

PHYS 410 Project 2

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Introduction

In this project, the time-dependent Schrödinger equation is solved numerically in both one dimension and two dimensions. In both cases, solutions account for a time-independent potential term V , which takes the form of a rectangular barrier or well, a double slit (in 2d only), or is zero everywhere. The MATLAB script `sch_1d_cn.m` implements the Crank-Nicolson discretization approach to solve the Schrödinger equation in 1d, while the script `sch_2d_adi.m` implements the alternating-direction-implicit (ADI) method to solve the equation in 2d.

The 1d case is tested by conducting convergence testing in the file `ctest_1d.m` which checks for solution convergence among increasing discretization levels. A similar convergence test is done for two dimensions in the file `ctest_2d.m`. For the 1d case, the solution "excess fractional probability" is also examined in the files `barrier_survey.m` and `well_survey.m`, which provides insights into how much time the quantum particle is spending in a certain location. Lastly, videos of the 2d wave function scattering off a rectangular barrier or well, and producing self-interference through a double slit are created using the scripts `video_rec_bar.m`, `video_rec_well.m`, and `video_double_slit.m`.

Review of Theory

1d Schrödinger Equation

The 1d Schrödinger Equation PDE is given by the following equation:

$$i\psi(x, t)_t = -\psi_{xx} + V(x, t)\psi \quad (1)$$

where the wave function, $\psi(x, t)$, is complex. The equation is to be solved on the domain

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

subject to initial and boundary conditions

$$\psi(x, 0) = \psi_0(x) \quad (2)$$

$$\psi(0, t) = \psi(1, t) = 0 \quad (3)$$

The family of exact solutions to (1) is

$$\psi(x, t) = e^{-im^2\pi^2t} \sin(m\pi x) \quad (4)$$

where m is a positive integer.

Since the modulus squared of the wave function represents the probability density, $\rho = |\psi|^2 = \psi\psi^*$, the "running integral" of the probability density represents the probability that the particle is to the left of x at any given time t :

$$P(x, t) = \int_0^x \psi(\tilde{x}, t)\psi^*(\tilde{x}, t)d\tilde{x} \quad (5)$$

Note that equation (5) only computes the correct probability if the wave function is properly normalized such that $P(1, t) = 1$. Even if it is not so normalized, we should have

$$P(1, t) = \text{conserved to level of solution error}$$

2d Schrödinger Equation

The 2d Schrödinger Equation PDE is given by the following equation:

$$\psi_t = i(\psi_{xx} + \psi_{yy}) - iV(x, y)\psi \quad (6)$$

where the wave function, $\psi(x, y, t)$, is complex. The equation is to be solved on the domain

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

subject to initial and boundary conditions

$$\psi(x, y, 0) = \psi_0(x, y) \quad (7)$$

$$\psi(0, y, t) = \psi(1, y, t) = \psi(x, 0, t) = \psi(x, 1, t) = 0 \quad (8)$$

A family of exact solutions to (6) is given by

$$\psi(x, y, t) = e^{-i(m_x^2 + m_y^2)\pi^2 t} \sin(m_x \pi x) \sin(m_y \pi y) \quad (9)$$

Numerical Approach

1d Schrödinger Equation

$$i \frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = \frac{1}{2} \left(\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{\Delta x^2} + \frac{\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n}{\Delta x^2} \right) \quad (10)$$

$$+ \frac{1}{2} V_j^{n+\frac{1}{2}} (\psi_j^{n+1} + \psi_j^n), \quad j = 2, 3, \dots, n_x - 1, \quad n = 1, 2, \dots, n_t - 1, \quad (11)$$

$$\psi_1^{n+1} = \psi_{n_x}^{n+1} = 0, \quad n = 1, 2, \dots, n_t - 1, \quad (12)$$

$$\psi_j^1 = \psi_0(x_j), \quad j = 1, 2, \dots, n_x. \quad (13)$$

2d Schrödinger Equation

$$\partial_{xx}^h u_{i,j}^n \equiv \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2},$$

$$\partial_{yy}^h u_{i,j}^n \equiv \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2}.$$

$$\left(1 - i\frac{\Delta t}{2}\partial_{xx}^h\right)\psi_{i,j}^{n+\frac{1}{2}} = \left(1 + i\frac{\Delta t}{2}\partial_{xx}^h\right)\left(1 + i\frac{\Delta t}{2}\partial_{yy}^h - i\frac{\Delta t}{2}V_{i,j}\right)\psi_{i,j}^n, \\ i = 2, 3, \dots, n_x - 1, \quad j = 2, 3, \dots, n_y - 1, \quad n = 1, 2, \dots, n_t - 1. \quad (14)$$

$$\left(1 - i\frac{\Delta t}{2}\partial_{yy}^h + i\frac{\Delta t}{2}V_{i,j}\right)\psi_{i,j}^{n+1} = \psi_{i,j}^{n+\frac{1}{2}}, \\ i = 2, 3, \dots, n_x - 1, \quad j = 2, 3, \dots, n_y - 1, \quad n = 1, 2, \dots, n_t - 1. \quad (15)$$

Implementation

1d Tridiagonal System

2d Tridiagonal System

Results

1d Schrödinger Equation

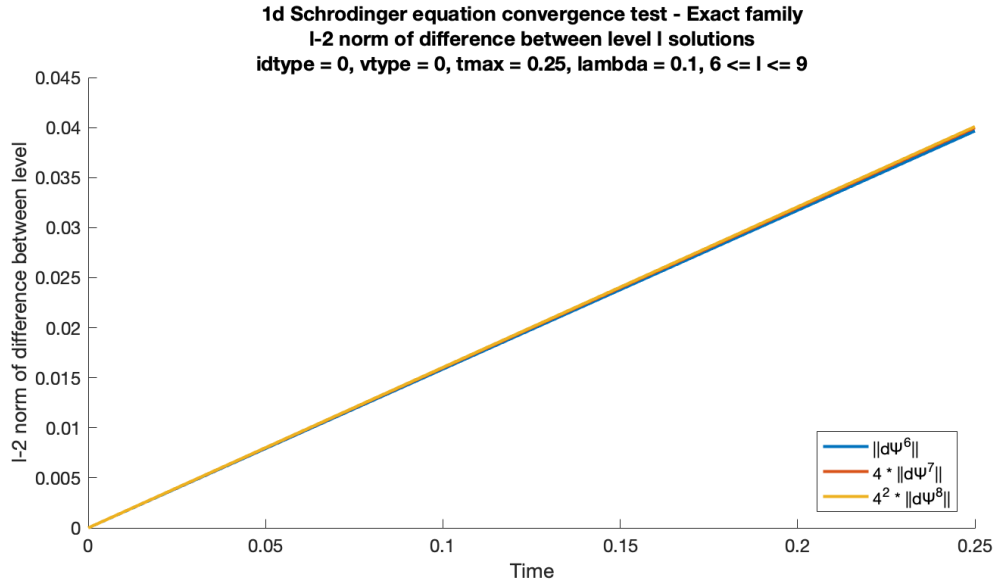


Figure 1: Output 1 of `ctest_1d.m` - l-2 norm of difference between discretization level solutions for exact family initial conditions.

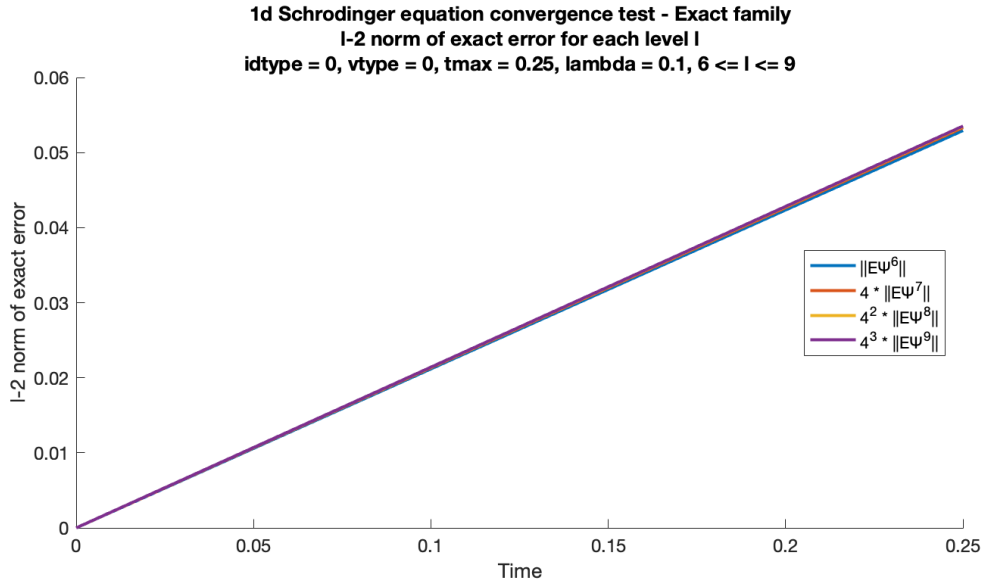


Figure 2: Output 2 of `ctest_1d.m` - l-2 norm of exact error at each discretization level for exact family initial conditions.

