* A - 1 5 2 0 *

A-1520

M. Sc. (Sem. III) Examination

March / April – 2015

Physics : PH (T) - 534

(Computational & Simulation Methods in Physics)

Time : **3** Hours] [Total Marks : **70**

Instructions :

(1)

નીચે દર્શાવેલ ☛ નિશાનીવાળી વિગતો ઉત્તરવહી પર અવશ્ય લખવી.
Fillup strictly the details of ☛ signs on your answer book.

Name of the Examination :

☛ **M. SC. (SEM. 3)**

Name of the Subject :

☛ **PHYSICS : PH (T) - 534**

☛ Subject Code No. : **1 5 2 0** ☛ Section No. (1, 2,.....) : **Nil**

Seat No. :

Student's Signature

(2) Attempt all questions.

(3) Symbols used have their usual meaning.

(4) Figures to the **right** indicate marks.

(5) Non-programmable scientific calculator may be used.

1 Attempt any **two** questions :

(i) (a) Discuss in detail the Crout LU decomposition method to find the solution of system of linear equations. **3**

(b) Fit a cubic spline curve that passes through (0, 0.0), (1, 0.5), (2, 2.0), (3, 1.5) with the natural boundary conditions $S''(0)=0;\ S''(3)=0.$ **4**

(ii) (a) Discuss the least-square method to fit a data to a curve $y=mx+c.$ **3**

(b) Perform LU decomposition of the following matrix and hence find its inverse matrix : **4**

$$\begin{bmatrix} 2 & -5 & 1 \\ -1 & 3 & -1 \\ 3 & -4 & 2 \end{bmatrix}.$$

(iii) (a) What is meant by cubic spline ? What are the conditions required to evaluate the unknown parameters in the spline equations ? **3**

(b) Using the principles of least squares, find an equation of the form $y = ae^{bx}$ that fits the following data : **4**

x:	1	2	3	4	5
y:	0.6	1.9	4.3	7.6	12.6

2 Attempt any **two** questions :

(i) (a) Discuss advantages and disadvantages of various methods for eigenvalue problem. **3**

(b) Using Romberg's integration method, find the value of $\int_1^{1.8} f(x)\,dx$ correct to $O(h^4)$ starting with Trapezoidal rule, for the tabular values : **4**

x :	1.0	1.2	1.4	1.6	1.8
$f(x)$:	1.543	1.811	2.151	2.577	3.107

(ii) (a) What is meant by improper integrals ? How are they evaluated ? **3**

(b) Compute $\int_2^4 \left(x^4 + 1\right) dx$ using three point Gauss quadrature method. **4**

(iii) (a) List the two ways by which the accuracy of numerical integration process can be improved. Discuss Romberg integration procedure and how is it related to Richardson extrapolation. **3**

(b) Find the largest eigenvalue and corresponding eigenvector of the matrix $\begin{bmatrix} 3.556 & -1.778 & 0 \\ -1.778 & 3.556 & -1.778 \\ 0 & -1.778 & 3.556 \end{bmatrix}$ by Power method up to three iterations. **4**

3 Attempt any **two** questions :

(i) (a) What is meant by Fast Fourier Transform ? Discuss an algorithm for FFT. **3**

(b) Explain elliptic, parabolic and hyperbolic categories of linear, second-order partial differential equations with one physical example in each case. **4**

(ii) (a) Explain how FFT is different from DFT. **3**

(b) Derive the finite difference formula corresponds to the Poisson equation in two dimensions. **4**

(iii) (a) What is the central idea behind the fast Fourier Transforms ? **3**

(b) Use the explicit method to find the temperature distribution at t = 0.1 s and 0.2 s of a long, thin rod with a length of 10 cm and the following values : $k = 0.49 cal/(s.cm.^{\circ}C)$, $\Delta x = 2 cm$ and $\Delta t = 0.1 s$. At $t = 0$, the temperature of the rod is zero and the boundary conditions are fixed for all times at $T(0) = 100^{\circ}C$ and $T(10) = 50^{\circ}C$. The rod is of Aluminium with $C = 0.2174\ cal/(g.^{\circ}C)$ and $\rho = 2.7\, g/cm^3$, $k = 0.835\, cm^2/s$ and $\lambda = 0.020875$. **4**

4 Attempt any **two** questions :

(i) (a) Discuss the simulation problem of a harmonic oscillator with damping. **3**

(b) Discuss the simulation algorithm for projectile motion with variable gravitational force. **4**

(ii) (a) Write an algorithm for motion of car with limited power and gears. **3**

(b) Apply Kirchhoff's loop rule to a RC circuit and write an algorithm to determine current $i(t)$ in the loop. **4**

(iii) (a) Discuss the problem of a falling object near the surface of earth without neglecting air resistance. **3**

(b) Apply Kirchhoff's loop rule to a LRC circuit and write an algorithm to determine current $i(t)$ in the loop. **4**

5 Attempt any **two** questions :

(i) (a) Mention some areas of applications of the molecular dynamics method. **3**

(b) Discuss the need for periodic boundary conditions in *Molecular Dynamics* simulations of classical systems. How it is implemented in 2-dimensions ? **4**

(ii) (a) What are the boundary conditions used in simulation of a quantum mechanical system ? **2**

(b) Discuss the Euler-Cromer algorithm for finding energy eigen values and eigen functions for a particle in a one-dimensional harmonic oscillator potential using time-independent Schrödinger equation. **5**

(iii) Discuss a mathematical model of radioactivity and a simulation algorithm for the same. **7**
