Computational Physics Homework 9

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1 Problem 1

This problem concerns using the Crank-Nicolson method to solve the full time-dependent Schrodinger equation for a particle of mass M with no potential energy in one dimension - this equation is given by:

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

We put the particle in a box with impenetrable walls so that we only have to solve the equation within a finite-sized space, forcing the wavefunction to become zero at the walls i.e. we have $\psi = 0$ at $x = 0$ and $x = L$. Replacing the second derivative in the above equation with a finite difference and applying Euler's method we eventually (after some manipulation) arrive at the Crank-Nicolson equations, which are of the form:

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

where h is the size of the time-step and $\mathbf{A}$ and $\mathbf{B}$ are both symmetric and tridiagonal:

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

with:

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

For the purposes of this problem we considered an electron of mass $M = 9.109 \times 10^{-31}$kg in a box of length $L = 0^{-8}$m. At $t = 0$ the electron wavefunction has the form:

$$\psi(x, 0) = \exp\left[-\frac{(x - x_0)^2}{2\sigma^2}\right] \mathrm{e}^{\mathrm{ikx}} \tag{5}$$

where:

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

The first part of this problem involved writing a program performing a single step of the Crank-Nicolson method for this electron, calculating $\boldsymbol{\psi}(t)$ given the initial wavefunction above and using $N = 1000$ spatial slices with $a = \frac{L}{N}$. Following this, the linear system was solved, yielding the new value for $\boldsymbol{\psi}$. The program was then extended to perform repeated steps and hence solve for ψ at a sequence of times a separation h apart.

Following this, the solution to the wavefunction was plotted for various different times as seen on the following page in *Figure 1.* At $t = 0$ we see the electron's wavefunction centralised within the potential well (as imposed by our initial condition). As we start the numerical calculation and have $t > 0$ we see that the wavefunction moves to the right (and rebounds at the boundary) and then as time increases further starts to

spread out and decrease in amplitude until it fills the whole well with oscillations of a similar amplitude. This makes sense due to the fact that at $t = 0$ we knew that the electron was localised in the centre of the well, however as time increased this position becomes more uncertain hence the spreading out of the wavefunction.

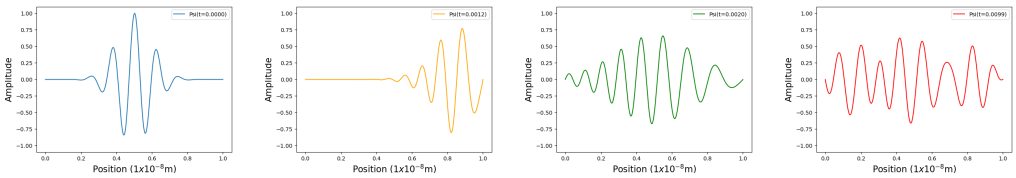

Figure 1: From left to right: Wavefunctions for times $t = 0.0000$s, $t = 0.0012$s, $t = 0.0020$s, $t = 0.0099$s