

Wavefunction of an electron in an arbitrary Potential

Phys 338: Individual Project Report

Khaled Hasan 1210265

Course: Computational Physics

July 3, 2024

Contents

1	Abstract	2
2	Theory	2
3	Computational methods	3
4	Test cases	3
4.1	Infinite Square well:	4
4.2	Harmonic Oscillator	4
5	Results	5
5.1	Dispersion:	5
5.2	Gaussian in an infinite well	6
5.3	Tunneling	6
5.4	Double slit experiment	8
6	Conclusion	9
6.1	Boundaries	9
7	References	9
8	Appendicies	9
8.1	The Code	9

1 Abstract

The wave function is a complex function that describes the probability density of the existence of an electron in certain position in space (that is upon taking the norm squared of it), this suggests a dual behaviour of an electron, and that it acts as a wave. The dual behaviour of electrons that was proposed by de Broglie, using the Schrodinger equation which describes the wave function of an electron in a potential energy given by the potential operator $V(x, y, z)$. As the potential changes, the solution of the wave function changes, and due to the complexity of the partial differential equations, wave functions tends to get more and more complicated, even for simple potentials such as the harmonic oscillator. The solution is hard to treat analytically, and can only be solved using special functions ("Hermite Polynomials").

This Problem of having complicated solutions that are easily effected by the small changes in potential, encourages the use of computational methods, in order to solve for the wave function of the electron.

In this project, the Schrodinger equation was solved in one and two dimensions, for arbitrary potential.

2 Theory

The Schrodinger Equation

$$i\hbar \frac{\partial_x |\psi(x, y, z, t)\rangle}{\partial t} = \hat{H} |\psi(x, y, z, t)\rangle \quad (1)$$

Where H is the hameltonian defined as:

$$\hat{H} = \frac{-\hbar^2}{2m} \nabla^2 + V(x, y, z) \quad (2)$$

from here on, the position parameters are dropped.

The Taylor expansion of $|\psi(t)\rangle$

$$|\psi(t)\rangle = |\psi(0)\rangle + t \frac{\partial |\psi(t)\rangle}{\partial t} |_{t=0} + \frac{t^2}{2!} \frac{\partial^2 |\psi(t)\rangle}{\partial t^2} |_{t=0} + \dots \quad (3)$$

substituting from equation 2:

$$|\psi(t)\rangle = |\psi(0)\rangle + t \frac{-i\hat{H}}{\hbar} |\psi(0)\rangle + \frac{t^2}{2!} \left(\frac{-i\hat{H}}{\hbar} \right)^2 |\psi(0)\rangle + \dots \quad (4)$$

This can then be reduced to:

$$|\psi(t)\rangle = e^{-i\frac{\hat{H}}{\hbar}t} |\psi(0)\rangle \quad (5)$$

$$e^{-i/\hbar \hat{H}} = \sum_{n=0}^{\infty} \frac{-i/\hbar \hat{H}^n}{n!} \quad (6)$$

by diagonalizing \hat{H} :

$$\hat{H} = \hat{A}\hat{D}\hat{A}^{-1} \quad (7)$$

where \hat{D} is a diagonal matrix, whose elements are the eigenvalues of $-i/\hbar\hat{H}$, and A is a matrix whose columns are the eigenvectors, since the eigenvectors are orthonormal, $\hat{A}^{-1} = \hat{A}^\dagger$.

Then it follows that:

$$\hat{H}^n = \hat{A}\hat{D}^n\hat{A}^\dagger \quad (8)$$

and thus:

$$\begin{aligned}
 e^{-i/\hbar\hat{H}} &= \sum_{n=0}^{\infty} \frac{(-it/\hbar)^n}{n!} \hat{A}\hat{D}^n\hat{A}^\dagger \\
 &= \hat{A} \left(\sum_{n=0}^{\infty} \frac{(-it/\hbar)^n}{n!} \hat{D}^n \right) \hat{A}^\dagger \\
 &= \hat{A} \left(e^{-it/\hbar\hat{D}} \right) \hat{A}^\dagger
 \end{aligned} \quad (9)$$

But since the matrix \hat{D} is diagonal, $(e^{-it/\hbar\hat{D}})$ is the same as a diagonal matrix whose n^{th} diagonal element is $e^{-iE_n t/\hbar}$, where E_n is the n^{th} eigenvalue of \hat{H} .

