COMPUTATIONAL PHYSICS LAB

(PH49012)

SPRING-2021, IIT KGP

Lab Exam
Date: April 5, 2021
Time duration: 3 Hrs (From 2 PM to 5 PM)

Instructions:

(1) Write the algorithms / your plans to go about the assigned problems: Sketch briefly the mathematical expressions / governing equations and show the discretization (if it is used).
(2) **Implementation of the above instruction carries 4 points for each question**.
(3) Plots should be self explanatory with proper labels and legends. **Plotting in each question carries another four marks.**
(4) Marks distribution for each question: 4 (See point: 2) + 12 (Coding + Viva) + 4 (see point 3)

Q1. Particle in a potential well

Let us consider the system of a particle in a 1D box. The time-independent Schrödinger equation corresponding to the system is given by

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

where $V(x)$ is the potential defined as

$$V(x) = \begin{cases} 0 & \text{if} \quad 0 \le x \le a \\ \infty & \text{otherwise} \end{cases} \tag{2}$$

The energy eigen values of the particle are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}, \quad n = 1, 2, 3, ... \tag{3}$$

Write a pragram to solve Eqn. (1) for the region $0 \le x \le a$ for ground state and first three excited states, and plot the corresponding probability densities ($|\psi|^2$) on a single page using subplots. Don't forget to normalize your wave function once you update it, otherwise your solution will blow up. To normalize your wave function in python, you may simply use the following

$$\psi_N = \frac{\langle\psi|\psi\rangle}{\text{numpy.trapz}(\langle\psi|\psi\rangle)}$$

Consider $\hbar = m = 1$, $a = 1$, and 500 slices to discretize the domain.

(20 points)

Q2. The nonlinear pendulum

Let us consider the equation of motion of a nonlinear pendulum given by

$$\frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} = -\frac{g}{l}\sin\theta \tag{4}$$

Because it is nonlinear it is not easy to solve this equation analytically. But a solution on the computer is straightforward. We first use the following trick to convert it into two first order differential equations.

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = \omega, \qquad \frac{\mathrm{d}\omega}{\mathrm{d}t} = -\frac{g}{l}\sin\theta \tag{5(a, b)}$$

You may consider an array $\mathbf{r} = (\theta, \omega)$ and use 4th order Runge-Kutta method in vector form to solve the two equations simultaneously. The method gives us the solution for both, but we can simply ignore the value of ω if we don't need it. Use your program to calculate the angle θ of displacement for several periods of the pendulum when it is released from a standstill at $\theta = 179^0$ from the vertical. Make a graph of θ as a function of time.

(20 points)
