UNIVERSITY OF LONDON

BSc and MSci EXAMINATIONS (MATHEMATICS)

May-June 2006

This paper is also taken for the relevant examination for the Associateship.

M3A5

Statistical Mechanics and Complex Systems I

Date: Tuesday, 9th May 2006 Time: 10 am – 12 noon

Credit will be given for all questions attempted but extra credit will be given for complete or nearly complete answers.

Calculators may not be used.

1. A system is defined in terms of the Hamiltonian

$$H = \epsilon \sum_{i=1}^{N} n_i, \quad n_i \in \{0, 1, 2\}.$$

(i) Calculate the partition function.

(ii) Calculate the equilibrium energy.

(iii) Calculate the Helmholtz free energy.

(iv) Calculate the entropy and determine the limits $\lim_{T\to 0} S(T)$ and $\lim_{T\to\infty} S(T)$.

2. (i) Use the classical equipartition theorem to explain why the molar heat capacity of a monoatomic gas is

$$C_V = \frac{3}{2}R$$

and of a diatomic gas made up of rigid molecules is

$$C_V = \frac{5}{2}R.$$

(ii) According to thermodynamics the entropy at temperature T relative to that at some reference temperature T_0 is given by

$$S(T) = S(T_0) + \int_{T_0}^{T} \frac{C_V}{T} dT.$$

The Third Law of thermodynamics states that $S(T) \to 0$ as $T \to 0$. Show that the results in part (i) are inconsistent with the Third Law.

(iii) Explain how Einstein by use of Quantum Mechanics resolved the inconsistency between i) and ii).

3. In a certain system the free energy $F(\phi, T)$ is an even function of an order parameter ϕ, so that $F(\phi, T) = F(-\phi, T)$.

(i) Expand the free energy up to fourth order in ϕ and describe the assumptions about the temperature dependence of the coefficients that lead to a second order phase transition at a critical temperature T_c. Derive the equilibrium temperature dependence of ϕ under these assumptions.

(ii) Show that the *equilibrium* free energy is twice differentiable with respect to T, with continuous first derivative, and discontinuous second derivative.

(iii) Explain Landau's argument for the absence of a phase transition at non-zero temperature in one dimension for models with short range interaction, as for example the Ising chain.

4. Consider a branching process defined in terms of the branching probabilities

$$p_k = \frac{e^{-x}x^k}{k!} \, .$$

(i) Calculate the generator function for the branching probabilities.

(ii) Determine the average branching ratio σ.

Consider a stochastic variable

$$S_N = \chi_1 + \chi_2 + \cdots + \chi_N \, ,$$

where χ_i are all independent and identically distributed and the number of terms N is fluctuating independently. The generator functions for S_N, χ and N satisfy

$$g_{S_N} = g_N(g_\chi(s)) \, .$$

(iii) Express the average size Z_n of generation number n of a branching process in terms of the branching ratio σ.

Let the stochastic variable B assume positive integer values. Consider $A = 1 + B$.

(iv) Show that the generator functions for A and B are related in the following way

$$g_A(s) = s g_B(s).$$

(v) Use the result in (iv) to show that the average tree size is given by

$$\langle Y_\infty \rangle = \frac{1}{1-\sigma} \, .$$

5. Consider the one dimensional Ising model

$$H = -J \sum_{i=1}^{N} S_i S_{i+1} + NJ,$$

with $S_i = \pm 1$ for $i = 1, \ldots, N+1$.

(i) Calculate the energy E_1 of the first excited state of the system in which the spin configuration can be described in terms of a single kink.

(ii) Assume that the chain in a higher excited state can be described by a gas of non-interacting kinks distributed along the chain. Show that the partition function is given by

$$Z = [1 + e^{-\beta E_1}]^N.$$

(iii) Show that the average number of kinks $\langle n \rangle$ is given by

$$\langle n \rangle = -\frac{1}{E_1} \frac{\partial}{\partial \beta} \ln Z \, .$$

(iv) Consider $\langle l \rangle = N / \langle n \rangle$ to be a measure of the correlation length and derive its temperature dependence. Comment on the limits $T \to 0$ and $T \to \infty$.