PS 10 - Numerical Solutions of the Schrödinger Equation

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Codes:

The Python codes used in this report can be found at the following link: GitHub Repository.

Introduction

This report explores numerical solutions of the time-dependent Schrödinger equation for a particle in a one-dimensional infinite potential well. Two methods are utilized: the Crank-Nicolson method (Question 1) and the spectral method (Question 2). Both approaches demonstrate the evolution of a Gaussian wave packet under quantum mechanical principles, such as spreading, reflection, and interference.

Methods

Crank-Nicolson Method (Question 1)

The Crank-Nicolson method combines stability and second-order accuracy by discretizing the Schrödinger equation as:

$$A\psi(t + \Delta t) = B\psi(t),$$

where A and B are tridiagonal matrices. The wavefunction is updated iteratively using these matrices.

Simulation parameters include:

- Time step: $\Delta t = 10^{-17}$ s.
- Box length: $L = 10^{-8}$ m.
- Electron mass: $M = 9.109 \times 10^{-31}$ kg.
- Number of grid points: $N = 1000$.

The initial wavefunction is a Gaussian wave packet:

$$\psi(x, 0) = \exp\left(-\frac{(x - x_0)^2}{2\sigma^2}\right) e^{ik_0 x},$$

where $x_0 = L/2$, $\sigma = 10^{-10}$ m, and $k_0 = 5 \times 10^{10}$ m^{-1}. The evolution of the wavefunction is visualized by updating the real part at each time step.

Spectral Method (Question 2)

The spectral method expands the wavefunction in terms of sine basis functions:

$$\psi_k(x,t) = \sin\left(\frac{k\pi x}{L}\right) e^{iE_k t/\hbar},$$

where $E_k = \frac{k^2\pi^2\hbar^2}{2ML^2}$. The full wavefunction is a linear combination of these basis functions:

$$\psi(x,t) = \sum_k b_k \sin\left(\frac{k\pi x}{L}\right) e^{iE_k t/\hbar}.$$

Simulation parameters:

- Time step: $\Delta t = 2 \times 10^{-18}$ s.
- Box length: $L = 10^{-8}$ m.
- Electron mass: $M = 9.109 \times 10^{-31}$ kg.
- Number of grid points: $N = 1000$.

The coefficients b_k are calculated from the initial wavefunction using the discrete sine transform (DST) and evolved over time. The wavefunction is reconstructed using the inverse DST, allowing visualization of its real part.

Results

Crank-Nicolson Method (Question 1)

The evolution of the wavefunction using the Crank-Nicolson method is shown below:

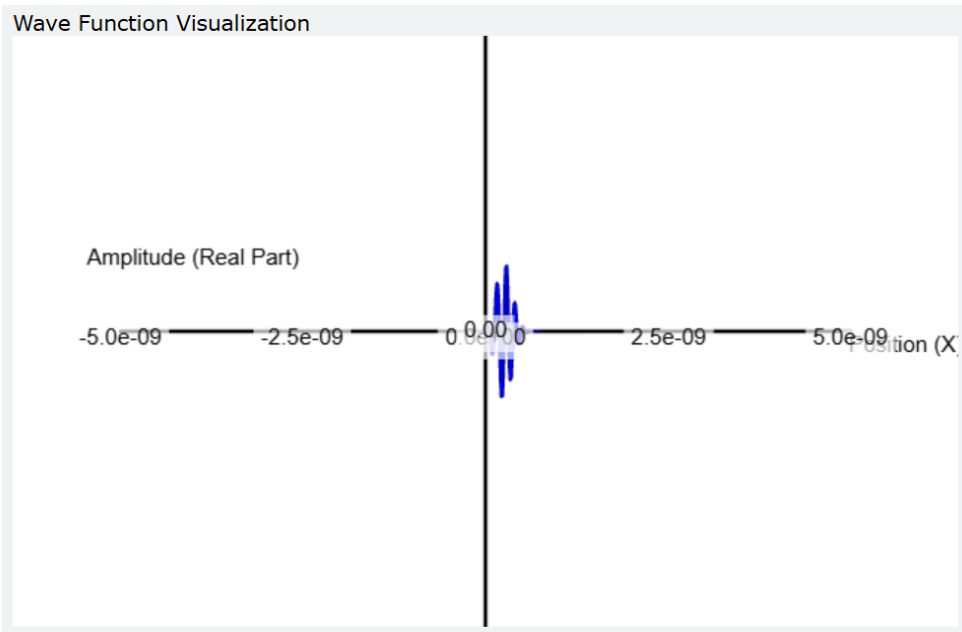

Figure 1: Initial Gaussian wave packet centered in the box (Method 1: Crank-Nicolson).

