Numerical Double Slit Experiment

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The code used in this study is available here: https://github.com/vebjoro/fys4150_project5.

Abstract

We have solved the Schrödinger equation for a single electron numerically in order to study the wave-like nature of electrons by replicating the double slit experiment. We used the Crank-Nicolson method to do the simulation and implemented a wall and slits through the potential $V(\mathbf{r})$. The initial condition used was a Gaussian wave packet with a sharply defined momentum, and the simulation was run until the wave function hit the back wall of the domain, at which time we assume the electron has hit the screen. The results accurately reproduced the wave-like behaviour of electrons and the characteristic diffraction pattern well known from earlier experiments.

1 Introduction

The double slit experiment was first conducted by Thomas Young in 1802 demonstrating that light had the properties of waves.[1] In 1927, Davisson and Germer performed a diffraction experiment on nickel, demonstrating that electrons also have wave like properties, confirming de Broglies wave hypothesis.[2] The double slit experiment was first performed on electrons in 1961. [3] The wave-particle duality, though experimentally well-founded, is still a highly mysterious aspect of modern physics. In this study, we will simulate the Schrödinger equation for a single electron wave function to replicate the double-slit experiment. Although the results are well known, this study can serve to demonstrate the wave-like properties of electrons. By performing the experiment numerically, we can access the physical process at any stage of the experiment without concern for how measurements interfere with the system. This leaves out some aspects of real quantum systems, such as the collapse of the wave function.[1] Nonehteless, it allows us to study the entire wave function at once, not just the collapsed state, as well as the interaction with the wall leading up to the electron hitting the wall. After a brief introduction to the Schrödinger equation, we present the Crank-Nicolson method for solving partial differential equations (PDEs) and derive the discretized version of the Schrödinger equation according to this method. Then, we present the experimental set-up to be simulated before discussing the results we obtained.

[1] However you would like to interpret that.

2 Theory and Method

2.1 The Schrödinger Equation

All the information about a quantum system is contained in the wave function Ψ. The evolution of the wave function over time is described by the time-dependent Schrödinger equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\Psi\right\rangle = \hat{H}\left|\Psi\right\rangle, \tag{1}$$

where $\hat{H}$ is the Hamiltonian operator. In this study the system of interest is an electron confined in a box with a central wall with one, two or three slits. In this case the Hamiltonian of the system is

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}),$$

where $V(\mathbf{r})$ is the potential in the box, which is constructed to representing the walls and the slits inside the domain. On dimensionless form the Schrödinger equation can be written as

$$i\frac{\partial u(\mathbf{r},t)}{\partial t} = -\nabla^2 u(\mathbf{r},t) + v(\mathbf{r})u(\mathbf{r},t), \tag{2}$$

Where function u has substituted the wave function and v is a dimensionless time-independent potential. Although solving equation 2 will give a complete description the system it will not predict the outcome of single measurements. The probability density for finding the electron at any given position is given by the Born rule,

$$p(\mathbf{r},t) = \Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t). \tag{3}$$

2.2 Crank-Nicolson

We will use the Crank-Nicolson method to solve the partial differential equation (PDE) 1. It is second order accurate in time and space as well as yielding stable solutions for any step size Δt or Δx.

To start off deriving the Crank-Nicolson scheme we consider a $1+1$ dimensional function $u(x,t)$ that fulfil the equation

$$\frac{\partial u}{\partial u} = F(x,t),$$

where $F(x,t)$ is some function.

Two intuitive ways to discretize this equation are to use forward differencing and backward differencing in time. This would yield

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = F_i^n \tag{4}$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = F_i^{n+1}, \tag{5}$$

where n indicates the time step and i indicate the nodes in the x-direction. If we were to derive a numerical scheme from the equations 4 and 5, we would find that the explicit scheme based on 4 is conditionally stable, whereas the implicit scheme, using 5, is unconditionally stable. The Crank-Nicolson scheme can be obtained as a linear combination of the forward differencing scheme and the backward differencing scheme, giving each of them a weight of a half

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{2}\left(F_i^{n+1} + F_i^n\right). \tag{6}$$

In the case of the dimensionless Schrödinger equation 2 in 2D we can express the function $F(x,y,t)$ as

$$F = i\nabla^2 u(x,y,t) - iv(x,y)u(x,y,t).$$

Approximating the second derivative we get a discrete approximation for $F(x,y,t)$

$$F_{ij}^n = \left[\frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2} + \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2}\right] - v_{i,j}u_{i,j}^n.$$

