Report file - Problem Set #10

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Abstract

This is the report for the problem set #10. Since the problem set is composed of two exercises, we divide the report into two sections, one for each problem. The scripts (labelled as ps_10.'problem number') and the raw file of the animation in `GIF` format are stored in this directory, while here we report only some fixed-time snapshots.

1 Problem 1

1.1 Formulation of the problem

In this problem, we are going to use the Crank-Nicolson method to solve the full time-dependent Schrödinger equation in one dimension:

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

1.2 Computational methods

After some mathematical manipulation shown in [1] (finite difference, Euler's method and averaging between FTCSs) the problem of a particle in a box of finite dimension L takes the form:

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

where $\mathbf{A}$ and $\mathbf{B}$ are both symmetric tridiagonal matrices:

$$\mathbf{A} = \begin{pmatrix} a_1 & a_2 & & & \\ a_2 & a_1 & a_2 & & \\ & a_2 & a_1 & a_2 & \\ & & a_2 & a_1 & \\ & & & & \ddots \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_1 & b_2 & & & \\ b_2 & b_1 & b_2 & & \\ & b_2 & b_1 & b_2 & \\ & & b_2 & b_1 & \\ & & & & \ddots \end{pmatrix} \tag{3}$$

with

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

This is a matrix inversion problem that can be solved using the (tridiagonal version of the) Gaussian elimination (found using the Crank-Nicolson method).

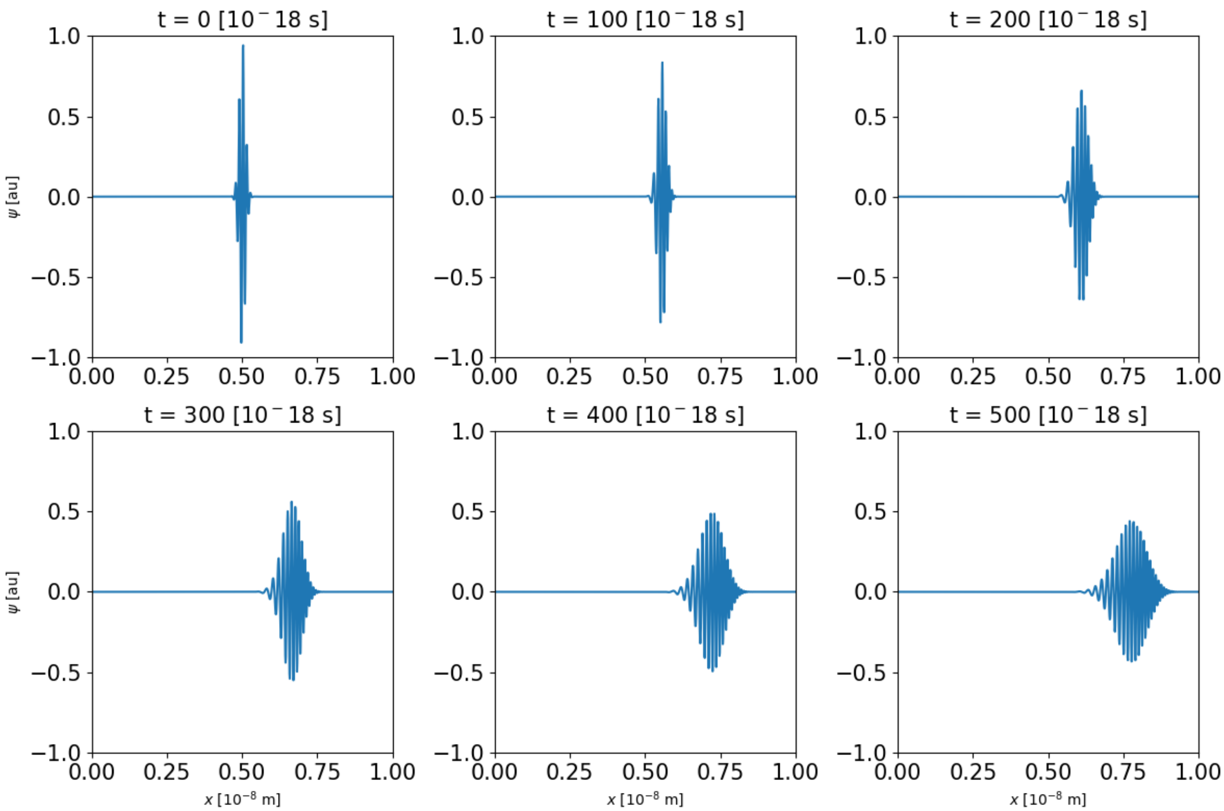

Figure 1: Different time snapshots of the numerical solution of the Schrödinger equation of a particle in a box with parameters and initial conditions as in eq. (5) using the Crank-Nicolson method.

