Problem Set 9

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Abstract

In this problem set, we apply the Crank-Nicolson method to solve the Schrodinger equation for a particle trapped in an infinite square well potential as well as plot the time development of the wavefunction for this system.

1 Introduction

Partial differential equations can be classified based on the conditions given in the problem, giving rise to boundary value and initial value problems. These two groups are not mutually exclusive, as shown by the Schrodinger equation for an infinite square well potential, a potential whose value is 0 for $0 < x < L$ and infinity for the remaining region. The Schrodinger equation within the range $0 < x < L$ is given by the following:

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

Because of the infinite potential outside of the well, the wavefunction must be 0 on the boundaries. On physical grounds the boundary conditions for this problem are the following:

$$\Psi(0) = 0 \qquad \Psi(L) = 0$$

At the same time, however, we need the initial condition of the wavefunction in order to determine how it changes with time. This occurs because any solution to the infinite square well potential can be written as follows:

$$\Psi(x,t) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} c_n \sin\big(\frac{n\pi x}{L}\big) e^{-i\frac{n^2\pi^2\hbar}{2mL^2}t}$$

Knowing the initial conditions will allow us to use orthonormality to determine the coefficients c_n. For this problem set, the initial wavefunction is the following Gaussian distribution with an initial nonzero momentum, as seen by the position dependent phase:

$$\Psi(x,0) = \exp\big[-\frac{(x-x_0)^2}{2\sigma^2}\big] e^{i\kappa x}$$

where $x_0 = \frac{L}{2}$, $\sigma = 1 \times 10^{-10}$ meters, $L = 10^{-8}$ meters, and $\kappa = 5 \times 10^{10}$ inverse meters. For the present problem set, the massive particle is an electron and since the standard deviation of the Gaussian is 1 Angstrom, we see that the exercise seeks to model an electron in an atom by ignoring electrostatic attraction.

We present our methods as well as our outputs.

2 Methods

When the Crank-Nicolson method is applied to the aforementioned Schrodinger equation, the average of the following two finite difference equations is taken. We note that h is represents the timestep, which we chose to be 10^{-18} seconds.

$$\Psi(x, t+h) = \Psi(x, t) + h\frac{i\hbar}{2ma^2}\Big[\Psi(x+a, t) + \Psi(x-a, t) - 2\Psi(x, t)\Big]$$

$$\Psi(x, t+h) - h\frac{i\hbar}{2ma^2}\Big[\Psi(x+a, t+h) + \Psi(x-a, t+h) - 2\Psi(x, t+h)\Big] = \Psi(x, t)$$

The average of these two equations can be represented by the matrix equation $A\Psi(x+t) = B\Psi(t)$, where A and B are defined as follows. We note that Ψ is a vector of wavefunction values on a spatial grid.

$$A = \begin{pmatrix} a_1 & a_2 & 0 & 0 & 0 & 0 & 0... \\ a_2 & a_1 & a_2 & 0 & 0 & 0 & 0... \\ 0 & a_2 & a_1 & a_2 & 0 & 0 & 0... \\ 0 & 0 & a_2 & a_1 & a_2 & 0 & 0... \\ ... & ... & ... & ... & ... & ... & ... \end{pmatrix} \tag{1}$$