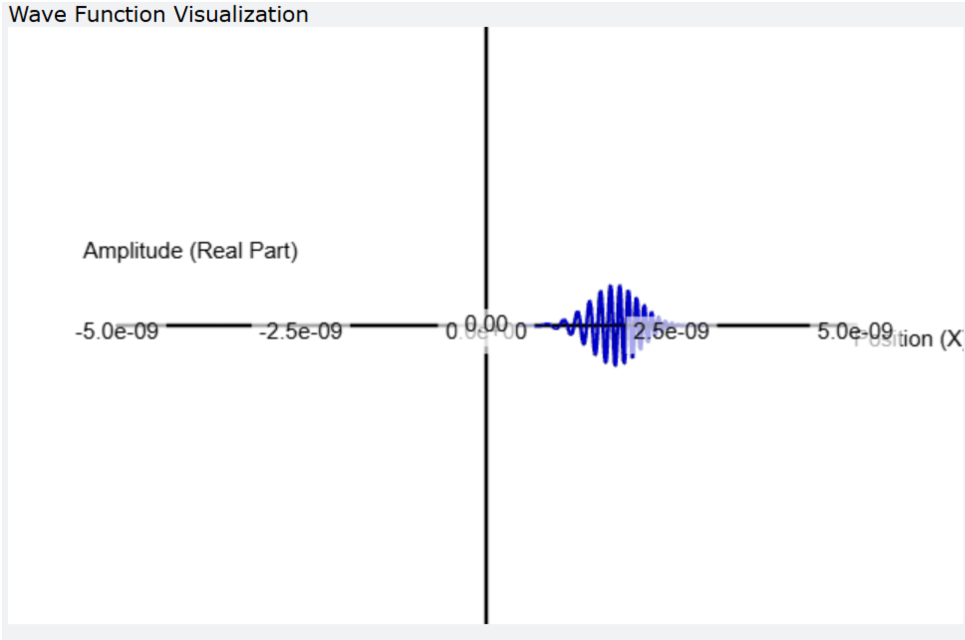

Figure 2: Wave packet starts propagating to the right (Method 1: Crank-Nicolson).

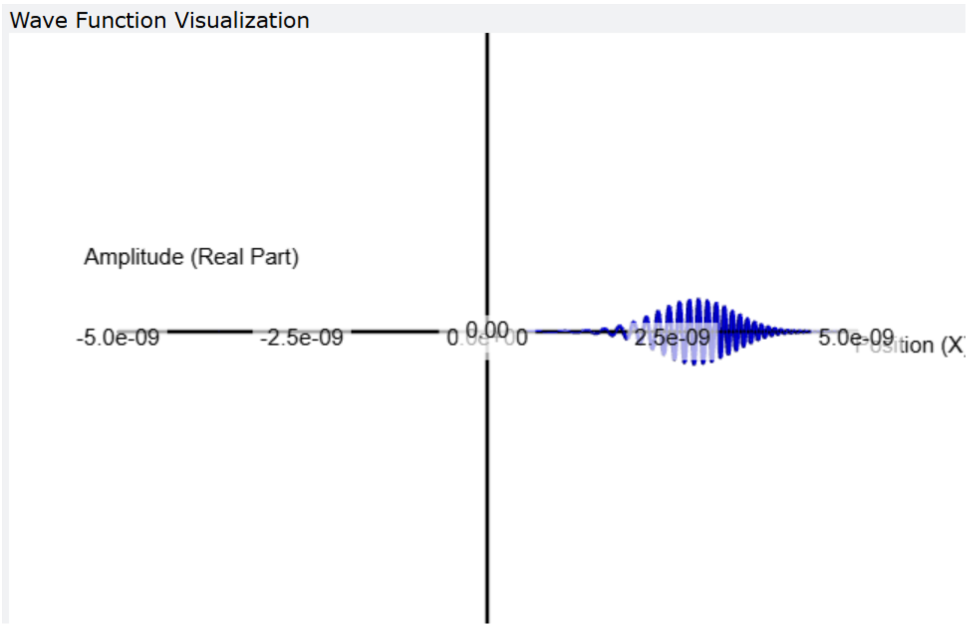

Figure 3: Wave packet reflects off the boundary at $x = L$ and starts moving to the left (Method 1: Crank-Nicolson).

Spectral Method (Question 2)

The evolution of the wavefunction using the spectral method is shown below:

These images demonstrate the oscillatory and reflective nature of the wavefunction in the infinite potential well. Interference patterns arise due to the superposition of reflected waves.

These images highlight the wavefunction's spreading, reflection, and interference patterns. The spectral method ensures numerical stability, producing smooth and symmetric evolution.

