Computational Simulation of a Quantum Particle Interacting with Various Potential Barriers

Aim

The purpose of this report was to produce a computational model of the time-dependent Schrödinger equation. This was achieved using the programming language Python and involved taking the work previously done on simulating a quantum particle in free space and adding both interactions with different barrier potentials and a more adequate time evolution of the particle which can be adjusted to reach any point in time using small discrete time steps.

Background

As aforementioned in my first report (Timms, 2023) electrons exhibit both particle and wavelike characteristics. Why this is the case comes from Young's postulate about light being a wave in 1801. (Britannica, 2023) In order to test his postulate, he designed the double slit experiment which should produce an interference pattern due to the superposition property of waves.

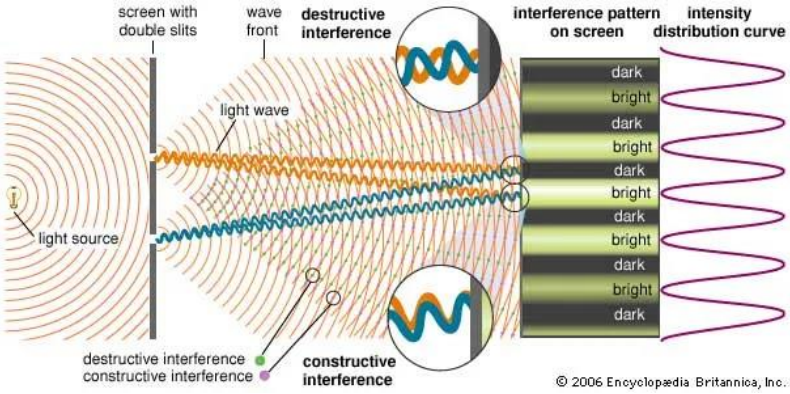

Figure 1: A demonstration Young's double slit experiment showing the wavelike nature of light and the interference pattern displayed on the screen as a result. (Britannica, 2023)

This experiment was the impetus of another experiment which instead of using light uses an electron (a quantum particle) in order to determine whether it is a wave or a particle. This was first done by the Davisson-Germer experiment (H.GERMER & C.DAVISSON, 1927) by firing electrons into a crystal of nickel and observing a diffraction pattern which was similar to the diffraction pattern shown in Young's experiment.

Methods

Using Python, the following mathematical expressions were used with coordinate arrays to produce a computational model.

The time-dependent Schrödinger equation has the form:

$$i\,\hbar\partial_t\psi = \left[\frac{-\hbar^2}{2m}\,\nabla^2 + V\right]\psi$$

Equation 1: Where V is a potential, ψ is the wavefunction, ∇^2 denotes the Laplacian, m is the mass, $\hbar$ and i are both constants and t is time.

In this second report, the potential V will be set to something non-zero. To do this, you will use a technique called the split-operator method.

With the potential V, the formal solution to this equation is $\psi(t)$ at later times $t > 0$ is:

$$\psi(t) = e^{-\frac{it}{\hbar}\left[\frac{-\hbar^2}{2m}\nabla^2+V\right]}\psi(t=0)$$

Equation 2: Where V is a potential, ψ is the wavefunction, ∇^2 denotes the Laplacian, m is the mass, $\hbar$ and i are both constants and t is time.

Note the argument of the exponential is an operator. The exponential of an operator is given by the Taylor series expansion of the exponential, but we won't use that here. A difficulty with exponentials of operators is that $e^{A+B} \neq e^{A}e^{B}$, unless A and B commute. For operators that don't commute, the Campbell-Baker-Hausdorf relation holds.

$$e^{A}e^{B} = e^{At+Bt+\frac{1}{2}[A,B]t^2+\frac{1}{12}[A[A,B]]t^3+\cdots}$$

Equation 3: The Campbell-Baker-Hausdorf relation, where the "…" indicates higher order terms.

The split operator method employs **very short time steps Δt** so that Equation 2 can be approximately written:

$$\psi(\Delta t) \approx e^{\frac{-i\hbar\Delta t}{2m}\nabla^2}e^{-\frac{i\Delta t}{\hbar}V}\psi(t=0)$$

Equation 4: The discrete approximation of the Schrödinger equation.

The operator $e^{-\frac{i\Delta t}{\hbar}V}$ is easy to evaluate, because V is just a function. It's simply the exponential of a function. While the propagation term $e^{\frac{-i\hbar\Delta t}{2m}\nabla^2}$ was solved in the first report.

To simulate a longer time evolution, equation 4 must be applied iteratively. I.e. we build up a long time by advancing the wave function in lots of tiny steps. The wave function at iteration $i+1$ is calculated from the wave function at iteration i:

$$\psi((i+1)\Delta t) \approx e^{\frac{-i\hbar\Delta t}{2m}\nabla^2}e^{-\frac{i\Delta t}{\hbar}V}\psi(i\,\Delta t)$$

Equation 5: The iterative function which calculates the next wavefunction based on the previous wavefunction.

