

PC5215, Numerical Recipes with Applications

Lab 4, due Friday 13 November 2015

1. In this last lab, we consider solving 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 what is the probability $T(E)$ (transmission probability) that the electron passes through the barrier, as a function of incoming electron energy E . The equation is

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

We choose two forms of the potential

$$V_1(x) = \begin{cases} 0, & x < 0, \\ V_0, & 0 \leq x < a, \\ 0, & x \geq a. \end{cases} \quad V_2(x) = \begin{cases} 0, & x < 0, \\ \frac{4V_0}{a^2}(a-x)x, & 0 \leq x < a, \\ 0, & x \geq a. \end{cases}$$

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.

- a. First, we solve the problem with the rectangular potential V_1 analytically as a check for part (b) and (c) 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 and evolve the wavepacket in time for 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 center around p_0 ,

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

To do this, we use the “operator splitting method”. First, note that formally, the solution can be found by $\Psi(t + \Delta t) = e^{-\frac{i}{\hbar} H \Delta t} \Psi(t)$. We then use Trotter-Suzuki formula

$$e^{A+B} \approx e^A e^B$$

where A and B are arbitrary operators but small of order Δt (a more accurate one is $e^{A+B} \approx e^{A/2} e^B e^{A/2}$). We take the kinetic energy term as A and potential energy

term as B . In coordinate representation, $e^B \Psi = e^{-\frac{i}{\hbar} \Delta t V(x)} \Psi(x)$, which is very easy, but the kinetic energy part is hard because it is a differential operator. However, it will be easy if we work in momentum representation. Then it becomes

$e^A \Psi = e^{-\frac{i}{\hbar} \Delta t \frac{p^2}{2m}} \Psi(p)$. The relationship between coordinate and momentum representation is obtained by Fourier transform:

$$\Psi(p) = \langle p | \Psi \rangle = \int_{-\infty}^{+\infty} dx \langle p | x \rangle \langle x | \Psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \Psi(x) e^{-i\frac{px}{\hbar}} dx.$$

To implement a Schrödinger equation solver on computer, (i) discretize the coordinate x and momentum p appropriately so that FFT can be conveniently performed. (ii) multiply the associated phase factor for the Trotter-Suzuki decomposition to evolve Ψ in time, changing the representations whenever it is needed. Compare your answers for $T(E)$ with the exact one find in part (a). Pay attention to unspecified parameters such as x_0 , σ , Δt , discretization steps for x and p and number of sampling point N in FFT, so that your answers are reasonably accurate.

- c. Repeat the same calculation as in (b) with the parabolic potential V_2 . Compare and discuss the result.
- d. Alternative possibly better methods not using FFT: Crank-Nicholson method. This will be a bonus question if some of you wish to try and compare with FFT/Trotter-Suzuki method in part b.