trapped inside the potential well:

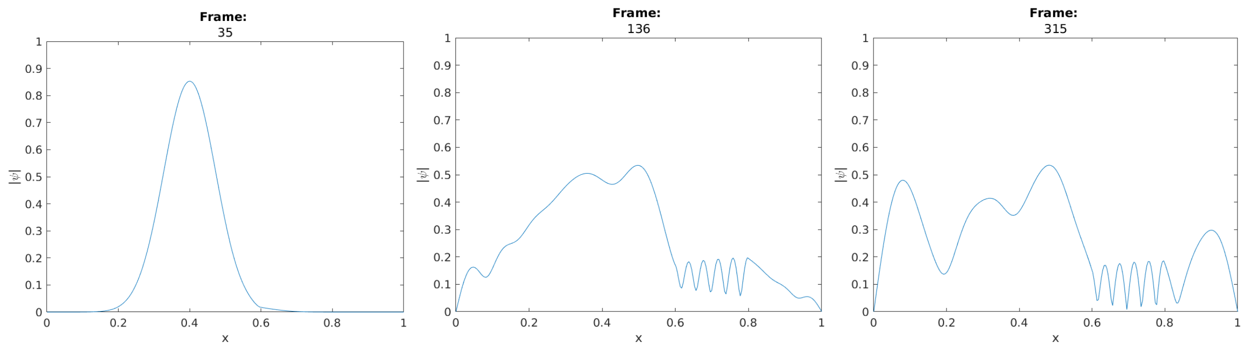

Fig. 11. Simulation results in case of potential well

You can find the animation of the above plots in the animations folder (“PotentialWell.avi”).
And finally in the following plot you can find the plot of excess fraction vs. the height of potential barrier.

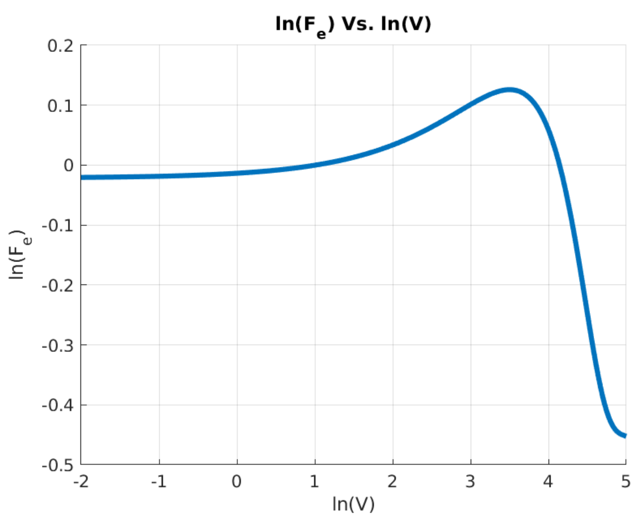

Fig. 12. Plot of excess fraction Vs. strength of potential barrier

My Explanation:
We know that a free particle would spend some of its time in interval [0.6,0.8]. But as we increase the depth of the potential well, some of the wave function gets trapped inside the potential well. So the probability for a particle to spend its time in interval [0.6,0.8] increases. But this increase in probability will not increase forever. For deeper potential wells, a particle spends even less time than a free particle in interval [0.6,0.8]. The reason for that is that we should note that the particle inside a potential well can only have discrete values of energy levels. Because of the finite initial energy of the particle, possible energy configurations for the particle inside the well decreases. So for deeper wells, the particle spends less time than a free particle inside the well located at [0.6,0.8]

Problem 2:

1 Theory and Derivation

In this section I will be simulating a 2D schrodinger equation. To do that I will be using the ADI method.

The differential equation that I am going to solve is:

$$i\frac{\partial\psi}{\partial t} = -(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2}) + V(x,y,t)\psi$$

Let's apply the Crank-Nicolson discretization:

$$i(\psi_{i,j}^{n+1} - \psi_{i,j}^{n}) = -\frac{\Delta t}{2\Delta x^2}(\delta_x^2 + \delta_y^2)(\psi_{i,j}^{n} + \psi_{i,j}^{n+1}) + \frac{V_{i,j}^{n+1/2}}{2}(\psi_{i,j}^{n} + \psi_{i,j}^{n+1})$$