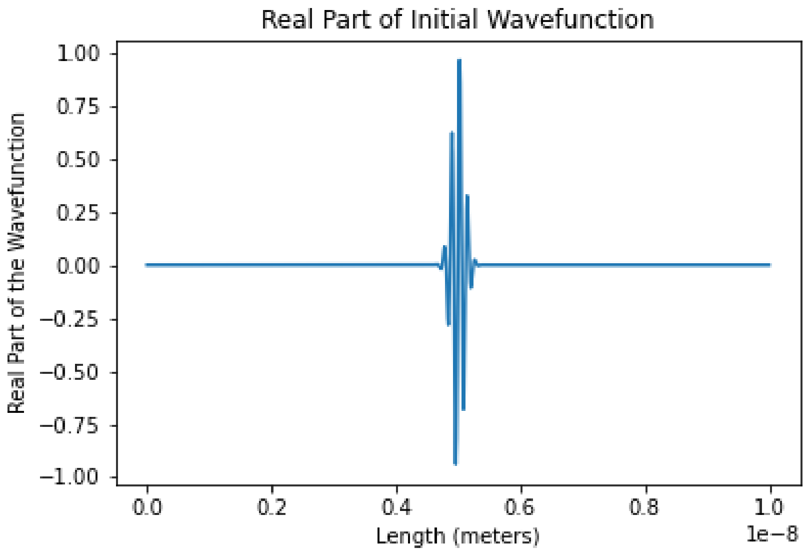
$$B = \begin{pmatrix} b_1 & b_2 & 0 & 0 & 0 & 0 & 0... \\ b_2 & b_1 & b_2 & 0 & 0 & 0 & 0... \\ 0 & b_2 & b_1 & b_2 & 0 & 0 & 0... \\ 0 & 0 & b_2 & b_1 & b_2 & 0 & 0... \\ ... & ... & ... & ... & ... & ... & ... \end{pmatrix} \tag{2}$$

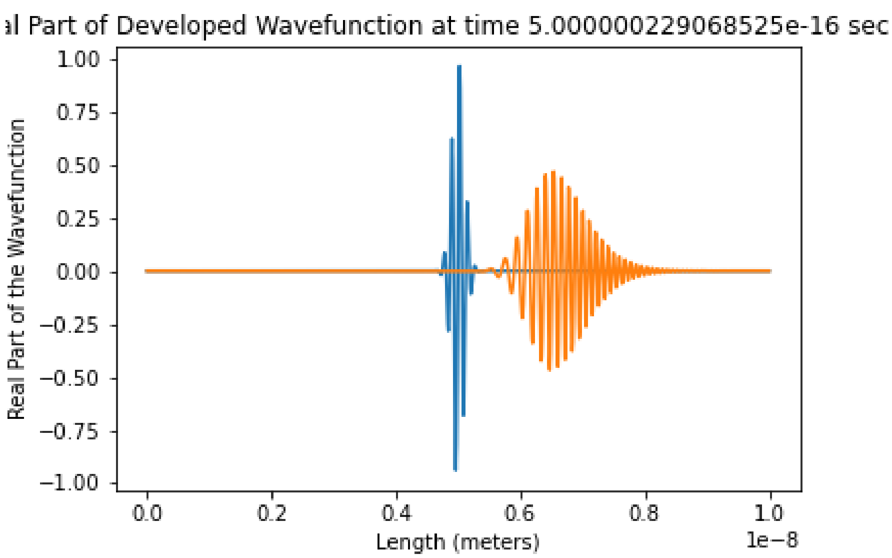
Here $a_1 = 1 + h\frac{i\hbar}{2ma^2}$, $a_2 = -h\frac{i\hbar}{4ma^2}$, $b_1 = 1 - h\frac{i\hbar}{2ma^2}$, and $a_2 = h\frac{i\hbar}{4ma^2}$.

