Simulating the two-dimensional time-dependent Schrödinger equation for the double slit using the Crank-Nicolson scheme

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Simulating a wave packet in the double slit experiment is done using the Crank-Nicholson scheme on Schrödinger's equation in $2 + 1$ dimensions. The partial differential equation, assuming Dirichlet boundary conditions, is solved on matrix form using Armadillo's built in solver class. The initial state is specified by a normalized Gaussian wave packet, ensuring a normalized wave packet at all times t. For a total simulation time $T = 0.008$, the deviation from a normalized wave packet is minimal, and of order 10^{-15}. The simulation results in colourplots and an animation illustrating the probability function of the wave packet at times $t = 0.0$, $t = 0.001$, $t = 0.002$, and for the entire time interval $t \in [0, T]$. The probability of a particle's position along the y-axis, when measured to be in the position $x = 0.8$ at time $t = 0.002$, is simulated for one, two and three slit openings. The resulting plots show interference for two and three slits, and a normal probability distribution for the single slit simulation.

https://github.com/sunnikbe/comfys/tree/main/Project5

I. INTRODUCTION

Solving partial difference equations (PDEs) help our understanding of physical processes such as diffusion, fluid dynamics and quantum mechanics. The Crank-Nicolson (N-C) method is an implicit method for solving partial differential equations, such as the heat equation [3]. By simulating the double slit experiment [1], with electrons, using the N-C method in $2 + 1$ dimensions on the Schrödinger wave equation, we will obtain and study a double-slit-in-a-box model and how it evolves over time.

In section II, we will present the methodology of how we will construct and develop our simulation model. We will simulate a double-slit model over time, with the initial state generated by a normalized Gaussian wave packet. The results will be presented in section III, which will include plots of how the norm deviates as a function of time for both without a slit, and with a double slit. In addition, we will present a plot of the absolute value of the state, i.e. the probability of the state in 2D space for different times of the double slit simulation. We will also be plotting the real and imaginary parts of the state in 2D space for the same times. Then, finally we will run three simulations, from one to three slits, where we will investigate the probability of a particle's y position, measured at a specific point along the x-axis at a specific time. In section III, we will also discuss our results and in section IV, their implications along with a brief summary.

II. METHOD

Assuming dimensionless variables, we have the Schrödinger equation on the form

$$i\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} + v(x, y)u, \tag{1}$$

where $u(x, y, t)$ is the "wave function" and $v(x, y)$ is a time-independent potential.

We will be using $x \in [0, 1]$, $y \in [0, 1]$ and $t \in [0, T]$. In both the x, and the y direction, our stepsize is equal and denoted by h. In the simulations, $h = 0.005$, while the time-step-size $dt = 2.5 \times 10^{-5}$. This means that we will have $M = 201$ steps along the x and y axes with the boundary conditions. We will run the simulations for the times $T = 0.008$ and $T = 0.002$, which gives us $N_t = 321$ timesteps for $T = 0.008$ and $N_t = 81$ timesteps for $T = 0.002$. Notation used:

- $x \to x_i = ih$ for $i = 0, 1, ..., M - 1$.
- $y \to y_j = jh$ for $j = 0, 1, ..., M - 1$.
- $t \to t_n = n\Delta t$ for $n = 0, 1, ..., N_t - 1$.
- $u(x, y, t) \to u(ih, jh, n\Delta t) \equiv u^n_{ij}$.
- $v(x, y) \to v(ih, jh) \equiv v_{ij}$.
- U^n is a matrix with elements u^n_{ij}.
- V is a matrix with elements v_{ij}.

