NATIONAL UNIVERSITY OF SINGAPORE

PC5202 ADVANCED STATISTICAL MECHANICS

(Semester II: AY 2013-14)

Time Allowed: 2 Hours

INSTRUCTIONS TO CANDIDATES

1. This assessment 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. Write each question on a new page.
4. This is a CLOSED BOOK examination.
5. Each question carries 20 marks.

1. Answer or explain briefly the following questions/concepts:
    a. The difference between steady state and equilibrium state.
    b. The Kelvin temperature scale.
    c. Duality for the Ising model.
    d. The eutectic point.
    e. Curie-Weiss law.

a) The steady state is characterized by ρ, the density matrix or classical distribution, "independent of time", so that all thermodynamic observables are time-independent. Equilibrium is the same plus more restrictive conditions, such as no currents exist. Examples of equilibrium states are the canonical distribution and micro-canonical distribution.

b) Temperature 0 K is fixed by 3rd law; the triple point of water is fixed at the value 273.16K; other temperatures can be calibrated by Carnot cycle (through measuring heat).

c) Duality has two aspects, one, dual lattice can be defined for planar graphs, two, the low temperature expansion and high temperature expansion of partition function of a nearest neighbor Ising model are related by the duality relation.

d) Eutectic point is the lowest temperature point for which the mixture of alloy stays in liquid phase for a specific concentrate. It is best to show a phase diagram to illustrate this, see Callen book (2nd ed) on page 250 figure 9.18.

e) The magnetic susceptibility is given by $\chi = C/(T-T_C)$, according to Curie and Weiss, which is, of course, not true near critical point.

2. The heat capacities can behave differently in canonical ensemble and micro-canonical ensemble in a finite system of N degrees of freedom. We elaborate this point with the following questions.
    a. Express the heat capacity, $C_1 = \mathrm{d}U/\mathrm{d}T$, in terms of the fluctuation of the energy, $\langle H^2\rangle - \langle H\rangle^2$, where the average is over the canonical distribution. Other model parameters, such as system volume, external field, etc., are fixed. Show that $C_1 \geq 0$.
    b. Suppose that the entropy is calculated as a function of energy as, $S = S(U)$, in a micro-canonical ensemble. Derive a formula relating the heat capacity C_2 to the entropy function.
    c. Discuss the condition for $C_1 = C_2$. Is it possible that $C_2 < 0$, and why?

a) The required relation between C_1 and the fluctuation is $C_1 = [<H^2>-<H>^2]/(k_BT^2) = <(H-<H>)^2>/(k_BT^2) \geq 0$. This is obtained by differentiating the average energy $U = <H>$, where $<H>$ is the canonical distribution average, i.e., $< \ldots > = \sum \ldots \exp(-H/(k_BT))/Z$. Z is partition function. Since $k_B > 0$, $T^2 > 0$, and an average of a positive quantity $(H-<H>)^2$ is positive, so C_1 must be positive.

b) *The entropy function S(U) gives us inverse temperature 1/T = dS(U)/dU=S'(U). This means we have a relation of T as a function of U, i.e., T =T(U) = 1/(dS(U)/dU). The heat capacity* $C_2 = dU/dT = 1/(dT/dU) = -1/(T^2 d^2 S/dU^2) = -1/(T^2 S''(U)) = -S'(U)^2/S''(U)$*, which is obtained by differentiate with respect to U on both side of the equation 1/T = S'(U). That is,* C_2 *is expressed by first and second derivatives of S with respect to U.*

c) *Ensemble equivalence occurs only in the thermodynamic limit,* $N \to \infty$*, so we expect* C_1 *and* C_2 *are equal only in that limit. We have proved that* $C_1 \geq 0$ *in (a), but no similar prove can be given within finite N statistical mechanics without evoking the thermodynamic arguments (such as concavity of S, which may be true only in the thermodynamics limit). So within statistical mechanics of finite N,* $C_2 < 0$ *is possible, and not against any known laws.*

3. Consider the standard ferromagnetic Ising model with nearest neighbor interactions in a magnetic field,

$$H(\sigma) = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j - h\sum_{i=1}^{N}\sigma_i ,$$

where each nearest neighbor interaction with coupling constant J is summed once only. We derive the mean-field equation in the following way different from the methods used in class.

   a. First, split the Hamiltonian into two terms of the form, $H(\sigma) = H_{\text{cavity}} - \sigma_i h_i$, where H_{cavity} is the cavity Hamiltonian, and h_i depends on the spins of nearest neighbors of site i only. Give the explicit forms of H_{cavity} and h_i. This will be helpful for the next step.

   b. Prove an exact identity, known as the Callen identity:

$$\langle\sigma_i\rangle = \left\langle \tanh\left[\beta\left(h + J\sum_{j\in\text{ nn of } i}\sigma_j\right)\right]\right\rangle,$$

   where $\beta = 1/(k_B T)$. The average has the usual meaning of $\langle\cdots\rangle = \sum_{\{\sigma\}}\cdots e^{-\beta H}/Z$ and the summation is over the nearest neighbor sites j of a fixed center site i.

   c. Assuming that the spins are uncorrelated, in the sense, $\langle\sigma_i\sigma_j\cdots\sigma_k\rangle = \langle\sigma_i\rangle\langle\sigma_j\rangle\cdots\langle\sigma_k\rangle$, for any number of spins, show that the usual mean-field equation is recovered.

a) *Let the site of interest i be called 0 instead of i. Then* $h_0 = h + J\sum_{j\in\text{nearest neighbors of site }0}\sigma_j$.