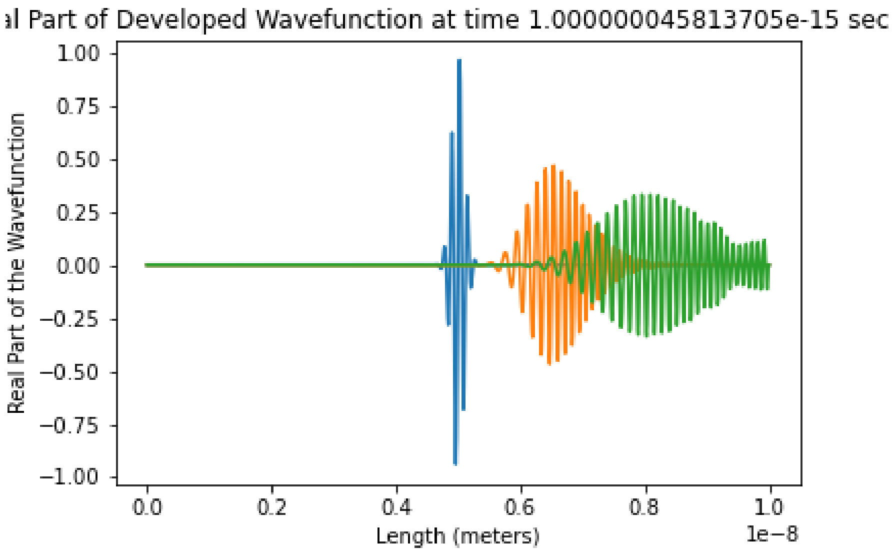
We first perform one step of the Crank-Nicolson method by determining the vector $B\Psi$. We then solve the matrix vector equation $Ax = B\Psi$ for the vector x, yielding the wavefunction values at the next increment. We repeat this procedure for 5000 iterations and plot the real part of the wavefunction at every 500-th iteration.

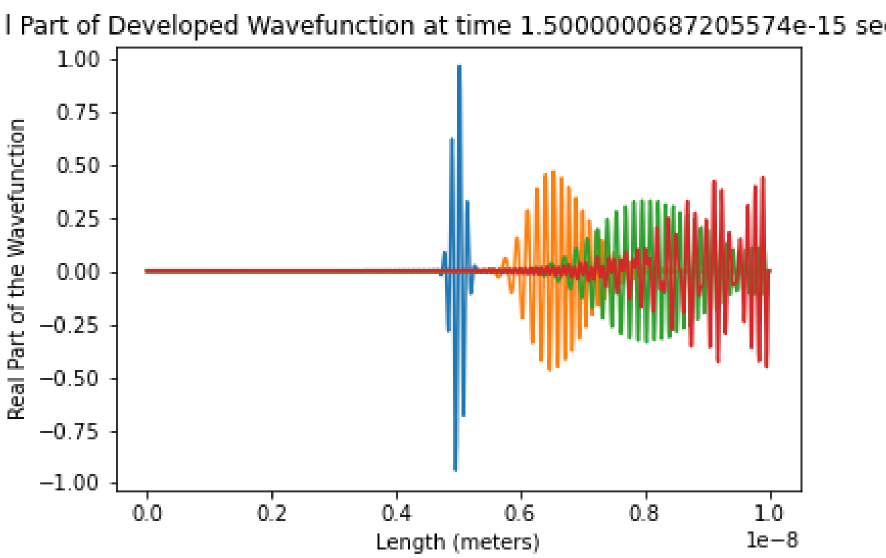
3 Results

Here are the plots of the real part of the wavefunctions for various times. Each plot contains the wavefunctions of the previous plots.


Real Part of Initial Wavefunction
Real Part of the Wavefunction
Length (meters)
1e−8
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0.0
0.2
0.4
0.6
0.8
1.0


al Part of Developed Wavefunction at time 5.000000229068525e-16 sec
Real Part of the Wavefunction
Length (meters)
1e−8
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0.0
0.2
0.4
0.6
0.8
1.0