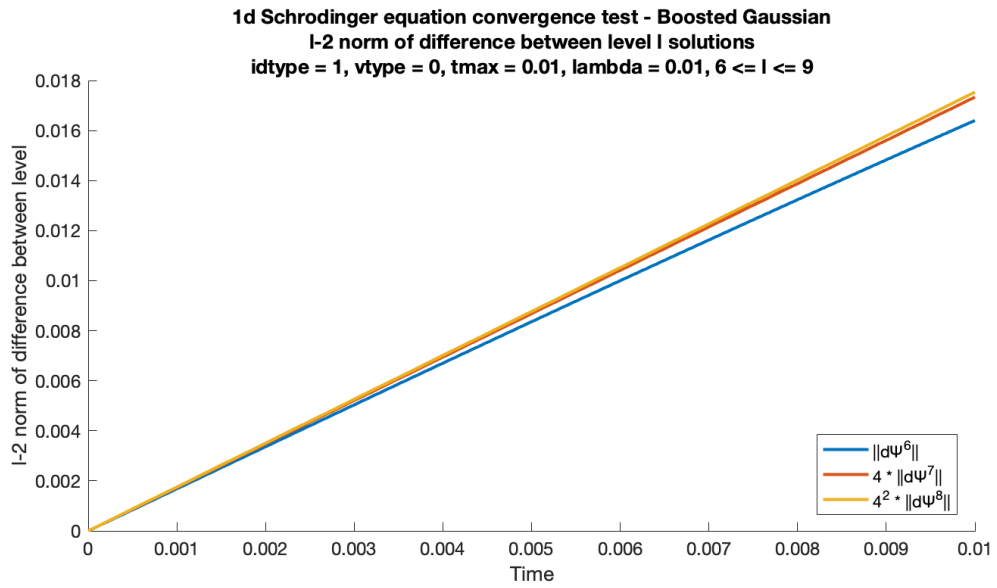


Figure 3: Output 3 of `ctest_1d.m` - l-2 norm of difference between discretization level solutions for boosted Gaussian initial conditions.

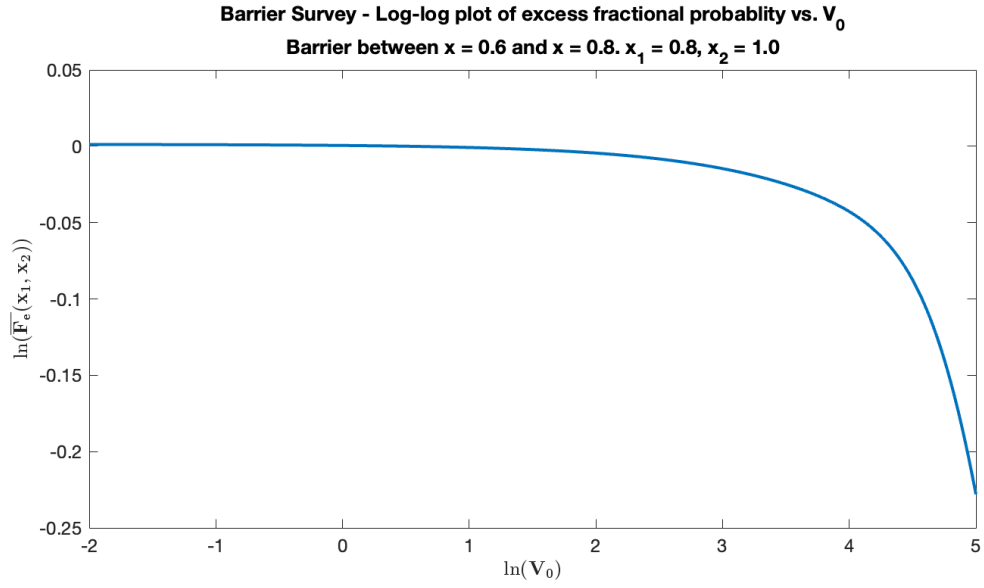


Figure 4: Output of `barrier_1d.m` - Log-log plot of excess fractional probability vs. V_0 for 1d potential barrier.

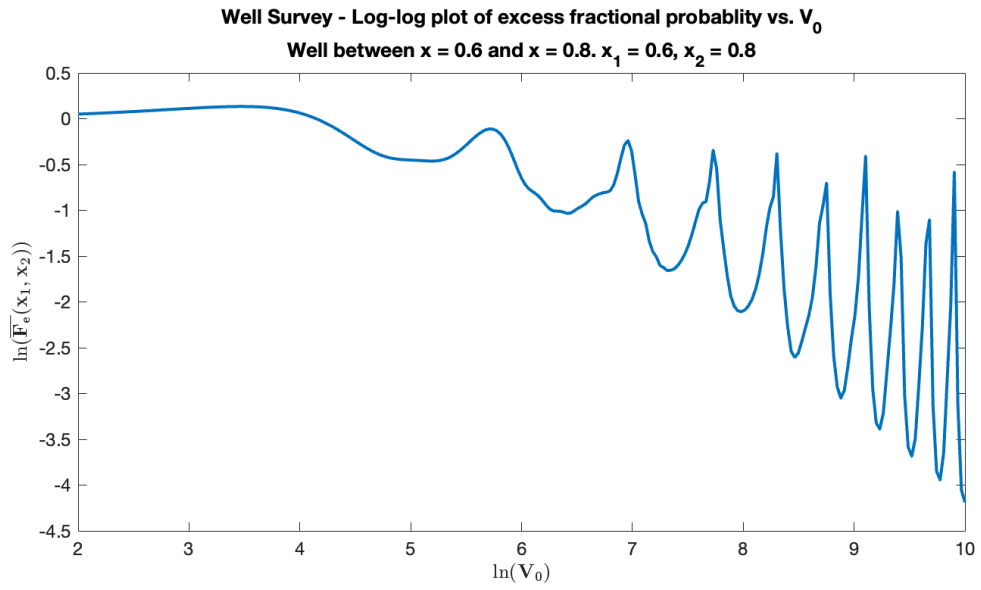


Figure 5: Output of `well_1d.m` - Log-log plot of excess fractional probability vs. V_0 for 1d potential well.

2d Schrödinger Equation

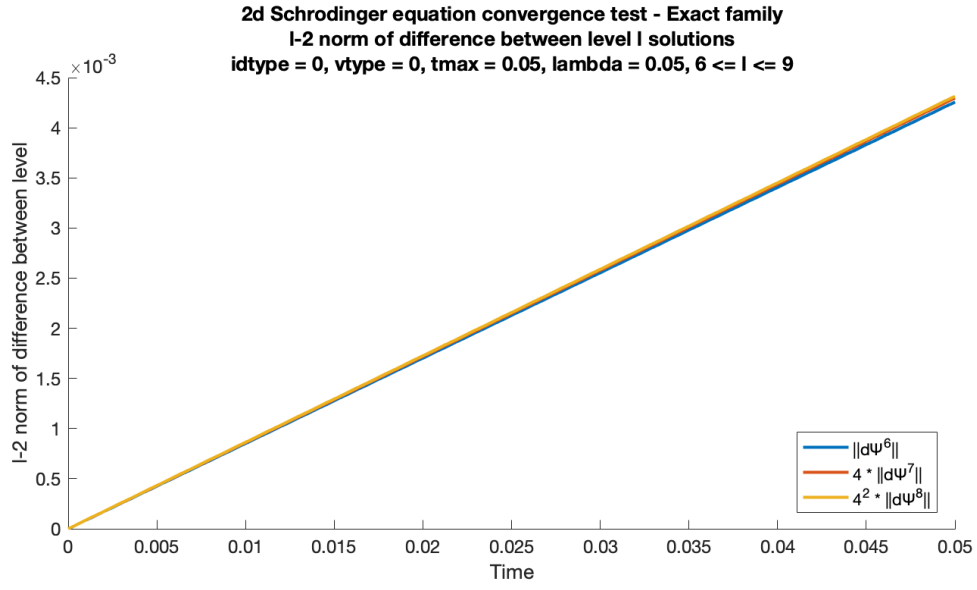


Figure 6: Output 1 of `ctest_2d.m` - l-2 norm of difference between discretization level solutions.