M is the number of points along the x and y axis and N_t-1 is the number of timesteps within the time interval. To discretize equation 1, we introduce the parameter θ, which is equal to $1/2$ for the C-N method. To simplify,

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2} &\approx \frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h^2} = F_i,\\ \frac{\partial^2 u}{\partial y^2} &\approx \frac{u_{i,j+1} - 2u_{ij} + u_{i,j-1}}{h^2} = F_j.\end{aligned} \tag{2}$$

Combining the forward and backward time derivatives gives the equation

$$i\frac{u_{ij}^{n+1}-u_{\mathrm{ij}}^{n}}{\Delta t} = -\theta(F_i^{n+1}+F_i^n)-\theta(F_j^{n+1}+F_j^n) + \theta(v_{i,j}u_{ij}^{n+1}+v_{i,j}u_{ij}^{n}), \tag{3}$$

which yields

$$\begin{aligned} u_{ij}^{n+1} &- r\left[u_{i+1,j}^{n+1}-2u_{ij}^{n+1}+u_{i-1,j}^{n+1}\right] \\ &- r\left[u_{i,j+1}^{n+1}-2u_{ij}^{n+1}+u_{i,j-1}^{n+1}\right]+\frac{i\Delta t}{2}v_{ij}u_{ij}^{n+1} \\ &= u_{ij}^{n}+r\left[u_{i+1,j}^{n}-2u_{ij}^{n}+u_{i-1,j}^{n}\right] \\ &\quad + r\left[u_{i,j+1}^{n}-2u_{ij}^{n}+u_{i,j-1}^{n}\right]-\frac{i\Delta t}{2}v_{ij}u_{ij}^{n}, \end{aligned} \tag{4}$$

where $r \equiv \frac{i\Delta t}{2h^2}$. Full analytical solution is found in appendix A 1

We will assume Dirichlet boundary conditions in the xy plane:

- u(x = 0, y, t) = 0.
- u(x = 1, y, t) = 0.
- u(x, y = 0, t) = 0.
- u(x, y = 1, t) = 0.

Equation 4 can be expressed in matrix form as

$$A\mathbf{u}^{n+1} = B\mathbf{u}^{n}, \tag{5}$$

where the vectors $\mathbf{u}^{n+1}$ and $\mathbf{u}^{n}$, with size $(M-2)^2$, contains the u_{ij}^n values for all the internal points of the xy grid at time step n. This makes the A and B matrices be of a size $(M-2)^2 \times (M-2)^2$, which is very large, but since they mostly consist of zeros we don't need as much memory to store the matrices as if they were dense.

To find the next vector $\mathbf{u}^{n+1}$, from $\mathbf{u}^{n}$, we need to find the vector $\mathbf{b}$

$$B\mathbf{u}^{n} = \mathbf{b}, \tag{6}$$

and solve

$$A\mathbf{u}^{n+1} = \mathbf{b} \tag{7}$$

for $\mathbf{u}^{n+1}$.

The initial state u_{ij}^0 of the wave function is given by a Gaussian wave packet

$$u(x,y,0) = e^{-\frac{(x-x_c)^2}{2\sigma_x^2}-\frac{(y-y_c)^2}{2\sigma_y^2}+ip_x(x-x_c)+ip_y(y-y_c)}, \tag{8}$$

where x_c and y_c are the centre coordinates of the initial wave packet, σ_x and σ_y are the initial widths, and p_x and p_y are the wave packet momenta. We will use the following values

- $x_c = 0.25$
- $\sigma_x = 0.05$
- $p_x = 200$
- $y_c = 0.5$
- $\sigma_y = 0.5$
- $p_y = 0$

All of these values will be held constant over all the simulations, except for σ_y which we will change to 0.1 for computing the deviation for the normalization with two slits. We set $p_y = 0$ as we want the wave packet to hit the slits head on. By normalizing the initial state by requiring

$$\sum_{i,j} u_{ij}^{0*}u_{ij}^{0} = 1, \tag{9}$$

the probability function given by the Born rule [2]

$$p_{ij}^{n} = u_{ij}^{n*}u_{ij}^{n}, \tag{10}$$

will be normalized at $t = 0$. This allows us to check for a deviation in the total probability over time.

We will use the following double-slit configuration:

- Wall thickness (x-direction): 0.02.
- Wall position (centre in x-direction): 0.5.
- Distance between slits (y-direction): 0.05.
- Slit aperture (opening in y-direction): 0.05.
- Middle of slit setup (centre in y-direction): 0.5.

The same configurations will be used for our single-slit and triple-slit configurations.

A. The algorithm

The C-N method in $2+1$ dimensions will be applied to solve our partial differential equation (eq. 1). Details on using the C-N method are found in algorithm 1.