To determine the wave function at a time $t = t_0 + n\Delta t$, we repeat equation 5 n times. Formally we can write this as

$$\psi(t_0 + n\Delta t) \approx \left[e^{\frac{-i\hbar\Delta t}{2m}\nabla^2}e^{-\frac{i\Delta t}{\hbar}V}\right]^n \psi(t_0)$$

Equation 6: The general equation for any wavefunction at time t after repeating the calculation n times.

The wavefunction used to simulate an electron was the gaussian as it satisfies all the requirements mathematically that wavefunctions require and is also an approximation of the form of the electron when not bound by the nucleus. There also exists a method using gaussian wavefunctions of stationary electrons to approximately calculate any configuration of an atom (S.F.Boys, 1950).

Results

In order to understand this experiment a few parameters need to be defined to interpret the results. In table 1 below each parameter and constant used in the simulation is recorded down with their units specified. Some notable changes of values which differ from the first paper proceeding this (Timms, 2023) are the potential term V, Grid size N, movement constant k, the change in time Δt and total time t.

Table 1: A table detailing all the values used for the following simulation in figure 2 and their associated units as discussed.

Symbol:	Definition:	Value:
N	Grid length	200 cells
V	Potential	10^{100} J
σ	Wavefunction width	$0.05\sqrt{\ln(\mathrm{m})}$
k	Spatial movement constant	-10^{8}
$\hbar$	Reduced planks constant	1.0545×10^{-34} J s
m	Mass	$9.109537944498001 \times 10^{-31}$ kg
Δt	Change in time	0.1 s
t	Total time	600 s

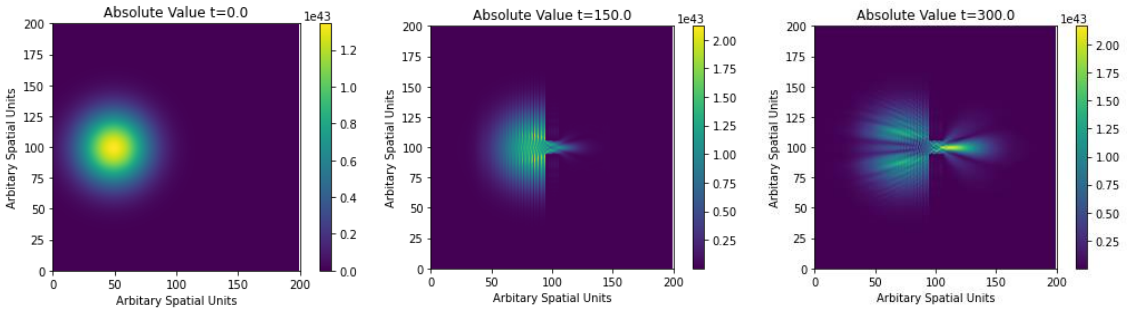

Figure 2: Evolution of a quantum particle (electron) over time at t = 0, 150 and 300 interacting with the single slit barrier potential. The simulation's parameters in are found in table 1 with the particle existing in a space of arbitrary size and length.

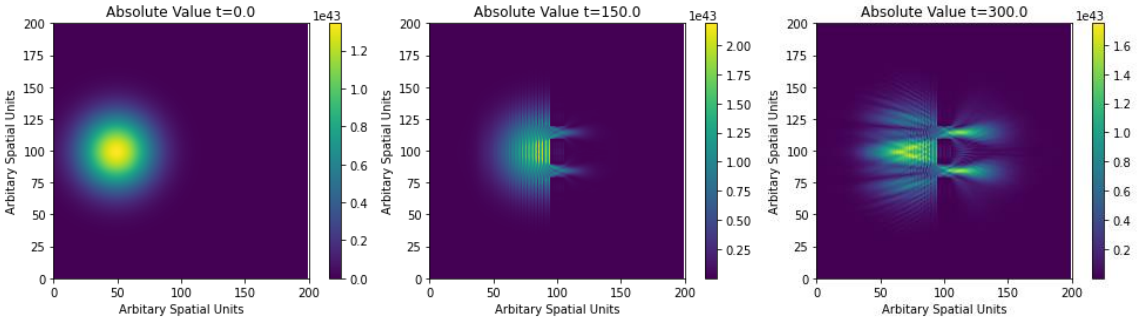

Figure 3: Evolution of a quantum particle (electron) over time at t = 0, 150 and 300 interacting with the double slit barrier potential. The simulation's parameters in are found in table 1 with the particle existing in a space of arbitrary size and length.

The addition of a barrier for the quantum particle to interact with means the strength of that barrier needs to be defined. The strength or the potential energy of that barrier is defined by the potential energy constant V with an associated value of 10^{100} J. Ideally, we would use an infinite potential energy as to create an impenetrable barrier but in place of that a generic large number is chosen in this case a googol which is by far larger than the energy of the particle partially interacting with the barrier (Figure 5). Another value we introduced was the total time t, this is due to the new design of our simulation where now the program will continue to run and move the particle forward by Δt until it reaches a specified time, t.