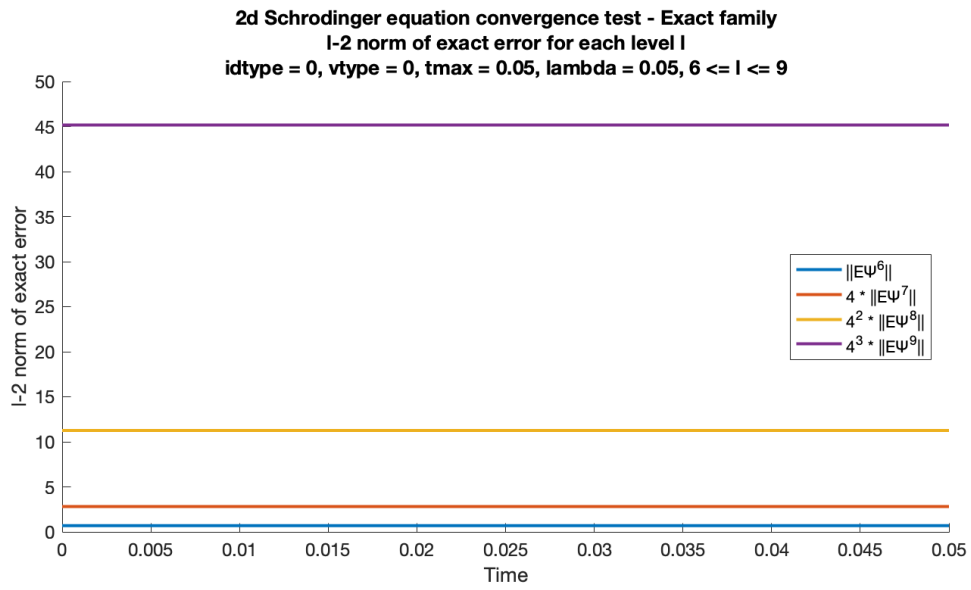


Figure 7: Output 2 of `ctest_2d.m` - l-2 norm of exact error at each discretization level.

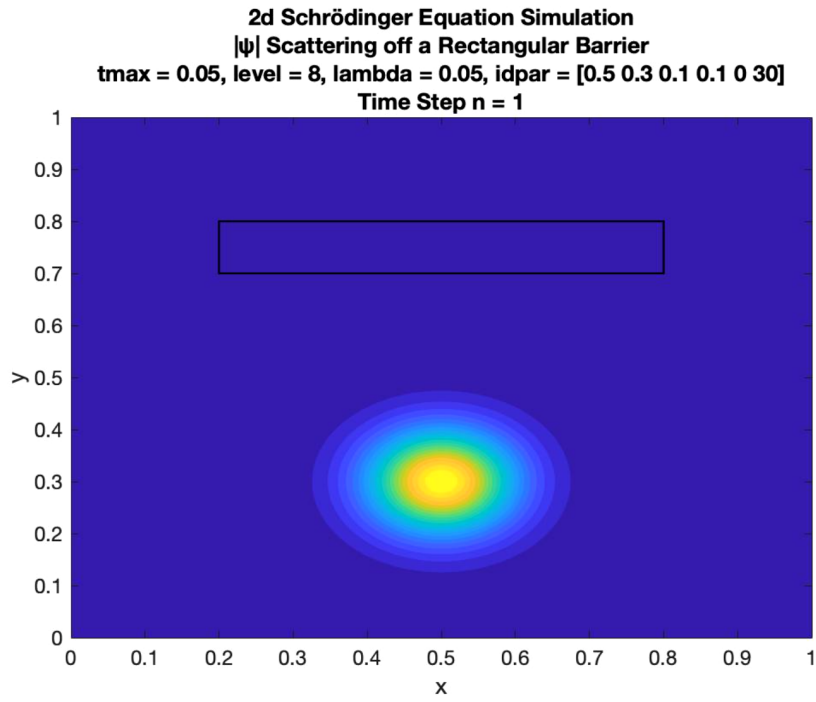


Figure 8: Screenshot of video produced by `video_rec_bar.m` - Initial conditions.

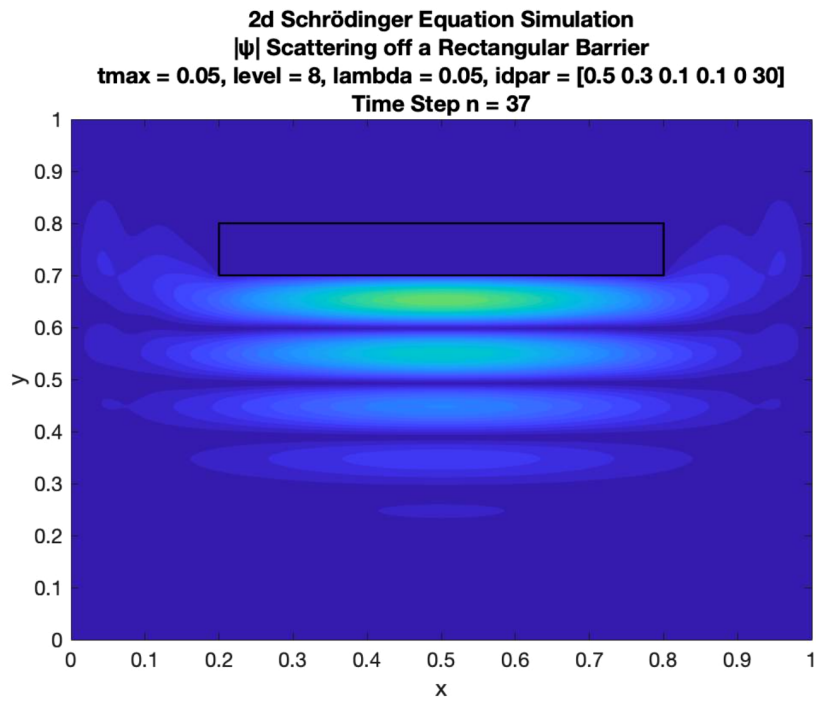


Figure 9: Screenshot of video produced by `video_rec_bar.m` - Scattering off barrier.

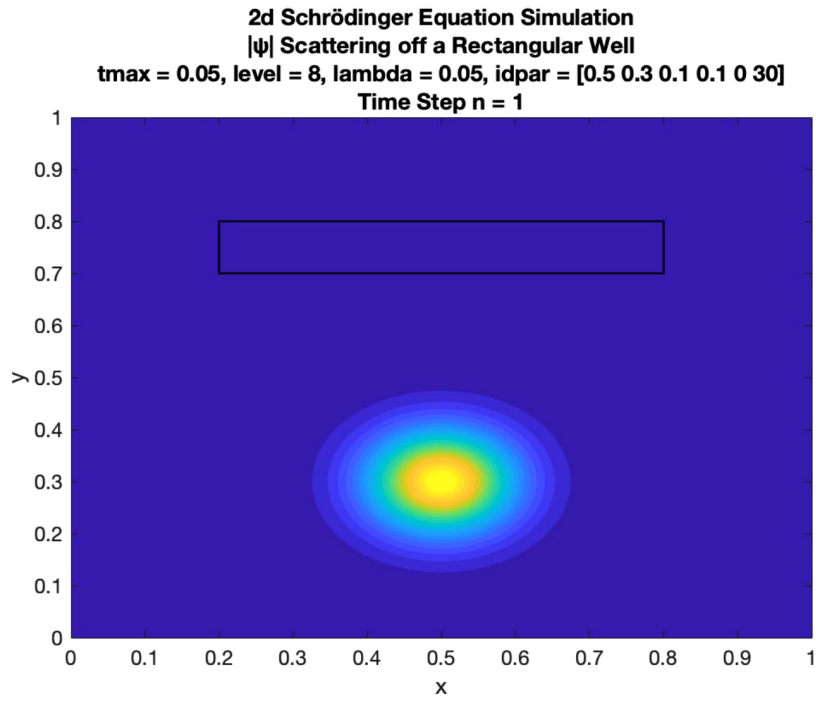


Figure 10: Screenshot of video produced by `video_rec_well.m` - Initial conditions.

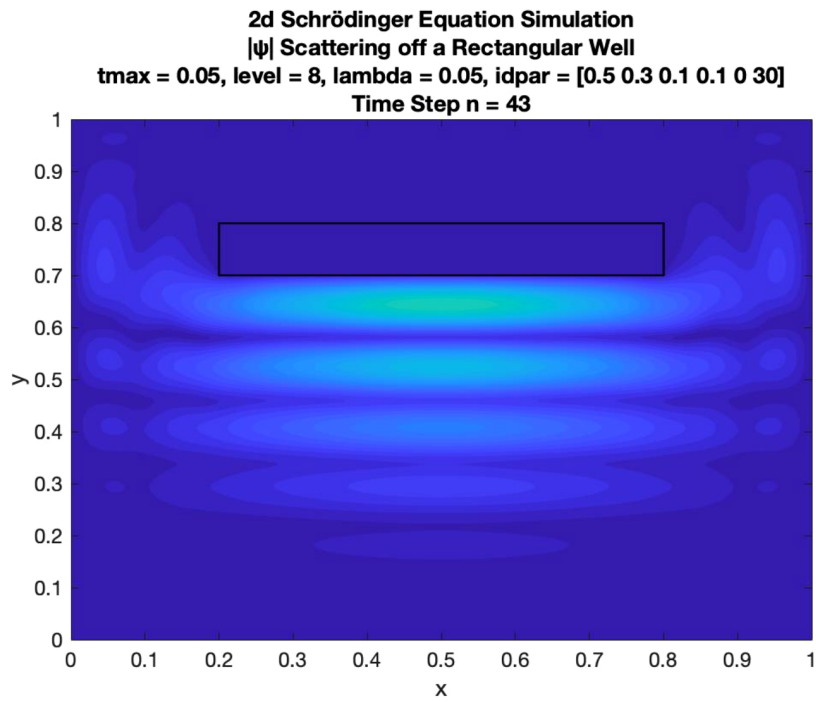


Figure 11: Screenshot of video produced by `video_rec_well.m` - Scattering off well.