In which:

$$\delta^2\psi_i^n = \psi_{i-1}^n - 2\psi_i^n + \psi_{i+1}^n$$

(Note that δ_x^2 acts on i component and δ_y^2 acts on j component.) After a little bit of simplification we will have:

$$(i + \frac{R}{2}(\delta_x^2 + \delta_y^2) - \frac{\Delta t}{2}V_{i,j}^{n+1/2})\psi_{i,j}^{n+1} = (i - \frac{R}{2}(\delta_x^2 + \delta_y^2) + \frac{\Delta t}{2}V_{i,j}^{n+1/2})\psi_{i,j}^{n}$$

In which

$$R = \frac{\Delta t}{\Delta x^2}$$

Using the expansion idea of ADI method ($\delta^2\delta^2 \approx 0$), We can write:

$$\psi_{i,j}^{n+1} = (1 - i\frac{R}{2}\bar{\delta}_x^2)^{-1}(1 + i\frac{R}{2}\delta_x^2)(1 - i\frac{R}{2}\delta_y^2)^{-1}(1 + i\frac{R}{2}\bar{\delta}_y^2)\psi_{i,j}^{n}$$

In which:

$$\bar{\delta}_x^2 = \delta_x^2 - \frac{\Delta t}{R}V_{i,j}^{n+1/2}$$
$$\bar{\delta}_y^2 = \delta_y^2 - \frac{\Delta t}{R}V_{i,j}^{n+1/2}$$

Note that to preserve the symmetry, I have one merged the potential term with δ_x^2 and one other time I have merged with δ_y^2.

To achieve more computation performance it is better to write the update rules in from of matrix multiplication. To do that we introduce the following matrices:

$$\bar{D}_y^2 = \Delta^2 - \frac{\Delta t}{R} V$$
$$\bar{D}_x^2 = \Delta^2 - \frac{\Delta t}{R} V^T$$

In which Δ^2 is the following tridiagonal matrix:

$$\Delta^2 = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 \end{pmatrix}$$

So in conclusion we can write:

$$\Psi^{n+1} = [(1 - i\frac{R}{2}\bar{D}_x^2)^{-1}(1 + i\frac{R}{2}D_x^2)[(1 - i\frac{R}{2}D_y^2)^{-1}(1 + i\frac{R}{2}\bar{D}_y^2)\Psi^n]^T]^T$$

In which T operator denotes matrix transpose operation. We can write the above equation in more compact form by introducing the following new variables:

$$M_x = 1 - i\frac{R}{2}\bar{D}_x^2$$
$$M_p = 1 + i\frac{R}{2}D_x^2$$
$$M_m = 1 - i\frac{R}{2}D_y^2$$
$$M_y = 1 + i\frac{R}{2}\bar{D}_y^2$$

So the final update rule will be:

$$\Psi^{n+1} = M_m^{-1} M_y \Psi^n (M_x^{-1} M_p)^T$$

2 Code Exploration

sch_2d_adi.m: Solver of 2D schrodinger equation using ADI method (the theory is described in above section)
main.m: This script is the starting point to reproduce the results.
Experiment{n}.m: Scripts that generate data corresponding to each of the experiments described in this report.
Experiment{n}_plots.m: Scripts to generate appropriate plots for each experiment.
ConvergenceTest.m: Performs 4 level convergence test
ConvergenceTest_plots.m: Generates appropriate plots for the 4 level convergence test.
ConvergenceTestExact.m: Performs convergence test with comparing the numerical solution with exact solution.
ConvergenceTestExact_plot.m: Generates appropriate plots for convergence test using exact solution

3 Convergence Test

To perform the convergence test, I use the following approach. I define $d\psi^l$ as:

$$d\psi_l = \psi^{l+1} - \psi^l$$

In which l denotes the discretization level. Using the following formula for the second norm, we can calculate the norm of $d\psi^l$ as the function of time.

$$||v|| = \sqrt{\frac{\sum_{j=1}^{n} |v^j|^2}{n}}$$

3.1 Standard Convergence Test

In this section I perform 4 level standard convergence tests. In the following figure you can see that as we increase the level of discretization, numerical error goes down:

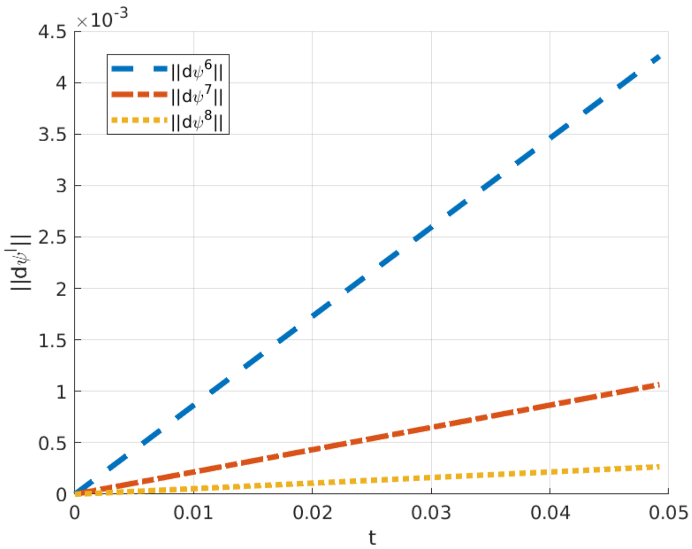

Fig. 13. Numerical error for different discretization of the same plot

But to better see by how much the error decreases, I will plot the scaled errors as well.

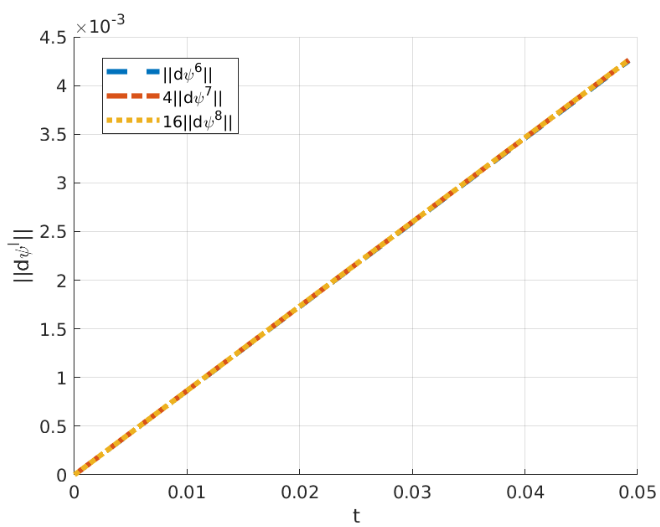

Fig. 14. Scaled numerical errors

As you can see the error rate goes down with power of 4 as we decrease discretization level.

3.2 Comparison with the exact solution

Since for idtype=0 we have the exact solution of the schrodinger equations, we can use that to verify our model. In the following plot you can see that the error goes down with decreasing the discretization level.

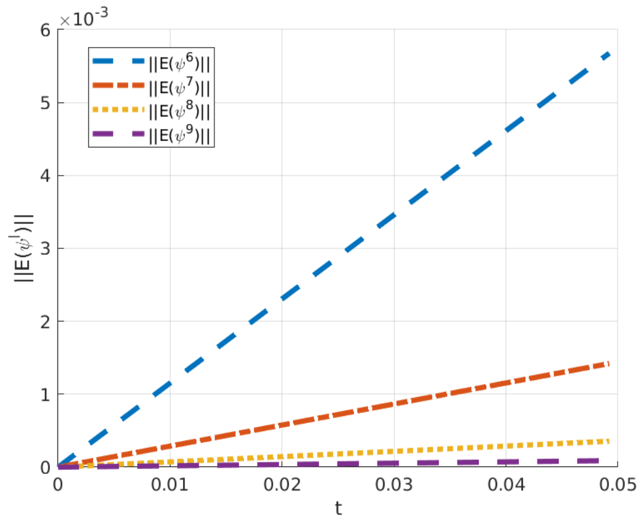

Fig. 15. Numerical error with respect to the exact solution

Like above, we can also plot the scaled numerical error:

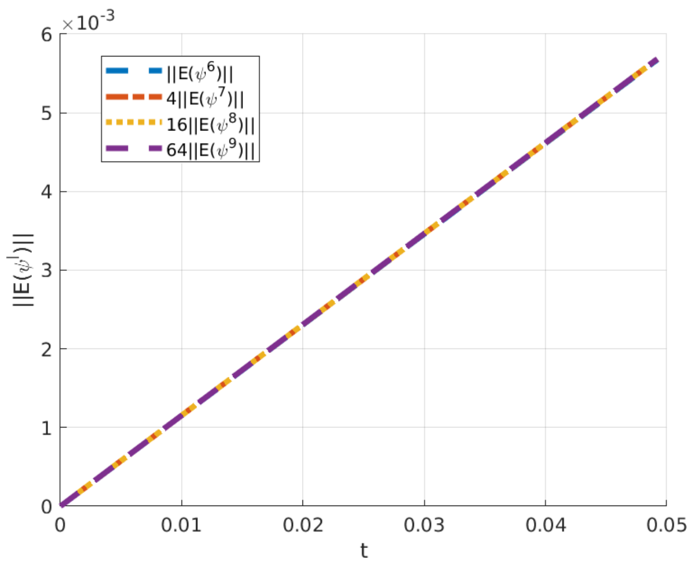

Fig. 16. Numerical error with respect to the exact solution

As you can see the scaled numerical errors match each other perfectly. This indicates that the solution is O(h^4) accurate.

3 Numerical Experiments

3.1 Potential Well:

For this section I put particles just at the middle of a potential well with depth -50. Here are the initial values I have used for this experiment.

idtype = 1;

vtype = 1;

idpar = [0.5,0.5,0.07,0.07,0,0];

vpar = [0.25,0.75,0.25,0.75,-50];

tmax = 0.004;

lambda = 0.001;

level = 7;

Here are some snapshots of the particle inside well (I have plotted the absolute value of wave function)

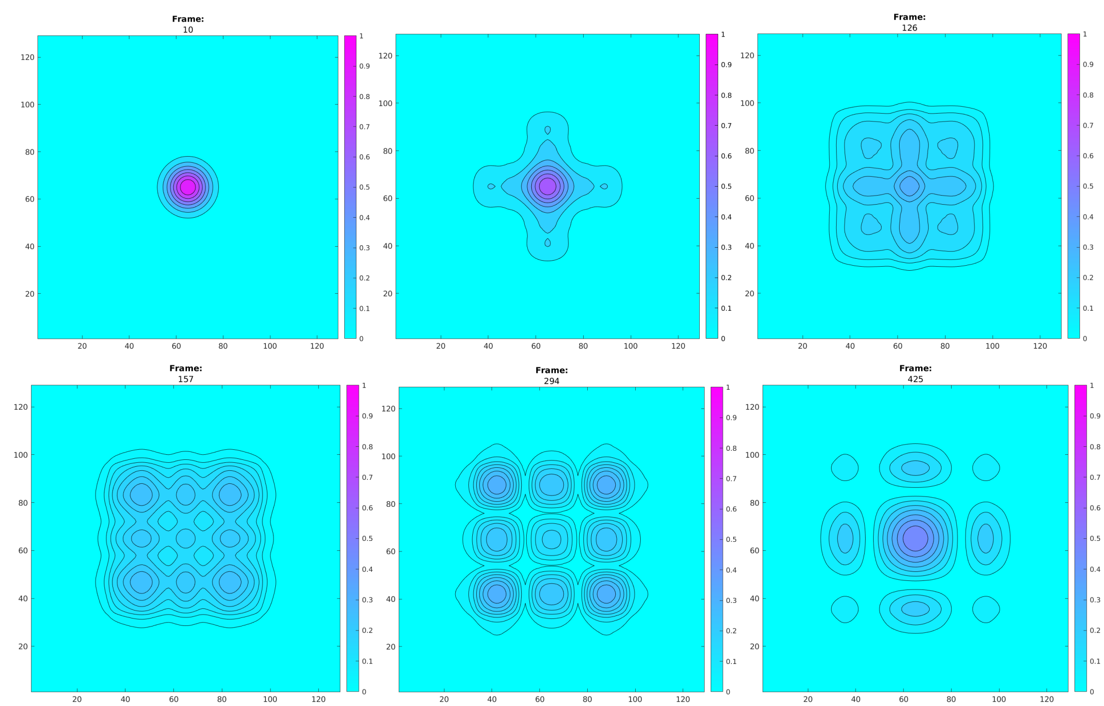

Fig. 17. Time evolution of the absolute value of wave function located at middle of a potential well.

You can find the animation of this experiment at animations folder with name "2D_potentialWell.avi".

