NATIONAL UNIVERSITY OF SINGAPORE

PC5202 Advanced Statistical Mechanics

(Semester II: AY 2007-08, 5 May 08)

Time Allowed: 2 Hours

INSTRUCTIONS TO CANDIDATES

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

1. Choose only one (A, or B, or C) among the alternatives that is the most accurate statement. Notations are those used in class.

(1). A typical time scale associated with atomic motions (e.g. vibration in solids) is of the order of,

A. 10^{-17} s,
B. 10^{-14} s,
C. 10^{-10} s.

(2). Callen's second postulate says that entropy S of a system is a maximum in comparison with the entropies of

A. other nonequilibrium states,
B. unconstrained states,
C. constrained equilibrium states.

(3). Which of the statements is incorrect: entropy is defined by,

A. $1/T = \partial S/\partial U$,
B. $dS = dQ/T$,
C. $S = k_B \ln \Omega$.

(4). Liouville's theorem states:

A. $\partial\rho/\partial t = -(H, \rho)$,
B. $dA/dt = (A, H)$,
C. $d\Gamma_t =$ const.

(5). Single out the inaccurate statement: in a microcanonical ensemble, the system is distributed in phase space,

A. on a constant energy surface (H=const) with equal probability,
B. on an energy shell $E < H < E + \Delta$ with equal probability,
C. on a constant energy surface with probability proportional to $d\sigma/|\nabla H|$.

(6). Canonical ensemble is valid for a single particle

A. in contact with a heat bath,
B. in isolation,
C. in isothermal processes.

(7). The heat capacity C of an Einstein solid

A. decreases with temperature T linearly,
B. decreases with T exponentially,
C. approaches a constant as $T \to 0$.

(8). The spontaneous magnetization of a ferromagnet is the

A. average magnetic moments when magnetic field is present,
B. average magnetic moments when temperature is low,
C. average magnetic moments when a magnetic field is absent.

(9). Which of the following is correct:

A. triangular lattice is self-dual,
B. rectangular lattice is self-dual,
C. face-centered cubic lattice is self-dual.

(10). Einstein relation in the theory of Brownian motion means that:

A. noise correlation is related to frictional force,
B. the viscous force is proportional to the velocity,
C. the diffusion constant is proportional to mobility.

(1) B, (2) C, (3) A, (4) C, (5) A, (6) A, (7) B, (8) C, (9) B, (10) C.

2. Consider N non-interacting point particles moving between a fixed, permeable, and diathermal wall of two compartments of volumes V_1 and V_2 with $V_1 = V_2 = V$. The Hamiltonian of the combined system can be written as

$$H = \sum_{i=1}^{N} \left(\frac{\mathbf{p}_i^2}{2m} + u(\mathbf{r}_i) \right).$$

The single particle potential energy $u(\mathbf{r})$ is $+\infty$ for $\mathbf{r}$ outside the two compartments, and is 0 in the first compartment, but is a constant u_0 in the second compartment.

(a) Are the temperatures of the gas in the two compartments equal?
(b) Which of the ensembles among the microcanonical, canonical, and grand-canonical is most suited for this problem?
(c) Calculate the average number of particles N_1 and N_2 in each compartment, expressed in terms of the temperature T of the compartment, the potential u_0, and the total number of particles N.
(d) Compute the pressure P_1 and P_2 in each compartment.

(a) Yes, $T_1=T_2=T$, since two compartments are separated by a diathermal wall (i.e. heat conducting wall).

(b) Canonical. Taking the system as a whole, volume V_1+V_2 and total number of particles N are fixed.

*(c) Consider only one particle, $Exp[-\beta(p^2/(2m) + u(\mathbf{r}))]d\mathbf{p}d\mathbf{r}$ gives the (unnormalized) probability that it has momentum **p** and position **r**. Integrating over **p**, we find that the probability of finding the particle at **r** is just proportional to $Exp[-\beta\, u(\mathbf{r})]\, d\mathbf{r}$. Integration over the volume of V_1 or V_2, we find the ratio of probability for it in the 1st to 2nd volume is 1 to $\exp(-\beta u_0)$. Since particles are non-interacting, the ratio is the same as a whole, i.e.,*

$N_1 + N_2 = N, \quad N_1/N_2 = 1/\exp(-\beta u_0), \quad \beta=1/(k_B T).$

Solve the equations, we find $N_1=N/(1+\exp(-\beta u_0))$, $N_2= N/(1+\exp(\beta u_0))$.

(d) Use ideal gas law, we find $P_1=N_1kT/V_1$, $P_2=N_2kT/V_2$. Alternatively, one can also find the partition function first, $Z = z^N/N!$.

$z = (2\pi m k_B T/h^2)^{3/2}\, [V_1+V_2 \exp(-\beta\, u_0)].$

P_1 or P_2 is obtained by taking partial derivative with respective to V_1 or V_2 of the free energy $F = -k_BT \ln Z$, then set $V_1=V_2=V$.

3. Consider a one-dimensional three-state Potts model with periodic boundary condition. The Hamiltonian of the system is given by

$$H(s) = -J\sum_{i=1}^{N}\delta_{s_i,s_{i+1}}, \quad s_i = -1,0,1\ ,$$

where the spins take three different values, and δ is the Kronecker delta symbol, i.e., $\delta_{a,b} = 0$ if $a \neq b$, and 1 if $a = b$. Use the transfer matrix method to solve this problem.