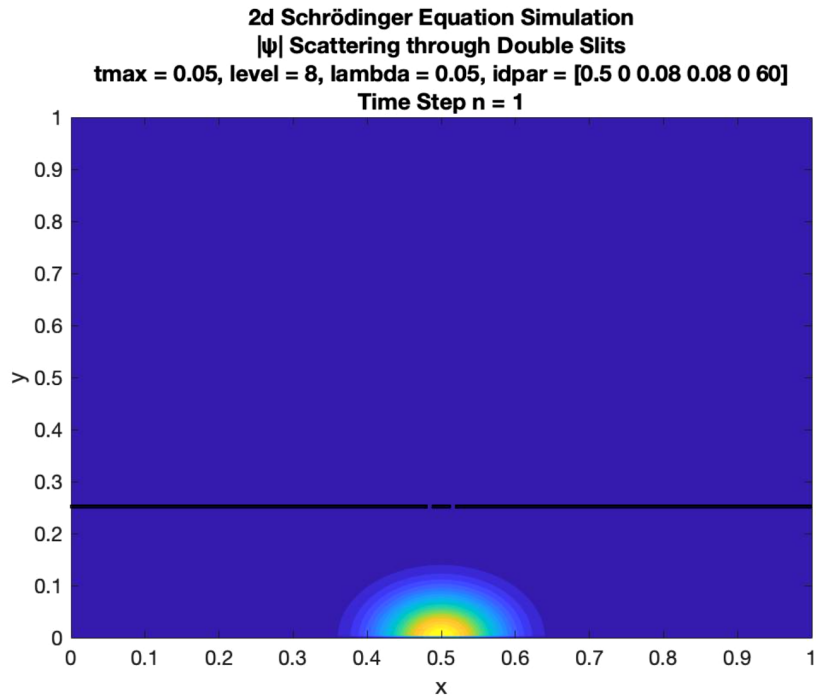


Figure 12: Screenshot of video produced by `double_slit_well.m` - Initial conditions.

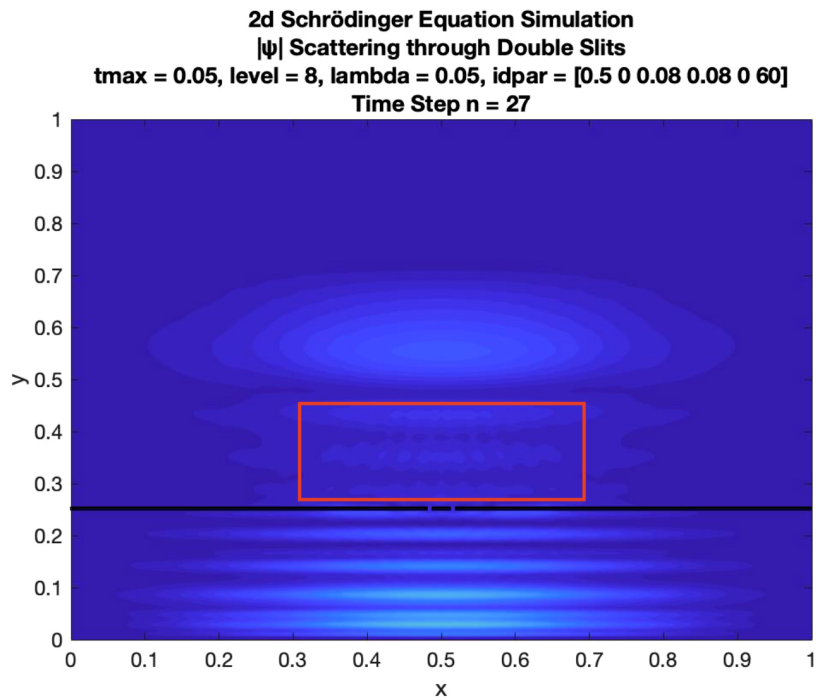


Figure 13: Screenshot of video produced by `double_slit_well.m` - Self interference through slits.

Conclusions

Generative AI was used to help with understanding how to use MATLAB's `contourf` function for making videos of numerical experiments in 2d. It was also used for help with typesetting this document.

Appendix A - sch_1d_cn.m Code

```

1 % sch_1d_cn: Solves 1D Schrödinger equation using  $O(dt^2, dx^2)$ 
2 % Crank–Nicolson implicit scheme.
3 %
4 % Inputs:
5 %
6 %   tmax:    Maximum integration time
7 %   level:   Discretization level
8 %   lambda:  dt/dx
9 %   idtype:  Selects initial data type
10 %   idpar:   Vector of initial data parameters
11 %   vtype:   Selects potential type
12 %   vpar:    Vector of potential parameters
13 %
14 % Outputs:
15 %
16 %   x:       Column vector of x coordinates [nx]
17 %   t:       Column vector of t coordinates [nt]
18 %   psi:     Array of computed psi values [nt x nx]
19 %   psire:   Array of computed psi_re values [nt x nx]
20 %   psiim:   Array of computed psi_im values [nt x nx]
21 %   psimod:  Array of computed sqrt(psi psi*) values [nt x nx]
22 %   prob:    Array of computed running integral values [nt x nx]
23 %   v:       Column vector of potential values [nx]
24 function [x t psi psire psiim psimod prob v] = ...
25     sch_1d_cn(tmax, level, lambda, idtype, idpar, vtype, vpar)
26
27 % Define mesh and derived parameters
28 nx = 2^level + 1;
29 x = linspace(0.0, 1.0, nx);
30 dx = x(2) - x(1);
31 dt = lambda * dx;
32 nt = round(tmax / dt) + 1;
33 t = (0 : nt-1) * dt;
34
35 % Initialize solution, and set initial data
36 psi = zeros(nt, nx);
37 if idtype == 0
38     % Exact family
39     psi(1, :) = sin(idpar(1) * pi * x);
40 elseif idtype == 1
41     % Boosted Gaussian
42     psi(1, :) = exp(1i * idpar(3) * x) .* ...
43         exp(-((x - idpar(1)) ./ idpar(2)).^ 2);
44 else
45     fprintf('sch_1d_cn: Invalid idtype=%d\n', idtype);
46     return
47 end
48 % Set first and last values of initial data to zero
49 psi(1, 1) = 0;
50 psi(1, nx) = 0;
51
52 % Initial storage for prob and calculate for initial time
53 prob = zeros(nt, nx);
54 for j = 2 : nx
55     prob(1, j) = trapz(x(1:j), abs(psi(1, 1:j)).^2);
56 end

```

```

57
58 % Initialize potential
59 v = zeros(1,nx);
60 if vtype == 0
61     % No potential – leave unchanged
62 elseif vtype == 1
63     % Rectangular barrier or well
64     v(x > vpar(1) & x < vpar(2)) = vpar(3);
65 else
66     fprintf('sch_1d_cn: Invalid vtype=%d\n', vtype);
67     return
68 end
69
70 % Initialize storage for RHS
71 f = zeros(nx,1);
72
73 % Set up tridiagonal system
74 dl = 0.5/dx^2 * ones(nx, 1);
75 d = (1i/dt - 1/dx^2 - 0.5*v.') .* ones(nx,1);
76 du = dl;
77 % Fix up boundary cases
78 d(1) = 1.0;
79 du(2) = 0.0;
80 dl(nx-1) = 0.0;
81 d(nx) = 1.0;
82 % Define sparse matrix
83 A = spdiags([dl d du], -1:1, nx, nx);
84
85 % Compute solution using CN scheme
86 for n = 1 : nt-1
87     % Define RHS of linear system
88     f(2:nx-1) = psi(n, 2:nx-1) .* (1i/dt + 1/dx^2 + 0.5*v(2:nx-1)) ...
89         + (-0.5/dx^2) * (psi(n, 1:nx-2) + psi(n, 3:nx));
90     f(1) = 0.0;
91     f(nx) = 0.0;
92     % Solve system, thus updating approximation to next time step
93     psi(n+1, :) = A \ f;
94     % Set first and last values to zero
95     psi(n+1, 1) = 0;
96     psi(n+1, nx) = 0;
97
98     % Calculate prob each time step
99     for j = 2 : nx
100         prob(n+1, j) = trapz(x(1:j), abs(psi(n+1, 1:j)).^2);
101     end
102 end
103
104 % Compute real, imaginary, and modulus of each entry in psi
105 psire = real(psi);
106 psiim = imag(psi);
107 psimod = abs(psi);
108
109 % Convert to column vectors
110 x = x.';
111 t = t.';
112 v = v.';
113 end