3 Computational methods

The main task for the computational part was to find the eigenvectors and eigenvalues of \hat{H} in order to find both \hat{A} and \hat{D} , and the used functions were:

- For the case of 1D, the Python function in Scipy module `scipy.linalg.eightridiagonal` was used to calculate the eigenvalues and eigenvectors of \hat{H} .
- For the case of 2D, the Python function in Scipy module `scipy.Sparse.linalg.eigs` was used to calculate the eigenvalues and eigenvectors of \hat{H} .

other required matrices multiplicaions were done using numpy library.

4 Test cases

To test the solution, the eigenvalues were compared to the ones calculated analytically in the cases of infinite square well and the harmonic oscillator:

4.1 Infinite Square well:

values of $\frac{2ma^2 E_n}{\pi^2 \hbar^2}$:

n	theoretical	Computational
1	1	0.99800279
2	4	3.99200871
3	9	8.98201038
4	16	15.9679955
5	25	24.9499469
6	36	35.9278424
7	49	48.9016551

4.2 Harmonic Oscillator

values of $\frac{E_n}{\omega \hbar}$:

n	theoretical	Computational
0	0.5	0.49999745
1	1.5	1.49998727
2	2.5	2.49996691
3	3.5	3.49993636
4	4.5	4.49989564
5	5.5	5.49984473
6	6.5	6.49978364
7	7.5	7.49971236

5 Results

Most of the results were on forms of animations, depicting the time evolution of a wave function. However here are some of the figures that showed some of the results:

5.1 Dispersion:

Any wave packet is a combination of many different waves, each with specific wavelength, in the case of electron wave function, the speed (Phase velocity) of each of the waves differ with the wavelength, which results in a spread of the wave-packet in question, this is depicted in the following 2 figures:

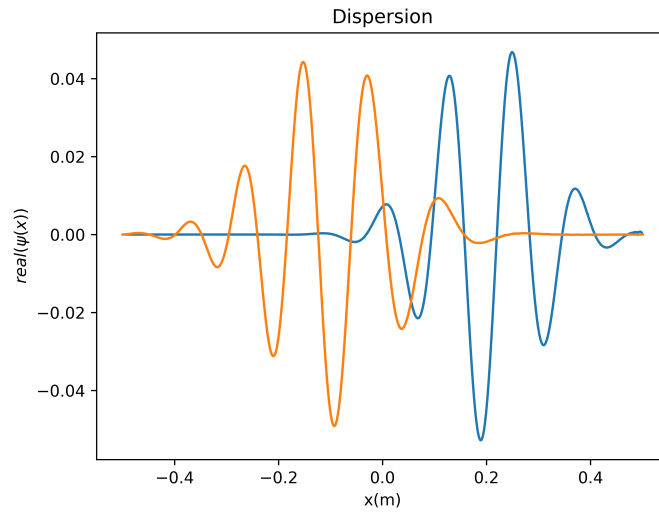


Figure 1: the real part of a wavefunction of an electron moving in as it disperse, $k = 200$, $dt = 2.5 \times 10^{-2}$

