Problem Set 10

Dario Loprete

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GitHub link

`https://github.com/dariolop76/phys-ga2000`

1 Problem 1

We follow the instructions given by the prompt. We apply the Crank-Nicolson method to obtain the time evolution of the wave function, given the initial condition

$$\psi(x,0) = \exp\Big[-\frac{(x-x0)^2}{2\sigma^2}\Big]e^{i\kappa x}. \tag{1}$$

We solve the equation

$$A\vec{\psi}(t+h) = v, \tag{2}$$

for $\vec{\psi}(t+h)$ using the module `banded.py`, where $v = B\vec{\psi}(t)$ and the matrices A, B are given in the prompt.

Fig. 1 shows six different snapshots of the real part of the wavefunctions.

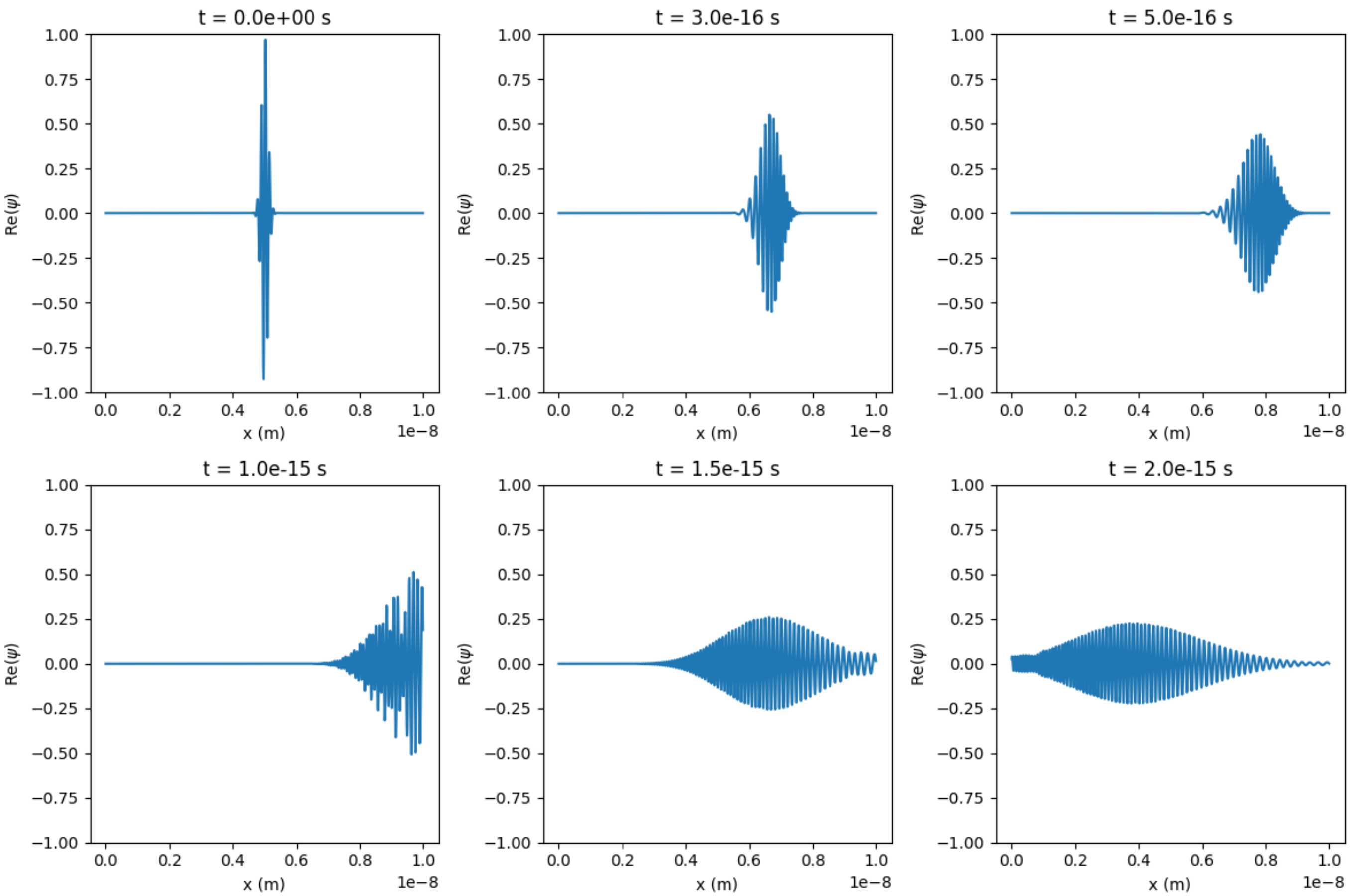

Figure 1: Real part of the wavefunction for six different times, obtained using the Crank-Nicolson method.