```

Appendix B - ctest_1d.m Code

```

1 %% 1.4 - 1d Convergence Testing
2
3 close all;
4 clear; clc;
5 format long;
6
7 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
8 % Convergence Test #1
9 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
10
11 % Simulation maximum time
12 tmax = 0.25;
13 % Discretization levels
14 minlevel = 6;
15 maxlevel = 9;
16 % Delta t by Delta x ratio
17 lambda = 0.1;
18
19 % idtype = 0    -> Exact family (sine wave)
20 % idtype = 1    -> Boosted Gaussian
21 idtype = 0;
22 idpar = [3]; % m = 3
23
24 % vtype = 0     -> No potential
25 % vtype = 1     -> Rectangular barrier or well
26 vtype = 0;
27 vpar = zeros(1,3);
28
29 % Perform computation at various levels of discretization, store
30 % results in cell arrays ...
31 for l = minlevel : maxlevel
32     % Compute the solution
33     [x{l} t{l} psi{l} psire{l} psiim{l} psimod{l} prob{l} v{l}] ...
34     = sch_1d_cn(tmax, l, lambda, idtype, idpar, vtype, vpar)
35
36     [nt{l}, nx{l}] = size(psi{l});
37
38     % Since idtype == 0, compute exact solution
39     psixct{l} = zeros(nt{l}, nx{l});
40     for n = 1 : nt{l}
41         psixct{l}(n,:) = exp(-1i * idpar(1)^2 * pi^2 * t{l}(n)) ...
42             * sin(idpar(1) * pi * x{l});
43     end
44     % Compute exact errors and their rms values for later
45     Epsi{l} = psixct{l} - psi{l};
46     rms_Epsi{l} = rms(abs(Epsi{l}), 2);
47 end
48
49 % Calculating the level-to-level differences, taking every second
50 % value of the larger length array
51 dpsi6 = downsample(downsample(psi{7}, 2).', 2).' - psi{6};
52 dpsi7 = downsample(downsample(psi{8}, 2).', 2).' - psi{7};
53 dpsi8 = downsample(downsample(psi{9}, 2).', 2).' - psi{8};
54
55 % Compute l-2 norm of each dpsi, resulting in functions of t
56 rms_dpsi6 = rms(abs(dpsi6), 2);

```

```

57 rms_dpsi7 = rms(abs(dpsi7), 2);
58 rms_dpsi8 = rms(abs(dpsi8), 2);
59
60 % Plot scaled errors for different discretization levels
61 fig1 = figure;
62 rho = 4;
63 hold on
64 plot(t{6}, rms_dpsi6, 'LineWidth', 2);
65 plot(t{7}, rho*rms_dpsi7, 'LineWidth', 2);
66 plot(t{8}, rho^2*rms_dpsi8, 'LineWidth', 2);
67 xlabel("Time");
68 ylabel("l-2 norm of difference between level");
69 legend('||dΨ^6||', '4 * ||dΨ^7||', '4^2 * ||dΨ^8||', 'Location', 'best');
70 title("1d Schrodinger equation convergence test - Exact family"
71       "l-2 norm of difference between level 1 solutions"
72       "idtype = 0, vtype = 0, tmax = 0.25, lambda = 0.1, 6 <= l <= 9");
73 ax = gca;
74 ax.FontSize = 12;
75
76 % Plot scaled exact errors for different discretization levels
77 fig2 = figure;
78 rho = 4;
79 hold on
80 plot(t{6}, rms_Epsi{6}, 'LineWidth', 2);
81 plot(t{7}, rho*rms_Epsi{7}, 'LineWidth', 2);
82 plot(t{8}, rho^2*rms_Epsi{8}, 'LineWidth', 2);
83 plot(t{9}, rho^3*rms_Epsi{9}, 'LineWidth', 2);
84 xlabel("Time");
85 ylabel("l-2 norm of exact error");
86 legend('||EΨ^6||', '4 * ||EΨ^7||', '4^2 * ||EΨ^8||', '4^3 * ||EΨ^9||'...
87       , 'Location', 'best');
88 title("1d Schrodinger equation convergence test - Exact family"
89       "l-2 norm of exact error for each level l"
90       "idtype = 0, vtype = 0, tmax = 0.25, lambda = 0.1, 6 <= l <= 9");
91 ax = gca;
92 ax.FontSize = 12;
93
94
95 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
96 % Convergence Test #2
97 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
98
99 clear;
100
101 % Simulation maximum time
102 tmax = 0.01;
103 % Discretization levels
104 minlevel = 6;
105 maxlevel = 9;
106 % Delta t by Delta x ratio
107 lambda = 0.01;
108
109 % idtype = 0    -> Exact family (sine wave)
110 % idtype = 1    -> Boosted Gaussian
111 idtype = 1;
112 idpar = [0.50 0.075 0.0];
113
114 % vtype = 0     -> No potential

```

```

115 % vtype = 1    -> Rectangular barrier or well
116 vtype = 0;
117 vpar = zeros(1,3);
118
119 % Perform computation at various levels of discretization, store
120 % results in cell arrays ...
121 for l = minlevel : maxlevel
122     % Compute the solution
123     [x{1} t{1} psi{1} psire{1} psiim{1} psimod{1} prob{1} v{1}] ...
124     = sch_1d_cn(tmax, l, lambda, idtype, idpar, vtype, vpar);
125
126     [nt{1}, nx{1}] = size(psi{1});
127 end
128
129 % Calculating the level-to-level differences, taking every second
130 % value of the larger length array
131 dpsi6 = downsample(downsample(psi{7}, 2).', 2).' - psi{6};
132 dpsi7 = downsample(downsample(psi{8}, 2).', 2).' - psi{7};
133 dpsi8 = downsample(downsample(psi{9}, 2).', 2).' - psi{8};
134
135 % Compute l-2 norm of each dpsi, resulting in functions of t
136 rms_dpsi6 = rms(abs(dpsi6), 2);
137 rms_dpsi7 = rms(abs(dpsi7), 2);
138 rms_dpsi8 = rms(abs(dpsi8), 2);
139
140 % Plot scaled errors for different discretization levels
141 fig3 = figure;
142 rho = 4;
143 hold on
144 plot(t{6}, rms_dpsi6, 'LineWidth', 2);
145 plot(t{7}, rho*rms_dpsi7, 'LineWidth', 2);
146 plot(t{8}, rho^2*rms_dpsi8, 'LineWidth', 2);
147 xlabel("Time");
148 ylabel("l-2 norm of difference between level");
149 legend('||dΨ^6||', '4 * ||dΨ^7||', '4^2 * ||dΨ^8||', 'Location', 'best');
150 title({"1d Schrodinger equation convergence test - Boosted Gaussian"
151        "l-2 norm of difference between level l solutions"
152        "idtype = 1, vtype = 0, tmax = 0.01, lambda = 0.01, 6 <= l <= 9"});
153 ax = gca;
154 ax.FontSize = 12;

```

Appendix C - barrier_survey.m Code

```
1 %% 1.5.1 - 1d Barrier Survey
2
3 close all;
4 clear; clc;
5 format long;
6
7 % Simulation maximum time
8 tmax = 0.10;
9 % Discretization level
10 level = 9;
11 % Delta t by Delta x ratio
12 lambda = 0.01;
13
14 % idtype = 0 -> Exact family (sine wave)
15 % idtype = 1 -> Boosted Gaussian
16 idtype = 1;
17 idpar = [0.40, 0.075, 20.0];
18
19 % vtype = 0 -> No potential
20 % vtype = 1 -> Rectangular barrier or well
21 vtype = 1;
22 xmin = 0.6;
23 xmax = 0.8;
24 lnV0 = linspace(-2, 5, 251);
25
26 % Survey range
27 x1 = 0.8;
28 x2 = 1.0;
29
30 for idx = 1 : length(lnV0)
31     % Get this iteration's vpar
32     vpar = [xmin, xmax, exp(lnV0(idx))];
33
34     % Compute the solution
35     [x{idx} t{idx} psi{idx} psire{idx} psiim{idx} psimod{idx} prob{idx} v{
36         idx}] ...
37         = sch_1d_cn(tmax, level, lambda, idtype, idpar, vtype, vpar);
38
39     % Compute temporal average of probability matrix
40     P_bar{idx} = mean(prob{idx});
41     % Normalize the temporal average
42     P_bar{idx} = P_bar{idx} / P_bar{idx}(end);
43
44     % Compute indices of x1 and x2 in the array x
45     % This only needs to be done once
46     if idx == 1
47         [~, x1_loc] = min(abs(x{idx} - x1));
48         [~, x2_loc] = min(abs(x{idx} - x2));
49     end
50
51     % Compute excess fractional probability and its logarithm
52     Fe_bar{idx} = (P_bar{idx}(x2_loc) - P_bar{idx}(x1_loc)) / ...
53         (x{idx}(x2_loc) - x{idx}(x1_loc));
54     lnFe_bar{idx} = log(Fe_bar{idx})
55 end
```

```

56 fig1 = figure;
57 plot(lnV0, cell2mat(lnFe_bar), 'LineWidth', 2)
58 title({"Barrier Survey – Log–log plot of excess fractional probablity vs.
      V_0"
59       "Barrier between x = 0.6 and x = 0.8. x_1 = 0.8, x_2 = 1.0"})
60 xlabel('$$\mathbf{\ln(V_0)}$$', 'interpreter', 'latex')
61 ylabel('$$\mathbf{\ln(\overline{F_e}(x_1, x_2))}$$', 'interpreter', 'latex'
62 )
63 ax = gca;
64 ax.FontSize = 12;