Algorithm 1 The Crank-Nicolson method

On a 2D grid of x and y values to evolve in time

1. Compute potential matrix V
2. Find A and B by creating diagonal matrices where:
   - The main diagonals are given by:
     for $k(= i = j) = 0, 1, 2, ..., (M - 2)$ **do**
     $a_k = 1 + 4r + \frac{i\Delta t}{2} v_{ij}$
     $b_k = 1 - 4r + \frac{i\Delta t}{2} v_{ij}$
   - The superdiagonal and the subdiagonal are given by a vector of r-values, where every third value is zero. The vector is negative in B and positive in A.
   - The third superdiagonal and subdiagonal are given by a vector of only r-values. The vector is negative in B and positive in A.
3. Find initial state matrix $U = U^0$
4. **for** $n = 0, 1, 2, ..., N_t - 1$ **do**
   Compute $\mathbf{b}$ from $B\mathbf{u}^n = \mathbf{b}$
   Solve $A\mathbf{u}^{n+1} = \mathbf{b}$ for $\mathbf{u}^{n+1}$
   Update state matrix $U = U^{n+1}$

III. RESULTS & DISCUSSION

Matrices A and B from equations 5, 6 and 7, are based on submatrices of size $(M - 2) \times (M - 2)$, and can be deconstructed into one diagonal matrix, one lower triangular matrix, and one upper triangular matrix. Given that A and B are not on a tridiagonal form, elimination methods such as LU decomposition, are not a practical choice. However, Jacobi's method or the Gauss-Seidel methods are preferable for solving equation 7 [7].

Equation 7 was solved using the built in solver in Armadillo for a hermitian matrix [5]. Based on the AI of the Armadillo solver class and our matrix A, it is likely that the solver class will use Cholesky decomposition. Regardless, it will choose the most efficient method. As previously stated, the probability function (eq. 10), is normalized at $t = 0$. Plot showing the deviation from the total probability over time without the double-slit barrier is found in figure 1. To compare, plot showing the deviation from the probability over time with the double-slit barrier and the potential switched on is found in figure 2. The deviation of the total probability from 1.0 over time is within the 15'th decimal place in both figures (fig. 1 and 2). Given that a 64-byte floating-point number represented in a modern computer have approximately 15-17 significant decimal digits [4], our simulation holds an acceptable consistency. We do expect, that since the initial state is normalized, then the time evolved states should also be normalized. Since we are simulating numerically there will always be an error from the numerical computations. Since we use one of Armadillos solvers instead of creating our own, we can expect that the error will be a lot smaller.

Colourmap plots illustrating the time evolution of the

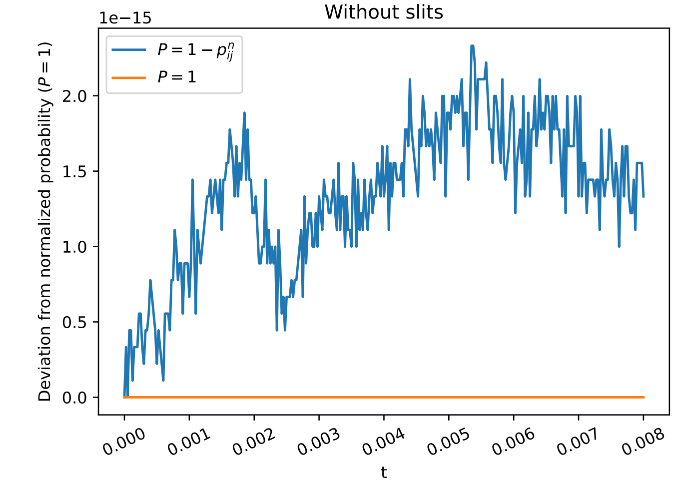

FIG. 1. Plot showing deviation from the normalized probability of 1 over time without a double-slit barrier and with the width of the wave packet in y-direction $\sigma_y = 0.05$.

