

Duration 90 minutes

Max Marks 20

1. The interatomic Lennard-Jones potential has a strongly repulsive part and an attractive part which is usually written as

$$V_{\text{int}}(r) \sim -\frac{c_0}{r^6}.$$

What is the reason for the dependence to be  $r^{-6}$ ? Under what circumstance can this be  $r^{-3}$ ? (2 marks)

2. Consider the one dimensional Ising model with nearest neighbor coupling described by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - h \sum_i S_i.$$

Here  $h$  is the applied external field. Given that the transfer matrix has the eigenvalues

$$\lambda_{1,2} = e^K \left[ \cosh \beta h \pm \sqrt{\sinh^2 \beta h + e^{-4\beta J}} \right]$$

and the partition function  $Z = \lambda_1^N + \lambda_2^N$ , show that the system has a phase transition at  $T = 0$  and at  $T \neq 0$  only, i.e., the free energy is a non-analytic function of the magnetic field  $h$  at  $T = 0$ .

(4 marks)

3. Determine the critical exponent for the function  $f(t) = At^2 e^{-t}$  as  $t \rightarrow 0$ .

(2 marks)

4. Consider the Ising model on a square lattice but now also including the next nearest neighbour ( $\langle mn \rangle$ ) interactions.

$$H = -|J_1| \sum_{\langle mn \rangle} S_i S_j - J_2 \sum_{\langle mn \rangle} S_i S_j - h \sum_{i=1}^N S_i$$

Here  $J_1$  and  $J_2$  are the two coupling constants. Solve the problem using a mean field approach. What should be the value of  $J_2$  if the transition temperature has to become twice of what it is when there are no next nearest neighbour interactions?

(Note: Next nearest neighbours are along the diagonals.)

(7 marks)

5. Given that the number fluctuations in the grand canonical ensemble

$$\langle (N - \langle N \rangle)^2 \rangle = \frac{\langle N \rangle^2 k_B T}{V} \kappa_T, \quad (1)$$

where  $\kappa_T$  is the isothermal compressibility, show that

$$\int d^3r G(r) = \frac{\langle N \rangle^2 k_B T}{V^2} \kappa_T. \quad (2)$$

Here  $G(r)$  is the density-density correlation function. Write the relations analogous to equations (1) and (2) for spins.

(3 marks)

6. Give a heuristic argument for the existence of a phase transition at  $T \neq 0$  for the 2D Ising model on a square lattice along with a rough estimate of the transition temperature.

(2 marks)