The other constants that were changed were Δt and k. The change in time Δt is now required to be very small compared to the total time it will run for (t) as instead of having an equation for the state of the system we are now iterating an initial wavefunction as seen in equation 4 until it reaches a desired time. The smaller these iterations the less errors will be generated. A high value for Δt can be seen used in figure 4. For the movement constant we had to increase its value tremendously as the Δt dropped to see a notable change in subsequent iterations.

Lastly, the grid size dictated by the N value had to be decreased to keep the runtime of the program to reasonable times. An N value of 200 still creates a 40 000-pixel image which is still large enough to avoid any resolution errors as seen in the first report. (Timms, 2023)

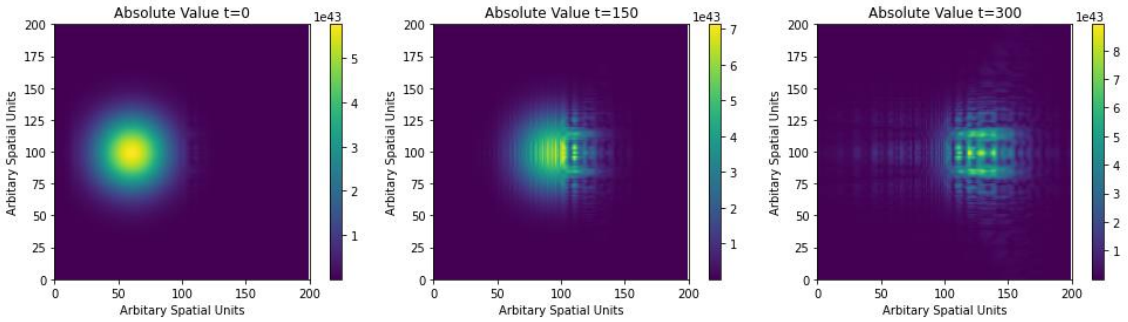

Figure 4: Evolution of a quantum particle (electron) over time at t = 0, 150 and 300 interacting with the double slit barrier potential. The simulation's parameters in are found in table 1 although with Δt set to 50 s. The particle exists in a space of arbitrary size and length.

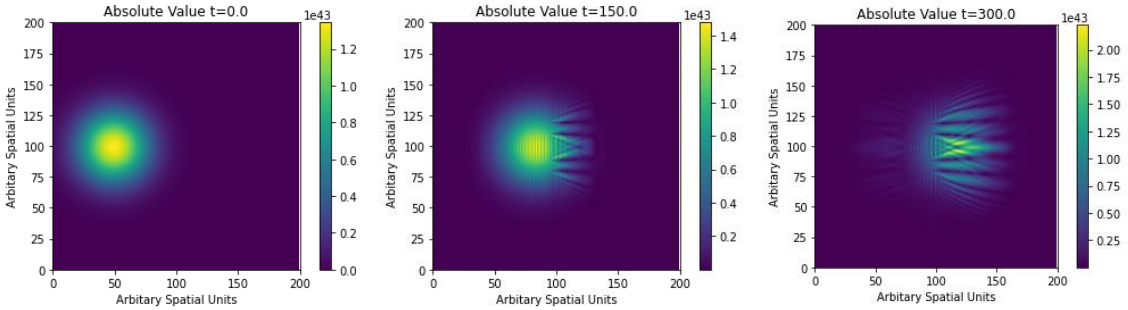

Figure 5: Evolution of a quantum particle (electron) over time at t = 0, 150 and 300 interacting with the double slit barrier potential. The simulation's parameters in are found in table 1 although with V set to 10^{-35} J. The particle exists in a space of arbitrary size and length.

The other interesting result we can find is the probability of the electron we are simulating passing through the barrier if it does not contain any gaps. This is what we call quantum tunnelling and can be seen in figure 6.