Inserted into 6 at times n and $n+1$, and assuming the same step size in x and y direction, $\Delta x = \Delta y = h$, we get the following equation

$$u_{i,j}^{n+1} - \frac{i\Delta t}{2h^2}\left[u_{i+1,j}^{n+1} - 2u_{i,j}^{n+1} + u_{i-1,j}^{n+1} + u_{1,j+1}^{n+1} - 2u_{i,j}^{n+1} + u_{i,j-1}^{n+1}\right] + \frac{i\Delta t}{2}v_{ij}u_{ij}^{n+1}$$
$$=$$
$$u_{i,j}^n + \frac{i\Delta t}{2h^2}\left[u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n + u_{1,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n\right] - \frac{i\Delta t}{2}v_{ij}u_{ij}^n, \quad (7)$$

which can be solved for $u_{i,j}^{n+1}$. Equation 7 can also be written in a more compact format as a matrix equation

$$A\mathbf{u}^{n+1} = B\mathbf{u}^n. \quad (8)$$

Here the vector $\mathbf{u}^n$ contains the rows of the matrix $u_{i,j}^n$ from equation 7. It looks something like

$$\mathbf{u}^n = \left[\left(u_{1,1}^n, u_{2,1}^n, \ldots, u_{M-2,1}^n\right), \left(u_{1,2}^n, u_{2,2}^n, \ldots u_{M-2,2}^n\right), \ldots, \left(u_{1,M-2}^n \ldots u_{M-2,M-2}^n\right)\right], \quad (9)$$

where the parentheses indicate the which elements belong to the same row of $u_{i,j}^n$. Say that we discretize the domain using M nodes in say the x-direction, including the boundary points, the A matrix consists of sub matrices of size $(M-2)\times(M-2)$. Along the centre diagonal of A the submatrices are given by

$$\mathrm{D} = \begin{pmatrix} a_k & -r & 0 & \cdots & & & & \\ & \ddots & & & & & & \\ & & \ddots & & & & & \\ & & & \ddots & & & & \\ & \cdots & 0 & -r & a_k & -r & 0 & \cdots \\ & & & & & \ddots & & \\ & & & & & & \ddots & \\ & & & & \cdots & 0 & -r & a_k \\ . & & & & & & & \end{pmatrix}$$

The off second diagonals contain submatrices given by

$$\mathrm{R} = \begin{pmatrix} -r & \cdots & \\ \cdots & -r & \cdots \\ & \cdots & -r \end{pmatrix},$$

where all the off diagonal elements are zero.

We can illustrate the form of the A-matrix in the 3×3 case. Using the submatrices D and R defined above it can be written as

$$\mathrm{A} = \begin{pmatrix} \begin{bmatrix} & \mathrm{D} & \end{bmatrix} & \begin{bmatrix} & \mathrm{R} & \end{bmatrix} & \begin{bmatrix} & 0 & \end{bmatrix} \\ \begin{bmatrix} & \mathrm{R} & \end{bmatrix} & \begin{bmatrix} & \mathrm{D} & \end{bmatrix} & \begin{bmatrix} & \mathrm{R} & \end{bmatrix} \\ \begin{bmatrix} & 0 & \end{bmatrix} & \begin{bmatrix} & \mathrm{R} & \end{bmatrix} & \begin{bmatrix} & \mathrm{D} & \end{bmatrix} \end{pmatrix}.$$

The overall structure of A is tridiagonal, with D-matrices on the first diagonal and R-matrices on the second diagonals. The rest of the matrix contains only zeros. For a domain of size $(M-2)\times(M-2)$, we would get a supermatrix A of $(L-2)\times(L-2)$ submatrices. Note that the diagonal elements in D are different for each row of A, not of D. The D-matrices in A are not all the same. The diagonal of A is given by a vector of length $(M-2)^2$.

