Ps 9

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Abstract

This short paper will show some plots and discuss implementing the Crank-Nicholson method for solving the Schrodinger equation for an electron in an infinite square well.

1 Introduction

The Shrodinger equation lies at the heart of quantum mechanics. It is a linear partial differential equation that describes the time evolution of a wave function. Solving partial differential equations isn't always easy so it's nice to be able to solve them computationally. I solve an electron in an infinite box (free particle with boundary conditions) using the Crank-Nicholson method.

2 Methods

Crank-Nicholson is a finite difference method used for solving partial differential equations similar to the heat equation, aka, where a single time derivative is related to a double spatial derivative. It is solved by taking the average of the forward Euler and backwards Euler methods. That looks like this:

$$\psi(x,t+h)-h\frac{i\hbar}{4ma^2}[\psi(x+a,t+h)+\psi(x-a,t+h)-2\psi(x,t+h)] = \psi(x,y)+h\frac{i\hbar}{4ma^2}[\psi(x+a,t)+\psi(x-a,t)-2\psi(x,t)] \tag{1}$$

Which I do not know how to get onto two split lines nicely in latex. This can be rewritten as a matrix equation.

$$A\psi(t+h) = B\psi(t) \tag{2}$$

where A and B are bounded and constant matrices. Do some initial condition for psi (in our case a gaussian) and solve the matrix equation by applying the correct matrix transformation over and over. The constants associated in this problem aren't good to use because they are too small or differ too much. The main difference is non-dimensionalizing some units and changing the length scale from meters to nanometers. See code for details of the change from the actual values for an electron.

The problem statement recommended a time step of 10^{-18} which is machine precision. After changing the physical values I used a time step of order 10^{-4} to 10^{-6} and saw no difference so I take this to be fine.

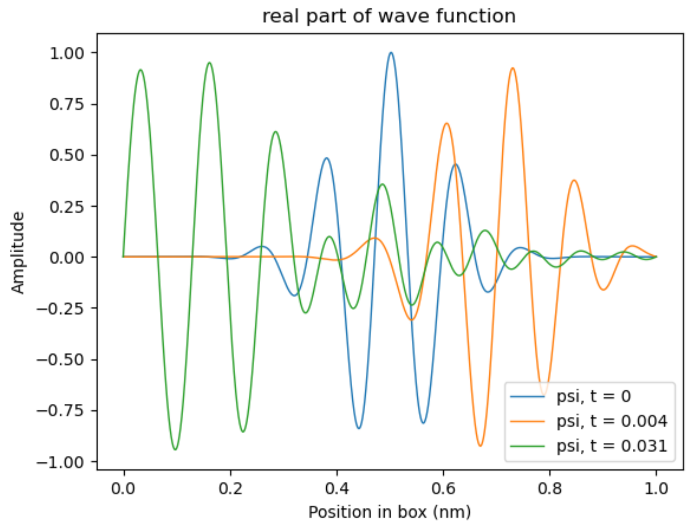

Figure 1

3 Results

The wave function evolves over time, while maintaining its total probability amplitude. Which means that the method used should be physically accurate.

4 Discussion

This is a very simple case, but it should also apply in general. For example, if the box were larger, we could watch the wave function spread out over time. Because of our boundaries the wave moves back and forth instead. This problem worked well because I was able to vectorize the calculation for python, but even with that it still took a bit to run. I can see how with only slightly more complicated systems that solving would become computationally difficult to impossible.