PHYS 325: Computational Physics III

Winter 2023

Exercise 10.2

1. Modify the scripts presented in class to solve the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

for the potential

$$V(x) = \begin{cases} 0 & (x < 0)\,, \\ V_0 & (0 < x < a)\,, \\ 0 & (x > a)\,, \end{cases}$$

where V_0 may be positive, negative, or zero. As discussed in class,

- All quantities become complex. See the course web page for how to handle this.
- Crank-Nicholson differencing of the Schrödinger equation gives

$$\begin{aligned} -\tfrac{1}{2}i\alpha\,\psi_{j-1}^{n+1} + \left[1 + i\alpha + \tfrac{1}{2}iV(x_j)\Delta t/\hbar\right]\psi_j^{n+1} - \tfrac{1}{2}i\alpha\,\psi_{j+1}^{n+1} \\ = \tfrac{1}{2}i\alpha\,\psi_{j-1}^{n} + \left[1 - i\alpha - \tfrac{1}{2}iV(x_j)\Delta t/\hbar\right]\psi_j^{n} + \tfrac{1}{2}i\alpha\,\psi_{j+1}^{n}\,, \end{aligned}$$

  where $\alpha = \hbar\Delta t/(2m\Delta x^2)$. Thus the arrays `a`, `b`, and `c` are constant in time, with

$$\begin{aligned} a_j &= -\tfrac{1}{2}i\alpha \\ b_j &= 1 + i\alpha + \tfrac{1}{2}iV(x_j)\Delta t/\hbar \\ c_j &= -\tfrac{1}{2}i\alpha \end{aligned}$$

  for $j = 1, \ldots, J-2$. (The values for $j = 0$ and $j = J-1$ are set by the boundary conditions, as described below.) The array `r` is defined by the right-hand side of the above difference equation (again for $j = 1, \ldots, J-2$).

- We will choose the simplest possible boundary conditions: $\psi_0 = \psi_{J-1} = 0$. These are imposed by suitable choices of $b_0, c_0, r_0, a_{J-1}, b_{J-1}$, and c_{J-1}:

$$\begin{aligned} b_0 &= b_{J-1} &= 1 \\ c_0 &= a_{J-1} &= 0 \\ r_0 &= r_{J-1} &= 0 \end{aligned}$$

- The initial state will be a normalized *Gaussian wave packet*:

$$\psi(x,0) = \left[2\pi\delta x^2\right]^{-1/4}\exp\left\{-\frac{(x-\bar{x})^2}{4\delta x^2} + \frac{i\bar{p}x}{\hbar}\right\}\,,$$

  where $\bar{x}$ is the initial position of the packet center, δx is the packet width, and $\bar{p}$ is the packet's momentum (so the energy is $\langle E\rangle = \bar{p}^2/2m$).

Make the following parameter choices in your program: $\hbar = 1$, $m = 1$, $\delta x = 2$, $\bar{x} = -5$, $\bar{p} = 5$, $a = 1$, and run the calculation on a grid of J points for $-20 \le x \le 20$ with time step δt. Choose J and δt according to the criteria developed in Exercise 10.1.

Carry out the calculation for $V_0 = 4, 6, 8, \ldots, 20$. For the cases $V_0 = 8, 10, 12$, plot $|\psi(x,t)|^2$ as a function of x at $t = 0, 1, 2, 3, 4$.

Continue all runs until the solution clearly describes two well-defined reflected and transmitted parts. At this time, determine the transmission and reflection probabilities, defined respectively as

$$T = \int_a^{\infty} |\psi|^2 \mathrm{d}x, \qquad R = \int_{-\infty}^{0} |\psi|^2 \mathrm{d}x.$$

Plot the expressions for T and R from the time-independent theory (as presented in class), as functions of $\varepsilon = E/V_0$, and add points corresponding to the 9 time-dependent calculations you have just completed.