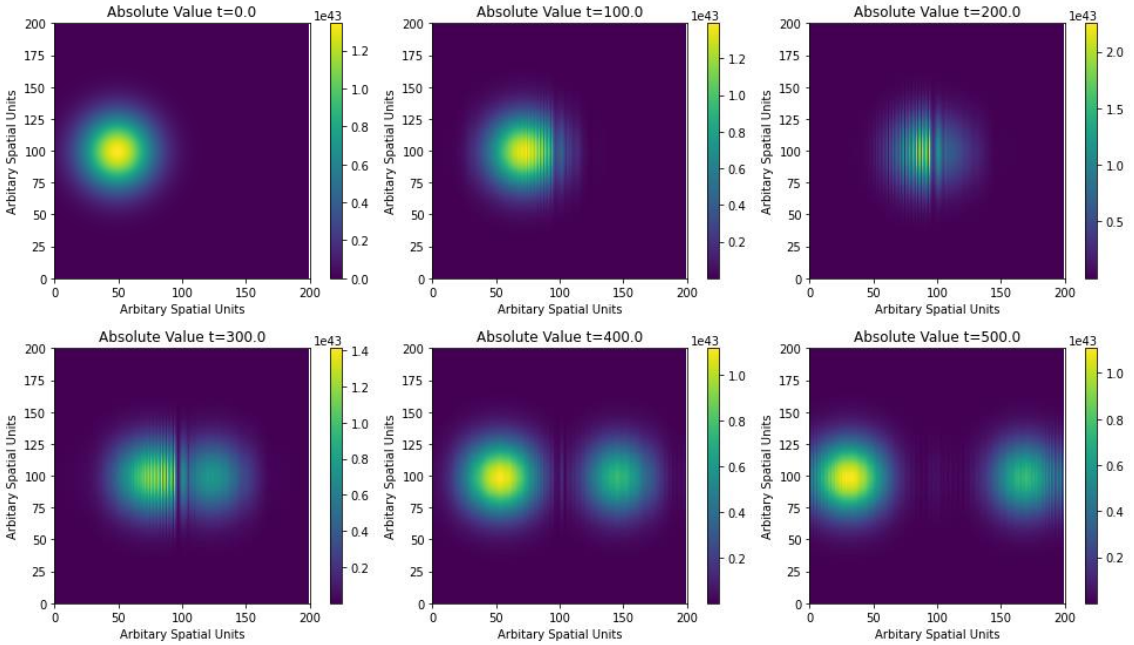

Figure 6: Evolution of a quantum particle (electron) over time at intervals of 100 interacting with a solid barrier potential. The simulation's parameters in are found in table 1 although with V set to 2.5 x 10^{-35} J. The particle exists in a space of arbitrary size and length.

As we can see the probability of the position of the electron is bifurcated as the electron partially could tunnel through the barrier or reflect off the barrier. This will be further discussed in the discussion below.

Discussion

Errors

As mentioned earlier in the results the time step Δt needs to be small as to avoid creating poor results. Why is this?

When comparing figure 3 with figure 4 you can see some resemblance to each other but with a lot more fringing in the latter figure. This particular fringing is due the approximation errors when using equation 4. This is from equation 2 which is used to calculate $\psi(\Delta t)$ which approximates the Schrödinger equation by use of a Taylor series expansion. The larger the Δt value is the less accurate the approximation equation 2 is because you are trying to make discrete function from a continuous one. These result in many numerical errors.

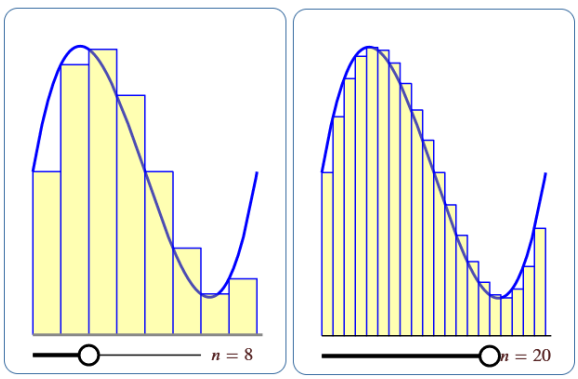

Figure 7: An example of using numerical integration using rectangles to approximate the area under the curve, where the number of rectangles is denoted by n. The higher the number of rectangles (n) the better the approximation. (Guichard, 2023)

Figure 7 is an example of numerical integration which is analogous to our numerical approximation in equation 4. We can think about the width of the rectangles as our Δt which is trying to approximate the Schrödinger equation represented by the curve. The more rectangles you use (n) the better the approximation curve you get. You can also see the more rectangles you use (n) the smaller the width of the rectangles has to be (Δt). Therefore Δt and n are related by the following equation which is a transform of the time function we used in equation 6.

$$\Delta t = \frac{t - t_0}{n}$$

Equation 7: The relationship between Δt (time step) and n (number of time steps) over the total time t which starts from 0.

To improve the accuracy of our wavefunction for a desired time instead of using a large time step to calculate the state at that desired time, we use a smaller timestep to hold the accuracy of equation 2 but repeat this equation many times until we reach the desired time t. The number of times this equation must be repeated (n) is the same as the number of time steps needed to reach the total time t.

The only other limitation of this simulation is the same as the first report (Timms, 2023) where boundary conditions cause any particle to leave the right of the image to appear on the left side.

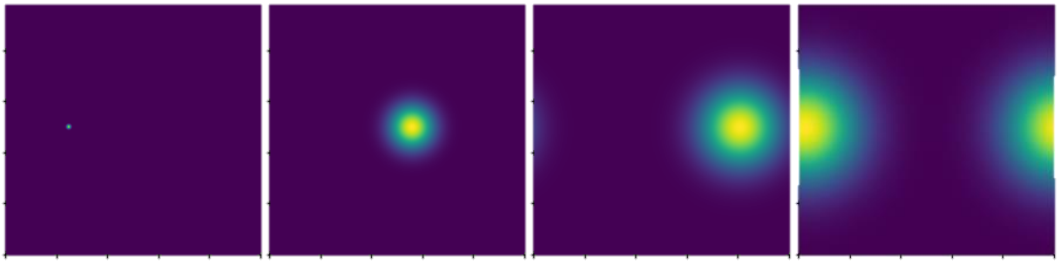

Figure 8: Images generated from the first report (Timms, 2023) of the simulation of an electron at different times: 0, 100, 180, 250. All special units used were arbitrary.

