PHYS-GA 2000 Computational Physics PS5

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1 Problem 1

In this problem, we use Crank-Nicolson method to solve the full time-dependent Schrödinger equation of a particle being trapped in a infinite square well potential and hence develop a picture of how a wave function evolve with time. We have the Schrödinger equation as followed here:

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

And we have the boundary condition on the bounds of the well which are:

$$\psi(0) = 0 \tag{2}$$

$$\psi(L) = 0 \tag{3}$$

And by applying Euler's method and similar way but in reverse, take the average, we get Crank-Nicolson equation:

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

This is the key method we will use today.

We arange the values of ψ at interior points into a vector, and rewrite the C-N equation in the form of:

$$A\psi(t+h) = B\psi(t) \tag{5}$$

With matrices A and B symmetric and tridiagonal:

$$\begin{bmatrix} a1 & a2 & 0 & 0 & ... \\ a2 & a1 & a2 & 0 & ... \\ 0 & a2 & a1 & a2 & ... \\ ... & ... & ... & ... & ... \end{bmatrix} \tag{6}$$

And B of the similar form with given:

$a_1 = 1 + h\frac{i\hbar}{2ma^2}, a2 = -h\frac{i\hbar}{4ma^2}, b1 = 1 - h\frac{i\hbar}{2ma^2}, b2 = h\frac{i\hbar}{4ma^2}$.

Now we repeat the C-N method for 10000 times, to see how the wave-function goes:

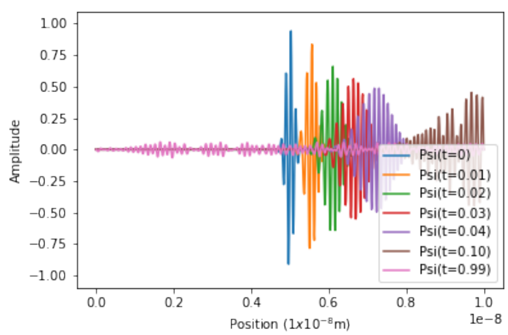

Figure 1: It is the plot of wave at different given time. We can see that the wave hit the wall and "bounce back". Which proves this method works fine.

The codes works well and gives figure above.

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