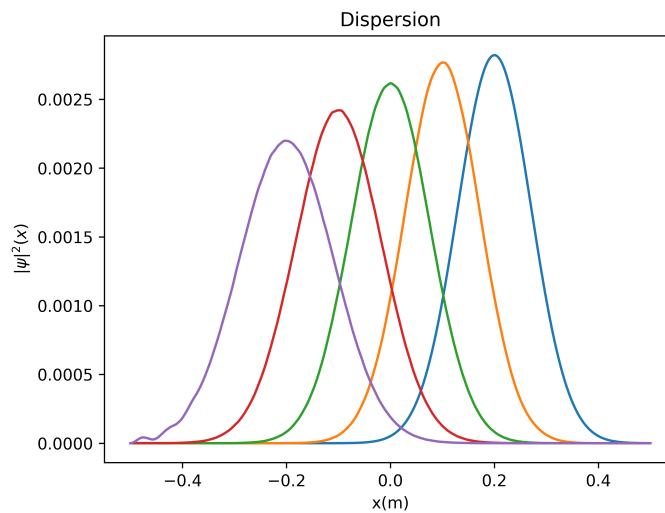


Figure 2: the probability density of an electron moving in as it disperse, $k = 200$, $dt = 5 \times 10^{-3}s$

5.2 Gaussian in an infinite well

The following figure shows the time evolution of a gaussian initial condition:

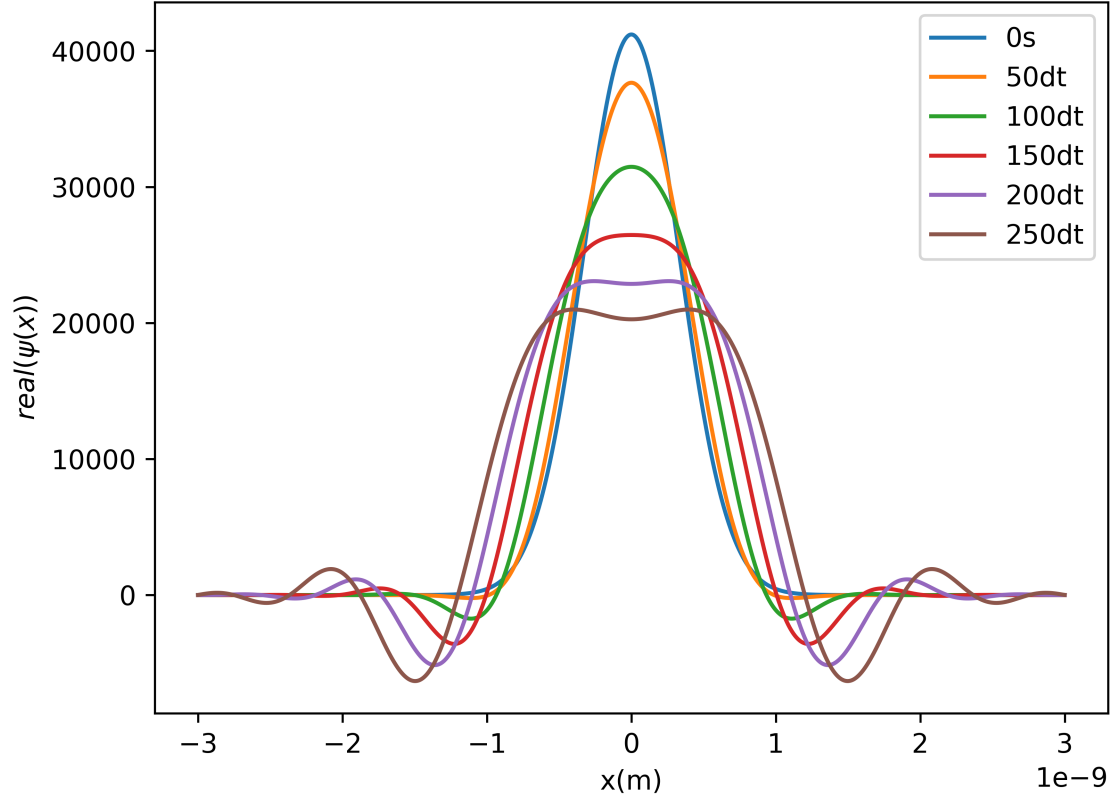


Figure 3: Particle in an infinite square potential well, $dt = 1 \times 10^{-17}$, $\sigma = \sqrt{\hbar/m_e}$.