(a) Give the transfer matrix P such that the partition function $Z = \mathrm{Tr}(P^N)$.

(b) Determine the equation for the eigenvalues λ, and find the eigenvalues of P [hint: to solve the polynomial equation, use a new variable $\alpha = e^K - 1 - \lambda$, where $K = J/(k_BT)$].

(c) Compute the free energy per spin in the thermodynamic limit.

(a) The partition function is

$$P = \exp(K\delta_{s_1,s_2}) = \begin{bmatrix} e^K & 1 & 1 \\ 1 & e^K & 1 \\ 1 & 1 & e^K \end{bmatrix}$$

(b) The eigenvalues are obtained from the secular equation $\det(P-\lambda I)=0$, which gives $(\alpha+1)^3-3\alpha-1 = 0$. Expanding the cubic term, $\alpha^3+3\alpha^2=0$, with solution $\alpha = 0, 0, -3$. Or $\lambda = e^K-1-\alpha = e^K-1$, e^K-1, or e^K+2. The last one is bigger.

(c) $f = -k_B T(\ln Z)/N = -k_B T \ln(e^K+2)$.

4. The magnetic susceptibility per spin is related to the two-point correlation function by

$$\chi = \frac{\partial m}{\partial h} = \beta\int d^d\mathbf{r}\, G(r), \quad \beta = \frac{1}{k_BT}\ .$$

The correlation function $G(r)$ takes the form

$$G(r) \sim \frac{e^{-r/\xi}}{r^{d-2+\eta}}$$

for an infinitely large lattice in d-dimensions.

(a) Show that, at the critical temperature T_c, on a finite lattice of hyper-volume L^d, the susceptibility diverges with the linear size L as $\chi \sim L^{2-\eta}$.

(b) The free energy of a finite system obeys a finite-size scaling near the critical point, $f(t,h,L) = b^{-d} f(b^y t, b^x h, b/L)$, where $b>0$ is an arbitrary scaling factor, x and y are some scaling exponents. Show that at the critical point, t = 0, h = 0, the susceptibility χ diverges with size L. Find the corresponding exponent, i.e., the power a in $\chi \sim L^a$.

(c) Based on the results of part (a) and (b), express the exponent η in terms of x, y, and d.

(a) At T_c, correlation length $\xi \to \infty$, so $G(r) \sim 1/r^{d-2+\eta}$. For a finite system of linear size L, the radius runs up to L, we get

$$\chi \sim \int^L \frac{1}{r^{d-2+\eta}} r^{d-1} dr \approx L^{2-\eta}.$$

(b) $\chi = \frac{\partial m}{\partial h} = -\frac{\partial^2 f}{\partial h^2}$. *Using the scaling relation for f, we find scaling for χ, by differentiation with respective to h twice, $\chi(t,h,L) = b^{2x-d}\chi(b^y t, b^x h, b/L)$. setting t=h=0, b=L, we get $\chi(0,0,L) = L^{2x-d}\chi(0,0,1)$, i.e., $\chi \sim L^{2x-d}$, $a = 2x-d$.*

(c) $2x-d=2-\eta$, so $\eta = 2-2x+d$.

5. Consider the Langevin equation in one dimension

$$m\frac{d^2x}{dt^2} = -kx - m\gamma\frac{dx}{dt} + R(t),$$
$$\langle R(t)\rangle = 0,$$
$$\langle R(t)R(t')\rangle = C\delta(t'-t).$$

This is a harmonic oscillator with mass m and spring constant k, subjected to damping and a random force (white noise).

(a) Let the Fourier transform of the coordinate x be

$$\tilde{x}[\omega] = \frac{1}{2\pi}\int_{-\infty}^{+\infty} x(t)e^{-i\omega t} dt.$$

Derive the algebraic equation that the Fourier component $\tilde{x}[\omega]$ must satisfy; solve the equation in terms of the Fourier transform of the random noise.

(b) Find the expression, $\tilde{F}[\omega]$, in terms of the model parameters (m, k, γ, C) and frequency ω, which is the Fourier transform of the correlation function, $F(t) = \langle x(t)x(0)\rangle$, [Hint: you may use the Wiener-Khintchine theorem].

(a) The inverse Fourier transform is

$$x(t) = \int_{-\infty}^{+\infty} \tilde{x}[\omega]e^{i\omega t} d\omega$$

Substituting into the differential equation, we get

$(i\omega)^2 m\tilde{x} = -k\tilde{x} - m\gamma(i\omega)\tilde{x} + \tilde{R}$, *which can be solved to get*

$$\tilde{x}[\omega] = \frac{\tilde{R}[\omega]}{k + im\gamma\omega - m\omega^2} .$$

(b) The Fourier transform of the correlation F(t) is given by the power spectrum of x. Applying the Wiener-Khinchine theorem, we found

$$\tilde{F}[\omega] = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\langle x(t)x(0)\rangle e^{-i\omega t}dt = \frac{C/(2\pi)}{\left|k + im\gamma\omega - m\omega^2\right|^2} .$$

Note that the power spectrum of random noise R is $C/(2\pi)$ for white noise.

-- the end --

[WJS, *6 May 2008*]