```


Appendix D - well_survey.m Code

```

1 %% 1.5.2 - 1d Well Survey
2
3 close all;
4 clear; clc;
5 format long;
6
7 % Simulation maximum time
8 tmax = 0.10;
9 % Discretization level
10 level = 9;
11 % Delta t by Delta x ratio
12 lambda = 0.01;
13
14 % idtype = 0 -> Exact family (sine wave)
15 % idtype = 1 -> Boosted Gaussian
16 idtype = 1;
17 idpar = [0.40, 0.075, 0.0];
18
19 % vtype = 0 -> No potential
20 % vtype = 1 -> Rectangular barrier or well
21 vtype = 1;
22 xmin = 0.6;
23 xmax = 0.8;
24 lnV0 = linspace(2, 10, 251);
25
26 % Survey range
27 x1 = 0.6;
28 x2 = 0.8;
29
30 for idx = 1 : length(lnV0)
31     % Get this iteration's vpar
32     vpar = [xmin, xmax, -exp(lnV0(idx))];
33
34     % Compute the solution
35     [x{idx} t{idx} psi{idx} psire{idx} psiim{idx} psimod{idx} prob{idx} v{
36         idx}] ...
37         = sch_1d_cn(tmax, level, lambda, idtype, idpar, vtype, vpar);
38
39     % Compute temporal average of probability matrix
40     P_bar{idx} = mean(prob{idx});
41     % Normalize the temporal average
42     P_bar{idx} = P_bar{idx} / P_bar{idx}(end);
43
44     % Compute indices of x1 and x2 in the array x
45     % This only needs to be done once
46     if idx == 1
47         [~, x1_loc] = min(abs(x{idx} - x1));
48         [~, x2_loc] = min(abs(x{idx} - x2));
49     end
50
51     % Compute excess fractional probability and its logarithm
52     Fe_bar{idx} = (P_bar{idx}(x2_loc) - P_bar{idx}(x1_loc)) / ...
53         (x{idx}(x2_loc) - x{idx}(x1_loc));
54     lnFe_bar{idx} = log(Fe_bar{idx})
55 end

```

```

56 fig2 = figure;
57 plot(lnV0, cell2mat(lnFe_bar), 'LineWidth', 2)
58 title({"Well Survey – Log–log plot of excess fractional probablity vs. V_0"
59       "Well between x = 0.6 and x = 0.8. x_1 = 0.6, x_2 = 0.8"})
60 xlabel('$$\mathbf{\ln(V_0)}$$', 'interpreter', 'latex')
61 ylabel('$$\mathbf{\ln(\overline{F_e}(x_1, x_2))}$$', 'interpreter', 'latex'
62       )
63 ax = gca;
64 ax.FontSize = 12;

```

Appendix E - sch_2d_adi.m Code

```

1 % sch_2d_adi: Solves 2D Schrödinger equation using ADI scheme.
2 %
3 % Inputs:
4 %
5 %   tmax:    Maximum integration time
6 %   level:   Discretization level
7 %   lambda:  dt/dx
8 %   idtype:  Selects initial data type
9 %   idpar:   Vector of initial data parameters
10 %  vtype:   Selects potential type
11 %  vpar:    Vector of potential parameters
12 %
13 % Outputs:
14 %
15 %   x:       Column vector of x coordinates [nx]
16 %   y:       Column vector of y coordinates [ny]
17 %   t:       Column vector of t coordinates [nt]
18 %   psi:     Array of computed psi values [nt x nx x ny]
19 %   psire:   Array of computed psi_re values [nt x nx x ny]
20 %   psiim:   Array of computed psi_im values [nt x nx x ny]
21 %   psimod:  Array of computed sqrt(psi psi*) values [nt x nx x ny]
22 %   v:       Array of potential values [nx x ny]
23 function [x y t psi psire psiim psimod v] = ...
24     sch_2d_adi(tmax, level, lambda, idtype, idpar, vtype, vpar)
25
26 % Define mesh and derived parameters
27 nx = 2^level + 1;          ny = nx;
28 x = linspace(0.0, 1.0, nx); y = x;
29 dx = x(2) - x(1);         dy = dx;
30 dt = lambda * dx;
31 nt = round(tmax / dt) + 1;
32 t = (0 : nt-1) * dt;
33
34 % Define meshgrid for populating psi(x,y,0) and V(x,y)
35 [X, Y] = meshgrid(x, y);
36
37 % Initialize solution, and set initial data
38 psi = zeros(nt, nx, ny);
39 if idtype == 0
40     % Exact family
41     psi(1, :, :) = sin(idpar(1)*pi*x)' * sin(idpar(2)*pi*y);
42 elseif idtype == 1
43     % Boosted Gaussian
44     % Create variable names for function parameters
45     x0 = idpar(1); y0 = idpar(2);
46     delta_x = idpar(3); delta_y = idpar(4);
47     p_x = idpar(5); p_y = idpar(6);
48
49     % Calculate psi(x, y, 0)
50     psi_0 = exp(1i*p_x*X) .* exp(1i*p_y*Y) ...
51         .* exp(-(((X - x0).^2)/delta_x^2 + ((Y - y0).^2)/delta_y^2));
52     psi(1, :, :) = reshape(psi_0, [1, nx, ny]);
53 else
54     fprintf('sch_2d_adi: Invalid idtype=%d\n', idtype);
55     return
56 end

```

```

57 % Set boundary conditions of initial data to zero
58 % t = 0:  $\psi(0,y,t) = \psi(1,y,t) = \psi(x,0,t) = \psi(x,1,t) = 0$ 
59 psi(1, 1, :) = 0;
60 psi(1, :, 1) = 0;
61 psi(1, nx, :) = 0;
62 psi(1, :, ny) = 0;
63
64 % Initialize time-independent potential
65 v = zeros(nx,ny);
66 if vtype == 0
67     % No potential – leave unchanged
68 elseif vtype == 1
69     % Rectangular barrier or well
70     % Create variable names for function parameters
71     x_min = vpar(1);    x_max = vpar(2);
72     y_min = vpar(3);    y_max = vpar(4);
73     Vc     = vpar(5);
74
75     % Calculate V(x, y)
76     v((X >= x_min & X <= x_max) & (Y >= y_min & Y <= y_max)) = Vc;
77 elseif vtype == 2
78     % Double slit
79     % Create variable names for function parameters
80     x1 = vpar(1);    x2 = vpar(2);
81     x3 = vpar(3);    x4 = vpar(4);
82     Vc = vpar(5);
83     j_prime = (ny - 1)/4 + 1;
84
85     % Calculate V(x, y)
86     Vc_indices = (x <= x1) | (x >= x2 & x <= x3) | (x >= x4);
87     v(j_prime, Vc_indices) = Vc;
88     v(j_prime + 1, Vc_indices) = Vc;
89 else
90     fprintf('sch_2d_adi: Invalid vtype=%d\n', vtype);
91     return
92 end
93
94 % Define sparse matrix diagonals for first ADI eqn
95 dl = (-1i*dt/(2*dx^2)) * ones(nx, 1);
96 d = (1 + 1i*dt/(dx^2)) * ones(nx, 1);
97 du = dl;
98 % Impose boundary conditions
99 d(1) = 1.0;
100 du(2) = 0.0;
101 dl(nx-1) = 0.0;
102 d(nx) = 1.0;
103 % Compute sparse matrix for first ADI eqn
104 A_half = spdiags([dl d du], -1:1, nx, nx);
105
106 % Loop that iterates each time step
107 for n = 1:nt-1
108     % reshape  $\psi$  to create a 2d matrix at this timestep
109     psi_n = reshape(psi(n,:,:), nx, ny);
110     % Create matrix for  $\psi^{(n+1/2)}$ 
111     psi_half = zeros(nx,ny);
112
113     % Solve tridiagonal system for each j (row)
114     for j = 2:ny-1

```

```

115 % Array for holding the RHS of the first ADI eqn
116 f = zeros(nx,1);
117
118 % Compute RHS of first ADI eqn in stages.
119 f(2:nx-1) = (1*dt/(2*dy^2)) * (psi_n(2:nx-1, j+1) + psi_n(2:nx
120 -1, j-1)) ...
121 + (1 - 1*dt*(1/dy^2 + v(2:nx-1,j)/2)) .* psi_n(2:nx
122 -1, j);
123 f(2:nx-1) = (1*dt/(2*dx^2)) * (f(1:nx-2) + f(3:nx)) + ...
124 (1 - 1*dt/dx^2) * f(2:nx-1);
125
126 % Impose boundary conditions
127 f(1) = 0.0;
128 f(nx) = 0.0;
129
130 % Solve first ADI system
131 psi_half(:,j) = A_half \ f;
132 % Impose boundary conditions
133 psi_half(1,:) = 0.0;
134 psi_half(:,1) = 0.0;
135 psi_half(nx,:) = 0.0;
136 psi_half(:,ny) = 0.0;
137 end
138
139 % Define upper and lower sparse matrix diagonals for second ADI eqn
140 dl = (-1*dt/(2*dy^2)) * ones(ny, 1);
141 du = dl;
142 % Impose boundary conditions
143 du(2) = 0.0;
144 dl(ny-1) = 0.0;
145
146 % Solve tridiagonal system for each i (column)
147 for i = 2:nx-1
148 % Define middle sparse matrix diagonal for second ADI eqn
149 v_i = reshape(v(i,:), ny, 1);
150 d = 1 + 1*dt/dy^2 + (1*dt/2)*v_i;
151 % Impose boundary conditions
152 d(1) = 1.0;
153 d(ny) = 1.0;
154
155 % Compute sparse matrix for second ADI eqn
156 A_full = spdiags([dl d du], -1:1, ny, ny);
157
158 % Compute RHS of second ADI eqn. BCs already imposed previously
159 f = reshape(psi_half(i,:), ny, 1);
160
161 % Solve second ADI system
162 psi(n+1, i, :) = A_full \ f;
163 % Impose boundary conditions
164 psi(n+1, 1, :) = 0.0;
165 psi(n+1, :, 1) = 0.0;
166 psi(n+1, nx, :) = 0.0;
167 psi(n+1, :, ny) = 0.0;
168 end
169 end
170
171 % Compute real, imaginary, and modulus of each entry in psi
172 psire = real(psi);

