PC5215, Numerical Recipes with Applications

Lab 4, due Tuesday 13 November 2018

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

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

We choose two forms of the potential

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

For numerical computation, we take V_0 = 1 eV, and take the distance of the barrier a such that $\frac{\hbar^2}{2ma^2} = \frac{1}{100}$ 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 $E = \frac{p_0^2}{2m}$ 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, as initial condition to the time-dependent Schrödinger equation:

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

To evolve the wavepacket, 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 computationally, 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 the 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. [Hint: σ should be large otherwise it is not close to a plane wave; N should be of the order 10^4. 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.

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.