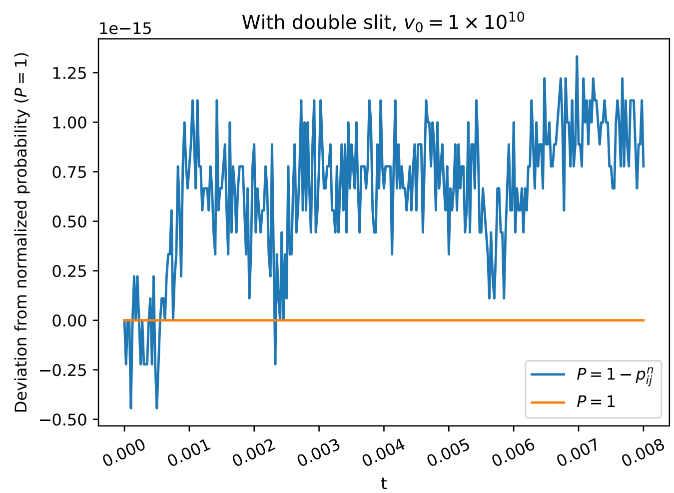

FIG. 2. Plot showing deviation from the normalized probability of 1 over time with the double-slit barrier switched on and a potential matrix V constructed by $v_0 = 1 \times 10^{10}$. While also the width of the wave packet in the y-direction $\sigma_y = 0.1$

2D probability function (eq. 10), at times $t = 0.0$, $t = 0.001$ and $t = 0.002$ are shown in figures 3, 4 and 5 respectively. An animation of the full time evolution can be found at `https://github.com/sunnikbe/comfys/blob/main/Project5/animation.mp4`.

From the plots in figures 3, 4 and 5, we follow the wave packet as it interacts with the double slit with the timesteps $t = 0.0$, $t = 0.001$ and $t = 0.002$. We plot the absolute value for the state since the state itself is not a physical state, but the absolute value will give us the

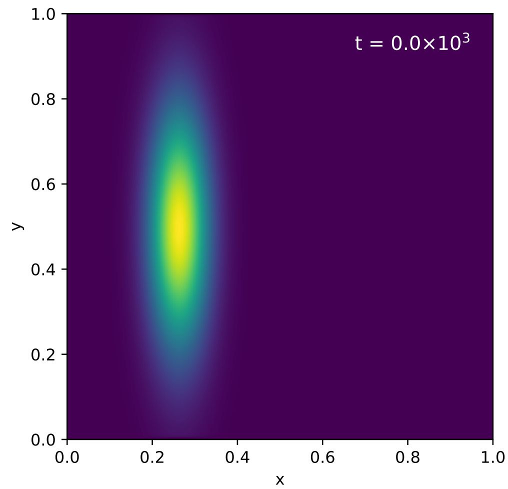

FIG. 3. Colourmap plot illustrating the 2D probability function p^n_{ij} (eq. 10) at time $t = 0.0$.

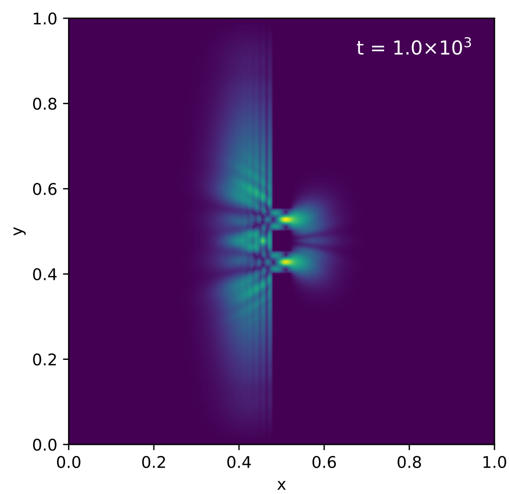

FIG. 4. Colourmap plot illustrating the 2D probability function p^n_{ij} (eq. 10) at time $t = 0.001$.

probability for measuring a particle in that position at that timestep. We see from the plots that the probability for the particles create an interference pattern after the double slit, as particles was discovered through quantum mechanics to have wave properties.

Colormaps showing both $Re(u_{ij})$ and $Im(u_{ij})$, for the same time steps are shown in figures 6, 7, 8, 9, 10 and 11.