3.2 Bouncing off from Walls:

In this section I am simulating the particle bouncing off the walls. Here is the initial values that I am using to setup the simulation:

idtype = 1;

vtype = 1;

idpar = [0.25,0.5,0.07,0.07,1000,600];

vpar = [0.5,1,0.5,1,0];

tmax = 0.01;

lambda = 0.001;

level = 7;

And here is the results:

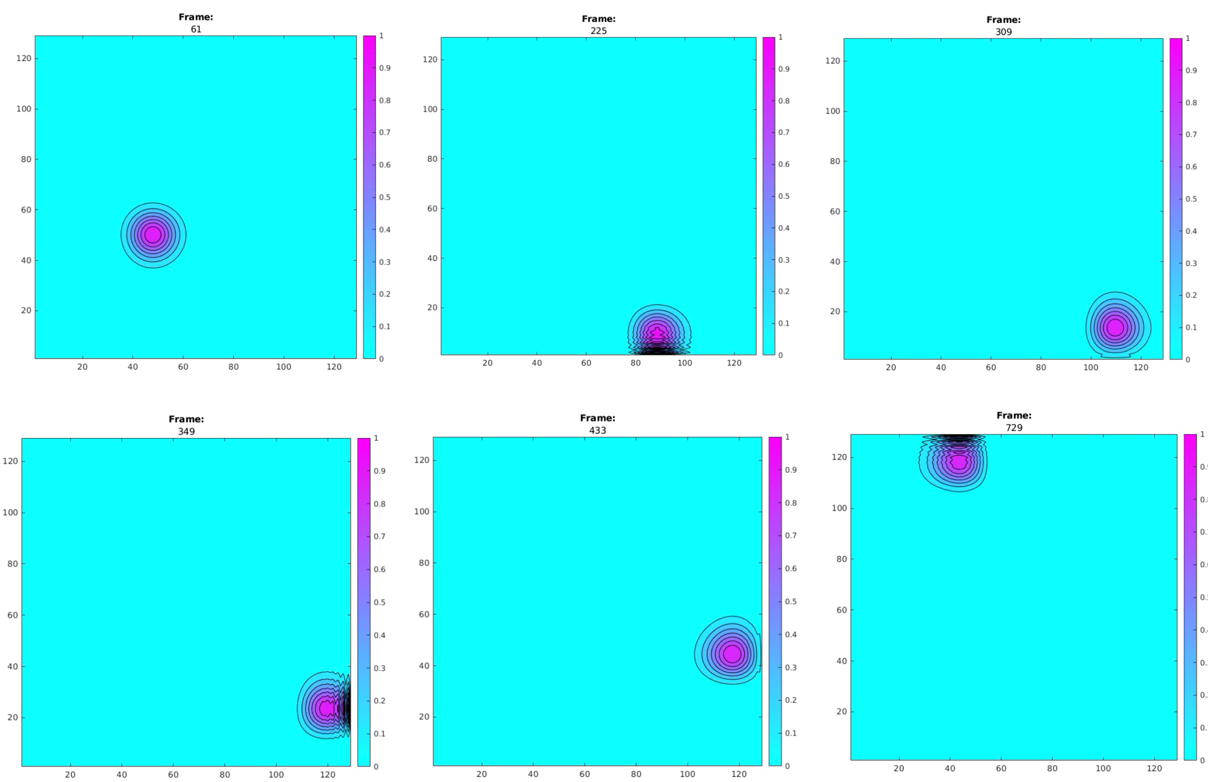

Fig. 18. Particle bouncing off the walls

You can see the animation of this experiment in the animations folder with name "2D_Bouncing.avi".

3.3 Potential Barrier:

In this experiment, I put a potential barrier with height of +50 in the middle of the box and put the initial value of the particle just at the middle of potential, i.e.:

idtype = 1;

vtype = 1;

idpar = [0.5,0.5,0.07,0.07,0,0];

vpar = [0.35,0.65,0.35,0.65,50];

tmax = 0.02;

lambda = 0.001;

level = 7;

In the following plots you can see the time evolution of the particle:

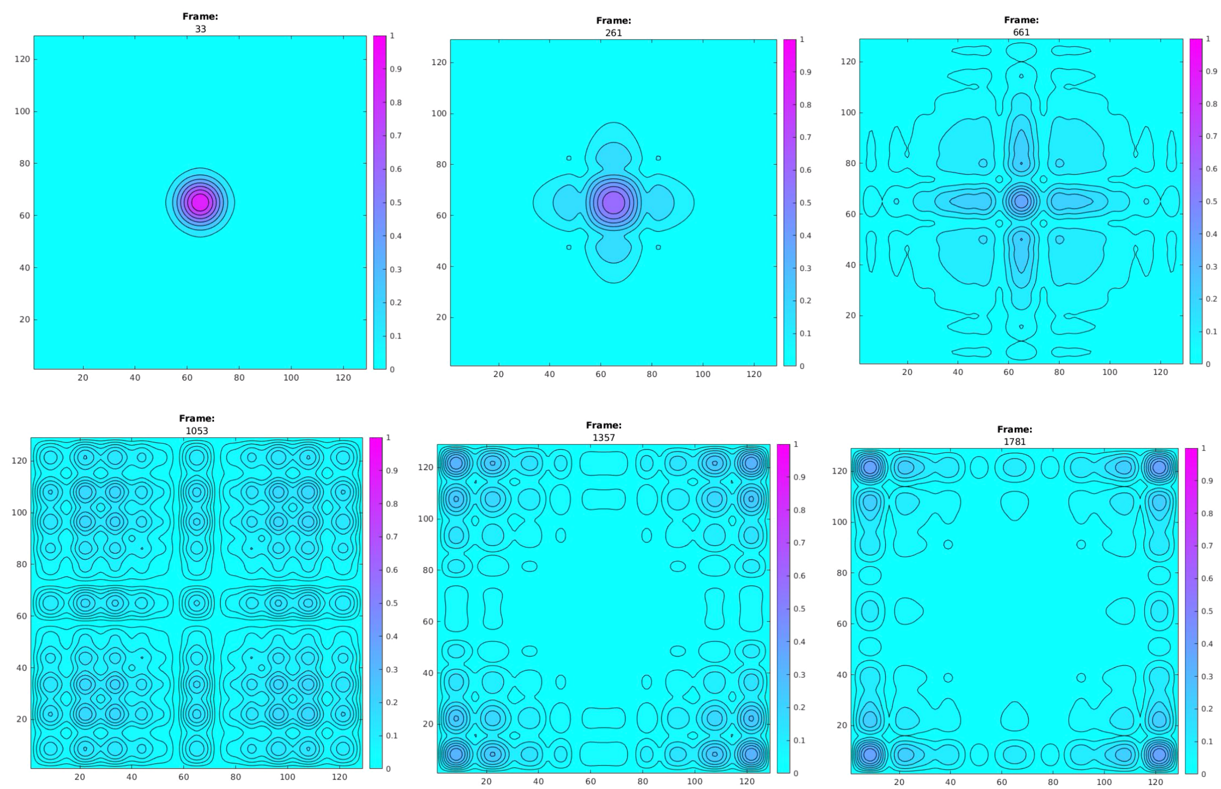

Fig. 19. Particle scattering off a rectangular barrier

Also you can find the animation of this numerical experiment in the animations. The name of the animation is “2D_PotentialBarrier.avi”.

3.4 Double Slit:

In this section I perform a standard double slit experiment. In the following figure you can see the configure of the double slit:

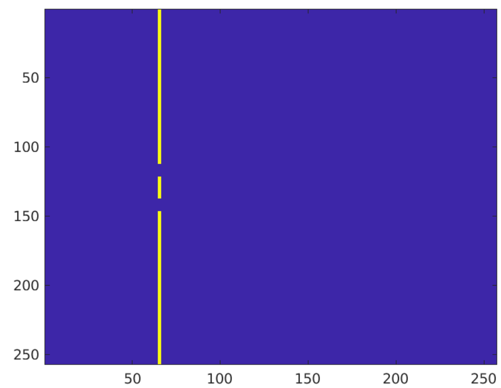

Fig. 20. Double Slit Configuration of the double slit experiment

Here is the initial values that I have used to generate these plots:

```
b = 7/100;
d = 3/100;
s = 0.5 -b/2 -d;
idtype = 1;
vtype = 2;
idpar = [0.1,0.5,0.07,0.07,40,0];
vpar = [s,s+d,s+d+b,s+2*d+b,100];
tmax = 0.01;
lambda = 0.01;
level = 8;
```

In which d is the opening of the slits, b is the distance between two slits, and lastly, s is the length of sides of slits (the distinct between the upper wall and first slit or equivalently, lower wall and the second slit).