I made the statement that you could consider this space curved as a result and as much this is a two-dimensional simulation, it acts as if the particle is moving along the surface of a sphere.

Physical interpretation

A range of different potentials were used and tested within this report, some of which pertaining to those seen in figures 2-6 which include barriers with no slits, one slit and two slits. Aside from the potentials which form a barrier that were used in the instructions of this report two other potential shapes were attempted. One which formed a tunnel for the electron to accelerate around in and one which features a chessboard pattern which simulates a grating. The images of these potentials can be seen in figure 9.

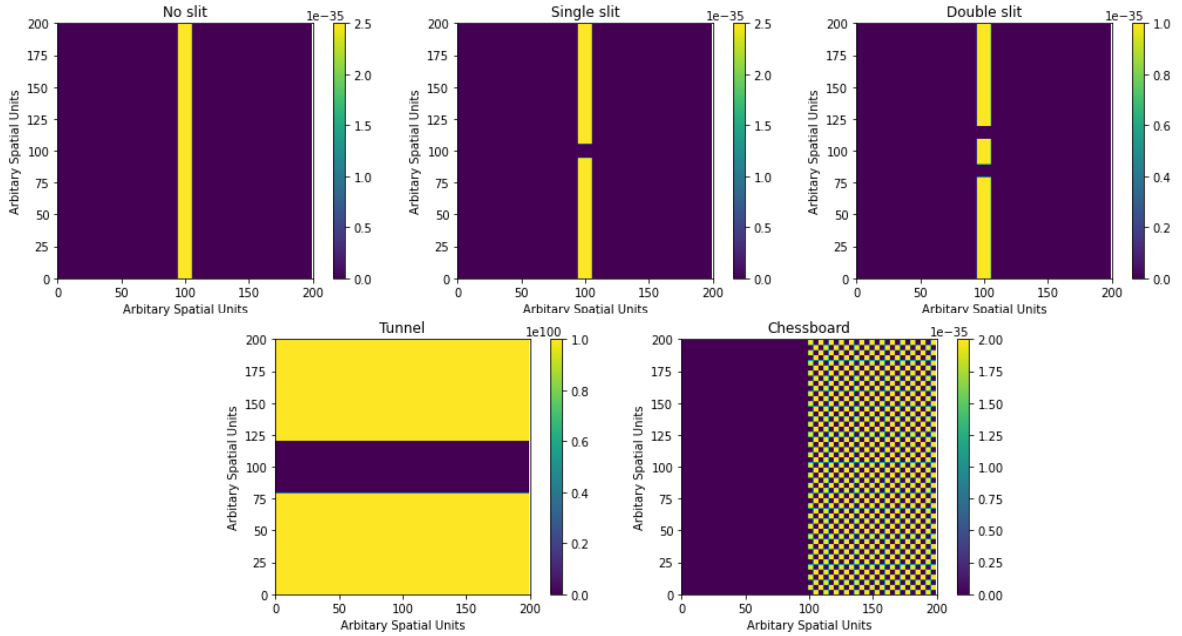

Figure 9: Images of the barriers with varying potential energies which are shown in the legend of each image. They feature simple barriers of no slits, one slit and two slits to some more unique ones like the tunnel or chessboard.

The simulated electron interacting with the first three potentials can be seen in the figures in the results already although if we examine these potentials further ahead in time the diffraction patterns can be seen more clearly.

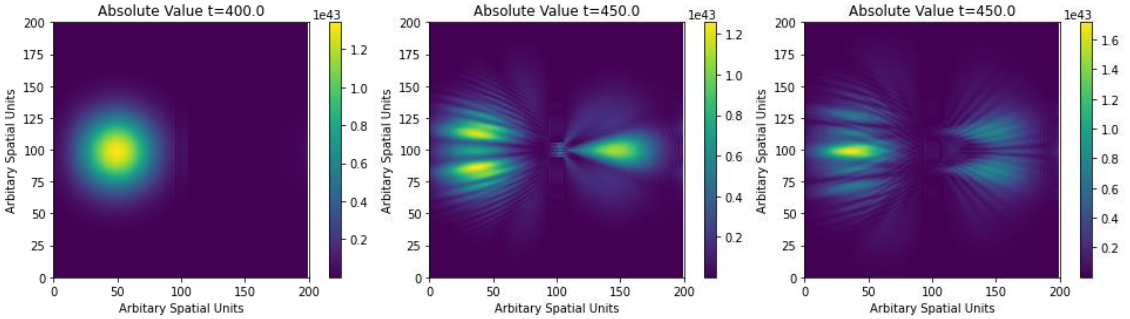

Figure 10: The electron after interaction with the first three potential barriers shown in figure 9 which are the barriers with no slit, one slit and two slits. Where V = 10^{100} J.

The first image contains the electron when it hits the solid barrier with no slit and an extremely high potential, now at t = 400 it approximately returns to the same position as it had at t = 0.0 found in figure 6. If the potential is low enough how ever like in figure 6 the electron can pass through the solid barrier. Unlike a possible error you could get if the Δt is too high, where the large time step causes the electron to skip over the barrier, the particle is interacting with the barrier and is able to tunnel through. The probability that the electron can pass through the barrier is related to the potential energy of the barrier which is what causes the bifurcation of the probability of the position of the electron. In our case it is still more likely that the electron reflects to the left but there is notable probability that it passes straight through.