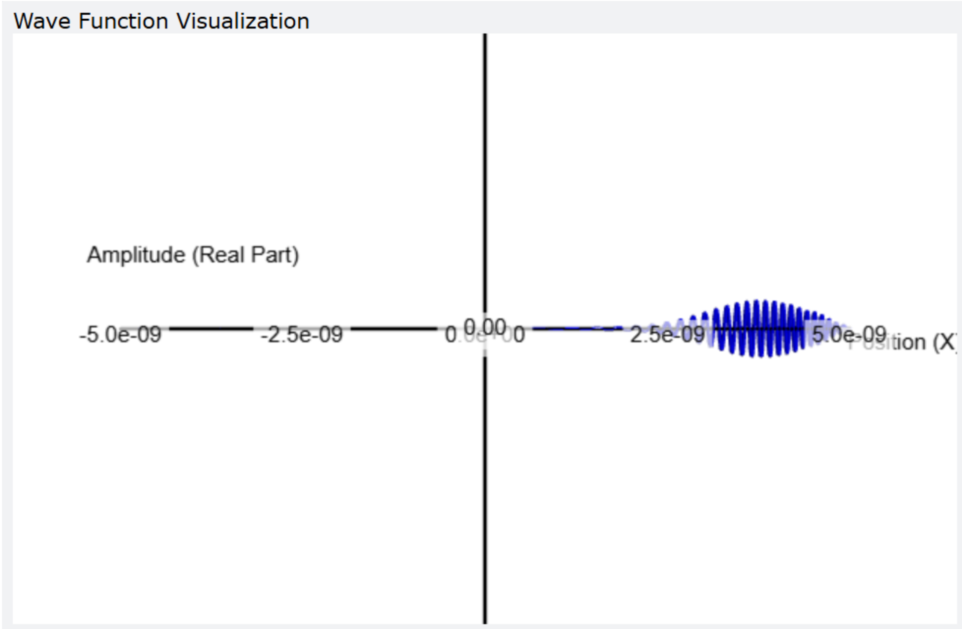

Figure 4: Wave packet interference as it propagates back to the left boundary (Method 1: Crank-Nicolson).

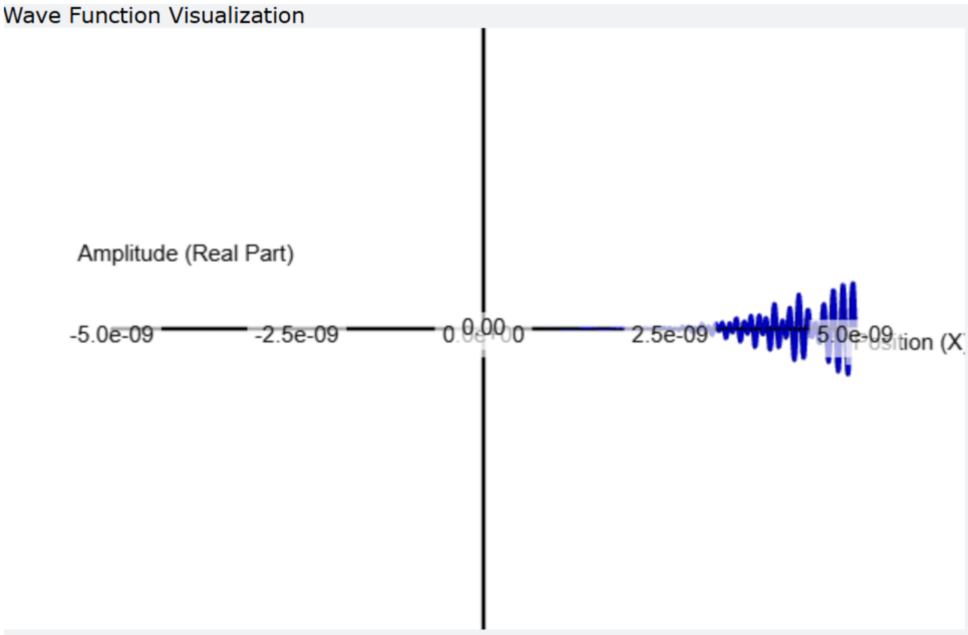

Figure 5: The wave packet continues its oscillatory behavior within the box (Method 1: Crank-Nicolson).

Conclusion

The Crank-Nicolson and spectral methods both effectively solve the time-dependent Schrödinger equation for a particle in an infinite potential well. The Crank-Nicolson method operates in real space, while the spectral method works in the frequency domain, leveraging sine basis functions. Both methods capture key quantum mechanical behaviors, such as wave packet spreading, reflection, and interference, illustrating the unitary