As expected, the wavefunction starts its motion towards the right, it moves at constant group velocity while being subject to dispersion. Then it reaches the wall, where it is forced to be zero due to the boundary condition. Therefore, it bounces back and undergoes interference, continuing its motion towards the left, until it reaches the other side and repeats this process back and forth.

In the code, we also perform an animation, which can be displayed by setting True in the if condition and running the code.

2 Problem 2

We solve the same problem, but using the spectral method, namely exploiting the fact that any solution of the Schrodinger equation can be expanded in the eigenstates of the Hamiltonian, which in these case are sine functions. Therefore we can perform a discrete sine transform to obtain the coefficients b_k of this expansion (whose expression is in the prompt). Once we have these coefficients, we can either reconstruct the real part of the wavefunction as follows (method 1):

$$Re\Big(\psi(x_n,t)\Big)=\frac{1}{N}\sum_{k=1}^{N-1}\Big[Re\big(b_k\big)\cos\Big(\frac{\pi^2\hbar k^2}{2ML^2}t\Big)+Im\big(b_k\big)\sin\Big(\frac{\pi^2\hbar k^2}{2ML^2}t\Big)\Big]\sin\Big(\frac{\pi kn}{N}\Big) \tag{3}$$

or we can perform the inverse discrete sine transform on the time evolution of the Fourier coefficients (method 2). In the code, we perform both methods. Figures 2 and 3 show the evolution in time of the real part of the wavefunctions using these two methods.