As seen from the real and imaginary plots, we see more of the waves that build up the wave packet. Where the real and imaginary parts are in opposite phases to each other. It is noticeable that since the wave packet spreads more out along the x-direction while staying more packed

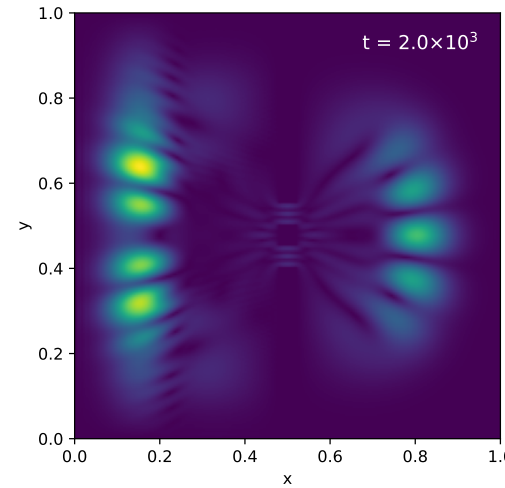

FIG. 5. Colourmap plot illustrating the 2D probability function p^n_{ij} (eq. 10) at time $t = 0.002$.

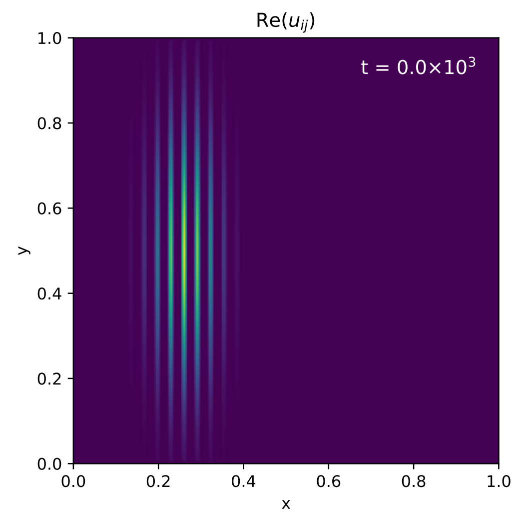

FIG. 6. Colourmap plot illustrating $Re(u_{ij})$ at time $t = 0.0$.

together in the y-direction, the ends of the wave packet have no effect from the slits and just get reflected back again, while most of the central bit of the wave gets either reflected back or sent through the slits. When the wave gets to the other side of the double slit, the wave spreads out across the space while being more intensive where the wave tops meet and less intensive where the waves split from the slits from destructive interference.

Figures 12, 13 and 14 show the probability of where the particle is along the y-axis if we were able to measure it at $x = 0.8$ at a time $t = 0.002$ for one, two and three slit openings. The maxima, i.e. the tops in the graphs, are created from interference, which is a wave property. It is noted that these values for probability only holds if we know that the particle is found at this x position, as the

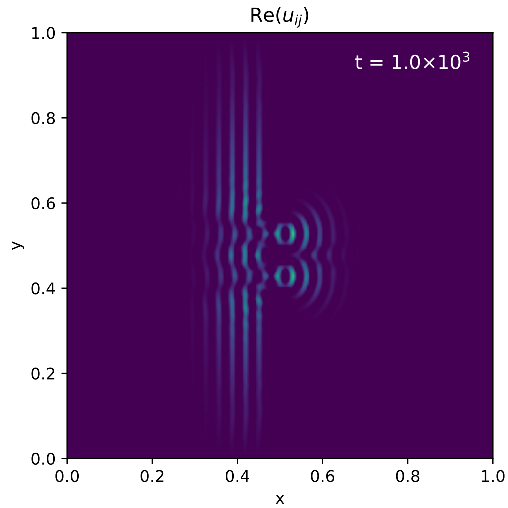

FIG. 7. Colourmap plot illustrating $Re(u_{ij})$ at time $t = 0.001$.