The next two images in figure 9 relate to the single slit and double slit experiments. In comparing these two we can see to the right of each barrier the different patterns they create. In the single slit experiment (figure 10), we see that there is a cone formed with the brightest spot in the middle of the cone and it slowly diminishing as it goes away from the centre. Interestingly, outside of this cone we

can also see secondary regions with a positive probability due to the electron interacting with the top and bottom of the slit as it passes through and bouncing off in the other direction it was traveling.

The double slit like the single slit generates this cone for each slit initially like seen in figure 3 before it is large enough to interact with each other. Later in time, when t = 450.0 (figure 10) the two slits interact with each other and cause an interference pattern of light areas and dark areas through constructive and destructive interference. Just like the Davisson-Germer experiment that proved electrons can make this interference pattern, showing the electron had wave-like properties and behaved just like the light did in Young's experiment.

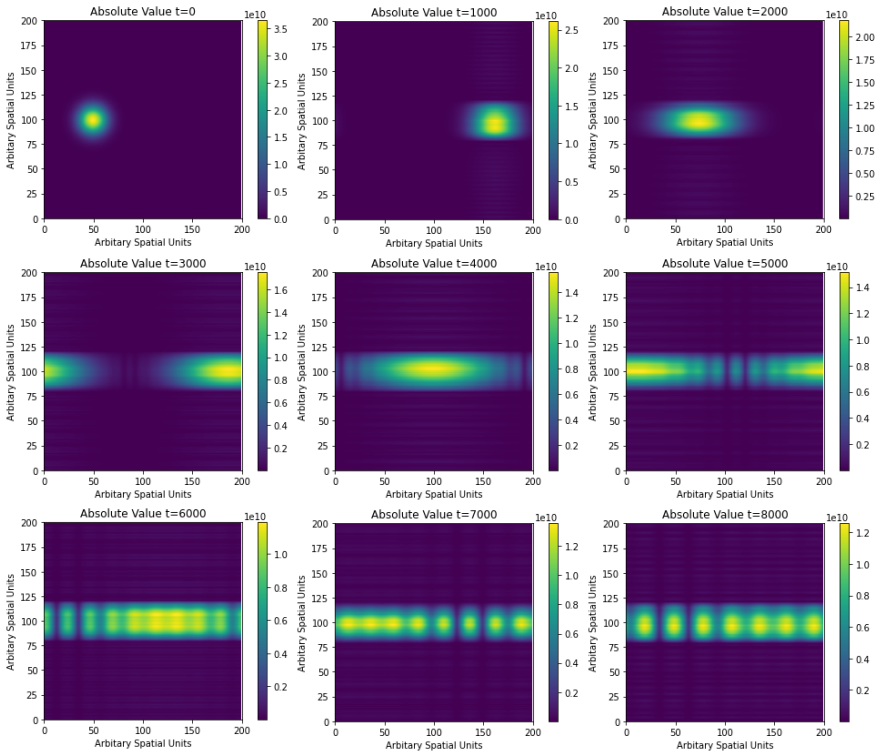

Figure 11: An electron as it continues to accelerate through the barrier tunnel at different points in time from t = 0 to t = 8000. Where V = 10^{100}.

Aside from proving the simulation can reproduce the results found in the original experiments which enabled many early quantum physicists to draw more conclusions about how the fundamental particles of our universe behaved. We also can subject the electron to whatever barrier configuration or potential energy of the barrier we like. The two that I tried out were, a tunnel similar to how synchrotrons would accelerate a charged particle and collimate it and a chessboard like grid or grate to see how the partial reflection or transmission via quantum tunnelling would be affected by distance.

As you can see in figure 11, the electron needs a lot more time before it evenly distributes its probability within the tunnel. The tunnel itself relative to the size of the electron is rather small and probably isn't a good simulation of a synchrotron but the effects that this has on the electron as it passes through time and stretches out as it goes at speed is an interesting result.

According to the Australian Synchrotron (Australian Synchrotron, 2023) the linear accelerator which accelerates the electron beam to an energy of 100 MeV over 10 m causes the beam to be separated into "discrete packets" with a consistent spacing. This is what we see at t = 8000 although of this single electron going through this small tunnel it is more likely that the electron has stretched to a size equal

or larger than the size of the tunnel and is interfering with itself just like the previous diffraction patterns. It still does mean though that the probability of finding this electron has been split up into discrete spots where it is more likely.