In the B-matrix the submatrices are given as

$$\mathrm{D} = \begin{pmatrix} b_k & r & 0 & \cdots & & & & \\ & \ddots & & & & & & \\ & & \ddots & & & & & \\ & & & \ddots & & & & \\ \cdots & 0 & r & b_k & r & 0 & \cdots & \\ & & & & \ddots & & & \\ & & & & & \ddots & & \\ & & & \cdots & 0 & r & b_k & \end{pmatrix}$$

$$\mathrm{R} = \begin{pmatrix} r & \cdots & \\ \cdots & r & \cdots \\ & \cdots & r \end{pmatrix},$$

The supermatrix B has the same structure as the A-matrix shown above. The elements along the diagonals of A and B are given by

$$\begin{aligned} a_k &= 1 + 4r + \frac{i\Delta t}{2} v_{ij} \\ b_k &= 1 - 4r - \frac{i\Delta t}{2} v_{ij}. \end{aligned}$$

The vector elements a_k and b_k are constructed from v_{ij} in the same manner as $\mathbf{u}^n$ is constructed from the matrix $u^n_{i,j}$. This means that the first diagonal submatrix of A and B have diagonals that correspond to the first row of v_{ij} and so forth. Now we can solve the equation 8 for the next time step $\mathbf{u}^{n+1}_{i,j}$. We do this in two steps: First performing a matrix multiplication to give the vector $\mathbf{b} = B\mathbf{u}^n$. Then solving the matrix equation $A\mathbf{u}^{n+1} = \mathbf{b}$. The full algorithm is presented in pseudocode as Algorithm 1.

Algorithm 1 Crank-Nicolson

Generate A and B matrices
$U[0] \leftarrow$ Inital state
for $j = 1, ..., n_s$Number of steps **do**
  procedure STEP(n)
    for $i = 1, ..., M-2$ **do**
      for $j = 1, ..., M-2$ **do** $\mathbf{u}[(i-1)*(M-2)+(j-1)] = U[n-1][i,j]$
    Solve linear system: $A\vec{u^{n+1}} = Bu$
    for $i = 1, ..., M-2$ **do**
      for $j = 1, ..., M-2$ **do** $U[n][i,j] = U\mathbf{u^{n+1}}[(i-1)*(M-2)+(j-1)]$

2.3 Parameters and experiments

We implement a wall of thickness $\Delta x = 0.02$ positioned at the center of our domain $x = 0.5$. The slits are placed with their centers a distance of 0.05 from the center of the wall and both have an aperture of $\Delta y = 0.05$. The wall is implemented through the potential V. We set the potential at the wall to a really high numner, approximating infinity, and zero everywhere else. In addition to the double-slit setup, we implement a single-slit wall and a triple-slit setup. The single slit is placed at the center of the wall at $y = 0.5$, and the two additional slits are placed with a distance of 0.1 from the center of the central slit, measured at their centers. All slits have the same aperture of $\Delta y = 0.05$.

The initial condition is a Gaussian wave packet with its center positioned at $(0.25, 0.5)$ and with width in the x-direction given by $\sigma_x = 0.06$. The momentum of the electron wave packet is set to $p_x = 200$. We first set the width in the y-direction to be $\sigma_y = 0.05$, then $\sigma_y = 0.10$. To test that our solver is working, we check whether it conserves the total probability. By integrating the probability density 3 over the entire domain, we should always get 1. We perform this test with and without the wall present before running the rest of our simulations. Two simulations are run, with and without the wall, until time $T = 0.008$ using a time step of $\Delta t = 2.5 \times 10^{-5}$ and a step length of $h = 0.005$.

Next, we simulate a wider wave packet with width $\sigma_y = 0.20$ until time $T = 0.002$. All other parameters for the electron are the same as before. We simulate the electron passing through a single, double, and triple slit.

3 Results and Discussion

3.1 Probability check

The results from our probability checks are shown in Figure 1. The total probability changes over time, however over the time span shown here the amplitude of the deviation from unity is on the order of 10^{-14}. Machine precision for doubles is about 10^{-16}, so we consider the changes in probability to be sufficiently close to machine precision that they can be neglected. The deviation is likely a result of numerical noise, which cannot be avoided. We also note that the deviation is not strictly increasing, but oscillating. This might indicate that the error does not accumulate over time, which would be desirable. Since the simulations we will be studying are run over a shorter time span than we have tested here, this is not a concern in this study. Within the time span of our simulations, we can neglect the change in total probability of the wave function and take our results to be physically reasonable in this regard.

