Draft version February 10, 2024
Typeset using LaTeX **RNAAS** style in AASTeX631

Calculating the Schrödinger Equation

Shannon Scofield[1] And Colin Madden[2]

[1] *Math Department, College of Natural Sciences, University of Texas at Austin, Austin, TX, 78712*
[2] *Aerospace Engineering Department, Cockrell School of Engineering, University of Texas at Austin, Austin, TX, 78712*

ABSTRACT

The Schrödinger equation was one of the most brilliant scientific breakthroughs in the 20th century. The equation is fundamental in the establishment of quantum mechanics, the rules that describe how very small particles move and interact, contrary to classical mechanics. Schrödinger published his findings 1926 and won the Nobel Prize in Physics in 1933. The Schrödinger equation is a linear partial differential equation that describes the wave function of a quantum mechanical system. The 'particle in a box' problem is a simple one-dimensional problem where Schrödinger's equation can be solved and used to describe the motion of the electron within the box. Two separate numerical methods for solving partial differential equations are presented and used in this paper to solve Schrödinger's equation to visualize the electron's movement in time and space.

INTRODUCTION

In quantum mechanics there are different methods to study quantum mechanical systems and make predictions. The Schrödinger equation is one of these ways, it predicts the form of wave functions which describe the movement of small particles and also describes how these functions are altered by external influences. Brittanica (2021) It is integral to Dirac's combination of matrix mechanics and the Schrödinger equation and is entangled with the path integral formulation. It has been used to compute the Hydrogen spectral series by computing the equation generated by an electron moving in a potential well created by a proton. Schrödinger (2001) Quantum mechanics is a unique field in that the different philosophical interpretations of quantum mechanics change how you interpret the results of the Schrödinger equation. The equation of a system can be viewed in the Copenhagen interpretation as statistical information about the system in that knowing the wave equation for a moment means that you can calculate the wave equation for all future times, with the after-measurement equation predicted using the Born Rule.I Omnès (1994) However Schrödinger's interpretation more closely aligned with the early version of Everett's many-worlds interpretation which holds that all possible post-measurements equations occur simultaneously in a multi-verse composed of mostly independent parallel universes. Bitbol (1996) Barrett (2018)

METHODOLOGY

The Schrödinger equation is a linear partial differential equation that governs the wave function of a quantum-mechanical system. The equation is show below:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = i\hbar\frac{\partial\Psi}{\partial t} \tag{1}$$

where $\hbar$ is the reduced Planck's constant, 1.054571817 x 10^{-34} $J \cdot s$, m is the mass of the body, and i is the imaginary unit.

In this paper, the Schrödinger equation is going to be solved to find the wave function of an electron with mass m = 9.109e-31 kg in a box of length 1.0e-8 m. There will be two methods presented to solve this partial differential equation, the Crank-Nicholson method and the spectral method utilizing the fast Fourier transform.

The spectral method employs the fast Fourier transform to transform Ψ as a function of space x and time t ($\Psi(x,t)$) to a function of spatial frequency, denoted by kappa, and time ($\hat{\Psi}(k,t)$). This results in the spatial derivatives Ψ_x and Ψ_{xx} becoming transformed as well where

$$\Psi_x = ik\hat{\Psi}$$

$$\Psi_{xx} = i^2k^2\hat{\Psi} = -k^2\hat{\Psi}$$

Note: derivatives are referenced by the subscript showing the variable of differentiation

