PHYS-GA2000-PS9

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1 Introduction

In this problem set, we are interested in solving the Schrodinger equation in one dimension using Crank-Nicolson method.

2 Method

The Crank-Nicolson equations can be written in the form

$$\boldsymbol{A}\boldsymbol{\Psi}(t+h) = \boldsymbol{B}\boldsymbol{\Psi}(t) \tag{1}$$

where $\boldsymbol{\Psi}(t)$ is the vector whose elements are the values of wave function at grid points and at time t. $\boldsymbol{A}$ and $\boldsymbol{B}$ are tridiagonal matrices whose main diagonal elements are a_1 and b_1 and those of upper and lower diagonal are a_2 and b_2, respectively.

$$\begin{aligned} a_1 &= 1 + \frac{hi\hbar}{2ma^2} \\ a_2 &= -\frac{hi\hbar}{4ma^2} \\ b_1 &= 1 - \frac{hi\hbar}{2ma^2} \\ b_2 &= \frac{hi\hbar}{4ma^2} \end{aligned} \tag{2}$$

where h is the time step and a is the distance between two grid points. Once we form matrices $\boldsymbol{A}$ and $\boldsymbol{B}$, what we need to do to find $\boldsymbol{\Psi}(t+h)$ is to solve linear system given by Eq.1. We can repeat this procedure to find $\boldsymbol{\Psi}(t)$ at later times.

3 Results

Norm and the real part of the wave function as of x at different times are presented in Figure 1 and 2, respectively. It is more intuitive to look at the animations to see what is going on in the well with impenetrable walls. As seen in Figure 1, the wave function is initially well-localized in the middle.

As time passes, it spreads over the region and the peak moves towards the right end. It is clear on the videos that wave function bounces back when it hits the impenetrable wall. Since the inital wave function is modulated by a gaussian function, there are infinitely many frequencies involved in general solution, which makes the solution look chaotic when the wave function hits the wall.

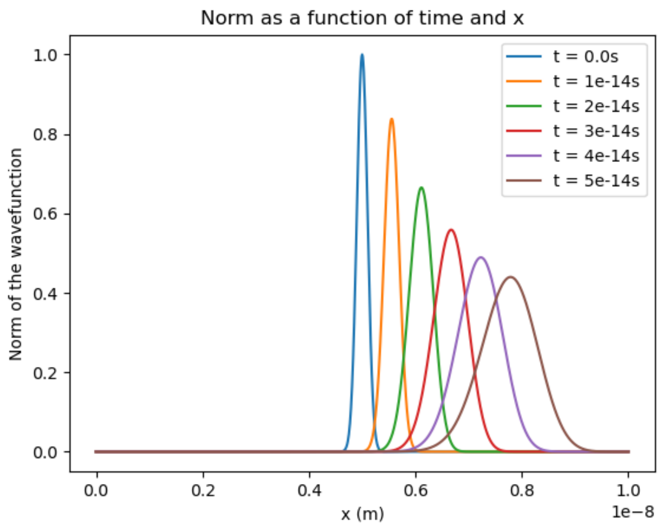

Figure 1: Norm of the wave function.

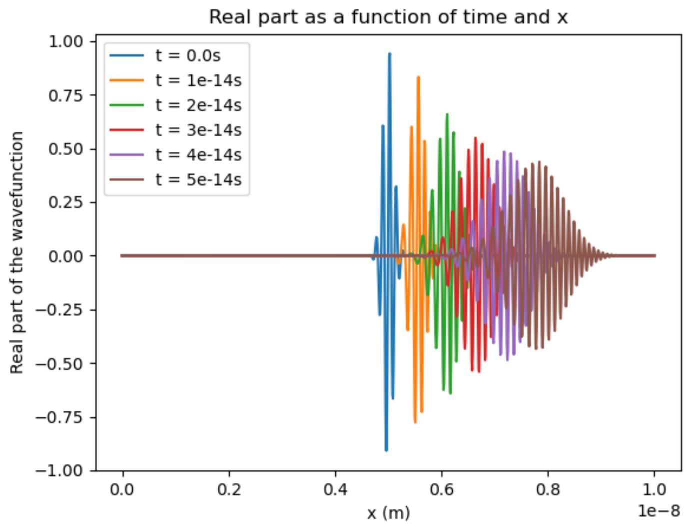

Figure 2: Real part of the wave function.