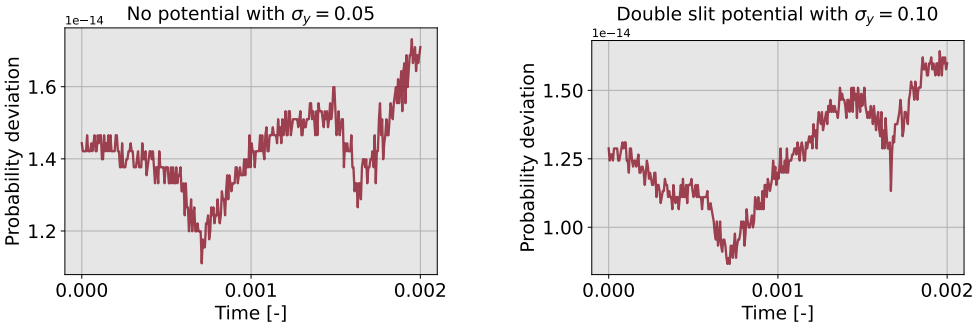

Figure 1: Deviation in total probability from unity from over time. On the left is the simulation of an empty box, on the right is a simulation with the wall potential switched on.

3.2 Time evolution of the wave function

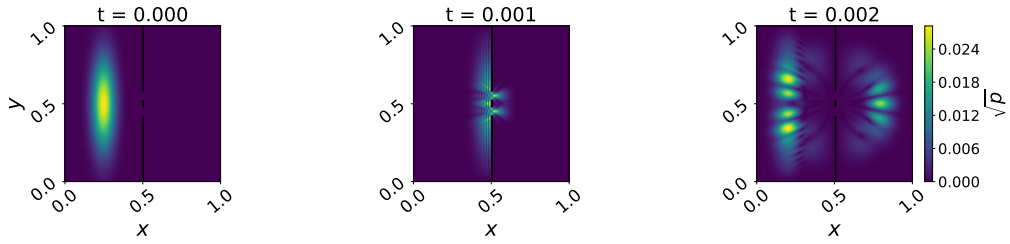

Figure 2: The time evolution of the wave probability density of finding the electron. From left to right the plots display times $t = 0$, $t = 0.001$ and $t = 0.002$

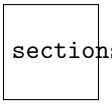

Figure 3: Zoomed-in view of the wave function at $t = 0.001$ as it passes through the slits.

The probability density of the electron's location is displayed in Figure 2. The Gaussian wave packet moves from left to right. In the middle image, we can see the electron passing through the slits. To obtain a more detailed view, we have zoomed in on the region around the two slits in Figure 3. The most probable scenarios are either that the electrons pass through the slits and continue more or less straight ahead, or that they are reflected by the wall. An interesting phenomenon to note is how the electron interacts with the edges of the slits. After passing through the slit, there is a non-zero probability that we will find the electron behind the wall. In classical wave theory, this could be explained through Huygens' principle, which states that any point of a wavefront can be considered an elementary wave expanding in all directions.[4]. Another possible explanation is through Heisenberg's uncertainty principle, which states that the momentum of the electron is not a sharply defined quantity. Even though that is how we initialize the simulation, setting $p_x = 200$, the momentum could spread out during the simulation. If there is some probability that the electron is travelling

at an angle to the wall, it will be possible to locate the electron behind the wall when it has just passed the slits. If the electron were a classical point particle, however, the probability of finding it behind the wall would be practically zero. In our simulation, the walls are point sharp, so the electron wouldn't notice a change in the potential unless it collided with them. It would then rebound every time, not pass over the top of the barrier. It is clear that the classical picture of marble like electrons are at odds with the dynamics we observe in our simulation, in this experiment electrons must be described as wave-like

In the last image we see a diffraction pattern spreading from the two slits. If we were to think of this as a single electron it would certainly challenge the idea that electrons are particles.

