PHYS516 ASSIGNMENT 5—TIME DEPENDENT SCHRÖDINGER EQUATION

Due: Monday, March 8, 2021

1. Derive the exponentiation of the kinetic energy operator, Eq. (20), in the lecture note on "Quantum Dynamics Basics". (Hint: Introduce the unitary transformation to diagonalize the 2×2 matrix; refer to the derivation of the asymptotic probability distribution of the 2-state system in the lecture note on "Monte Carlo Basics".)

2. Write a program that numerically integrates the time-dependent Schrödinger equation in 1 dimension, using the finite-difference method on N mesh points. Use the spectral method based on the fast Fourier transform algorithm as in the lecture note on "Quantum Dynamics Basics II—Spectral Method".

   The potential energy, $V_j = V(x_j)$ is defined as follows ($x_j = jdx$, where the mesh spacing $dx = L/N$, $j = 0, ..., N-1$, and L is the system length): $V_j = B_H$ if $(L - B_W)/2 < x_j < (L + B_W)/2$, E_H if $j = 0$ or $N-1$, and 0 otherwise. (B_H, B_W, and E_H are the barrier potential height, barrier width, and edge potential height, respectively.)

3. Run QD simulation for $N = 512$, $L = 50.0$, $\Delta t = 2\times10^{-3}$, $B_H = 5.0$, $B_W = 1.0$, and $E_H = 50.0$. Run the simulation for 4,000 time steps, starting with a Gaussian initial wave function,

   $$\psi(x,t=0) = C\exp\left(-\frac{(x-x_0)^2}{4\sigma^2}\right)\exp\left(i\sqrt{2E_0}x\right)$$

   (C is the pre-factor to normalize the probability to unity), where $x_0 = 12.5$, $\sigma = 3.0$ and $E_0 = 5.0$. Plot and report the following:

   (a) Plot the kinetic, potential and total energies as a function of time;

   (b) Plot the transmission coefficient $T(t)$ and reflection coefficient $R(t)$ as a function of time, and report their values at the last time step. Here, the transmission and reflection coefficients are defined as

   $$T(t) = \int_{(L+B_W)/2}^{L} dx\left|\psi(x,t)\right|^2 ,$$

   $$R(t) = \int_{0}^{(L-B_W)/2} dx\left|\psi(x,t)\right|^2 .$$

Submit your proof, a copy of your source code, and the plots.