BIRLA INSTITUTE OF TECHNOLOGY, MESRA, RANCHI
(END SEMESTER EXAMINATION)

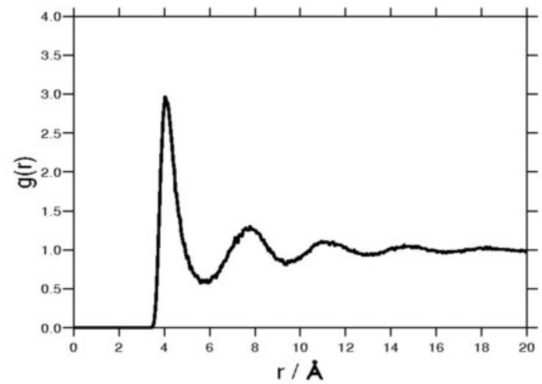
CLASS: I. M. Sc. **SEMESTER: X**
BRANCH: PHYSICS **SESSION: SP/2023**

SUBJECT: PH515 THEORETICAL AND COMPUTATIONAL CONDENSED MATTER PHYSICS
TIME: 3 Hours **FULL MARKS: 50**

INSTRUCTIONS:
1. The question paper contains 5 questions each of 10 marks and total 50 marks.
2. Attempt all questions.
3. The missing data, if any, may be assumed suitably.
4. Before attempting the question paper, be sure that you have got the correct question paper.
5. Tables/Data hand book/Graph paper etc. to be supplied to the candidates in the examination hall.

			CO	BL
Q.1(a)	What are the characteristics of a system with fractal dimensions?	[2]	1	1
Q.1(b)	What is the average mean squared displacement, $< r^2(t) >$, as a function of time for (I) random walks, (ii) self-avoided walks, and (iii) diffusion equations in two dimensions?	[3]	1	1
Q.1(c)	Outline the differences between the diffusion limited aggregation (DLA) and Eden cluster growth models. Illustrate with examples from two dimensions	[5]	1	2,4
Q.2(a)	Provide a pseudocode for the Metropolis-Hastings algorithm as applied to the study of second order phase transition in spin Hamiltonians.	[2]	1,2	3
Q.2(b)	Plot the behavior of the magnetization of the Ising ferromagnet as a function of the temperature, for three applied field cases: $h < 0$, $h = 0$, $h > 0$. Indicate the critical point.	[3]	2	1,2,4
Q.2(c)	Ising spin model with single ion anisotropy in the presence of external magnetic field h is given by: $$H = -J \sum_{<ij>} s_i \, s_j - D \sum_{i}^{N} (s_i)^2 - h \sum_{i}^{N} s_i ,$$ where $J > 0$ is the ferromagnetic coupling constant and D is the single-ion anisotropy that favors easy-axis magnetization for $D > 0$ and easy-plane magnetization for $D < 0$. Carry out the mean field analysis of the above Hamiltonian and obtain the mean field acting on the spins s_i .	[5]	2	3,5,6
Q.3(a)	Discuss the significance of velocity autocorrelation function for diffusion equation.	[3]	3,4	2,6
Q.3(b)	The energies of formation of Schottky and Frenkel defects in a material are 1eV/atom (1.6×10^{-19} J/atom) and 4 eV/atom (6.4×10^{-19} J/atom), respectively. What are the equilibrium concentrations of these defects at 900 K. [The Boltzmann constant is $k_B = 1.380649\times10^{-23}$ J·K^{-1}.]	[2]	4	6
Q.3(c)	Two molecules, separated by a distance of 3.0 angstroms, are found to have a σ value of 4.10 angstroms. By decreasing the separation distance between both molecules to 2.0 angstroms, the intermolecular potential between the molecules becomes more negative. Do these molecules follow the Lennard-Jones potential? Why or why not?	[5]	3	2,6
Q.4(a)	Describe the Verlet algorithm. How is it advantageous over the second and fourth order Runge-Kutta methods?	[5]	3	3,4
Q.4(b)	Discuss distinct types of defects in solids.	[5]	4	6

Q.5(a)	Consider a Lenard-Jones fluid composed of spherical particles and the corresponding pair correlation function $g(r)$. A typical plot of $g(r)$ is shown below.	[5]	1,3	5,6



(i) Explain the behavior of $g(r)$ in the $r \rightarrow 0$ and $r \rightarrow \infty$ limits.
(ii) What do the peaks and troughs correspond to?
(iii) Why do the peaks and troughs become less prominent with increasing distance.

Q.5(b)	Discuss the key features of Dissipative Particle Dynamics (DPD) and its applications.	[5]	5	6

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