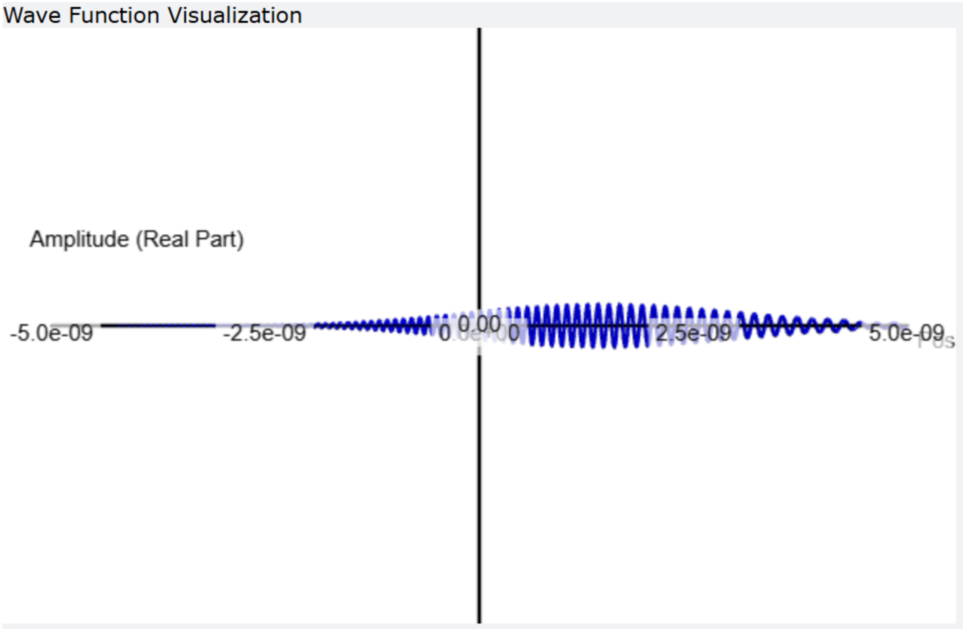

Figure 6: Wave packet interference as it propagates back to the left boundary (Method 1: Crank-Nicolson).

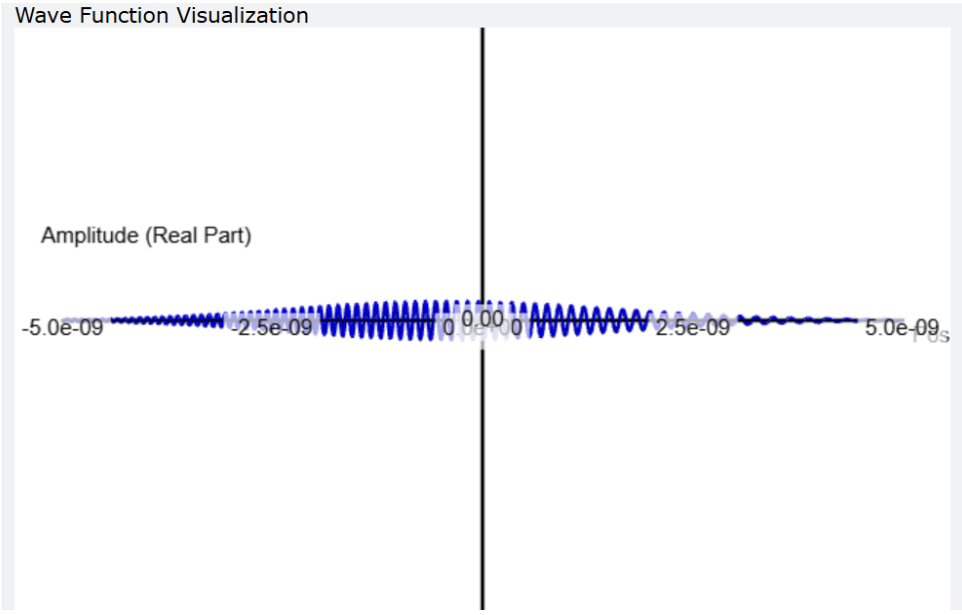

Figure 7: Wave packet interference as it propagates back to the left boundary (Method 1: Crank-Nicolson).

evolution of the wavefunction.

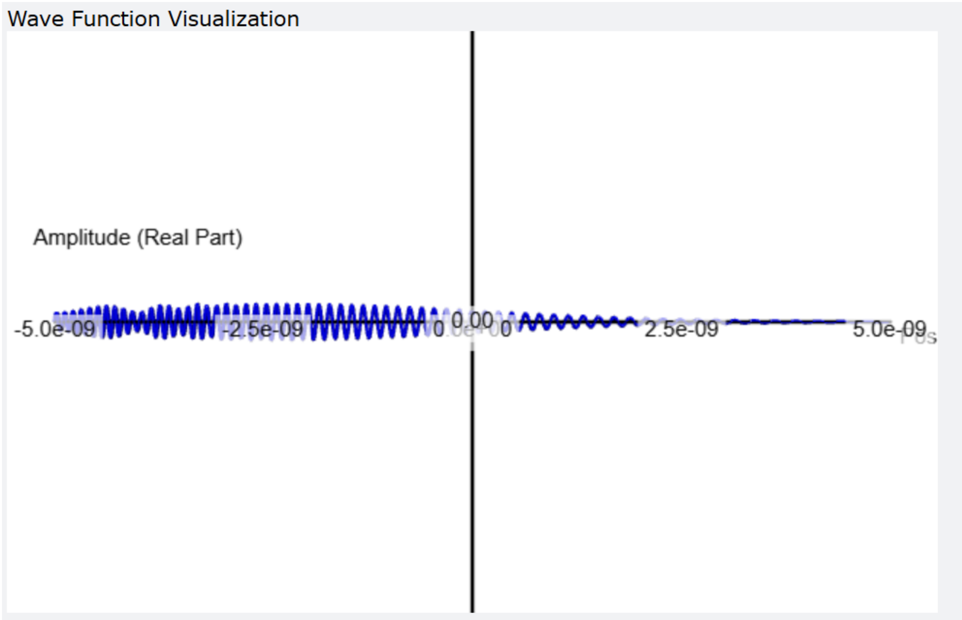

Figure 8: Wave packet interference as it propagates back to the left boundary (Method 1: Crank-Nicolson).

