

A-1520

M. Sc. (Sem. III) Examination March/April - 2015

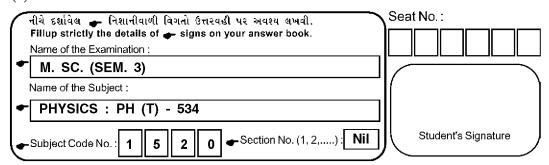
Physics: PH (T) - 534

(Computational & Simulation Methods in Physics)

Time: 3 Hours] [Total Marks: 70

Instructions:

(1)



- (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.
 - (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.

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- (ii) (a) Discuss the least-square method to fit a data to a curve y = mx + c.
 - (b) Perform LU decomposition of the following matrix 4 and hence find its inverse matrix:

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

- (iii) (a) What is meant by cubic spline? What are the conditions required to evaluate the unknown parameters in the spline equations?
 - (b) Using the principles of least squares, find an equation of the form $y = ae^{bx}$ that fits the following data:

<i>x</i> :	1	2	3	4	5
<i>y</i> :	0.6	1.9	4.3	7.6	12.6

- 2 Attempt any two questions:
 - (i) (a) Discuss advantages and disadvantages of various **3** methods for eigenvalue problem.
 - (b) Using Romberg's integration method, find the 4

value of $\int_{1}^{1.8} f(x) dx$ correct to $O(h^4)$ starting with

Trapezoidal rule, for the tabular values:

''' '	1.0		• -	· ·	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?
 - (b) Compute $\int_{2}^{4} (x^4 + 1) dx$ using three point Gauss 4 quadrature method.
- (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.
 - (b) Find the largest eigenvalue and corresponding 4

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.

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3	Attempt		any two questions:	
	(i)	(a)	What is meant by Fast Fourier Transform?	3
			Discuss an algorithm for FFT.	
		(b)	Explain elliptic, parabolic and hyperbolic	4
			categories of linear, second-order partial differential	
			equations with one physical example in each case.	
	(ii)	(a)	Explain how FFT is different from DFT.	3
		(b)	Derive the finite difference formula corresponds	4
			to the Poisson equation in two dimensions.	
	(iii)	(a)	What is the central idea behind the fast	3
			Fourier Transforms ?	
		(b)	Use the explicit method to find the temperature	4
			distribution at $t = 0.1 \text{ s}$ 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	
			$\Delta t = 0.1s$. 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	Atte	mpt	any two questions:	
	(i)	(a)	Discuss the simulation problem of a harmonic	3
		<i>a</i> >	oscillator with damping.	
		(b)	Discuss the simulation algorithm for projectile	4
	('')	()	motion with variable gravitational force.	
	(ii)	(a)	Write an algorithm for motion of car with limited	3
		<i>a</i> >	power and gears.	
		(b)	Apply Kirchhoff's loop rule to a RC circuit and	4
			write an algorithm to determine current $i(t)$ in the loo	_
	(iii)	(a)	Discuss the problem of a falling object near the	3
			surface of earth without neglecting air resistance.	
		(b)	Apply Kirchhoff's loop rule to a LRC circuit	4
			and write an algorithm to determine current $i(t)$ in	
			the loop.	

- 5 Attempt any two questions:
 - (i) (a) Mention some areas of applications of the molecular dynamics method.
 - (b) Discuss the need for periodic boundary conditions 4 in *Molecular Dynamics* simulations of classical systems. How it is implemented in 2-dimensions?

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- (ii) (a) What are the boundary conditions used in simulation of a quantum mechanical system?
 - (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.
- (iii) Discuss a mathematical model of radioactivity and a simulation algorithm for the same.

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