

Assignment 3

Course: *Computational Physics (PHYS4150/8150)* – Professor: *Prof. Zi Yang Meng*

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Due date: *Nov. 14th, 2025 (Friday)*

This assignment is also a project; you will need to form a group of 4 to 5 people and present your work on these questions during the class on **Nov. 14th**. The presentation should contain your answer to the questions, as well as how you solved them.

1. Consider again the problem of traffic flow. In this question, we simplify the flux as $F(x) = C * \rho(x)$ so we get an advection function $\frac{\partial \rho}{\partial t} = -C \frac{\partial \rho}{\partial x}$. We set $L = 400$ and $C = 1$. Use **Lax-Wendroff method** to see the different directions of flow for these initial conditions (the animation is needed for display).

$$(a) \rho(t = 0, x) = \rho_0(x) = \begin{cases} 4(x - \frac{L}{4})^2 / L^2, & \frac{L}{4} < x < \frac{L}{2}, \\ 0, & \text{else.} \end{cases}$$

$$(b) \rho(t = 0, x) = \rho_0(x) = \begin{cases} (\frac{L}{4} - |x - \frac{L}{2}|) \frac{4}{L}, & \frac{L}{4} < x < \frac{3L}{4}, \\ 0, & \text{else.} \end{cases}$$

- (c) Set $C = -1$ and use the $\rho(t = 0, x)$ in part (b), check the moving direction of the traffic flow

2. Conduct a von Neumann stability analysis on the following numerical schemes for the advection equation

$$\frac{\partial u}{\partial t} = -c \frac{\partial u}{\partial x} :$$

- (a) Forward Time Centered Space (FTCS)
- (b) Forward Time Forward Space (FTFS)
- (c) Centered Time Centered Space (CTCS, also known as the Leap-Frog method)
- (d) Lax-Wendroff

Please detail the stability analysis process for each scheme, as outlined in the lecture.

3. Tunneling is a quantum behavior where there is no classical counterpart. In this question, we study the tunneling behavior of a Gaussian wave packet.

Assuming a finite square potential barrier, and an initial right-moving Gaussian wave packet on the left of the barrier. Simulate the motion of the wave packet and answer the below questions.

The Gaussian wave packet has the form:

$$\psi(x) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{4}}} e^{-\frac{(x-x_0)^2}{(2\sigma)^2}} e^{ik_0x} \quad (1)$$

The recommended simulation details are:

- Range of the 1D box: [-200,200].
- Spatial step: 0.8.
- Time step: 0.5.
- Barrier center position: 0, Barrier height: 0.5, barrier width: 5.
- Gaussian wave packet $x_0 = -150, \sigma_0 = 5, k_0 = 1$.

- (a) Use the unitary discretization scheme to demonstrate the tunnelling process. An example of the probability amplitude of the wave function before and after the tunnelling is shown in Fig. 1.

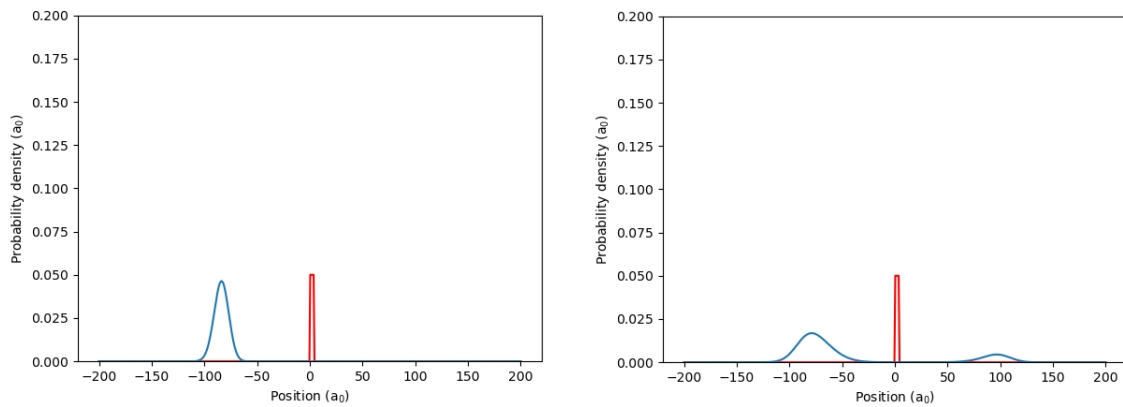


Figure 1: Snapshot of the motion of Gaussian wave packet before and after the collision with the barrier.

- (b) According to the analytical calculation of quantum mechanics, the transmission rate (the probability amplitude that penetrates the barrier) is:

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0-E)} \sinh^2 \frac{\sqrt{2m(V_0-E)}a}{\hbar}} \quad (2)$$

Here a and V_0 are the width and the height of the barrier separately, $E = \frac{\hbar^2 k^2}{2m} = \frac{1}{2}$ is the kinetic energy of the wavepacket. we choose $\hbar = 1, m = 1$. Perform simulations over different barrier widths and compare your result with theoretical prediction. See the example in Fig. 2.

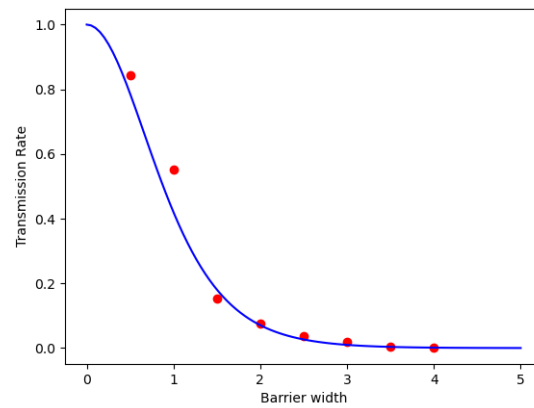


Figure 2: Theoretical prediction (in blue) and the numerical result of the transmission rate (in red).