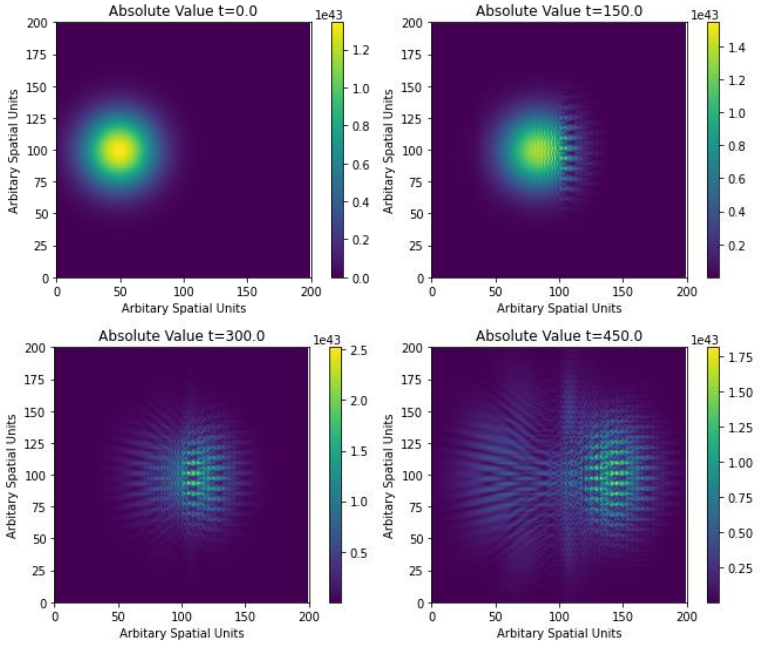

Figure 12: An electron as it interacts with a chessboard potential at different points in time from t = 0 to t = 450. Where V = 2 x 10^{-35}.

The last potential that was tested was a chessboard like pattern which forms a grate for the electron to pass in between. Unlike in figure 6, the potential of the pattern is slightly lower at 2 x 10^{-35}, and you can see the probability of the electron if favoured to tunnel as it appears brighter to the right. If we run the simulation for the barrier with no slit, we show a similar result.

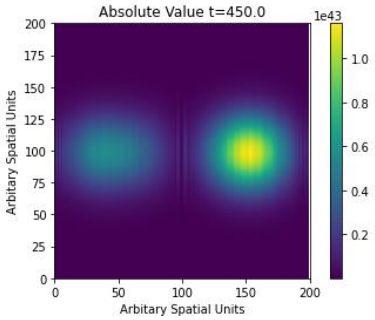

Figure 13: Evolution of an electron at a time of 450 interacting with a solid barrier potential. The simulation's parameters in are found in table 1 although with V set to 2 x 10^{-35} J. The particle exists in a space of arbitrary size and length.

It does seem that the electron penetrates both barriers with a comparable amount of transmission and reflection although in figure 12 the probability of the electron appearing in the pattern is less deep than in figure 13. Where the brightest part of the probability of the location of the electron is around 140 units while the brightest part in the solid potential is at around 160 units. This suggests that due to the wavelike nature of the electron it may slow down when passing through an area of uneven potential energy.

It also seems with so many opportunities for reflection and tunnelling of the wavelike particle there appears to be many diffraction patterns even overlayed on each other causing more intricate patterns.

Unlike previous simulations it is also much harder to determine the shape of the potential barrier just from the likely position of the electron.

Conclusions

Within this report the computational simulation of the time-dependent Schrödinger equation produced a variety of data and results both in reaffirming real world experiments on quantum mechanics and producing new and unique results.

Using this simulation, we were able to compare this to what has experimentally been achieved in the real world by key physicists in the birth of quantum mechanics. We simulated an impenetrable potential energy barrier with one and two slits to replicate Thomas Young's experimental set up and tried to prove the results of Davisson and Germer's experiments with the electron in which the electron is able to diffract through the slit and interfere with itself producing a diffraction pattern.

Aside from proving previous real-world results, the simulation was also used on a solid barrier with a low potential energy to observe quantum tunnelling and a chessboard like grating to observe how the electron handles a porous potential energy barrier. In each of these there is a partial interaction of transmission through the barrier and a reflection where it meets a potential barrier surface. The last potential barrier tested was the impenetrable barrier tunnel where the electron speeds up and collimates within the tunnel analogous to a synchrotron although our simulations have some limitations and differ to how a real synchrotron works.

References

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Appendix (printed code)