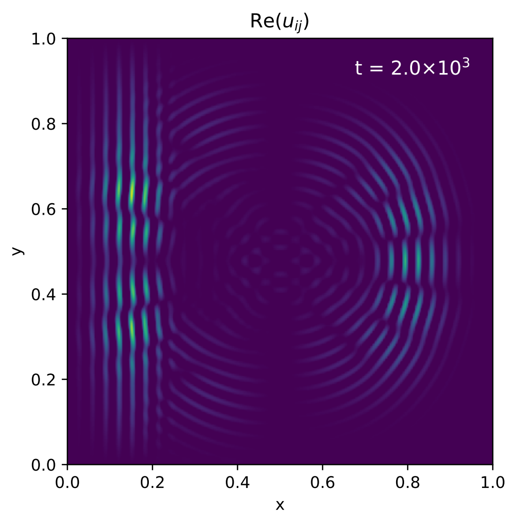

FIG. 8. Colourmap plot illustrating $Re(u_{ij})$ at time $t = 0.002$.

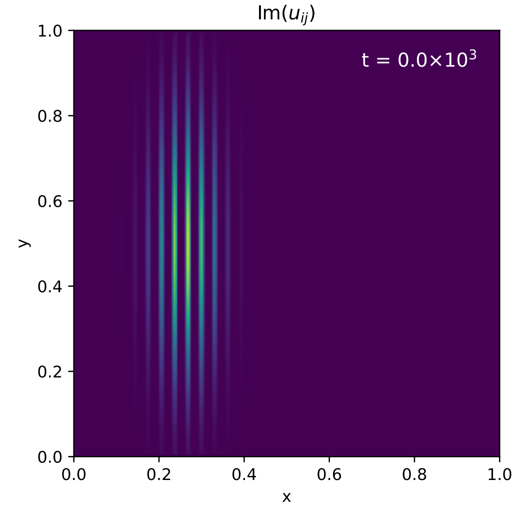

FIG. 9. Colourmap plot illustrating $Im(u_{ij})$ at time $t = 0.0$.

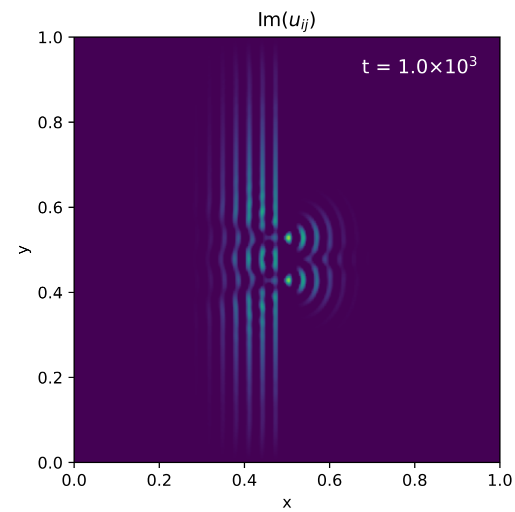

FIG. 10. Colourmap plot illustrating $Im(u_{ij})$ at time $t = 0.001$.

probability is normalized to 1.

For the first plot (fig 12), we get one central maxima, which deviates from most waves computed analytically, where we would have expected more than one maxima. Now, analytical computations have more assumptions used, considering that the slits we use in the simulations have a tunnel with a depth that can't be approximated to zero. We also send out a finite size wave packet in the x-direction, which would change the probability plot for different times, whereas analytically, we would use a constant beam for the wave and thus not have the probability plot change with time.

For number of slit holes larger than one we can see from the probability plot (figures 13 and 14), a better interference pattern, with more orders of maxima the more slits we use. While the triple slit have more orders of maxima than the double slit. We can also notice that the central maxima for the triple slit is more subdued at a level closer to the third order maxima. While for the double slit, the central maxima have the largest top.

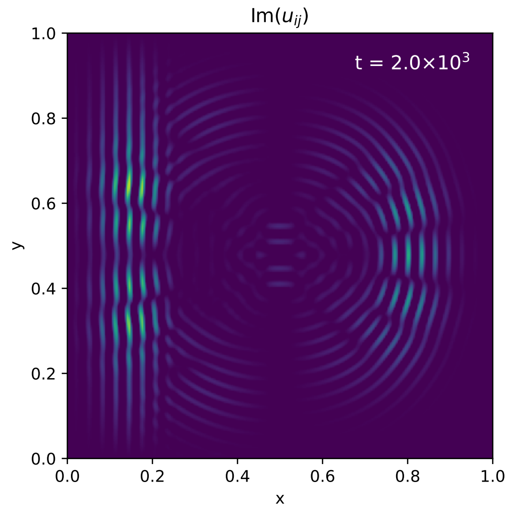

FIG. 11. Colourmap plot illustrating $Im(u_{ij})$ at time $t = 0.002$.

