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BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI

(I Semester 2016-17)

Mid Term Examination (Close Book)

Computational Physics (PHY F313)
Date: 08-10-2016 **Max Time: 60 min**
Max Marks: 60 **Weightage 20 %**

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Important:
Finding numerical answer is good but weightage will be given for correct procedure. Blindly finding the answer has no meaning.

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1. To find out the roots of any equation by NR method, the initial guess is very important. What should be your starting point for a function like $P_8(x)$ (*Legendre polynomial*) to solve? Justify your answer. **[5]**

$$P_8(x) = \frac{6435x^8 - 12012x^6 + 6930x^4 - 1260x^2 + 35}{128}$$

2. Consider a particle of mass m that is roaming between a solid wall at $x = \pm a/2$ of a 1 dimensional impenetrable box. The ground state wave function for this particle is

$$\Psi(x,t) = A\cos\left(\frac{\pi x}{a}\right)\exp\left(-\frac{-iEt}{\hbar}\right)$$

for the region $-a/2 < x < a/2$ and zero elsewhere. You may use this form of wave function to find out the average location of the particle between $-a/2 < x < a/2$ (*you might have found the exact solution for this problem earlier!*). This can be written as,

$$\overline{x} = (\overline{x^2})^{1/2} = \left[2A^2\int_0^{a/2} x^2\cos^2\left(\frac{\pi x}{a}\right)dx\right]^{1/2}$$

The exact solution to this problem is $0.18a$ ($A = \sqrt{2/a}$). Use the 10 point Gauss Legendre method to find out this integral for the two values of a: 1 & 3, and estimate the error in your calculations. **[20]**
The Gaussian points are:

± 0.9739065	± 0.8650634	± 0.6794096	± 0.4333954	± 0.1488743
0.0666713	0.1494514	0.2190864	0.2692667	0.2955242

3. The unnormalized radial probability density for the ground state of the hydrogen atom is given as,

$$P_{10}(r) = r^2\exp\left(-\frac{2r}{a_0}\right)$$

where $a_0(\approx 0.529$ Å) is the radius of the smallest orbit of hydrogen atom. Use suitable numerical method to find out the location at which the radial probability density is a maximum for the ground state of the hydrogen atom (*you have to make an intelligent initial guess to solve this problem!*). **[15]**

4. Consider a simple pendulum of mass m connected by a massless string to a rigid support. Assume that only two forces are acting on the bob, gravity and tension of the string. The equation of motion of this system can be written as,

$$\frac{d^2\theta}{dt^2} = -\frac{g}{l}\sin\theta.$$

If the bob is released from 15^0, find out its angular position at the end of 5 second. You may use the simplest method for ODE to solve by choosing a step size of 1 s. **[20]**

========== ALL THE BEST ==========

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BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI

(I Semester 2016-17)

Mid Term Examination (Open Source)

Computational Physics (PHY F313)

Date: 08-10-2016 **Max Time: 30 min**

Max Marks: 30 **Weightage 10 %**

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IMPORTANT

- The in-built functions of *MATLAB etc.* are **not allowed** to execute your codes.
- Once you are done, zip all the files in that folder as yourid.zip. *For eg*, if our ID is **2014B5A1345P**, the name of zip file should be, **2014B5A1345.zip**

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1. Repeat Q2 of part A by Monte Carlo method. **[12]**
2. Repeat Q4 of part A by RK-4 method and comment on your results. Plot the variation of θ with time. **[18]**

========== ALL THE BEST ==========