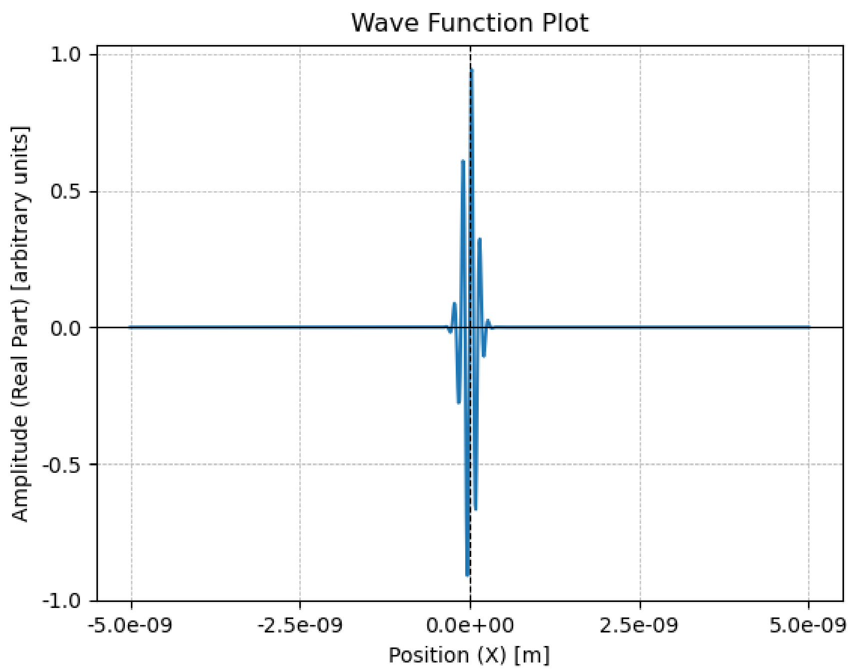

Figure 9: Initial Gaussian wave packet centered in the box (Method 2: Spectral Method).

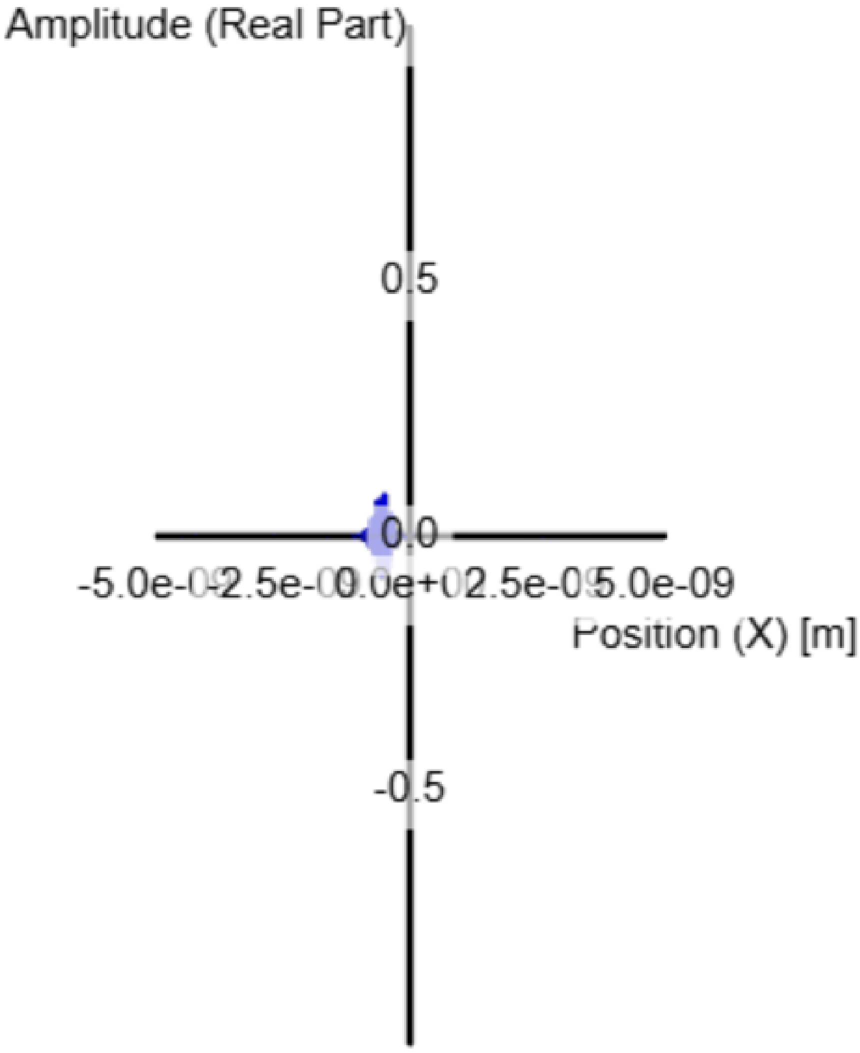

Figure 10: Wave packet spreads symmetrically within the box (Method 2: Spectral Method).

