PC5215, Numerical Recipes with Applications

Lab 4, due Thursday, 13 November 2025

1. In this last lab, we consider solving a one-dimensional time-dependent Schrödinger equation. It presents an electron scattering over a square potential barrier. We send an electron from the left side of the barrier $x \ll 0$, 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 for the wave function $\Psi(x,t)$, as a complex number, 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 the form of a potential

$$V_1(x) = \begin{cases} 0, & x < 0, \\ V_0, & 0 \le x < a, \\ 0, & x \ge a. \end{cases}$$

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

First, we solve the problem (not a requirement for the lab) with the rectangular potential V_1 analytically as a check for part a using numerical methods. This is a standard problem in quantum mechanics textbooks. 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. The transmission probability T is given by the analytic formula

$$T(E) = \frac{1}{1 + \frac{V_0^2 \sin^2 \sqrt{\frac{2ma^2(E-V_0)}{\hbar^2}}}{4E(E-V_0)}}.$$

Plot T as a function of E from 0 to 2 eV, together with your data points by the numerical simulation.

   a. In this lab, we solve the problem 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 for splitting into two pieces is to preserve wavefunction normalization. Verify numerically that the wavefunction is indeed normalized at all time, i.e., $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1$. 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 given. Pay attention to the unspecified parameters such as x_0, σ, Δt, Δx, number of points N, etc.

b. It is a good idea to make sequence of the plots (or even better, a jpeg movie) of the wavefunction squared $|\Psi(x,t)|^2$ to see if your parameters make sense, and the time choosing is propriate so that the transmission function $T(E)$ can be calculated correctly.