```

```
171     psiim = imag(psi);
172     psimod = abs(psi);
173
174     % Convert to column vectors
175     x = x.';
176     y = y.';
177     t = t.';
178 end
```

Appendix F - ctest_2d.m Code

```

1 %% 2.4 – 2d Convergence Testing
2
3 close all;
4 clear; clc;
5 format long;
6
7 % Simulation maximum time
8 tmax = 0.05;
9 % Discretization levels
10 minlevel = 6;
11 maxlevel = 9;
12 % Delta t by Delta x ratio
13 lambda = 0.05;
14
15 % idtype = 0    ->  Exact family (sine wave)
16 % idtype = 1    ->  Boosted Gaussian
17 idtype = 0;
18 idpar = [2, 3];
19 mx = idpar(1); my = idpar(2);
20
21 % vtype = 0     ->  No potential
22 % vtype = 1     ->  Rectangular barrier or well
23 vtype = 0;
24 vpar = zeros(1,5);
25
26 % Perform computation at various levels of discretization, store
27 % results in cell arrays ...
28 for l = minlevel : maxlevel
29     % Compute the solution
30     [x{l} y{l} t{l} psi{l} psire{l} psiim{l} psimod{l} v{l}] = ...
31         sch_2d_adi(tmax, l, lambda, idtype, idpar, vtype, vpar)
32
33     [nt{l}, nx{l}, ny{l}] = size(psi{l});
34
35     % Define meshgrid for computing exact psi(x,y,t)
36     [X{l}, Y{l}] = meshgrid(x{l}.' , y{l}.' );
37
38     % Compute exact solution
39     psixct{l} = zeros(nt{l}, nx{l}, ny{l});
40     for n = 1 : nt{l}
41         psixct_n{l} = exp(-1i*(mx^2 + my^2)*pi^2*t{l}(n)) * ...
42             sin(mx*pi*X{l}) .* sin(my*pi*Y{l});
43         % Enforce boundary conditions
44         psixct_n{l}(1, :) = 0.0;
45         psixct_n{l}(:, 1) = 0.0;
46         psixct_n{l}(nx{l}, :) = 0.0;
47         psixct_n{l}(:, ny{l}) = 0.0;
48         psixct{l}(n, :, :) = reshape(psixct_n{l}, [1, nx{l}, ny{l}]);
49     end
50
51     % Compute exact errors and their rms values for later
52     Epsi{l} = psixct{l} - psi{l};
53     Epsi_2d{l} = reshape(Epsi{l}, nt{l}, nx{l}*ny{l});
54     rms_Epsi{l} = rms(abs(Epsi_2d{l}), 2);
55
56     % Downsample each psi for differencing

```

```

57     psi_ds{1} = psi{1}(1:2:end, 1:2:end, 1:2:end);
58
59     % Flatten each 3d array into a 2d array
60     psi_2d{1} = reshape(psi{1}, nt{1}, nx{1}*ny{1});
61     psi_ds_2d{1} = reshape(psi_ds{1}, (nt{1}-1)/2+1, ...
62                             ((nx{1}-1)/2+1)*((ny{1}-1)/2+1));
63 end
64
65 % Calculating the level-to-level differences, taking every second
66 % value of the larger length array
67 dpsi6 = psi_ds_2d{7} - psi_2d{6};
68 dpsi7 = psi_ds_2d{8} - psi_2d{7};
69 dpsi8 = psi_ds_2d{9} - psi_2d{8};
70
71 % Compute l-2 norm of each dpsi, resulting in functions of t
72 rms_dpsi6 = rms(abs(dpsi6), 2);
73 rms_dpsi7 = rms(abs(dpsi7), 2);
74 rms_dpsi8 = rms(abs(dpsi8), 2);
75
76 % Plot scaled errors for different discretization levels
77 fig1 = figure;
78 rho = 4;
79 hold on
80 plot(t{6}, rms_dpsi6, 'LineWidth', 2);
81 plot(t{7}, rho*rms_dpsi7, 'LineWidth', 2);
82 plot(t{8}, rho^2*rms_dpsi8, 'LineWidth', 2);
83 xlabel("Time");
84 ylabel("l-2 norm of difference between level");
85 legend('||dΨ^6||', '4 * ||dΨ^7||', '4^2 * ||dΨ^8||', 'Location', 'best');
86 title({"2d Schrodinger equation convergence test - Exact family"
87        "l-2 norm of difference between level 1 solutions"
88        "idtype = 0, vtype = 0, tmax = 0.05, lambda = 0.05, 6 <= l <= 9"});
89 ax = gca;
90 ax.FontSize = 12;
91
92 % Plot scaled exact errors for different discretization levels
93 fig2 = figure;
94 rho = 4;
95 hold on
96 plot(t{6}, rms_Epsi{6}, 'LineWidth', 2);
97 plot(t{7}, rho*rms_Epsi{7}, 'LineWidth', 2);
98 plot(t{8}, rho^2*rms_Epsi{8}, 'LineWidth', 2);
99 plot(t{9}, rho^3*rms_Epsi{9}, 'LineWidth', 2);
100 xlabel("Time");
101 ylabel("l-2 norm of exact error");
102 legend('||EΨ^6||', '4 * ||EΨ^7||', '4^2 * ||EΨ^8||', '4^3 * ||EΨ^9||'...
103        , 'Location', 'best');
104 title({"2d Schrodinger equation convergence test - Exact family"
105        "l-2 norm of exact error for each level l"
106        "idtype = 0, vtype = 0, tmax = 0.05, lambda = 0.05, 6 <= l <= 9"});
107 ax = gca;
108 ax.FontSize = 12;

```


Appendix G - video_rec_bar.m Code

```

1 %% 2.5 - 2d Video of Scattering off Rectangular Barrier
2
3 close all;
4 clear; clc;
5 format long;
6
7 % Simulation maximum time
8 tmax = 0.05;
9 % Discretization level
10 level = 8;
11 % Delta t by Delta x ratio
12 lambda = 0.05;
13
14 % idtype = 0  -> Exact family (sine wave)
15 % idtype = 1  -> Boosted Gaussian
16 idtype = 1;
17 %x0      = idpar(1);      y0 = idpar(2);
18 %delta_x = idpar(3); delta_y = idpar(4);
19 %p_x     = idpar(5);      p_y = idpar(6);
20 idpar = [0.5, 0.3, 0.1, 0.1, 0.0, 30];
21
22 % vtype = 0  -> No potential
23 % vtype = 1  -> Rectangular barrier or well
24 % vtype = 2  -> Double Slit
25 vtype = 1;
26 x_min = 0.2;   x_max = 0.8;
27 y_min = 0.7;   y_max = 0.8;
28 %Vc     = vpar(5);
29 vpar = [x_min, x_max, y_min, y_max, 1e8];
30
31 % Compute solution
32 [x y t psi psire psiim psimod v] = ...
33     sch_2d_adi(tmax, level, lambda, idtype, idpar, vtype, vpar);
34
35 % Dimensions of matrix
36 [nt, nx, ny] = size(psimod);
37
38 % Create a VideoWriter object
39 video = VideoWriter(' ../output/problem2/rec_bar.avi ');
40 video.FrameRate = 30;
41 open(video);
42
43 % Create a figure and define where the rectangle indicating where
44 % the potential barrier is will be drawn
45 figure;
46 rect_xmin = x_min * (nx - 1) + 1;
47 rect_ymin = y_min * (ny - 1) + 1;
48 rect_xlen = (x_max - x_min) * (nx - 1);
49 rect_ylen = (y_max - y_min) * (ny - 1);
50
51 % Loop over time steps
52 for n = 1:nt
53     % reshape  $\psi$  to create a 2d matrix at this timestep
54     psi_n = reshape(psimod(n, :, :), nx, ny);
55
56     % Create filled contour plot