5.3 Tunneling

Tunneling is an interesting quantum phenomena, assuming a potential barrier (which can be thought of as a wall), if the energy of such a barrier is bigger than the energy of the electron arriving at it, from a classical point of view, the electron should never be able to pass such a barrier, however, from a quantum perspective, the electron has a probability of passing through (i.e some of the wave function passes through).

The probability of finding the electron after the barrier is represented by T .

E/V_0	$100T$
0.252	1.51
0.977	1.59
1.00	21.4
1.05	35.4
1.11	51.1
1.21	65.0
1.29	74.2
1.43	80.5
1.48	81.3
1.54	82.4
1.60	83.9
1.67	85.6
1.74	87.6
1.82	90.0
1.91	91.7
2.00	93.5

Table 1: The percentage of electron passing through a potential barrier

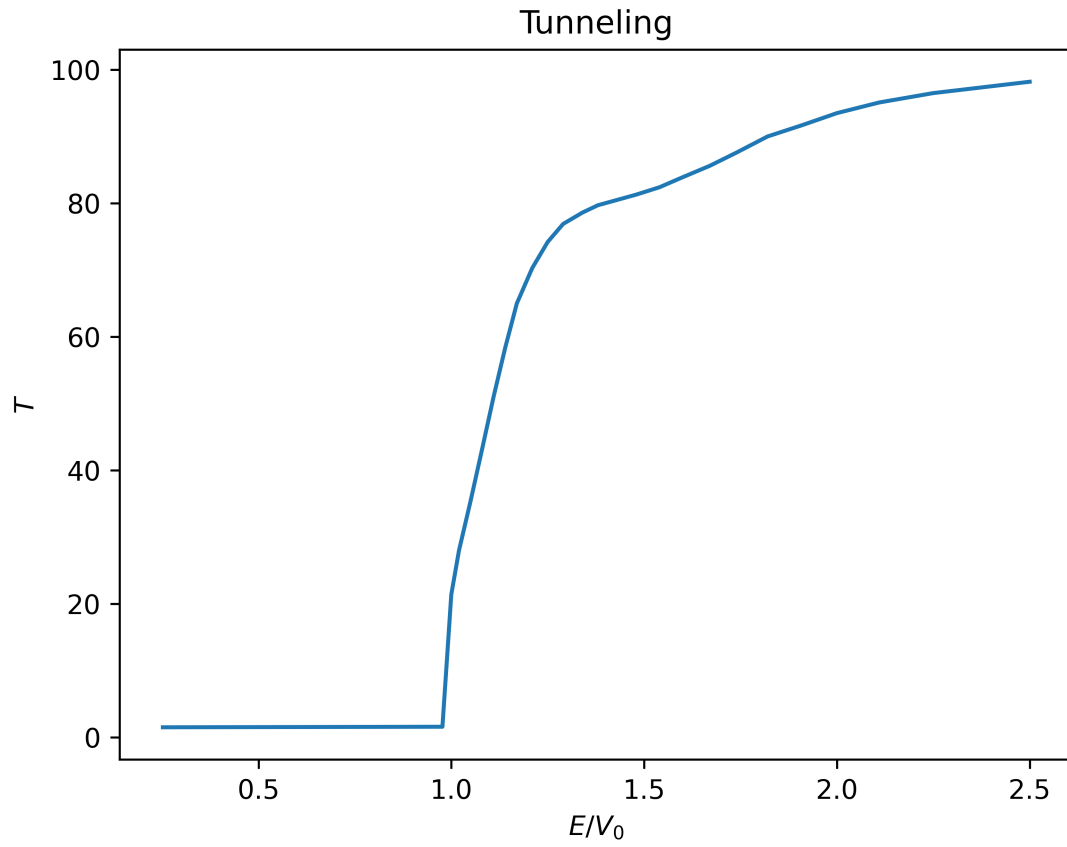


Figure 4: Data in Table 1

5.4 Double slit experiment

Perhaps the most popular quantum mechanics experiments that depicts the wave behaviour of the electron is the double slit experiment. Even if one electron was shot towards a double slit, the electron will be diffracted, and will result in an interference pattern. In this project, the code for solving the schrodinger equation in 2 dimensions was used to simulate the double slit experiment. Below are 2 figures depicting the resulting solution:

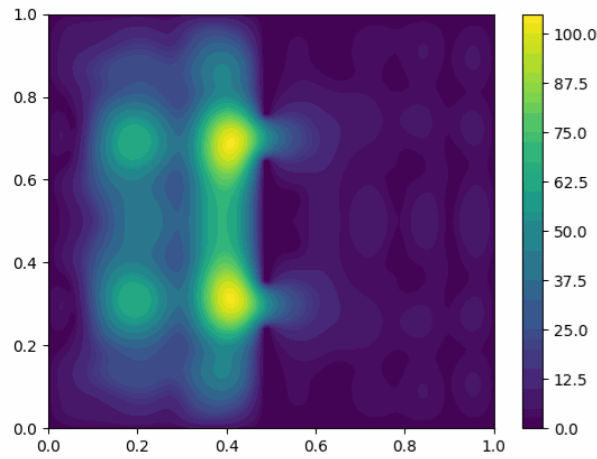


Figure 5: Double slit Experiment: one electron passing through double slit (the colour represents a value proportional to the absolute value of the wave function)

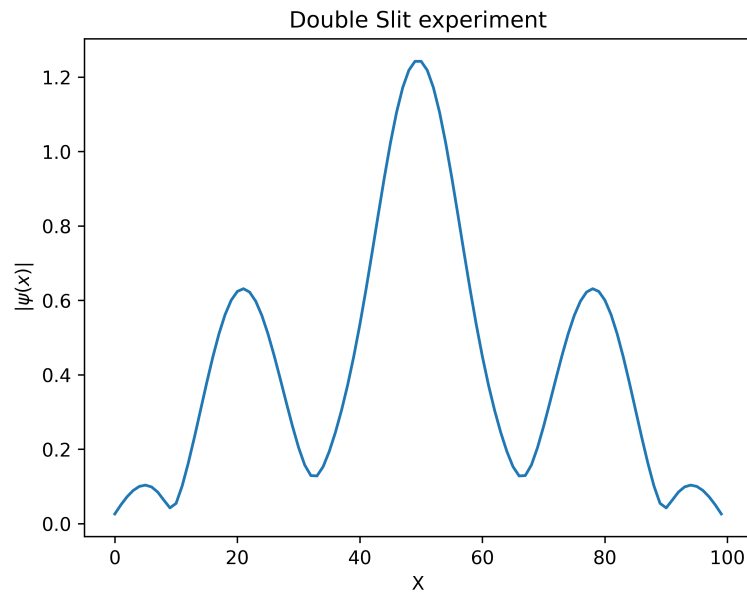


Figure 6: Double slit Experiment: the resulting interference pattern

6 Conclusion

Solving the Schrodinger equaiton using computational methods enables us to solve for the wave function of electron (or any quantum particle), in arbitrary potentials, and provides higher flexibility in solving it for various initial conditions, it also enable us to conduct many experiments, with lower costs than real life ones (such as the Double slit experiment).

6.1 Boundaries

All cases that were present in this project assumed the boundaries of an infinite square well, as the dimensions of such square gets bigger and bigger, electrons will behave more like an unbounded electron, or bounded by the defined potential, therefore, the

7 References

- MIT Opencourseware Physics 8.04 lectures by Prof. Allan Adams:https://www.youtube.com/watch?v=SsCeVABM4Mo&list=PLU14u3cNGP61-9PEhRognw5vrYrSEVLPr&index=13&t=2593s&ab_channel=MITOpenCourseWare
- Wave Packets:<https://scholar.harvard.edu/files/schwartz/files/lecture11-wavepackets.pdf>
- Quantum Tunneling: https://en.wikipedia.org/wiki/Quantum_tunnelling

8 Appendicies

8.1 The Code