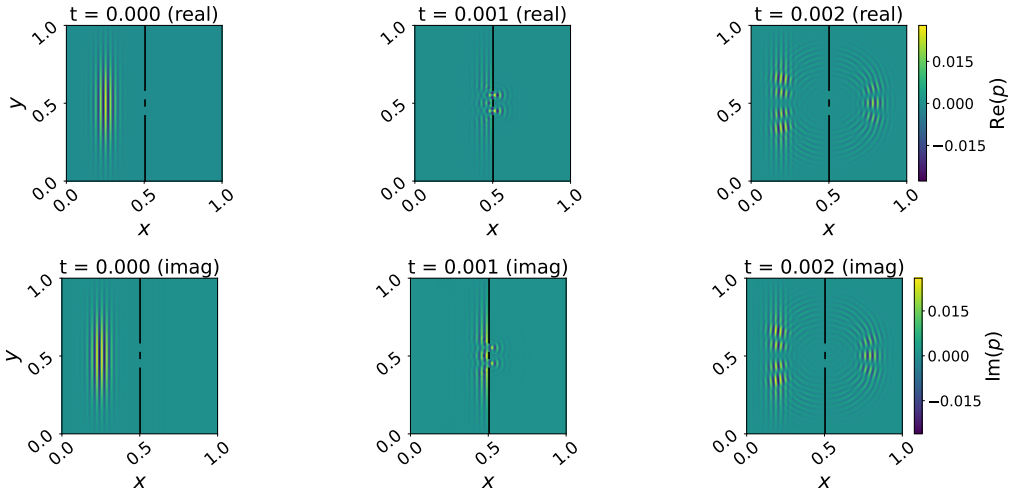

Figure 4: The time evolution of the real (above) and imaginary (below) part of the wave function. From left to right the wave function is displayed at time $t = 0$, $t = 0.001$ and $t = 0.002$.

The time evolution of the real and imaginary parts of the wave function is shown from left to right in Figure 4. We see that the smooth Gaussian wave packet consists of what looks reminiscent of plane waves travelling in the x-direction and with a limited extension in the y-direction. As the electron passes the slits in the middle image, we can see ripples spreading from the slits. In the image above Figure 2, this looks more like rays spreading out as many of these ripples cancel when we multiply the real part with the imaginary part. This is also clear in the last image, where separately the real and imaginary parts of the wave function look like waves in a pond.

3.3 Diffraction pattern

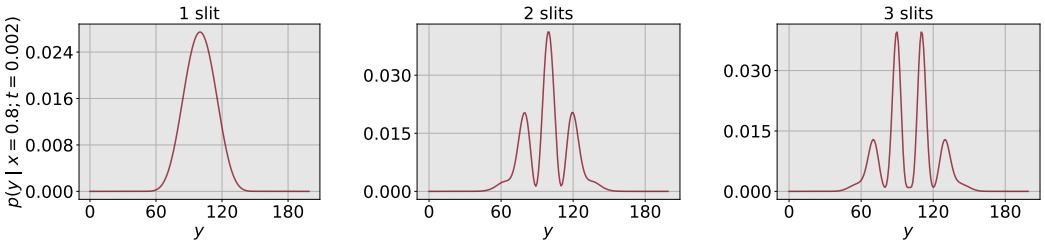

Figure 5: Probability of detecting the electron along $x = 0.8$ at $t = 0.008$ (assuming we do indeed detect it). Plots for one, two and three slits

The probability of where an electron would hit a wall at $x = 0.8$ at $t = 0.2$ was determined by extracting the slice of the wave function at this location and normalizing this part of the wave function to one. The wave function now gives the probability density of finding the electron at any y given that $x = 0.8$, i.e. given that the electron has hit the wall. The results showed a diffraction pattern, as expected, indicating wave-like behavior. The results are presented in figure 5. This pattern is the result of the interference of waves passing through the slits and spreading out in different directions. Let us emphasize, the patterns are result of the interaction of multiple waves, the electron is interacting with itself so to speak. Our results are in concord with previous experiments that have demonstrated the wave-like nature of electrons. The diffraction pattern is symmetrical, this is because the slits are equidistant from the centre of the wall and the electrons are emitted from a single point source in the centre of the domain heading straight towards the wall. This leads to constructive and destructive interference at the same points on the wall on either side of the central extrema. This phenomenon is known as Fraunhofer diffraction and is a well-known characteristic of waves passing through apertures.

3.4 Animation

We present an animation of the system to highlight the aesthetic beauty that can be achieved through the application of computer simulations to physical systems. The animation shows the wave function passing through the double slit wall and can be accessed through the following link: https://gifyu.com/image/Skvjb

4 Conclusions

We explored the Schrödinger equation using the Crank-Nicolson method to simulate the behaviour of a single electron in a double-slit experiment. The simulation showed the wave-like nature of electrons and the characteristic diffraction pattern that arises from the interference of waves passing through the slits. We have discussed the electrons interaction with the wall and its how the diffraction patters also seen in experiments on real world physical systems indicate that electrons do indeed have a wave-like nature. The technical aspect of implementing a wall and slits in the simulation through the potential $V(\mathbf{r})$ has also been briefly discussed. This simulation provides a valuable tool for studying the wave nature of electrons and can easily be generalized for other potentials to simulate other confined systems. By using the Crank-Nicolson method to solve the Schrödinger equation numerically, we are able to describe the physical processes throughout the experiment without disrupting

the system. This provides insights into the behaviour of electrons that would be challenging to obtain through traditional experiments.

References

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