Prior to the Fourier transform, the initial condition of the wave function at time 0, $\Psi(x,0)$, is expressed as:

$$\Psi(x,0) = e^{-\frac{(x-x_0)^2}{2\sigma^2}} * e^{ikx}$$

where $x_0 = \frac{L}{2}$, $\sigma = 10^{-10}$ m, and k=$5 * 10^{10}m^{-1}$. The Fourier transform of this vector initial conditions is then taken. When applying the fast Fourier transform, $\hat{\Psi}$ becomes a vector of Fourier coefficients and k becomes a vector of frequencies. The time derivative in Eq. 1 can also be expressed in terms of $\hat{\Psi}$ with the fast Fourier transform so that it becomes:

$$\hat{\Psi}_t = \frac{-\hbar^2}{2m} * k^2 * \hat{\Psi}$$

This results in n number of decoupled ordinary differential equations which can be numerically integrated, where n is the size of our domain. The derivatives are simulated in the Fourier frequency domain using SciPy's odeint function. To achieve values for Ψ, an inverse Fourier transform is employed to bring the values back from the frequency domain to the spatial domain. NumPy's fft and ifft function are utilized for the Fourier transforms. The values for Ψ are then plotted.

The Crank-Nicholson method is a finite difference method used to approximate the solution to a partial differential equation. The method uses the values surrounding a particular point to approximate the next step in time. Thus, the time derivative, $\frac{\partial\psi}{\partial t}$ can be approximated like so:

$$\frac{\partial\psi}{\partial t} = \frac{\psi(x,t+\Delta t) - \psi(x,t)}{\Delta t}$$

The spatial derivative for the Crank-Nicholson method uses the average of the forward difference and backwards difference schemes to result in a spatial second derivative:

$$\frac{\partial^2\psi}{\partial x^2} = \frac{[\psi(x+\Delta x,t) - 2\psi(x,t) + \psi(x-\Delta x,t)]}{\Delta x^2} + \frac{[\psi(x+\Delta x,t+\Delta t) - 2\psi(x,t+\Delta t) + \psi(x-\Delta x,t+\Delta t)]}{2\Delta x^2}$$

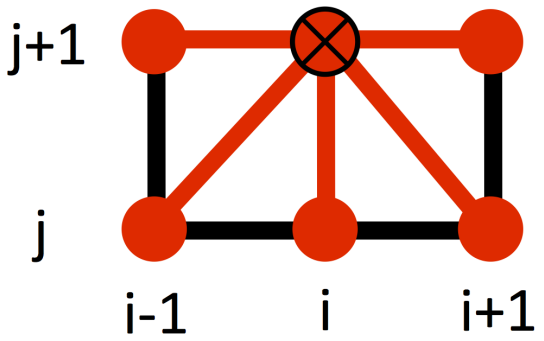

Figure 1. Stencil showing Crank-Nicholson finite difference method

The stencil for this method in shown in Figure 1. In the figure, our time step Δt is denoted with j and the spatial step Δx is denoted with i. The stencil shows how the values from surrounding points are used to approximate the value at position (t_{j+1}, x_i).

The wave function, Ψ, at time t+Δt can then be expressed as:

$$\psi(x,t+\Delta t)-\psi(x,t) = \frac{\Delta t}{4m\Delta x^2} i\hbar[\psi(x+\Delta x,t)-2\psi(x,t)+\psi(x-\Delta x,t)+\psi(x+\Delta x,t+\Delta t)-2\psi(x,t+\Delta t)+\psi(x-\Delta x,t+\Delta t)] \tag{2}$$

where is the mass of the electron, m = 9.109e-31 kg.

Using this, we can rewrite as a linear system $A\Psi(t+\Delta t) = B\Psi(t)$. A and B are square matrices of size N-1. The matrices have values only on three of their diagonals.

$$A = \begin{bmatrix} a1 & a2 & 0 & 0 & ... & 0 \\ a2 & a1 & a2 & 0 & ... & 0 \\ 0 & a2 & a1 & a2 & 0 & 0 \\ 0 & 0 & a2 & a1 & a2 & 0 \\ 0 & 0 & 0 & a2 & a1 & a2 \\ 0 & 0 & 0 & 0 & a2 & a1 \end{bmatrix}$$

$$B = \begin{bmatrix} b1 & b2 & 0 & 0 & ... & 0 \\ b2 & b1 & b2 & 0 & ... & 0 \\ 0 & b2 & b1 & b2 & 0 & 0 \\ 0 & 0 & b2 & b1 & b2 & 0 \\ 0 & 0 & 0 & b2 & b1 & b2 \\ 0 & 0 & 0 & 0 & b2 & b1 \end{bmatrix}$$

The values a1, a2, b1, and b2 are:

$a_1 = 1 + \Delta t \frac{i\hbar}{2m\Delta x^2}$

$a_2 = -\Delta t \frac{i\hbar}{4m\Delta x^2}$

$b_1 = 1 - \Delta t \frac{i\hbar}{2m\Delta x^2}$

$b_2 = \Delta t \frac{i\hbar}{4m\Delta x^2}$.