In the following figures you can see the time evolution of the numerical experiment.

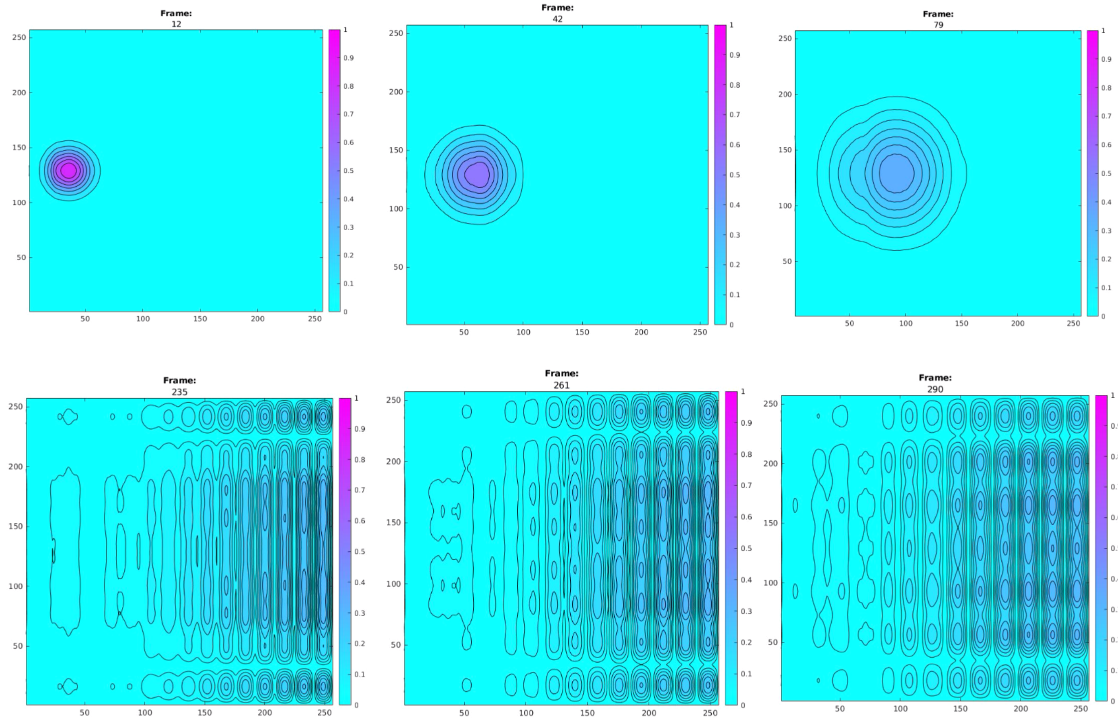

Fig. 21. Particle Scattering of a double slit.

We can clearly see the pattern of self interference on the right side of the box. To better see this, I have also plotted the cross section (parallel with y axis) in the following plot.

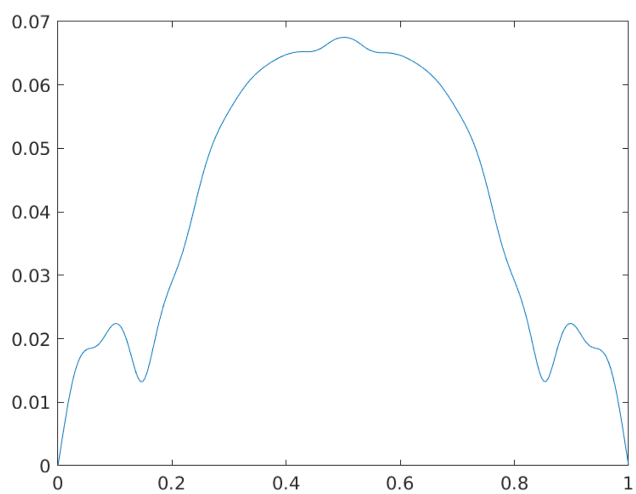

Fig. 22. Cross section of the right side of box to better see the diffraction pattern (for frame =150)

You can find the animation of this experiment in the animations folder. The name of animation is “2D_DoubleSlit.avi”.