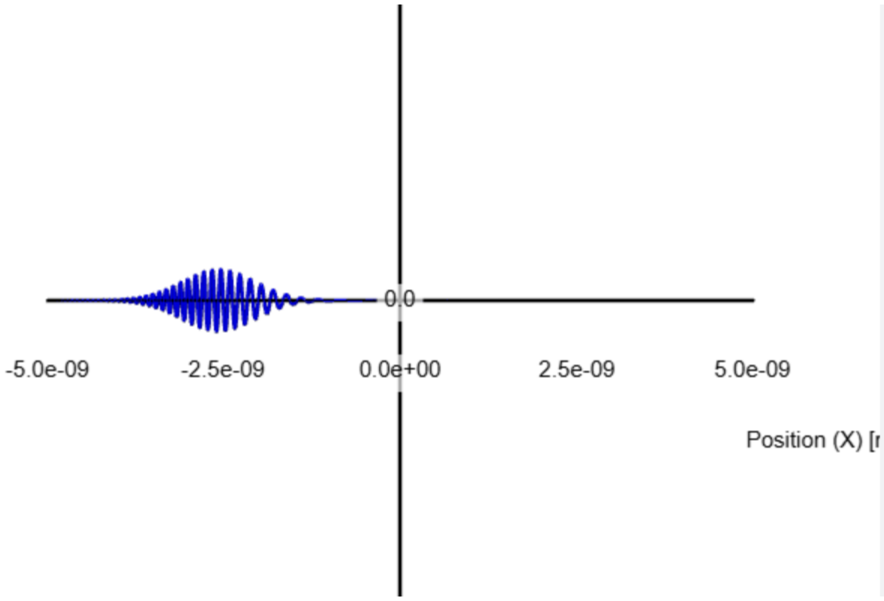

Figure 11: Interference patterns develop as the wave packet evolves (Method 2: Spectral Method).

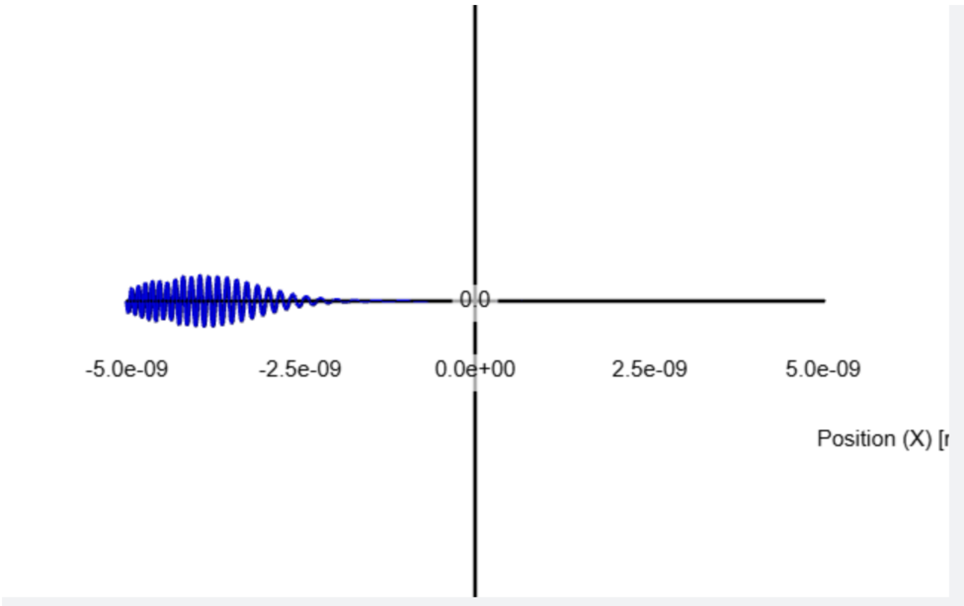

Figure 12: Wave packet reflects from the boundary, creating complex interference (Method 2: Spectral Method).

