

HW9

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Dec. 2023

1 Problem 1

This problem is simulation problem where we simulate the wave-function of a electron in a 1D box by solving the time dependent Schrodinger equation. The basic idea is to obtain the wave-function at next time step given the wave-function of previous time step, so if we have the initial condition for the wave-function, we are able to obtain a time evolution of the wave-function. The method is detailed described in book where they derived a Crank-Nicolson equation using Euler equation and FTCS equation. Basically, it forms the space dependent wave-function into a 1D matrix, where each row represents the value of wave-function at that position. There are two tridiagonal matrices A and B, where they satisfied the following equation:

$$A\phi(t+h) = B\phi(t)$$

where h is the time step. In this problem, we assume the initial wave-function of the electron have the following form:

$$\psi(x,0) = \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right] e^{ikx} \quad (1)$$

Using this setup, I formulated a python code that performs the simulation. Here's some simulation results of the wave-functions of electron at different time. One can see that the wave-function is spreading out as expected, and when it hit the wall, it kinda bounce back, which is pretty interesting. Also, the amplitude is decreases as the result of a more spreading wave-function.

2 Github

username: robertXi6 link: <https://github.com/robertXi6/phys-ua210>

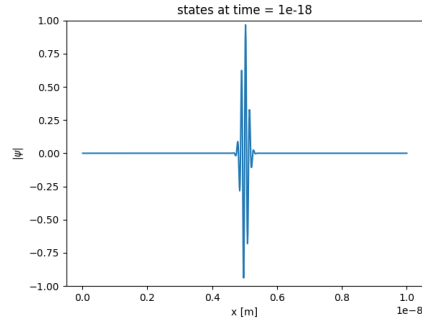


Figure 1: Wave-function of electron at time = 0s

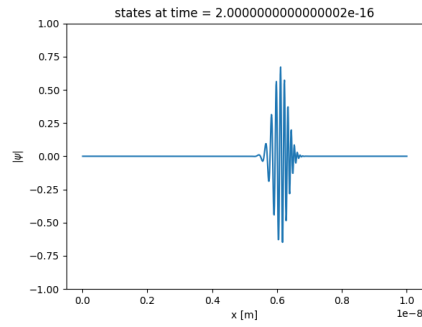


Figure 2: Wave-function of electron at time = 2e-16s

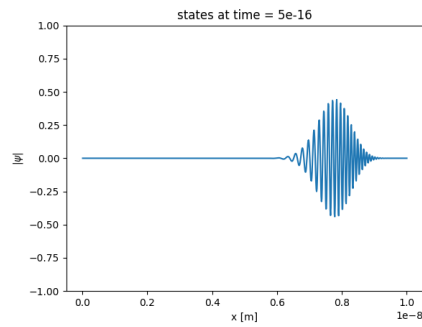


Figure 3: Wave-function of electron at time = 5e-16s

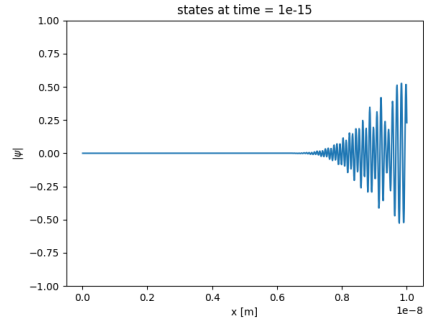


Figure 4: Wave-function of electron at time = 1e-15s

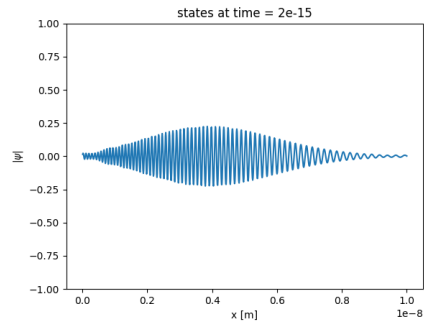


Figure 5: Wave-function of electron at time = 2e-15s

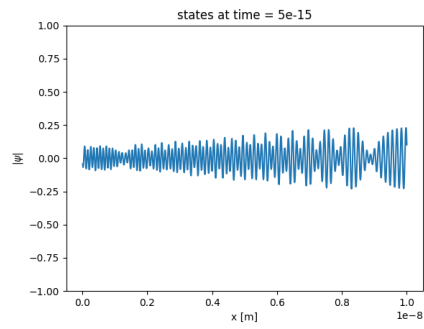


Figure 6: Wave-function of electron at time = 5e-15s