Now, a method for solving a linear system will yield the values of $\Psi(t)$. The solver used was NumPy's linalgsolve function.

DATA

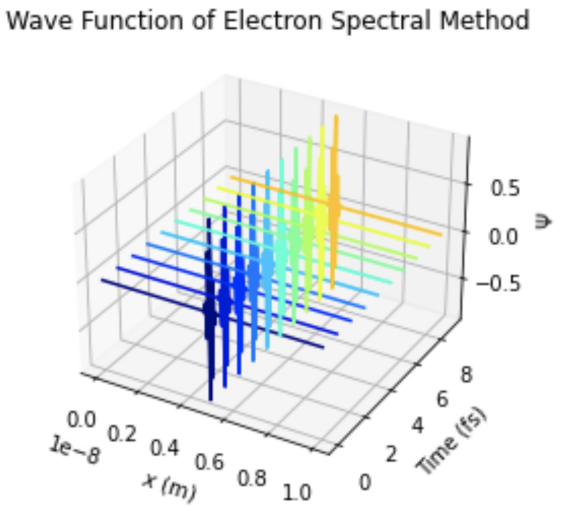

Figure 2. Wave Function of electron evaluated using spectral method with FFT

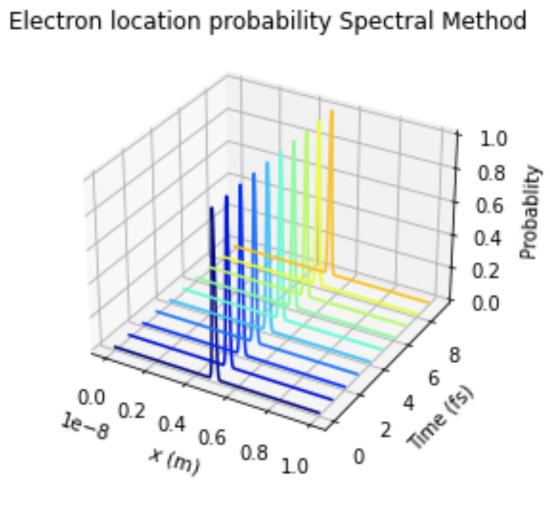

Figure 3. Probability of electron location evaluated using spectral method with FFT