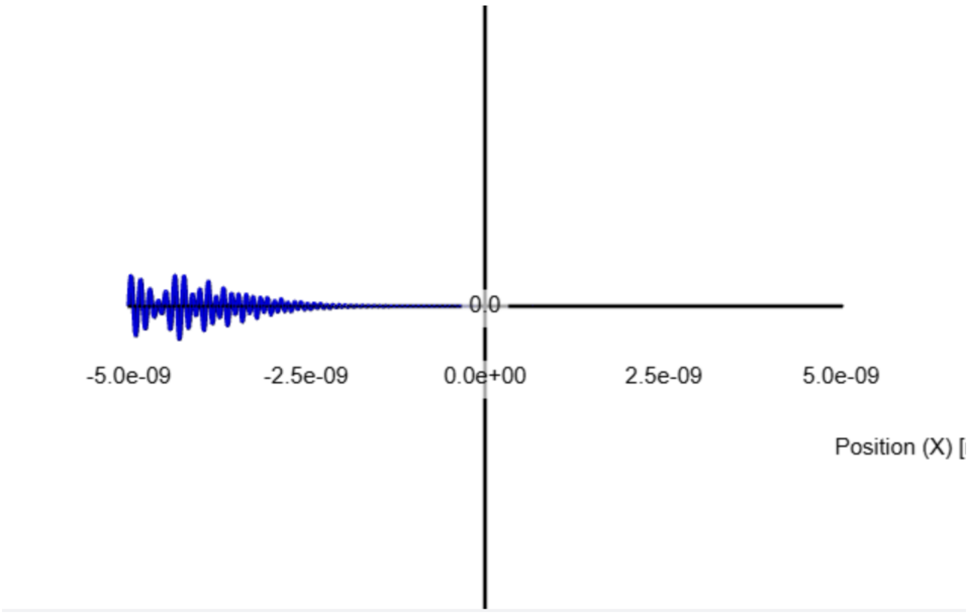

Figure 13: Further evolution shows oscillatory behavior and spreading (Method 2: Spectral Method).

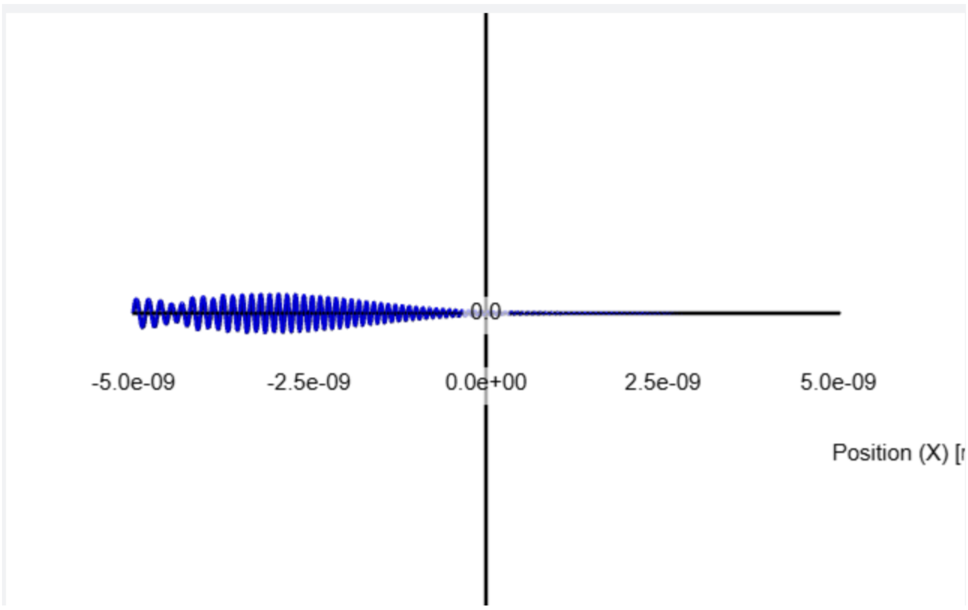

Figure 14: Further evolution shows oscillatory behavior and spreading (Method 2: Spectral Method).