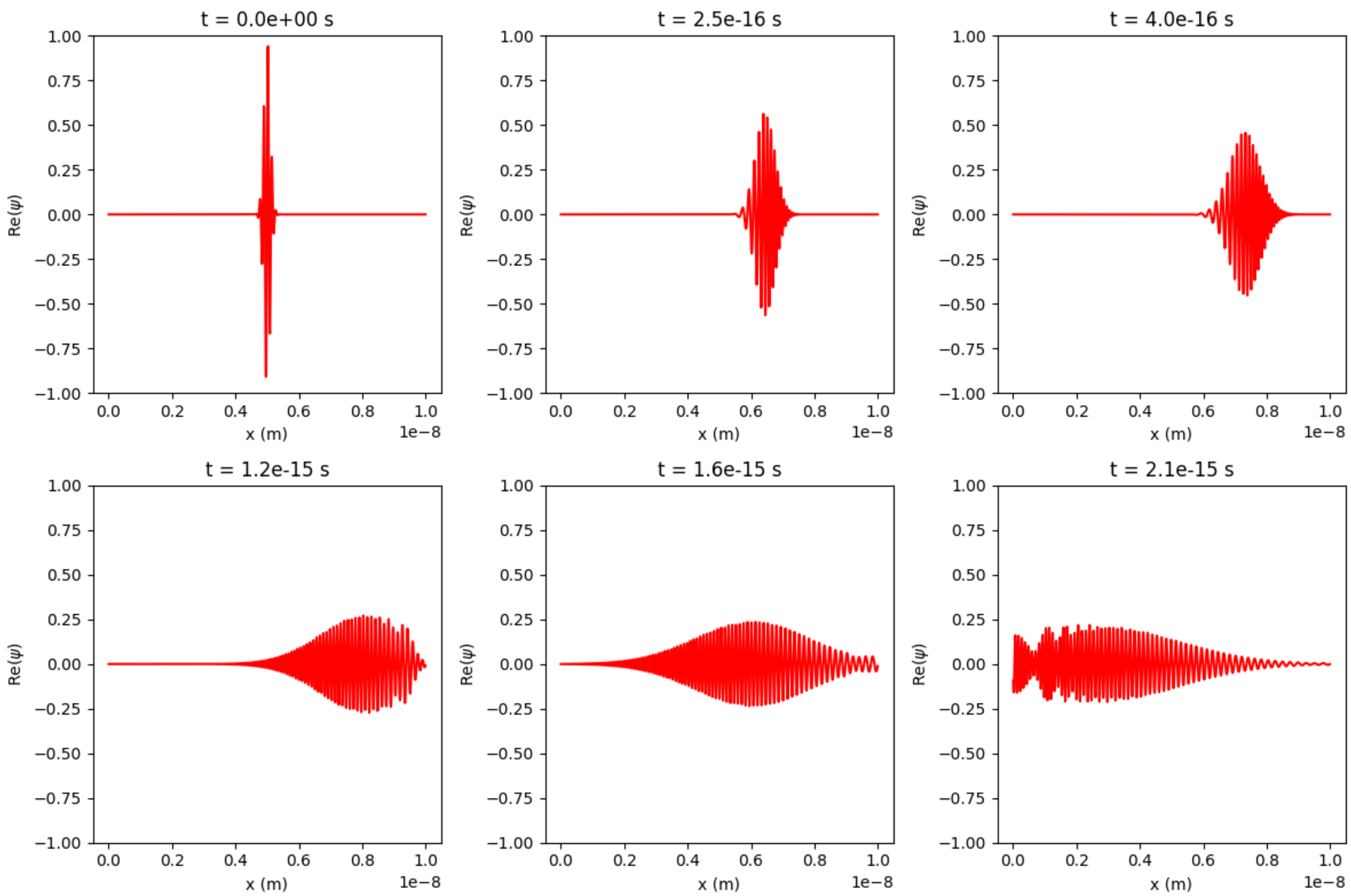

Figure 2: Real part of the wavefunction for six different times, obtained using method 1.

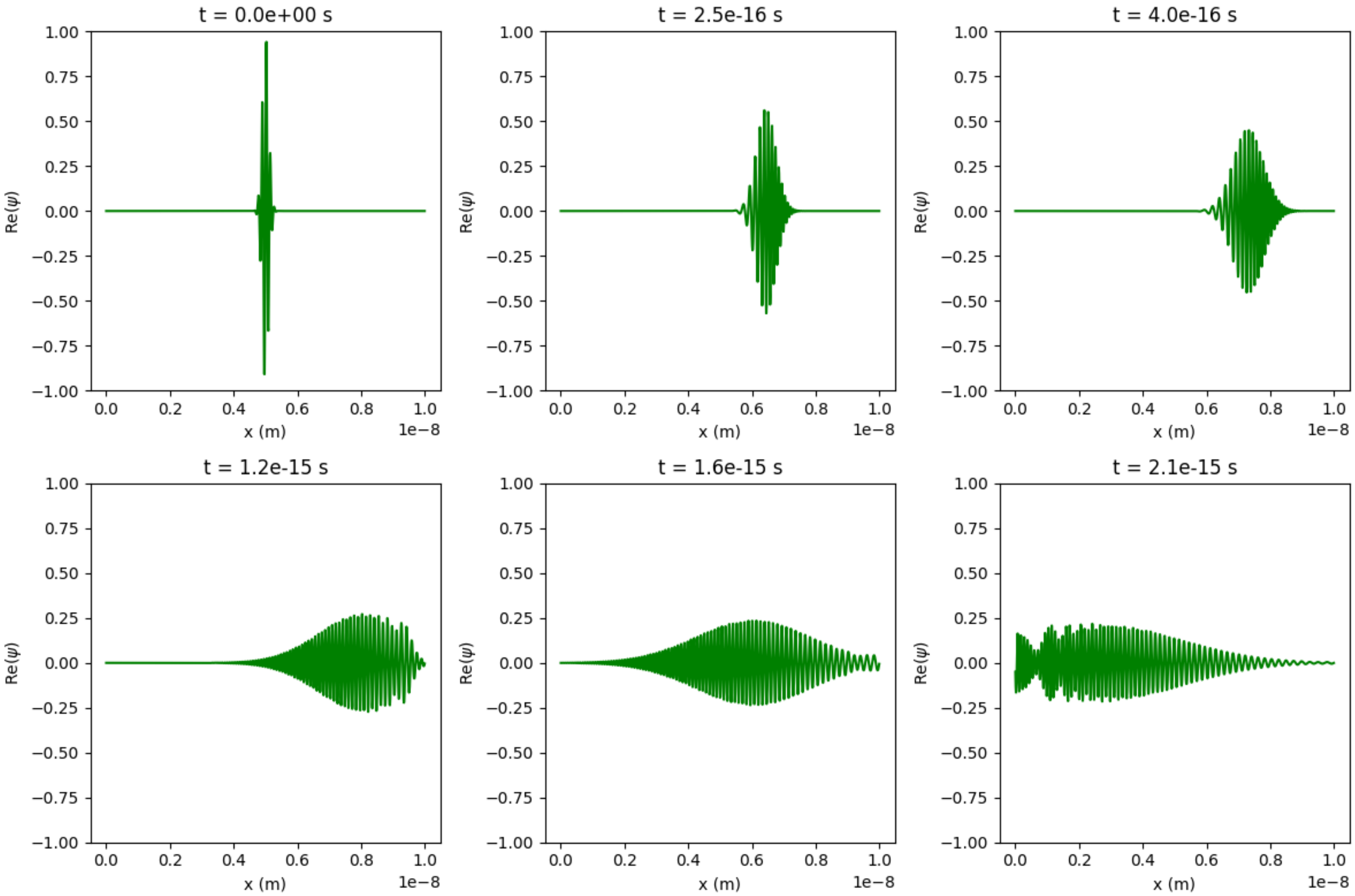

Figure 3: Real part of the wavefunction for six different times, obtained using method 2.