```

```

57     contourf(psi_n, 20, 'LineStyle', 'none');
58     colormap("default");
59     xlabel('x');
60     ylabel('y');
61     title({'2d Schrödinger Equation Simulation'
62           '| $\psi$ | Scattering off a Rectangular Barrier'
63           ['tmax = ', num2str(tmax), ', level = ', num2str(level), ...
64            ', lambda = ', num2str(lambda), ', idpar = [', ...
65             num2str(idpar(1)), ' ', num2str(idpar(2)), ' ', ...
66             num2str(idpar(3)), ' ', num2str(idpar(4)), ' ', ...
67             num2str(idpar(5)), ' ', num2str(idpar(6)), ']']
68           ['Time Step n = ', num2str(n)]]});
69     ax = gca;
70     ax.FontSize = 12;
71
72     % Set axis limits for consistency
73     axis([1 nx 1 ny]);
74     % Set color axis limits to match data range
75     clim([min(psimod(:)) max(psimod(:))]);
76
77     % Scale the axes tick labels to range from 0 to 1
78     xticks(linspace(1, nx, 11));
79     yticks(linspace(1, ny, 11));
80     xticklabels(linspace(0, 1, 11));
81     yticklabels(linspace(0, 1, 11));
82
83     % Draw rectangle where the potential is
84     rectangle('Position', [rect_xmin, rect_ymin, rect_xlen, rect_ylen], ...
85              'EdgeColor', 'black', 'LineWidth', 1);
86
87     % Write to video file
88     frame = getframe(gcf);
89     writeVideo(video, frame);
90 end
91
92 % Close the video file and figure
93 close(video);

```

Appendix H - video_rec_well.m Code

```

1 %% 2.5 - 2d Video of Scattering off Rectangular Well
2
3 close all;
4 clear; clc;
5 format long;
6
7 % Simulation maximum time
8 tmax = 0.05;
9 % Discretization level
10 level = 8;
11 % Delta t by Delta x ratio
12 lambda = 0.05;
13
14 % idtype = 0 -> Exact family (sine wave)
15 % idtype = 1 -> Boosted Gaussian
16 idtype = 1;
17 %x0 = idpar(1); y0 = idpar(2);
18 %delta_x = idpar(3); delta_y = idpar(4);
19 %p_x = idpar(5); p_y = idpar(6);
20 idpar = [0.5, 0.3, 0.1, 0.1, 0.0, 30];
21
22 % vtype = 0 -> No potential
23 % vtype = 1 -> Rectangular barrier or well
24 % vtype = 2 -> Double Slit
25 vtype = 1;
26 x_min = 0.2; x_max = 0.8;
27 y_min = 0.7; y_max = 0.8;
28 %Vc = vpar(5);
29 vpar = [x_min, x_max, y_min, y_max, -1e8];
30
31 % Compute solution
32 [x y t psi psire psiim psimod v] = ...
33     sch_2d_adi(tmax, level, lambda, idtype, idpar, vtype, vpar);
34
35 % Dimensions of matrix
36 [nt, nx, ny] = size(psimod);
37
38 % Create a VideoWriter object
39 video = VideoWriter(' ../output/problem2/well_bar.avi ');
40 video.FrameRate = 30;
41 open(video);
42
43 % Create a figure and define where the rectangle indicating where
44 % the potential barrier is will be drawn
45 figure;
46 rect_xmin = x_min * (nx - 1) + 1;
47 rect_ymin = y_min * (ny - 1) + 1;
48 rect_xlen = (x_max - x_min) * (nx - 1);
49 rect_ylen = (y_max - y_min) * (ny - 1);
50
51 % Loop over time steps
52 for n = 1:nt
53     % reshape  $\psi$  to create a 2d matrix at this timestep
54     psi_n = reshape(psimod(n, :, :), nx, ny);
55
56     % Create filled contour plot

```

```

57     contourf(psi_n, 20, 'LineStyle', 'none');
58     colormap("default");
59     xlabel('x');
60     ylabel('y');
61     title({'2d Schrödinger Equation Simulation'
62           '| $\psi$ | Scattering off a Rectangular Well'
63           ['tmax = ', num2str(tmax), ', level = ', num2str(level), ...
64            ', lambda = ', num2str(lambda), ', idpar = [', ...
65             num2str(idpar(1)), ' ', num2str(idpar(2)), ' ', ...
66             num2str(idpar(3)), ' ', num2str(idpar(4)), ' ', ...
67             num2str(idpar(5)), ' ', num2str(idpar(6)), ']']
68           ['Time Step n = ', num2str(n)]]});
69     ax = gca;
70     ax.FontSize = 12;
71
72     % Set axis limits for consistency
73     axis([1 nx 1 ny]);
74     % Set color axis limits to match data range
75     clim([min(psimod(:)) max(psimod(:))]);
76
77     % Scale the axes tick labels to range from 0 to 1
78     xticks(linspace(1, nx, 11));
79     yticks(linspace(1, ny, 11));
80     xticklabels(linspace(0, 1, 11));
81     yticklabels(linspace(0, 1, 11));
82
83     % Draw rectangle where the potential is
84     rectangle('Position', [rect_xmin, rect_ymin, rect_xlen, rect_ylen], ...
85              'EdgeColor', 'black', 'LineWidth', 1);
86
87     % Write to video file
88     frame = getframe(gcf);
89     writeVideo(video, frame);
90 end
91
92 % Close the video file and figure
93 close(video);

```

Appendix I - video_double_slit.m Code

```

1 %% 2.5 - 2d Video of Scattering through a Double Slit
2
3 close all;
4 clear; clc;
5 format long;
6
7 % Simulation maximum time
8 tmax = 0.05;
9 % Discretization level
10 level = 8;
11 % Delta t by Delta x ratio
12 lambda = 0.05;
13
14 % idtype = 0  -> Exact family (sine wave)
15 % idtype = 1  -> Boosted Gaussian
16 idtype = 1;
17 %x0      = idpar(1);      y0 = idpar(2);
18 %delta_x = idpar(3); delta_y = idpar(4);
19 %p_x     = idpar(5);      p_y = idpar(6);
20 idpar = [0.5, 0.0, 0.08, 0.08, 0.0, 60];
21
22 % vtype = 0  -> No potential
23 % vtype = 1  -> Rectangular barrier or well
24 % vtype = 2  -> Double Slit
25 vtype = 2;
26 x1 = 0.48;   x2 = 0.49;
27 x3 = 0.51;   x4 = 0.52;
28 %Vc      = vpar(5);
29 vpar = [x1, x2, x3, x4, 1e8];
30
31 % Compute solution
32 [x y t psi psire psiim psimod v] = ...
33     sch_2d_adi(tmax, level, lambda, idtype, idpar, vtype, vpar);
34
35 % Dimensions of matrix
36 [nt, nx, ny] = size(psimod);
37
38 % Create a VideoWriter object
39 video = VideoWriter(' ../output/problem2/double_slit.avi ');
40 video.FrameRate = 30;
41 open(video);
42
43 % Create a figure
44 figure;
45
46 % Loop over time steps
47 for n = 1:nt
48     % reshape  $\psi$  to create a 2d matrix at this timestep
49     psi_n = reshape(psimod(n,:,:), nx, ny);
50
51     % Create filled contour plot
52     contourf(psi_n, 20, 'LineStyle', 'none');
53     colormap("default");
54     xlabel('x');
55     ylabel('y');
56     title({'2d Schrödinger Equation Simulation'

```

```

57         '|ψ| Scattering through Double Slits'
58         ['tmax = ', num2str(tmax), ', level = ', num2str(level), ...
59         ', lambda = ', num2str(lambda), ', idpar = [', ...
60         num2str(idpar(1)), ', ', num2str(idpar(2)), ', ', ...
61         num2str(idpar(3)), ', ', num2str(idpar(4)), ', ', ...
62         num2str(idpar(5)), ', ', num2str(idpar(6)), ']' ]
63         ['Time Step n = ', num2str(n)]]});
64     ax = gca;
65     ax.FontSize = 12;
66
67     % Set axis limits for consistency
68     axis([1 nx 1 ny]);
69     % Set color axis limits to match data range
70     clim([min(psimod(:)) max(psimod(:))]);
71
72     % Scale the axes tick labels to range from 0 to 1
73     xticks(linspace(1, nx, 11));
74     yticks(linspace(1, ny, 11));
75     xticklabels(linspace(0, 1, 11));
76     yticklabels(linspace(0, 1, 11));
77
78     % Draw rectangles where the double slit potential is
79     hold on
80     rectangle('Position', [1, (ny - 1)/4 + 1, floor(x1*nx), 1], ...
81             'EdgeColor', 'black', 'LineWidth', 1);
82     rectangle('Position', [ceil(x2*nx), (ny - 1)/4 + 1, ceil((x3 - x2)*nx),
83             1], ...
84             'EdgeColor', 'black', 'LineWidth', 1);
85     rectangle('Position', [ceil(x4*nx), (ny - 1)/4 + 1, floor((1 - x4)*nx),
86             1], ...
87             'EdgeColor', 'black', 'LineWidth', 1);
88     hold off
89
90     % Write to video file
91     frame = getframe(gcf);
92     writeVideo(video, frame);
93 end
94
95 % Close the video file and figure
96 close(video);

```