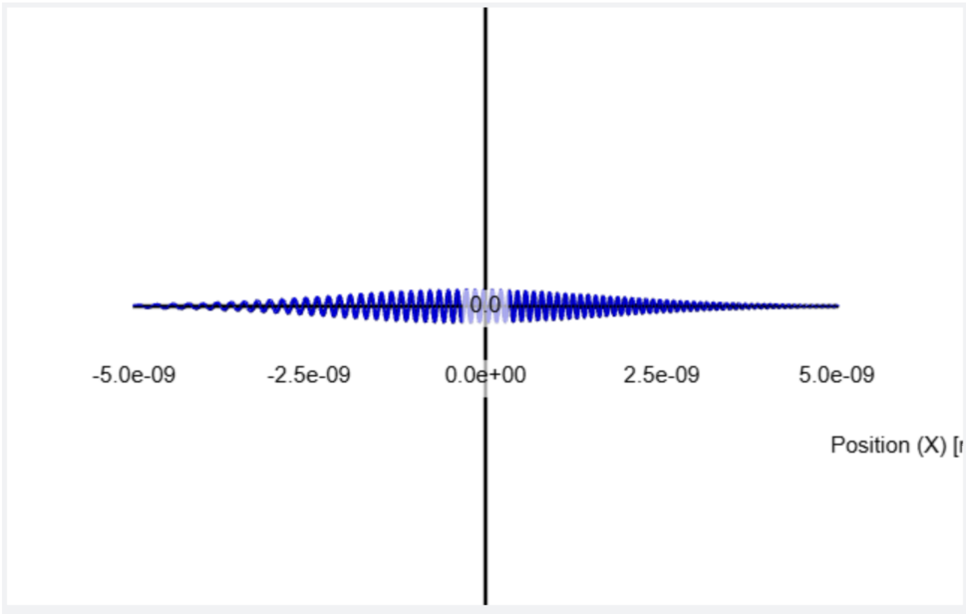

Figure 15: Further evolution shows oscillatory behavior and spreading (Method 2: Spectral Method).

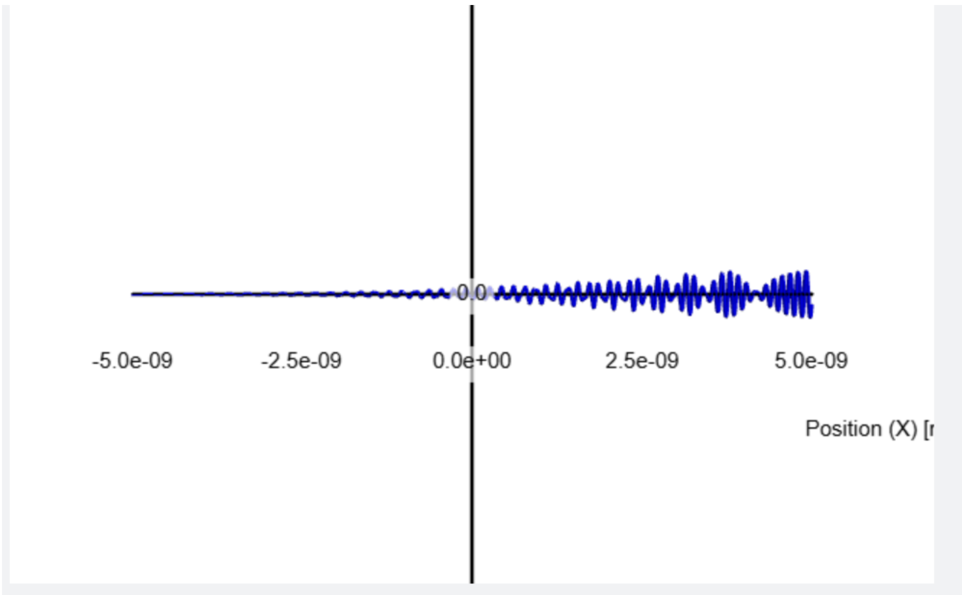

Figure 16: Further evolution shows oscillatory behavior and spreading (Method 2: Spectral Method).

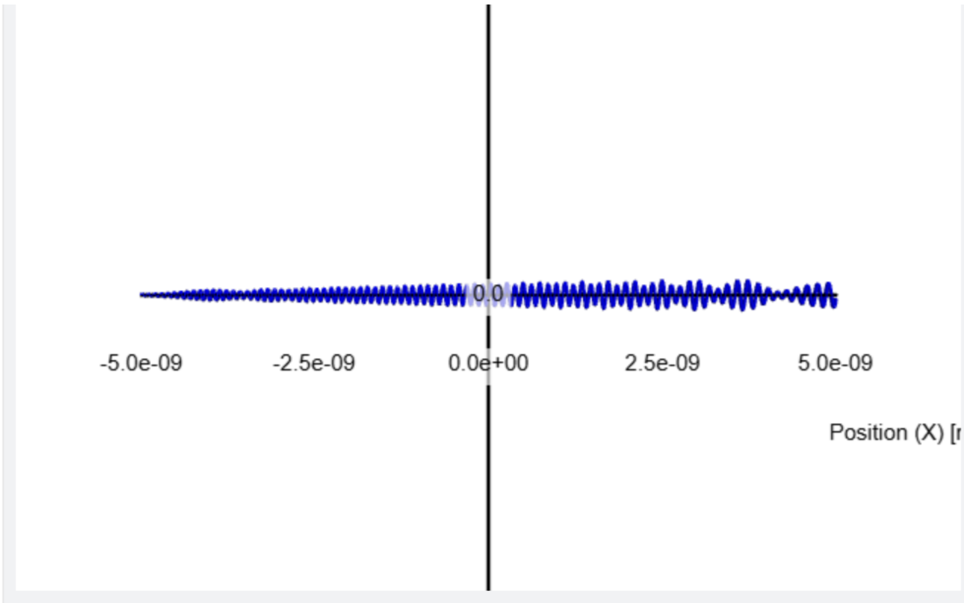

Figure 17: Further evolution shows oscillatory behavior and spreading (Method 2: Spectral Method).