PHYS-UA 210 Computational Physics
Problem Set 09

Sandhya Sharma

December 13, 2023

Solving the Time Dependent Schrödinger's Equation (Newman 9.8)

Time Dependent Schrödinger's Equation is given by:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\Psi(x,t)$$

In this problem, the following things are considered:
- No potential,
- Particle is in a box with impenetrable walls,
- Wave function ψ is zero at the walls,
- The walls are at $x = 0$ and $x = L$.

Crank-Nicolson Method
The Crank-Nicolson method is a numerical technique used for solving partial differential equations (PDEs). This method is applied on the TDSE to get the wave functions according to the following initial wave function:

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

where, $x_0 = \frac{L}{2}$, $\sigma = 10^{=10}$ m, $\kappa = 5 * 10^{10}\ m^{-1}$

This wave function is not normalized but because Schrödinger's equation is linear, the constant cancels out on both sides of the equation and plays no part in the solution.

Plotting the real part of wave function at a few time steps:

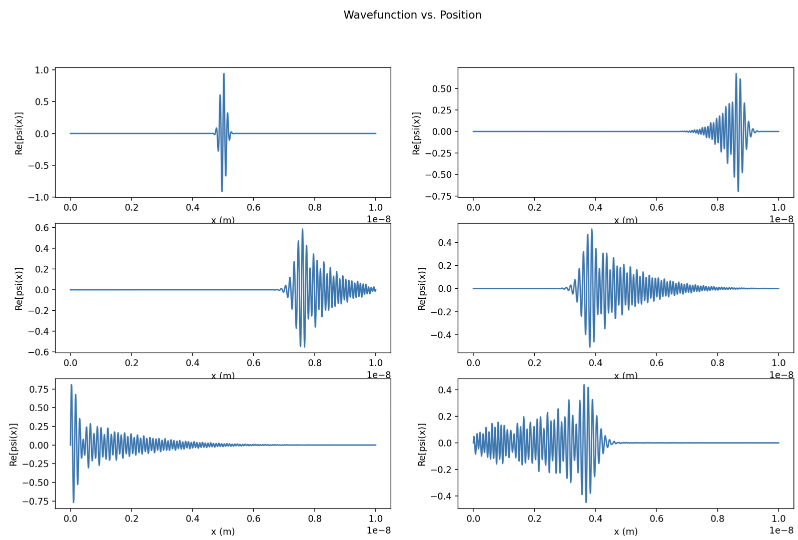

Figure 1: Time Evolution of Wave function with time-step = 10^{-17}

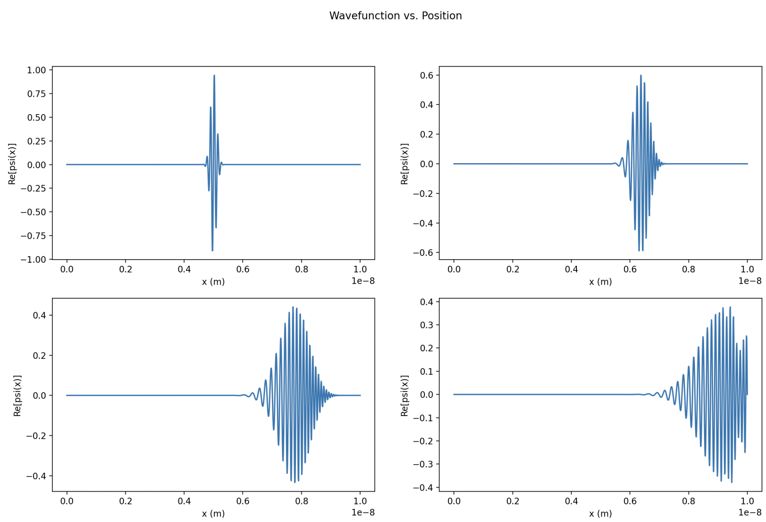

Figure 2: Time Evolution of Wave function with time-step = 10^{-18}

Analyzing the wave functions evolution over time:

This initial wave function is a Gaussian wave packet. The Gaussian part determines the spatial spread of the wave packet around while the exponential term contributes to the momentum or wave number of the wave packet. It is consistent with the initial conditions that the wave equation always vanishes at the walls of the finite box. At the boundaries, the wave function experiences reflections due to the abrupt change in the potential (from zero to infinite). The time evolution of the wave packet also causes the spread of the wave packet due to the uncertainty factor σ over time while the initial wave function is relatively localized. From the plots above, this behavior is very apparent.
Please find my GitHub repository through this: link.