The cavity Hamiltonian is the remaining terms which is an Ising model with site 0 and the interaction with it removed, i.e., $H_{\text{cavity}} = -J\sum_{<ij>, i\neq 0, j\neq 0}\sigma_i\sigma_j - h\sum_{i, i\neq 0}\sigma_i$.

b) *We have* $\langle \sigma_0 \rangle = \frac{1}{Z} \sum_{\{\sigma\}} \sigma_0 \exp\left[-\beta(H_{\text{cavity}} - \sigma_0 h_0)\right]$. *We split the sum over all spins into sum over only* σ_0 *and sum over the rest of the spins, then* $\langle \sigma_0 \rangle = \frac{1}{Z} \sum_{\{\sigma_i, i \neq 0\}} \left(e^{\beta h_0} - e^{-\beta h_0}\right) e^{-\beta H_{\text{cavity}}}$. *Now we multiply the summand by* $1 = \sum_{\sigma_0} e^{\beta \sigma_0 h_0} / \left(e^{\beta h_0} + e^{-\beta h_0}\right)$. *The required identity is proved.*

c) *Expand the tanh function as a power series, then expand* h_0 *and the final expression as a power series in σ, using the assumption given, we can move the average sign inside, to get* $\langle \sigma_i \rangle = \left\langle \tanh\left[\beta\left(h + J \sum_{j \in \text{nn of } i} \sigma_j\right)\right]\right\rangle = \tanh\left[\beta\left(h + J \sum_{j \in \text{nn of } i} < \sigma_j >\right)\right]$.

4. The finite-size scaling for an Ising ferromagnetic system takes the form

$$f(b^Y t, b^X h, b/L) = b^D f(t, h, L)$$

where f is the singular part of the free energy per site, $t = |T\text{-}T_c|/T_c$ is the relative deviation away from the critical temperature, h is magnetic field, and L is the linear size (length) of the system and D is dimension of the system. Exactly at the critical point when t=0 and h=0, show that

   a. Magnetization per spin $m \propto L^{\Delta_1}$ and determine the exponent Δ_1 in terms of X, Y, and D.
   b. Magnetic susceptibility $\chi \propto L^{\Delta_2}$ and also determine the exponent Δ_2.
   c. Finally, find (or argue) the exponent Δ_3 for the quantity $\dfrac{\left\langle \left(\sum_i \sigma_i\right)^4 \right\rangle}{\left\langle \left(\sum_i \sigma_i\right)^2 \right\rangle^2} \propto L^{\Delta_3}$.

a) $m = -\frac{\partial f}{\partial h}$, *we can set t=0, b=L, to get* $f(0, h, L) = L^{-D} f(0, L^X h, 1)$. *Differentiating with respect to h, then set h=0, assuming the limit h->0 exists, we get* $\Delta_1 = X - D$.

b) *Differentiate one more time with respect to h of f(0,h,L), we get* $\Delta_2 = 2X - D$.

c) *Differentiate 4 times, we get* $\langle M^4 \rangle / N = L^{4X-D}$, *and* $\chi = \frac{\partial m}{\partial h} = \langle M^2 \rangle / (k_B T N)$ *(assuming t>0), where* $N = L^D$, $M = \sum_i \sigma_i$. *Taking the ratio of 4-th moment to the second moment squared, we find* $\Delta_3 = 0$.

5. Consider a Langevin equation subject to two independent random noises $R_1(t)$ and $R_2(t)$, with the following equation:

$$m\frac{dv}{dt} = -m\gamma v + R_1(t) + R_2(t) \, ,$$

where $\langle R_\alpha(t) R_\beta(t') \rangle = C_\alpha \delta_{\alpha\beta} \delta(t-t')$, α, β = 1, 2, $\delta_{\alpha\beta}$ is the Kronecker delta and $\delta(t-t')$ is the Dirac delta function.

a. Derive the Fokker-Planck equation associated with the above Langevin equation. You can use standard well-known results without proof.
b. Based on the result in a, determine the steady-state solution (that is, when the average probability distribution does not change, $\partial \langle P(v,t) \rangle / \partial t = 0$).
c. Compute the steady-state average energy dissipation to the environment per unit time due to the damping force $-m\gamma v$, as a function of the model parameters m, γ, C_1, and C_2.

a) Let $R(t)=R_1(t) + R_2(t)$, we find $\langle R(t) R(t') \rangle = (C_1 + C_2)\delta(t-t')$. This means that the two independent noises are effectively equivalent to one noise with a new constant $C=C_1+C_2$. The Langevin equation is the same as the standard one, i.e.,

$$\frac{\partial P}{\partial t} = \gamma \frac{\partial}{\partial v}(vP) + \frac{C}{2m^2}\frac{\partial^2 P}{\partial v^2} \, .$$

b) Steady state means $\partial P/\partial t=0$, or $\gamma v P + \frac{C}{2m^2}\frac{\partial P}{\partial v} = \text{const}$. The constant must be 0 in order to be consistent with the fact that P is normalizable (integrable). The first order equation can be solved as $P = P_0 \exp\left(-\frac{\gamma m^2 v^2}{C}\right)$. P_0 can be determined by normalization.

c) The steady-state energy dissipation per unit time (power) is frictional force times velocity = $\langle m\gamma v\cdot v\rangle = m\gamma\langle v^2\rangle$. Since v is distributed according to Gaussian, $\langle v^2\rangle$ is its variance, which can be read off from the result in b), given $m\gamma\cdot C/(2\gamma m^2) = C/(2m)$.

---- End of Paper ---

[WJS]