1.3 Results

In fig. 1 we report the solution of eq. (1) for parameters and initial conditions:

$$M = 9.109 \times 10^{-31} \text{ kg}, \quad L = 10^{-8} \text{ m}, \quad \psi(t, 0) = \exp\left[-\frac{(x - x_0)^2}{2\sigma^2}\right] e^{i\kappa x}, \tag{5}$$

with

$$x_0 = \frac{L}{2}, \quad \sigma = 1 \times 10^{-10} \text{ m}, \quad \kappa = 5 \times 10^{10} \text{ m}^{-1}, \tag{6}$$

and $\psi = 0$ on the box walls at $x = 0, L$.

2 Problem 2

2.1 Formulation of the problem

In this problem, we are once again going to solve the full time-dependent Schrödinger equation in one dimension (eq. (1)) this time using the spectral method.

2.2 Computational methods

We start by writing a general solution of eq. (1) as a linear combination of normal modes:

$$\psi_k(x,t) = \sin\left(\frac{\pi k x}{L}\right) e^{-iE_k t/\hbar}, \quad E_k = \frac{\pi^2 \hbar^2 k^2}{2ML^2}, \quad \psi(x_n,t) = \frac{1}{N}\sum_{k=1}^{N-1} b_k \psi_k(x_n,t), \tag{7}$$

where $x_n = \frac{nL}{N}$ is a generic grid point.

Since the Schrödinger equation is first order in time we can just compute the FOurier coefficents $b_k = a_k + i\eta_k$ of the initial condition $\psi(x_n, 0)$ and directly compute the real part of the solution at a generic time t as the inverse sine transform with coefficients:

$$a_k \cos(E_k t/\hbar) + \eta_k \cos(E_k t/\hbar). \tag{8}$$

2.3 Results

In fig. 2 we report the solution of eq. (1) for parameters and initial conditions as eq. (5) (found using the spectral method).

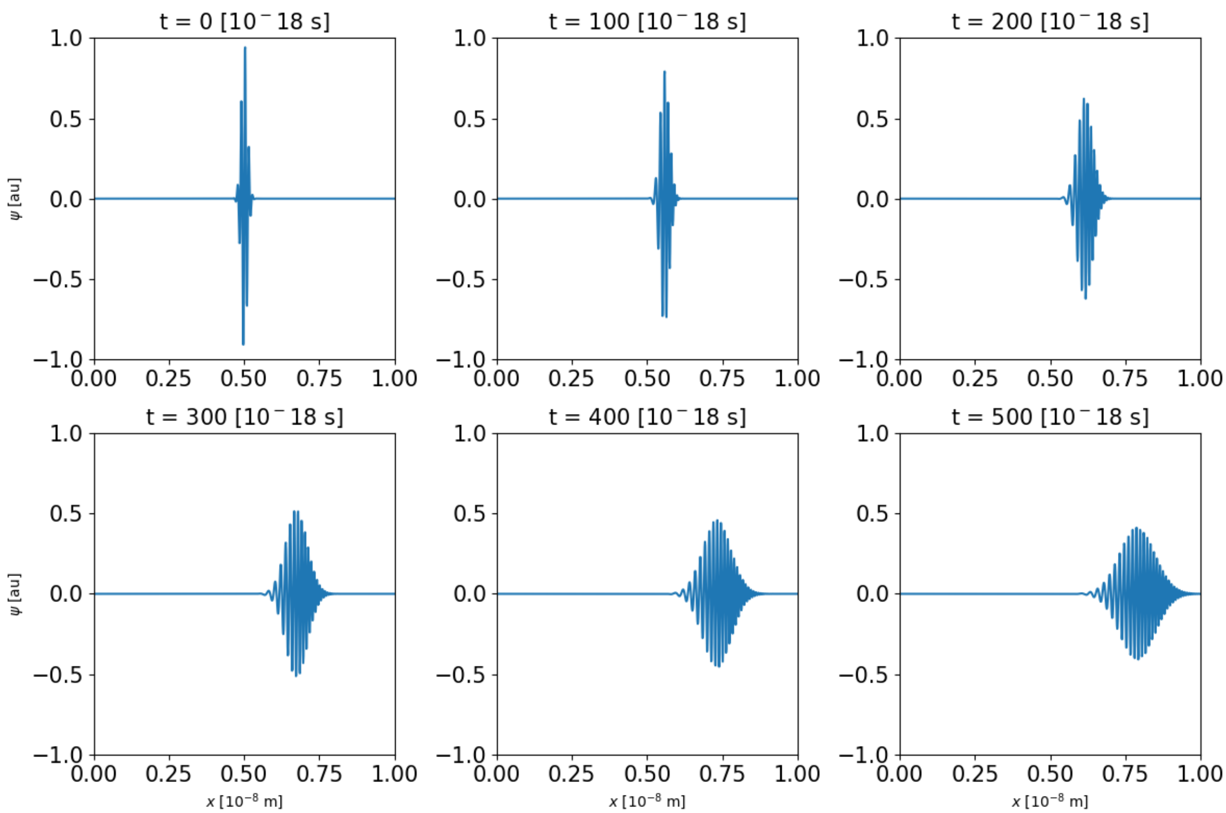

Figure 2: Different time snapshots of the numerical solution of the Schrödinger equation of a particle in a box with parameters and initial conditions as in eq. (5) using the spectral method.