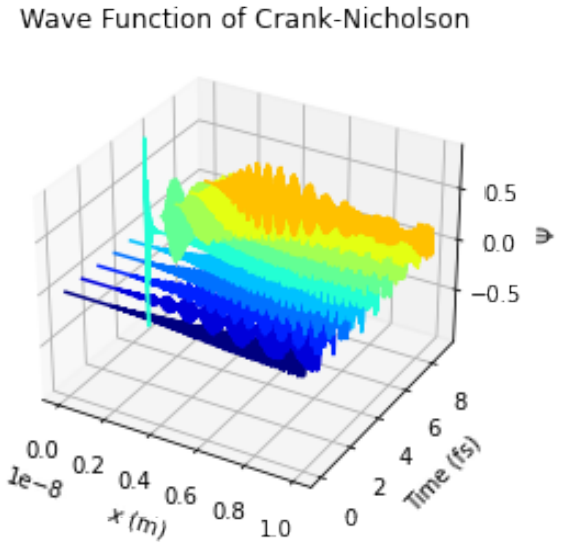

Figure 4. Wave Function of electron evaluated using Crank-Nicholson method

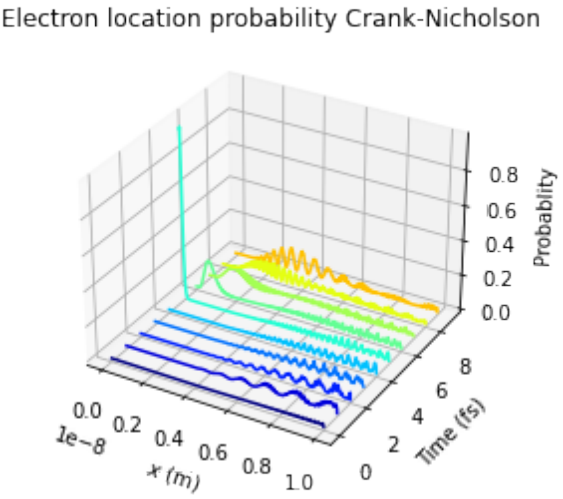

Figure 5. Probability of electron location evaluated using Crank-Nicholson method

RESULTS

The two different methods for solving this particular partial differential equation show two different scenarios. This suggests an error in one or both of the methods. The spectral method shows values of Ψ very near zero, with magnitudes of the order 10^{-200} or greater. Near L/2, the values get larger reaching a peak of $\pm$ 0.5. The results also show little variance with time. This can be explained by the very small time scale used; the time domain is in femtoseconds. The probability of finding the electron at any particular point is also plotted using $\Psi\Psi^*$, where Ψ^* is the complex conjugate of the complex-valued Ψ. The probability of finding the electron near the edges of the box is very low, but the probability increases towards the middle. This makes sense due to the fact if the electron is constantly

moving around, which is true given that it can not have zero energy, there will be more instances where the particle is moving through the middle as it chaotically moves around. The time for the spectral method to complete calculations was 0.08623623847961426 seconds. Meanwhile, the time it took the Crank-Nicholson to complete calculations was 127.68237113952637 seconds. The results for the Crank-Nicholson method differ from that of the spectral method in two separate ways. First, there is more variance in Ψ. The wave function of the electron changes in both space and time and shows oscillations. Secondly, the probability distribution is more widespread, showing more equal probabilities across the length of the box versus high probability in the center at L/2. The variance of the Crank-Nicholson method lends more credit to the veracity of its solution, which would reflect the electron's rapid, chaotic motion inside the box.

SUMMARY / CONCLUSION

The goal of this experiment was to solve the Schrödinger equation for the 'particle in a box' problem. Numerical methods were employed to solve the partial differential equation governing the electron's motion. The spectral method for solving PDE's was the most efficient out of the two methods tested, completing calculations in less than .1 seconds, while the Crank-Nicholson method took over 2 minutes. The two methods take different approaches to solving the differential equation. The spectral method relies on a fast Fourier transform, which allows it to quickly converge to a solution, while the Crank-Nicholson method relies on extensive linear algebra. The Crank-Nicholson results appears to have better accuracy due to the oscillations and time and space variance seen in Figure 4. Further work that could be done is solving the Schrödinger equation for a particle in a 2D box, where the electron is free to move in two directions as opposed to one. Even further, the electron can be placed in a 3D box where it is free to move in three directions.

REFERENCES

Barrett, J. 2018, Stanford Encyclopedia of Philosophy. https://plato.stanford.edu/entries/qm-everett/

Bitbol, M. 1996, Schrödinger's Philosophy of Quantum Mechanics (Springer Netherlands). http://public.ebookcentral.proquest.com/choice/publicfullrecord.aspx?p=3102458

Brittanica, T. E. o. E. 2021, Encyclopedia Britannica. https://www.britannica.com/science/Schrodinger-equation

Omnès, R. 1994, The interpretation of quantum mechanics, Princeton series in physics (Princeton University Press)

Schrödinger, E. 2001, Collected papers on wave mechanics: together with his Four lectures on wave mechanics, third (augmented) edition, new york 1982 edn. (AMS Chelsea Publishing, American Mathematical Society)