HW 14 Computational Physics
November 29, 2005 Due Noon on Friday, December 9

1. Implement the Crank-Nicholson scheme to calculate the quantum mechanical time evolution of a one-dimensional Gaussian wave packet with hard wall boundaries. (See Garcia §9.2 and §9.3.) Given the wavefunction $\mathbf{\Psi}$ at a time step t_n, the wavefunction at the next time step t_{n+1} is given by solving

$$\mathbf{Q}\boldsymbol{\chi} = \mathbf{\Psi} \tag{1}$$

for the vector $\boldsymbol{\chi}$, and then updating the wave function using

$$\mathbf{\Psi} = \boldsymbol{\chi} - \mathbf{\Psi}. \tag{2}$$

The new $\mathbf{\Psi}$ is the wavefunction at the next time step t_{n+1}. You must loop over time. You can be guided in your coding by the example in Garcia's Listing 9A.1. Notice, however, that you are not solving exactly the same problem.

Explanation:

A wave function $\psi(x,t)$ evolves in time according to Schrödinger's equation:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t).$$

Here $V(x)$ is the potential energy. For a system with $0 \le x \le L$, and considering times $0 \le t \le t_{\max}$, in discretized form we let

$$\begin{aligned}
x_j &= (j+1)h, \quad j = -1, 0, 1, 2, \ldots, j_{\max}, \quad \text{where } h = L/(j_{\max}+1),\\
t_n &= n\tau, \quad n = 0, 1, 2, \ldots, t_{\max}/\tau,\\
\psi_j^n &= \psi(x_j, t_n),\\
V_j &= V(x_j).
\end{aligned}$$

The CS approximation to the Hamiltonian is the matrix $\mathbf{H}$ with elements

$$H_{jk} = -\frac{\hbar^2}{2m}\frac{\delta_{j+1,k} + \delta_{j-1,k} - 2\delta_{jk}}{h^2} + V_j\delta_{jk}, \quad j,k = 0, 1, \ldots, j_{\max}-1.$$

Notice that $\mathbf{H}$ is tridiagonal, and that it implements the hard-wall boundary conditions. ($\mathbf{H}$ implicitly uses $\psi_{-1}^n = 0 = \psi_{j_{\max}}^n$.) The matrix $\mathbf{Q}$ in the Crank-Nicholson scheme is:

$$\mathbf{Q} = \frac{1}{2}\left[\mathbf{I} + \left(\frac{i\tau}{2\hbar}\right)\mathbf{H}\right].$$

$\mathbf{\Psi}$ on the right-hand-side of Eqs. (1) and (2) is the wavefunction at time t_n written as a vector:

$$\mathbf{\Psi} = \begin{pmatrix} \psi_0^n \\ \psi_1^n \\ \vdots \\ \psi_{j_{\max}-1}^n \end{pmatrix}.$$

$\mathbf{\Psi}$ on the left-hand side of Eq. (2) is similar but at time t_{n+1}.

Details:

- Notice that in the Crank-Nicholson scheme it is sufficient to store $\mathbf{\Psi}$ at only one time step (the latest). You *do not* need to store it at earlier times.
- Choose units so that $\hbar = m = 1$, and let $L = 200$.
- Choose values for $j_{\max}$ and τ.
- For this problem let $V(x) = 0$ so that you are investigating a free wave packet, but in a system with hard walls.
- You can solve for χ using `chi=solve_linear_equations(Q,psi)`. (You could instead use a function that takes advantage of the fact that $\mathbf{Q}$ is tridiagonal.)
- Choose the initial state to be a Gaussian wave packet

$$\psi(x, t = 0) = \frac{1}{\sqrt{\sigma_0\sqrt{\pi}}} e^{ik_0 x} e^{-(x-x_0)^2/2\sigma_0^2}.$$

  Here the wave vector k_0 is related to E_0, the expectation value of the wave packet's energy, by $E_0 = \hbar^2 k_0^2/2m$. Choose $x_0 = L/6$, $\sigma_0 = 4$ and $E_0 = 3$.
- $\boxed{\text{Plot } \operatorname{Re}\psi(x,0),\ \operatorname{Im}\psi(x,0), \text{ and } |\psi(x,0)| \textit{ vs. } x.}$
- In the absence of the confining walls at $x = 0, L$ there is a simple analytic expression for the time evolution of a Gaussian wave packet:

$$\psi(x, t) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} e^{ik_0(x-st/2)} e^{-(x-x_0-st)^2/2\sigma\sigma_0}.$$

  Here $s = \hbar k_0/m$ is the velocity's expectation value and

$$\sigma = \sigma_0 + \frac{i\hbar t}{m\sigma_0}.$$

- Plot occasional snapshots of the absolute values of the numerical and analytical results. You don't need to plot at every time step — plot often enough that you can see how the wave packets move in time. (Again: do not store Ψ at many times; instead, plot as time evolves.)
- Run your program long enough to watch the numerical wave packet bounce off the right and left walls. (The analytical wave packet of course doesn't know that the walls are there.)
- Your numerical and analytical results should be fairly close before the former hits the right-hand wall. Use this requirement to choose acceptable values for $j_{\max}$ and τ.
- $\boxed{\text{Hand in snapshots of } |\psi| \textit{ vs. } x \text{ at some representative times — enough to show the time evolution. Plot the numerical and analytical results together.}}$

2. Modify your code to add a potential

$$V(x) = \begin{cases} 1, & 0.5L \leq x \leq 0.52L \\ 0, & \text{otherwise} \end{cases} \quad .$$

Change your plots to show $V(x)$ as well as the wave function (and stop plotting the analytic results). Watch the wave packet as it bounces off the potential barrier. After a period of complicated interaction with the barrier, the packet ends up partially reflected and partially transmitted. Iterate for a long enough time that you have two outgoing wave packets, one on each side of the barrier.

Do the above for $E_0 = 4, 1.5, 1, 0.8$. For each energy hand in a plot of $\lvert\psi(x, t_{\max})\rvert$ *vs.* x at the final time.