Solving the time-independent Schrödinger's equation in one dimension: The Finite Difference Method for tunneling problem

In this problem, you will solve the time-independent Schrödinger's equation for a tunneling problem. In the given problem, we will be using a finite difference method on a grid.

- **Theory**

  We will discretize the wavefunction on a grid, instead of having that as a continuous function. For a regular grid, the x-axis value at each grid point is given by x_j=$j\ dx$. The integer values of j denote the "address" along the x-axis. Hence, the values of the wavefunction at each of these grid points are going to be $\psi(x_j) = \psi(j\ dx) \equiv \psi_j$.

  Here, we will apply the concept of "finite difference" from a wavefunction perspective. In the previous example, we applied the FD from the Hamiltonian perspective.

$$\frac{-\hbar^2}{2m}\psi''(x) + V(x)\psi(x) = E\psi(x) \tag{1}$$

$$\implies \psi''(x) + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0 \tag{2}$$

  Using finite-difference method, the Eq.2 can be rewritten as

$$\frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{dx^2} + \frac{2m}{\hbar^2}\left[E - V_j\right]\psi_j = 0. \tag{3}$$

  The above can be re-arranged to give

$$\psi_{j+1} = \left(2 - \frac{2m}{\hbar^2}\left[E - V_j\right]dx^2\right)\psi_j - \psi_{j-1}. \tag{4}$$

- We will take the incident wave as a plane wave, $c_0 e^{-ikx}$. The reflected wave will be $c_1 e^{ikx}$. Similarly, the transmitted wave will be $c_2 e^{-ikx}$. Here, the k values are taken to be the same, assuming an elastic transmission. k is related to the incident kinetic energy as $k = \sqrt{2mE/\hbar^2}$.

- Computing the tunneling probability

$$t = \left|\frac{c_2}{c_0}\right|^2 \tag{5}$$

$$r = \left|\frac{c_1}{c_0}\right|^2 \tag{6}$$

$$t + r = 1 \tag{7}$$

$$c_0^2 + c_1^2 \pm 2\left|c_0 c_1\right|^2 \tag{8}$$

$$P_{avg} = \left|c_0\right|^2 + \left|c_1\right|^2 \tag{9}$$

$$\tag{10}$$

$$\begin{aligned}
1 &= t + r && (11)\\
1 &= \frac{1}{|c_0|^2} + \frac{|c_1|^2}{|c_0|^2} && (12)\\
|c_0|^2 &= 1 + |c_1|^2 && (13)\\
|c_0|^2 &= 1 + P_{avg} - |c_0|^2 && (14)\\
|c_0|^2 &= \frac{1 + P_{avg}}{2} && (15)\\
\implies t &= \frac{2}{1 + P_{avg}} && (16)
\end{aligned}$$

- Calculation of P_{avg}: Find the maximum and minimum of the oscillations in the incident region, far away from the potential (let us say after 600th point). Then compute the average.

- Problem statement: Consider a PIB problem with the grid boundaries at 0 and 10, respectively. The potential is defined as

$$V(x) = \begin{cases} 0, & \text{if } x < 4 \\ 9, & \text{if } 4 \leq x \leq 5 \\ 0, & \text{if } 5 < x. \end{cases} \tag{17}$$

We will start with c_2=1, and hence, the calculation actually works backward in space to compute c_0 which should be consistent with c_2=1. In extreme left (where the wave is a free wave), the $\psi_{j=0}$ =$exp(-ikx) = 1$. Similarly, at $j = 1$ (at dx), $\psi_{j=1}$=$exp(-ik \times dx)$. Once, these two are known, we can calculate the others using the finite difference scheme. Use the following values: $\hbar$=1, m=1, dx=0.01. Write a Fortran code to compute the transmission probability as a function of incident kinetic energy. Vary the incident energy from 1 to 26 eV with $\Delta E = 0.1$ eV. Plot "transmission probability" vs "incident kinetic energy".

A zip file containing the following files has to be submitted

1. The code
2. Two output files, one for the wavefunction at E=9.0 eV as a function of x, and the other for the tunneling probability as a function of energy
3. Two figures

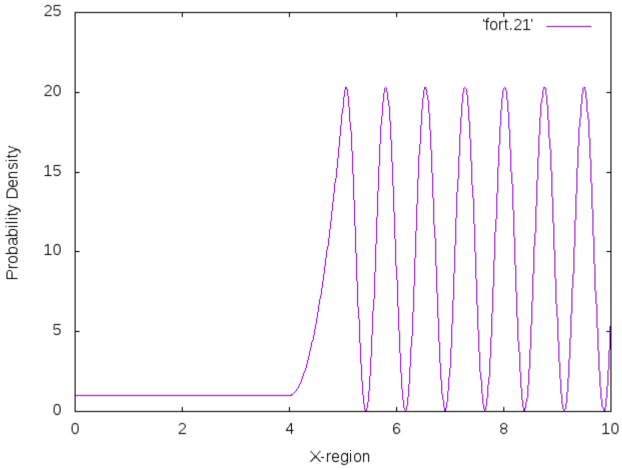

Figure 1: Tunneling Problem: Wavefunction oscillations

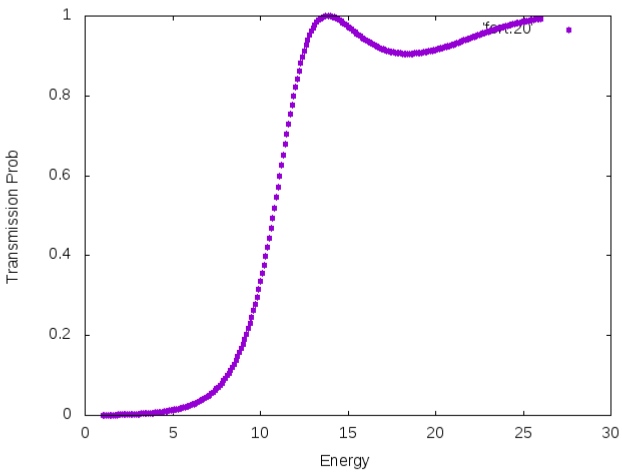

Figure 2: Tunneling Problem: Probability as a function of Kinetic energy