THE UNIVERSITY OF HONG KONG
DEPARTMENT OF PHYSICS

Assignment 3

Course: *Computational Physics (PHYS4150/8150)* – Professor: *Prof. Zi Yang Meng*
Tutor: *Mr. Tim Lok Chau, Mr. Min Long*
Due date: *14th November, 2024*

1. Stationary Schrödinger Equation.
Use the Numerov matrix method to solve the stationary Schrödinger equation with the following potential,

$$V(x) = \begin{cases} x & \text{if } x \geq 0 \\ 10^4 & \text{if } x < 0 \end{cases}$$

We set the term $\gamma^2 = 2m\omega/\hbar = 2$. The range of x is from -5 to 15 with $dx = 0.1$ and therefore $N = 200$. Please numerically solve the equation and complete the following questions.
(**Note:** for parts a) and b). The graphs are for you to benchmark the shape of the wave function and probability density function only. The **spacing is not exactly proportional to the energy difference**.)

(a) Plot the wave function $\psi_n(x)$ for $n = 1, 2, 3, 4, 5$. (Refer to Fig. 1a)

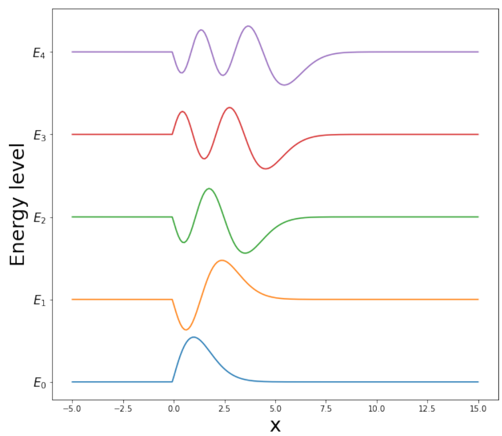

Figure 1: Wavefunction of first five eigenstates

(b) Plot the numerical probability density $P_n(x) = |\psi_n(x)|^2$ for $n = 1, 2, 3, 4, 5$. (Refer to Fig. 1b)

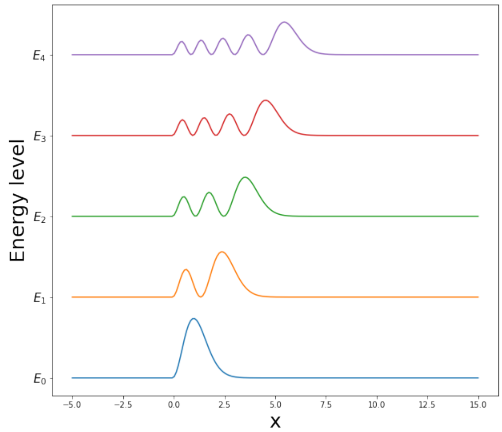

Figure 2: Probabiltiy density function of first five eigenstates

(c) Plot the eigenenergies as a function of n.

2. Time-dependent Schrödinger Equation.
Please use the Crank-Nicolson Scheme to solve the time-dependent Schrödinger equation numerically. Using the same variables setting as in the lecture: $\hbar = m = 1$, $x_0 = 0$, $L = 40$, $\sigma_0 = 1$, $k_0 = 7$, $N = 401$, $\tau = 0.03$ (time difference), $h = 0.1$ (spatial difference). The range of x is from -20 to 20, and the range of t is from 0 to 15. The initial condition is $\Psi(t=0,x) = \frac{1}{\sqrt{\sigma_0\sqrt{2\pi}}} e^{ik_0x} e^{-\frac{1}{2}\frac{(x-x_0)^2}{2\sigma_0^2}}$. The potential is as follows,

$$V(x) = \begin{cases} \frac{k_0^2}{2}\cos^2\left(\frac{\pi(x+6)}{8}\right) & \text{if } -10 < x < -2 \\ \frac{k_0^2}{2}\cos^2\left(\frac{\pi(x-6)}{8}\right) & \text{if } 2 < x < 10 \end{cases}$$

(a) Please use an animation to show the probability density $P(t,x) = |\Psi_n(t,x)|^2$ for t from 0 to 15. The screenshot at $t = 120\tau$ is shown in Fig 2.

(b) Show that the probability density P(t,x) is conserved during the evolution.

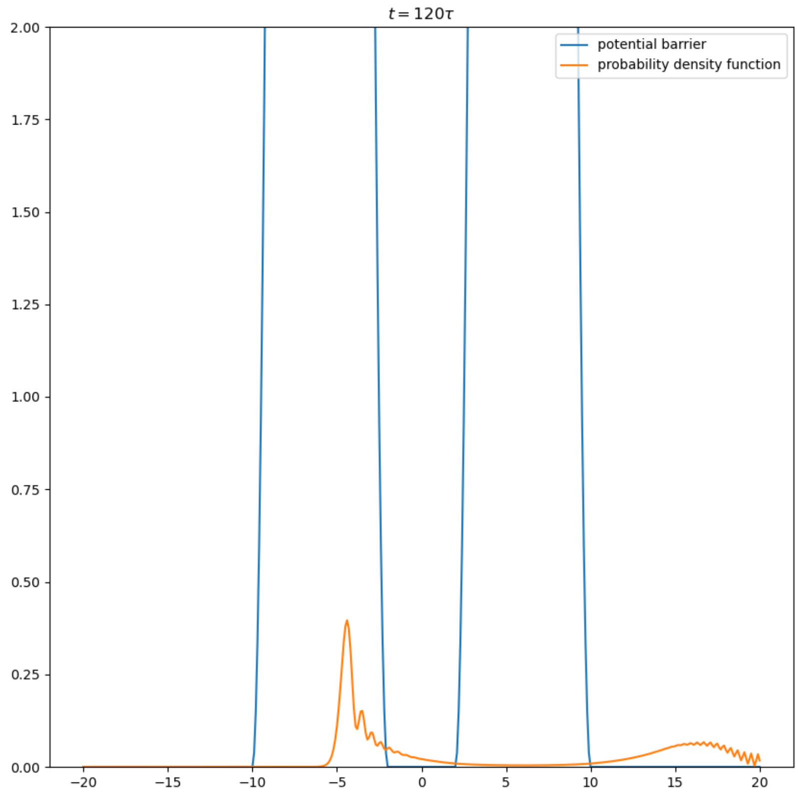

Figure 3: Screenshot of the animation at $t = 120\tau$.