PC5215, Numerical Recipes with Applications

Lab 4, due Tuesday 21 November 2023

1. In this last lab, we consider solving a one-electron time-dependent Schrödinger equation in one dimension scattering over a potential barrier. We send an electron from the left side of the barrier and ask the probability $T(E)$ (transmission probability) that the electron passes through the barrier, as a function of incoming electron energy E. The equation is

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi, \qquad \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

We choose two forms of the potential

$$V_1(x) = \begin{cases} 0, & x < 0, \\ V_0, & 0 \le x < a, \\ 0, & x \ge a. \end{cases} \qquad V_2(x) = \begin{cases} 0, & x < 0, \\ \dfrac{4V_0}{a^2}(a-x)x, & 0 \le x < a. \\ 0, & x \ge a. \end{cases}$$

For numerical computation, we take $V_0 = 1$ eV, and take the distance of the barrier a such that $\dfrac{\hbar^2}{2ma^2} = \dfrac{1}{100}$ eV.

a. First, we solve the problem with the rectangular potential V_1 analytically as a check for part (b) using numerical methods. To do this, use the plane wave as a trial solution $\Psi(x,t) = ce^{i(\pm px - Et)/\hbar}$ and match the boundary conditions (the function and its first derivative should be continuous) at 0 and a to find the whole solution. Determine the transmission probability by the absolute value square of the outgoing wave ($T = |c|^2$) if the incoming wave has amplitude 1. Note that $T + R = 1$, where R is the probability that the particle is reflected back to the left. Plot T as a function of E from 0 to 2 eV.

b. Next, we solve the same problem as in (a) numerically using "wave packet". The idea is that we send a wavepacket from the left side with energy centered around $E = \frac{p_0^2}{2m}$ and evolve the wavepacket in time for a sufficiently long time and then ask what is the total probability that the particle is on the right side. We use the following form for the Gaussian wavepacket with position centered around x_0 and momentum centered around p_0, as the initial condition to the time-dependent Schrödinger equation:

$$\Psi(x) \propto \exp\left(-\frac{1}{2\sigma^2}(x-x_0)^2 + \frac{i}{\hbar}p_0(x-x_0)\right).$$

Formally, the solution to the time-dependent Schrödinger equation can be obtained by $|\Psi(t)\rangle = e^{-it\hat{H}/\hbar}|\Psi(0)\rangle$. To evolve the wavepacket, we use the Crank-Nicholson method which is based on the evolution operator at small time intervals:

$$\left(1+i\frac{\Delta t\hat{H}}{2\hbar}\right)|\Psi(t+\Delta t)\rangle = \left(1-i\frac{\Delta t\hat{H}}{2\hbar}\right)|\Psi(t)\rangle .$$

The reason to split into two pieces is to preserve wavefunction normalization. Using the central difference for the second derivative with respect to position x, $f''(x) = \left[f(x+\Delta x) - 2f(x) + f(x-\Delta x)\right]/\Delta x^2$, derive a discrete scheme to solve a tri-diagonal linear system to get the new wavefunction, this solves the Schrödinger equation evolving in time, and then compute the probability that the particle is on the right-side.

Compare your answers for $T(E)$ with the exact one found in part (a). Pay attention to the unspecified parameters such as x_0, σ, Δt, Δx, number of points N, etc. You better make plots to see where your wavepacket is after a contain time step.]

c. Repeat the same calculation as in (b) with the parabolic potential V_2. Compare and discuss the result.