

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

CLASS: IMSc/MSc  
BRANCH: PHYSICS

SEMESTER : X/IV  
SESSION : SP/2025

**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 fundamental characteristics of (ideal/regular) fractals?	[2]	1	2
Q.1(b) What is the average mean squared displacement, $\langle r^2(t) \rangle$ , as a function of time for (i) random walks, (ii) self-avoided walks, and (iii) diffusion equations in two dimensions?	[3]	1	3
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
Q.2(a) Outline the algorithm to carry out Monte Carlo simulation for 2D Ising model using Metropolis-Hastings algorithm.	[5]	2	3
Q.2(b) For the 2D Ising model, plot (i) $M$ v/s $T$ ( $H=0$ ), (ii) $C_v$ v/s $T$ ( $H=0$ ), (iii) $\chi$ v/s $T$ ( $H=0$ ; FM exchange), (iv) $\chi$ v/s $T$ ( $H=0$ ; AF exchange), and (v) $M$ v/s $H$ ( $H \neq 0$ , $T < T_c$ ).	[5]	2	3
Q.3(a) What are correlation functions? Mention their types and their importance? Discuss the significance of velocity autocorrelation function for diffusion equation.	[5]	3	4
Q.3(b) What is Verlet algorithm? Compare the Verlet algorithm to standard Runge Kutta methods.	[5]	3	3
Q.4(a) Write down the form of the Leonard-Jones potential and discuss its physical significance.	[5]	3	1,2,4

The interaction potential between two neutral atoms is measured at various separations:

Distance (Angstrom)	Potential energy (eV)
5.0	+0.295
6.2	+0.001
7.0	-0.100
8.5	-0.024
10.0	-0.004
12.5	-0.001

Is the potential of the Lennard-Jones (LJ) form? Justify your answer. If yes, estimate the value of  $\sigma$  and identify the region(s) of attraction and repulsion.

Q.4(b) Discuss distinct types of defects in solids. How does the defect concentration in materials change with temperature?	[5]	4	3
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What will be the average concentration of vacancy defects in a sample at 300K if the defect formation energy is 100 meV?

Q.5 What is dissipative particle dynamics? Compare with Molecular dynamics simulations.	[10]	5	1,2,4
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