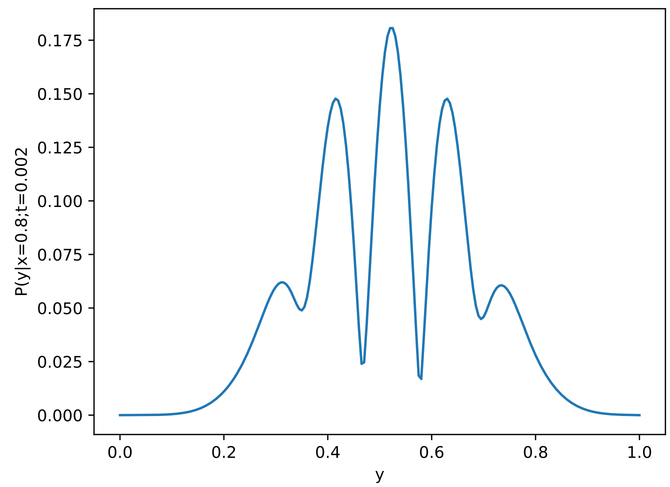

FIG. 13. A plot of the probability for the particle to be somewhere along $x = 0.8$ at a time $t = 0.002$ for a double slit. The probability is normalized to 1.

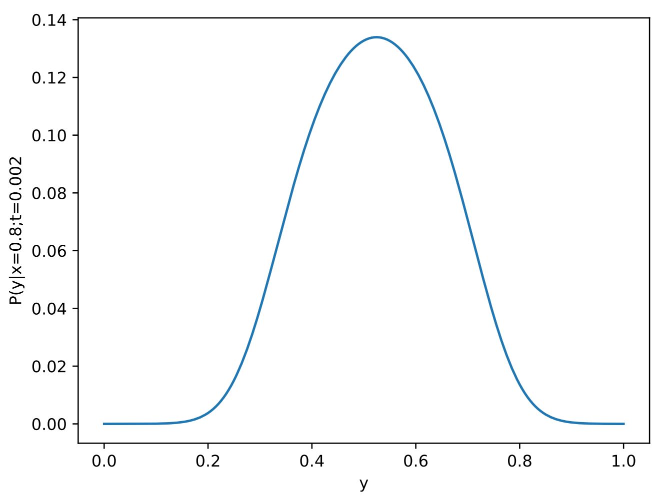

FIG. 12. A plot of the probability for the particle to be somewhere along $x = 0.8$ at a time $t = 0.002$ for a single slit. The probability is normalized to 1.

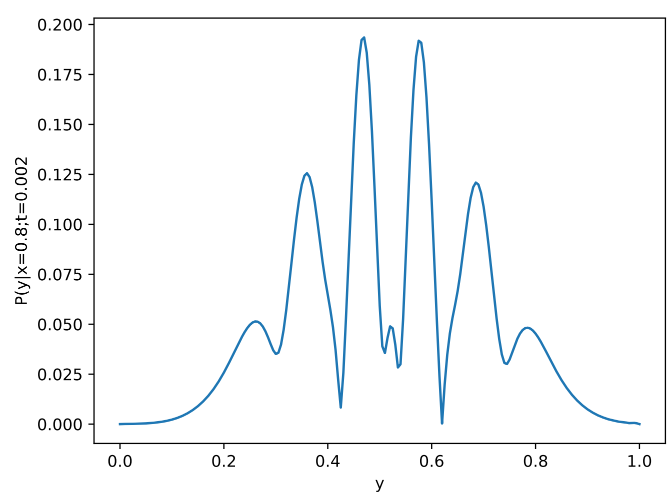

FIG. 14. A plot of the probability for the particle to be somewhere along $x = 0.8$ at a time $t = 0.002$ for a triple slit. The probability is normalized to 1.

