Homework 10 Solution

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December 10, 2024

This is my GitHub link: Nana Ama's GitHub Link

1 Introduction

In one-dimension(1D), the Schrodinger equation of a particle is expressed as

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

This particle, an electron, was then placed in a box with impenetrable walls in one dimension was solved in questions one and two using the Crank-Nicolson method and the spectral method. Boundary conditions of $\psi(x = 0) = \psi(x = L) = 0$ were applied in both cases. The mass of the electron is $M = 9.109 \times 10^{-31} kg$, in abox of length $L = 1 \times 10^{-8} m$. At time $t = 0$, the wavefunction of the electron is of the form

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

where $x_0 = \frac{L}{2}, \sigma = 1 \times 10^{-10} m$, and $k = 5 \times 10^{10} m^{-1}$

2 Crank-Nicolson Method

The Crank-Nicolson equations can be written in the form

$$A\psi(t + h) = B\psi(t) \tag{3}$$

with

$$\psi(t) = \begin{pmatrix} \psi(a, t) \\ \psi(2a, t) \\ \psi(3a, t) \\ \vdots \end{pmatrix} \tag{4}$$

where a is the spacing of the spacial grid points and h is the size of the time step and the matrices A and B are tridiagonal matrices

$$A = \begin{pmatrix} a_1 & a_2 & & & \\ a_2 & a_1 & a_2 & & \\ & a_2 & a_1 & a_2 & \\ & & a_2 & a_1 & \\ & & & \ddots & \end{pmatrix}, B = \begin{pmatrix} b_1 & b_2 & & & \\ b_2 & b_1 & b_2 & & \\ & b_2 & b_1 & b_2 & \\ & & b_2 & b_1 & \\ & & & \ddots & \end{pmatrix} \tag{5}$$

and

$$a_1 = 1 + h\frac{i\hbar}{2ma^2}, a_2 - h\frac{i\hbar}{4ma^2}, b_1 = 1 - h\frac{i\hbar}{2ma^2}, b_2 = h\frac{i\hbar}{4ma^2} \tag{6}$$

The vector $\psi(t)$ was calculated using the initial wavefunction above Equation .. numerically by

$$v = B\psi \tag{7}$$

with $N = 1000$ spatial slices and $a = L/N$ for a single step.
where

$$v_i = b_1\psi_i + b_2(\psi_{i+1} + \psi_{i-1}) \tag{8}$$

For the next step, the scipy.banded module was used to solve the linear system $Ax = v$, which gives the updated ψ It was then extended to perform repeated steps at a separation $h = 1 \times 10^{-18}s$. An animation of the solution was made at each time step.

3 Spectral Method

Th spectral method involves using a Fourier transform to solve for the k components. With the same 1D Schrodinger equation as in Equation ..., the potential solution to this equation is

$$\psi_k = \sin(\frac{\pi kx}{L}\exp(\frac{iEt}{\hbar})) \tag{9}$$

with

$$E = \frac{\pi^2\hbar^2k^2}{2ML^2} \tag{10}$$

with a full solution expressed as a linear combination of these individual solutions on grid points $x_n = \frac{nL}{N}$

$$\psi(x_n, t) = \frac{1}{N}\sum_{k=1}^{N-1}\sin(\frac{\pi kn}{N})\exp(i\frac{\pi^2\hbar k^2}{2ML^2}) \tag{11}$$

and $b_k = \alpha_k + i\eta_k$ with α_k being the real part and η_k, the imaginary part.

A programme was made to calculate these b_k coeffficients with the same parameters as those in the Crank-Nicolson method. Discrete sine transformations were performed on each initial wavefunction real and imaginary array at each grid point for all $k = 1, \cdots, N-1$. The real part of the wavefunction was taken and extended at an arbitrary time using the inverse discrete sine transformation. This programme was tested by making a graph of the wavefunction at time $t = 10^{-16}s$ as seen in Figure ... The programme was also extended to make an animation.

4 Discussion of Results

These 2 methods produced the same results as seen in Figure ....

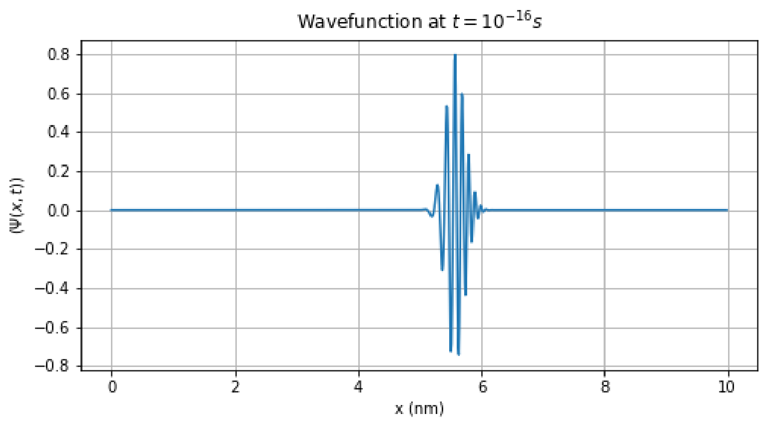

Figure 1: Waveform at $t = 1 \times 10^{-16}s$

The test at time $t = 1 \times 10^{-16}s$ yielded the plot in Figures 1 The progress of propagation of the wave can be seen in Figure 2 where it loses energy as it travels along the positive x direction and meets a boundary (that is the potential barrier), bounces back and travels along the negative x direction effectively changing its waveform.

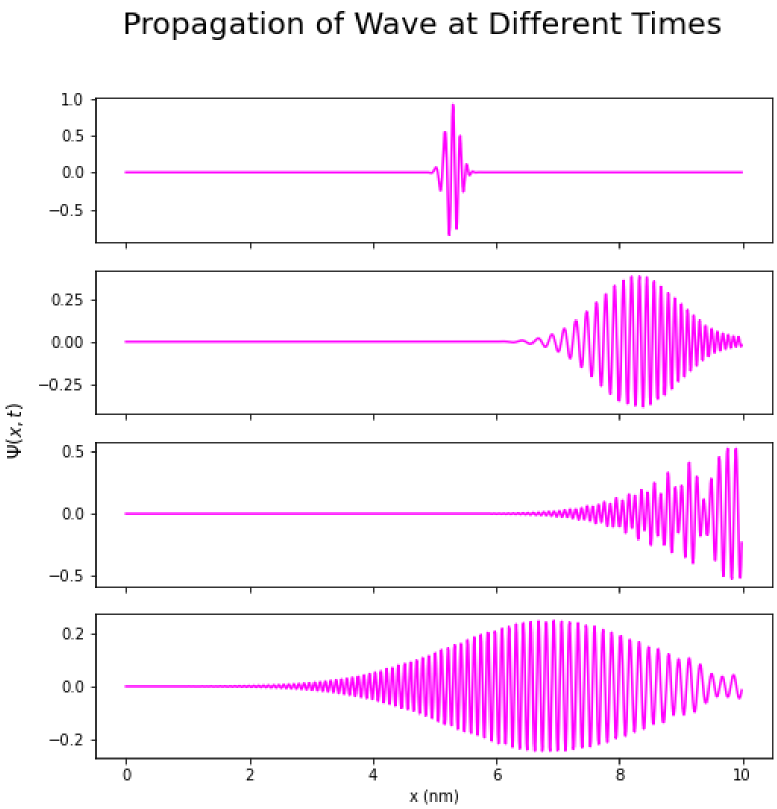

Figure 2: Crank-Nicolson Method