

**NATIONAL UNIVERSITY OF SINGAPORE**

PC5202 ADVANCED STATISTICAL MECHANICS

(Semester II: AY 2009 -10)

Time Allowed: 2 Hours

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**INSTRUCTIONS TO CANDIDATES**

1. This examination paper contains 5 questions and comprises 3 printed pages.
2. Answer ALL the questions.
3. Answers to the questions are to be written in the answer books.
4. This is an OPEN BOOK examination.
5. Each question carries 20 marks.

1. Answer briefly the following questions/concepts:
  - (a) Give quantum Liouville's equation (or the von Neumann equation) for density matrix and state how it is derived.
  - (b) Give the equation stating the ergodic hypothesis.
  - (c) Write down the global concavity condition (with respect to internal energy) on entropy.
  - (d) Define fugacity for gas.

(a)  $i\hbar dp/dt = [H, \rho]$ , derive from Schrödinger equation, (b) time average = ensemble average, (c)  $S(\lambda U_1 + (1-\lambda)U_2) > \lambda S(U_1) + (1-\lambda)S(U_2)$ , (d)  $z = e^{\beta\mu}$ .

2. Consider molecules moving in one dimension. The molecules are modeled as rigid rods of length  $a$ , they are confined between the walls within a space of length  $L$  (much larger than  $a$ ). The potential energy is 0 if the molecules do not overlap, and infinite if they overlap. The order of the molecules is maintained, i.e., they cannot pass through each other.
  - (a) Calculate the canonical configuration partition function  $Q$  if there is only one molecule in the system.
  - (b) Repeat the calculation if there are two molecules within the length  $L$ .
  - (c) Generalize the results to system with an arbitrary number of  $N$  molecules.
  - (d) Calculate the force exerted by the molecules on one of the walls for the case of one, two, or arbitrary  $N$  molecules.

(a)  $Q_1 = L - a$ , (b)  $Q_2 = (L - 2a)^2 / 2$ , (c)  $Q_N = (L - Na)^N / N!$ , (d)  $F_N = k_B T N / (L - Na)$ .

3. Consider the Potts model defined by the Hamiltonian

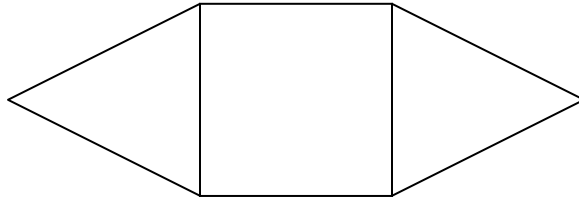
$$H = -J \sum_{i=1}^N \delta_{\sigma_i, \sigma_{i+1}}, \quad \sigma_i = 1, 2, \dots, q,$$

where the state is specified by discrete integers from 1 to  $q$ . The energy of the nearest neighbor is  $-J$  if the states are the same and 0 otherwise. Periodic boundary condition is assumed, that is,  $\sigma_{N+1} = \sigma_1$ .

- (a) Write down the transfer matrix  $P$  for the one-dimensional,  $q$ -state Potts model.
- (b) Find the largest eigenvalue of the transfer matrix  $P$ .
- (c) Write down expression for the free energy and correlation length of the model.

(a)  $P_{\sigma\sigma'} = \exp(\beta J \delta_{\sigma\sigma'})$ , (b)  $\lambda = e^{\beta J} + q - 1$ , (c)  $F = -k_B T N \ln \lambda$ ,  $\zeta^{-1} = \ln[(e^{\beta J} + q - 1) / (e^{\beta J} - 1)]$

4. Consider the Ising spins on a finite lattice (or graph) of one square and two triangles as shown in the figure below.
- Draw the dual lattice of the given lattice. Give the number of links  $L$ , number of sites  $N$ , and number of faces  $F$  (plaquettes) in both the original lattice and the dual lattice and show that Euler's relation is satisfied.
  - Draw the diagrams which have a nonzero contribution to the partition function  $Z$ . Give the high-temperature series expansion of  $Z$  in variable  $x = \tanh[J/(k_B T)]$ .
  - Use the duality relation to find the low temperature expansion of the partition function  $Z^*$  on the dual lattice.



$$(b) Z = 2^N (\cosh K)^L \{ 1 + 2x^3 + x^4 + 2x^5 + 2x^6 \}, N = F^* = 6, L = L^* = 8, F = N^* = 4.$$

5. Consider an over-damped Brownian particle governed by the stochastic differential equation

$$k \frac{dx}{dt} = R(t),$$

where  $k$  is the damping constant,  $x$  is the coordinate of the particle, and  $R$  is a Gaussian white noise satisfying the usual condition

$$\langle R(t) \rangle = 0 \text{ and } \langle R(t)R(t') \rangle = C\delta(t - t').$$

Derive the associated Fokker-Planck equation for the probability distribution  $\langle P(x, t) \rangle$  of the position  $x$  at time  $t$ .

$\langle P \rangle$  obeys the diffusion equation with diffusion constant  $C/(2k^2)$ .

[WJS]

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