IV. SUMMARY

We have now been able to simulate a wave packet for the double slit experiment. Using the Crank-Nicholson method to solve the Schrödinger's equation (eq. 1) for two spatial and one time dimension. Assuming Dirichlet boundary conditions, we were able to solve the partial differential equation on matrix form (eq. 5) using one of Armadillo's inbuilt solvers for equation 7. Using a normalized Gaussian wave packet (eq. 8) as our initial state, we should expect that the wave packet at a time t would also be normalized for all times t. With the solver we used we found that the deviation for the normalization over time for $T = 0.008$, was minimal of order 10^{-15}. Figures 3, 4 and 5 shows the probability for the wave packet at time $t = 0.0, 0.001, 0.002$. While figures 6, 7 and 8 shows the same for the real part of the state u_{ij} at the same times, and figures 9, 10 and 11 shows the same for the imaginary part for the state u_{ij}. These plots were simulated with two slit openings. Finally, we simulated the wave packet for one, two and three slit openings and made a plot of the probability for the position of a particle along the y-direction if we had measured the same particle to be in $x = 0.8$ at a time $t = 0.002$. These plots are shown in figures 12, 13 and 14.

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Appendix A: Calculations

1. Discretization of equation 1

$$i\,\frac{U_{ij}^{n+1}-U_{ij}^{n}}{\Delta t} = \frac{1}{2}\left[-\overset{(n+1\,+\,n)}{\underset{\equiv}{\frac{\partial^2 U}{\partial x^2}}} - \overset{(n+1+n)}{\underset{\equiv}{\frac{\partial^2 U}{\partial y^2}}} + \overset{(n+1\,+\,n)}{V(x,y)U}\right]$$

$$-\left(F_i^{n+1}+F_i^{n}\right)-\left(F_j^{n+1}+F_j^{n}\right)$$

$$\left(V_{ij}U_{ij}^{n+1} + V_{ij}U_{ij}^{n}\right)$$

$$\underset{\displaystyle V_{ij}^{n+1}}{\equiv} \qquad + \qquad \underset{\displaystyle V_{ij}^{n}}{\equiv}$$

$$\boxed{\begin{aligned} F_i &= \frac{U_{i+1,j}-2U_{ij}+U_{i-1,j}}{\Delta x^2} \\ F_j &= \frac{U_{i,j+1}-2U_{i,j}+U_{i,j-1}}{\Delta y^2} \end{aligned}}$$

$$x_i = ih \qquad y_j = jh$$

$$i\left(U_{ij}^{n+1}-U_{ij}^{n}\right) = \frac{\Delta t}{2}\left[-F_i^{n+1}-F_i^{n}-F_j^{n+1}-F_j^{n}+V_{ij}^{n+1}+V_{ij}^{n}\right] \quad \Big/\cdot i$$

$$-U_{ij}^{n+1}+U_{ij}^{n} = \frac{i\Delta t}{2}\left[-F_i^{n+1}-F_i^{n}-F_j^{n+1}-F_j^{n}+V_{ij}^{n+1}+V_{ij}^{n}\right]$$

$$U_{ij}^{n} + \frac{i\Delta t}{2}\left[F_i^{n}+F_j^{n}-V_{ij}^{n}\right] = U_{ij}^{n+1} + \frac{i\Delta t}{2}\left[-F_i^{n+1}-F_j^{n+1}+V_{ij}^{n+1}\right]$$

$$\Rightarrow \quad r \equiv \frac{i\Delta t}{2h^2} \quad \text{gives}$$

$$U_{ij}^{n+1} - r\left[U_{i+1,j}^{n+1}-2U_{ij}^{n+1}+U_{i-1,j}^{n+1}\right] - r\left[U_{i,j+1}^{n+1}-2U_{i,j}^{n+1}+U_{i,j-1}^{n+1}\right] + \frac{i\Delta t}{2}V_{ij}U_{ij}^{n+1}$$

$$= U_{ij}^{n} + r\left[U_{i+1,j}^{n}-2U_{ij}^{n}+U_{i-1,j}^{n}\right] - r\left[U_{i,j+1}^{n}-2U_{i,j}^{n}+U_{i,j-1}^{n}\right] + \frac{i\Delta t}{2}V_{ij}U_{ij}^{n}$$