al Part of Developed Wavefunction at time 1.000000045813705e-15 sec
Real Part of the Wavefunction
Length (meters)
1e−8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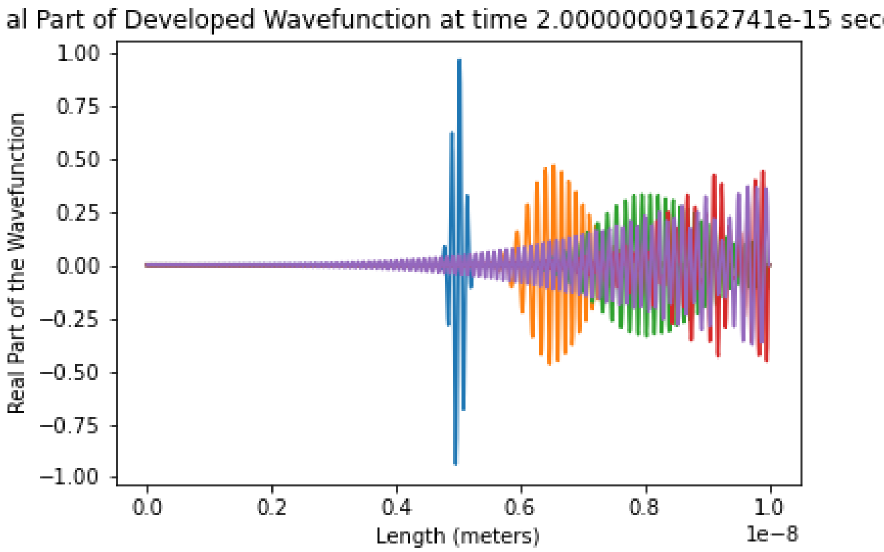
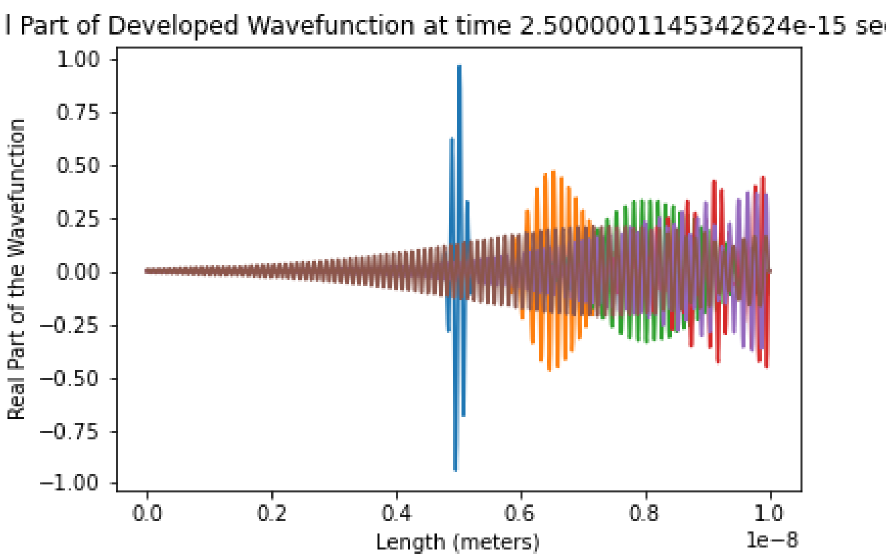
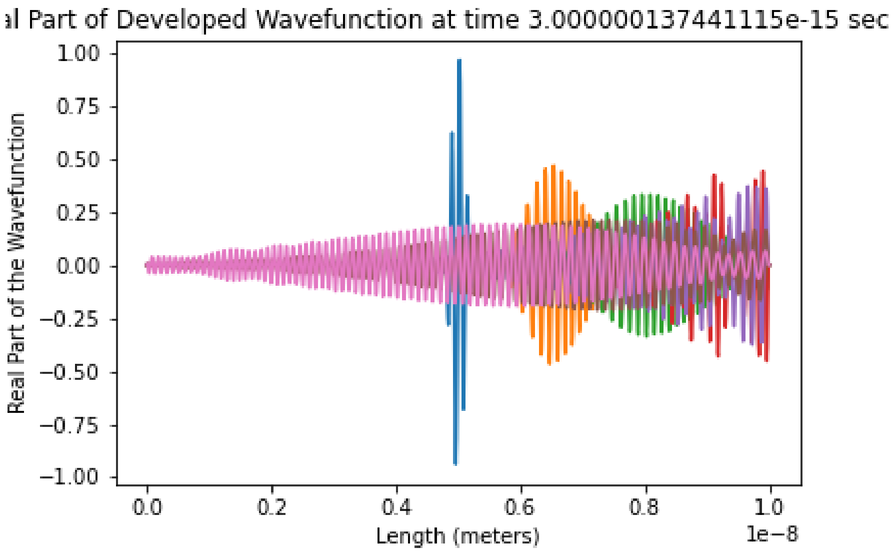
Real Part of the Wavefunction
Length (meters)
1e−8