The following code is of the double slit potential barrier only. Variations on this code to change the type of potential barrier faced is shown below this code and is replaced between lines 115. and 125.

```
# -*- coding: utf-8 -*-
"""
Created on Thu May 11 13:10:04 2023

@author: Campbell Timms
"""

import numpy as np
import matplotlib.pyplot as plt

# #Define values

N = 200
# # N = Number of pixels/grid size

sigma = 0.05
# #sigma value found in the Gaussian

delta_t = 0.1
# #change in time

k = -1e8
# #quickness in space

m = 9.109537944498001e-31
# #m-mass electron = 0.0005485803 (amu) * 1 amu =       1.660566E-27 kg  kg =
9.109537944498001e-31 kg

hbar = 1.054571817*10**-34
# #constant hbar: 1.054 571 817...x 10-34 J s or 6.582 119 569...  x 10-16 eV s

t_total = 650
# the end time that delta_t will stop at

pltfreq = 100
# #How frequent through the time step delta_t will a time be plotted

potential = 1e-35
# #Potential of the tophat middle, V

# # Bohr radius (m) Griff eq.4.72
a = 0.529e-10

# # Ground state of hydrogen eq.4.80 Griff
# psi100 = 1/(np.sqrt(np.pi*a**3))*np.exp(-r/a)

# defining the coordinates used
```

```
    xyarrays = np.mgrid[:N,:N]
    y = xyarrays[0]
    x = xyarrays[1]
    # z =
    Y = (y - y[N-1,N-1]/2)
    X = (x - x[N-1,N-1]/2)
    # Z =

    r = np.sqrt(X**2+Y**2)

    xyarrays = np.mgrid[:N,:N]

    q_x = xyarrays[0]
    q_y = xyarrays[1]
    #q_z = xyarrays[?]

    q_X = (q_x - q_x[N-1,N-1]/2)
    q_Y = (q_y - q_y[N-1,N-1]/2)
    # q_Z = (q_z - q_z[N-1,N-1]/2)

    shift = N//2
    q_xshift = np.roll( q_X, int(-shift), 0)
    q_yshift = np.roll( q_Y, int(-shift), 1)
    # q_zshift = np.roll( q_Z, int(-shift), ?)

    #Use the q-space arrays to make a complex array that stores the values of the
    free space equation
    qr2 = np.sqrt(q_xshift**2 + q_yshift**2)


    def kenetic (wavefunction, delta_t, N = 200, sigma = 0.05, k = -1e8, m =
    9.109537944498001e-31, hbar = 1.054571817*10**-34):

           Schro_time = np.exp((1j*hbar*delta_t/(2*m))*qr2**2)

           #Take the Fourier transform of the wavefunction at t=0.
           F_wavefunction = np.fft.fft2(wavefunction)

           # Multiply the Fourier transform of the wave function by the phase factor
           F_wavefunctiont = F_wavefunction*Schro_time

           # Take the inverse Fourier transform.
           wavefunctiont = np.fft.ifft2(F_wavefunctiont)

           return wavefunctiont

    # Wavefunction after time delta_t
    wavefuntion_out = kenetic(np.exp(-r**2/(2*sigma**2)), delta_t)

    # Input value of the tophat potential

    barrier_thickness_percentage = 0.05
    width = int(N*barrier_thickness_percentage)
    middle = N//2
```

```
95
96      tophat = np.zeros([N,N])
97      tophat[:,middle - width//2:middle + width//2 + 1] = potential
98
99      def potentialmultiplication(wf, V, delta_t, hbar = 1.054571817*10**-34):
100
101             potentialt = np.exp(((-1j*delta_t)/hbar)*V)
102
103             return wf*potentialt
104
105     wf = np.exp(-r**2/(2*sigma**2))
106     V = tophat
107
108     # Initialize the wave-function
109     N_constant = 1/np.sqrt(np.sum((wavefuntion_out)**2))
110     x0 = N//4
111     x_move = X+x0
112     int_wf = N_constant*np.exp((-(x_move**2+Y**2)/2*sigma**2)+1j*k*X)
113
114
115     #Create double slit in barrier
116     slit_1_start = N//2-2*width
117     slit_1_end = N//2-width
118
119     slit_2_start = (N//2)+width
120     slit_2_end = (N//2)+2*width
121
122     barrier_thickness_percentage = 0.05
123     width = int(N*barrier_thickness_percentage)
124     tophat[slit_1_start:slit_1_end,:] = 0
125     tophat[slit_2_start:slit_2_end,:] = 0
126
127     #image of the potential
128     plt.imshow(tophat)
129     plt.title('Double slit')
130     plt.xlim(0,N)
131     plt.xlabel('Arbitary Spatial Units')
132     plt.ylim(0,N)
133     plt.ylabel('Arbitary Spatial Units')
134     plt.colorbar()
135     plt.show()
136
137     n = int(t_total/delta_t)
138
139     for i in range(n):
140
141             wf_p = potentialmultiplication(int_wf, V, delta_t)
142             wf_t = kenetic(wf_p,delta_t)
143             int_wf = wf_t
144
145             if i%pltfreq == 0:
146                     plt.imshow(abs(wf_t))
147                     plt.title('Absolute Value' + ' ' + 't=' + str(delta_t*i))
148                     plt.xlim(0,N)
```

```
                    plt.xlabel('Arbitary Spatial Units')
                    plt.ylim(0,N)
                    plt.ylabel('Arbitary Spatial Units')
                    plt.colorbar()
                    plt.show()
```

```
#Single Slit
barrier_thickness_percentage = 0.05
width = int(N*barrier_thickness_percentage)
tophat[middle - width//2:middle + width//2 + 1,:] = 0

#Tunnel
barrier_thickness_percentage = 0.2
width = int(N*barrier_thickness_percentage)
tophat[middle - width//2:middle + width//2 + 1,:] = 0


#Chessboard
board = np.zeros((N, N))
square_size = 4
for i in range(N):
    for j in range(N):
        if (i // square_size + j // square_size) % 2 == 0:
            board[i, j] = potential
            board[:,0:N//2] = 0
```