al Part of Developed Wavefunction at time 2.00000009162741e-15 sec
Real Part of the Wavefunction
Length (meters)
1e−8


l Part of Developed Wavefunction at time 2.5000001145342624e-15 se
Real Part of the Wavefunction
Length (meters)
1e−8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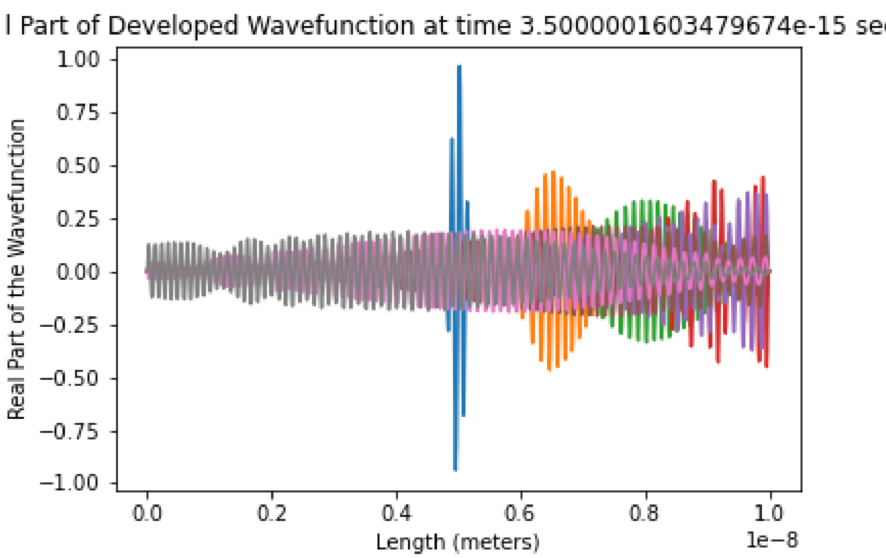
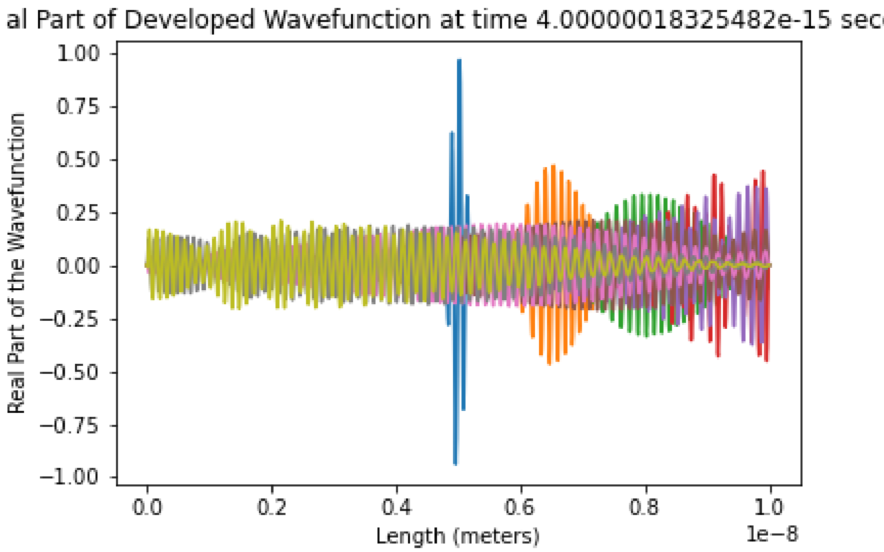
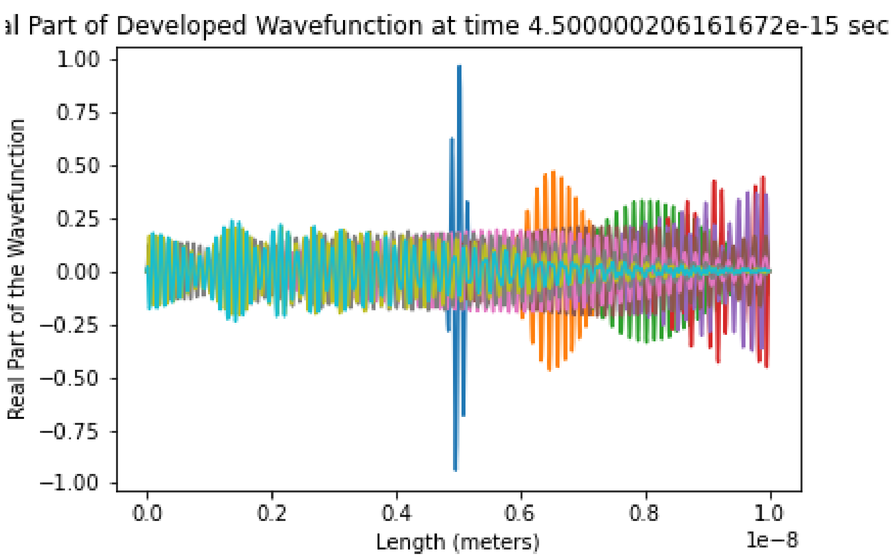
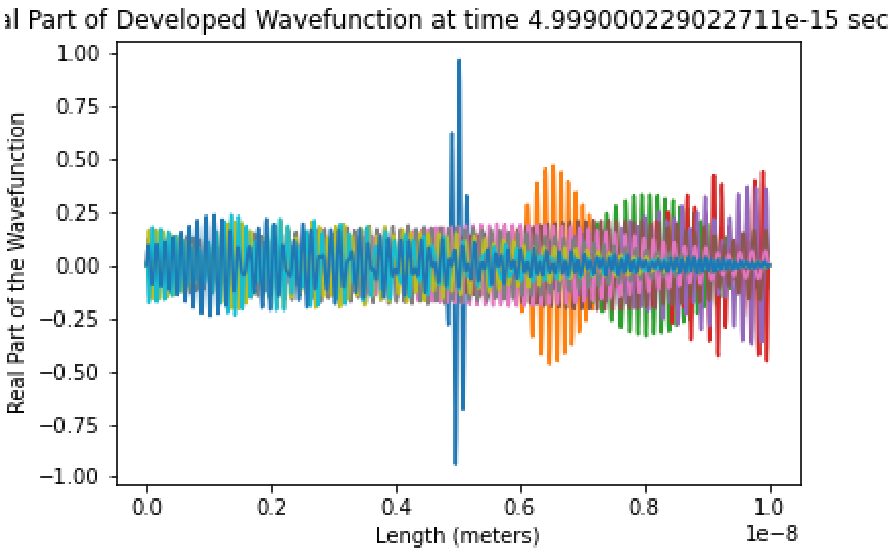
Real Part of the Wavefunction
Length (meters)
1e−8


l Part of Developed Wavefunction at time 3.5000001603479674e-15 sec
Real Part of the Wavefunction
Length (meters)
1e−8


al Part of Developed Wavefunction at time 4.00000018325482e-15 secc
Real Part of the Wavefunction
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0.0
0.2
0.4
0.6
0.8
1.0
1e−8
Length (meters)


al Part of Developed Wavefunction at time 4.500000206161672e-15 sec
Real Part of the Wavefunction
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0.0
0.2
0.4
0.6
0.8
1.0
1e−8
Length (meters)



4 Discussion

We see that the real part of the wavefunction travels in the position x direction. This is due to the positive x-dependent phase value κ present in the initial condition. The wavefunction then completing reflects after hitting the infinite barrier, spreading out after doing so. Because the potential barrier is infinitely high, the wavefunction cannot transmit. After doing so, the real part looks like a standing wave, but still goes to the other boundary and reflects.