NATIONAL UNIVERSITY OF SINGAPORE

PC5202 ADVANCED STATISTICAL MECHANICS

(Semester II: AY 2012-13)

Time Allowed: 2 Hours

INSTRUCTIONS TO CANDIDATES

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

1. Answer briefly:
    a. What is the Gibbs phase rule and how is it derived?
    b. State the equipartition theorem for classical systems and from this, derive the Dulong-Petit law for solids.
    c. Give the mathematical equation that states the global concavity property of the entropy S as a function of internal energy U.
    d. State the continuity equation (for probability, particle number, or electric charge). State the Fick's law. Combine the two to derive the diffusion equation.

a) $f = r - M + 2$, where r is the number of components (i.e., different types of molecules), M is the number of phases, and f is the number of intensive variables that can be varied and still is in that phase. It is derived by considering the Gibbs-Duhem relation in each phase.

b) In classical systems, each quadratic form of the term in the Hamiltonian gets a canonical average of $(1/2)k_BT$. In a solid lattice of N atoms, each atom has three kinetic energy terms and three potential energy terms and total average internal energy is $3Nk_BT$. Thus the heat capacity is $3Nk_B$: this is Dulong-Petit law.

c) $S(\lambda U_1 + (1-\lambda)U_2) \geq \lambda S(U_1) + (1-\lambda)S(U_2)$, $0 \leq \lambda \leq 1$.

d) $\dfrac{\partial n}{\partial t} + \nabla \cdot \mathbf{j} = 0, \quad \mathbf{j} = -D\nabla n, \quad \dfrac{\partial n}{\partial t} = D\nabla^2 n$.

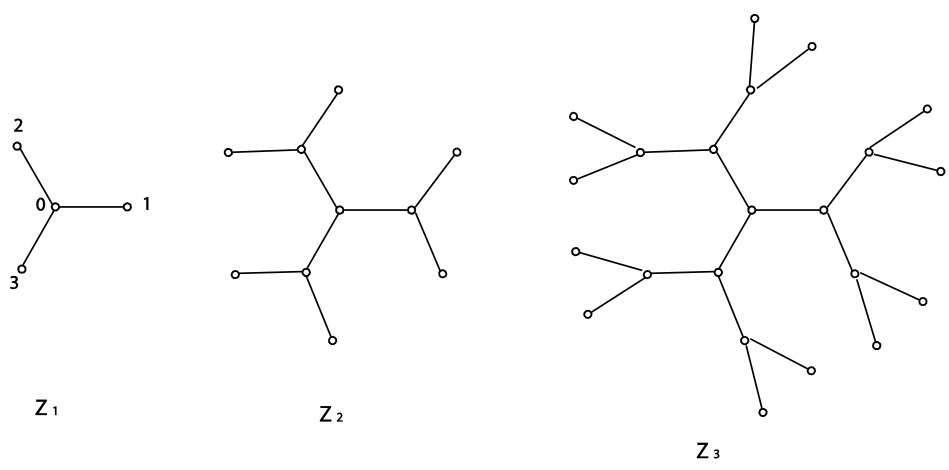
2. Consider one single particle of mass m moving in the one-dimensional domain $0 \leq x \leq L$. Except when the particle collides elastically with the boundaries, the particle moves freely with kinetic energy $p^2/(2m)$ and no potential energy.
    a. Compute the partition function Z at temperature T in a canonical ensemble. From this, determine the average kinetic energy $\left\langle p^2/(2m) \right\rangle$, heat capacity C, and the force f the particle exerts on one of the confining boundaries (walls).
    b. Calculate the phase-space volume $\Gamma(U)$ corresponding to the energies of the particle less than a given U. Assuming the Boltzmann entropy formula $S(U) = k_B \ln \dfrac{\Gamma(U)}{h}$, where k_B is the Boltzmann constant and h is the Planck constant, determine the system temperature T, heat capacity C, as well as force f exerted on the boundary by the particle.
    c. Discuss if the results in part a (canonical ensemble) and part b (micro-canonical ensemble) above are equivalent for the one particle problem. Explain why.

a) *The partition function is* $Z = \frac{1}{h}\int_0^L dx \int_{-\infty}^{+\infty} dp e^{-\beta p^2/(2m)} = \frac{L}{h}\sqrt{2\pi m k_B T}$. *$\beta=1/(k_BT)$. From Z we obtain* $U = \left\langle \frac{p^2}{2m} \right\rangle = -\frac{\partial \ln Z}{\partial \beta} = \frac{1}{2\beta} = \frac{1}{2}k_B T$. *$C=dU/dT = k_B/2$.* $f = -\frac{\partial F}{\partial L} = \frac{k_B T}{L}$ *($F = -k_BT \ln Z$).*

b) $\Gamma(U) = \int_0^L dx \int_{\frac{p^2}{2m}<U} dp = 2L\sqrt{2mU}$. *From this, $S=k_B \ln(\Gamma(U)/h)$, $1/T=\partial S/\partial U=k_B(2U)$, or $U=(1/2)k_BT$, and $C = dU/dT = (1/2) k_B$. $f = -\partial F/\partial L=k_BT/L$ (from $F=U-TS$).*

c) *Internal energy U, heat capacity C, and force f are the same, but the entropy S, free energy F are not. The two ensembles are not completely equivalent (since we are not in the thermodynamic limit). I think the fact U, C, f, are the same is accidental.*

3. Consider an Ising model defined on the graphs shown below in the next page, known as Cayley trees. The first three generations of the trees are shown. We assume that each site denoted by an open circle has an Ising spin $\sigma_i = \pm 1$ and each link has a nearest neighbor interaction, $-J\,\sigma_i\sigma_j$. For example, the first generation of the graph is associated with the energy $E = -J\,\sigma_0\sigma_1 - J\,\sigma_0\sigma_2 - J\,\sigma_0\sigma_3$.



a. Determine the canonical partition function Z_1 and Z_2 of the Ising model on the first and second generation Cayley trees.
b. Derive a general formula for Z_N for the N-th generation Cayley tree.

c. Discuss if the system has a phase transition at a finite temperature $T > 0$ when N approaches infinity.

a) *Sum over the out spins 1,2,3 first, we find ($K=\beta J=J/(k_B T)$)*

$$Z_1 = \sum_{\sigma_0}\left(\sum_{\sigma_1} e^{K\sigma_0\sigma_1}\sum_{\sigma_2} e^{K\sigma_0\sigma_2}\sum_{\sigma_3} e^{K\sigma_0\sigma_3}\right) = \sum_{\sigma_0}\left(e^{K\sigma_0}+e^{-K\sigma_0}\right)^3 = 2(e^K+e^{-K})^3.$$ *For Z_2 we also sum over the outer spins first, we find* $Z_2 = 2\left(e^K+e^{-K}\right)^9$.

b) *For the general case, we use high-temperature expansion. Since the tree graphs cannot have loops, all the* tanh*(x) parts are 0, and we only have the first term.* $Z_N=2^S\cosh^L(K)$ *where $S = L+1$ is the number of sites, and L is number of links,* $L=3(2^N-1)$.

c) *No phase transition as the partition function is the same, upto a constant factor, as the one-dimensional Ising model.*

4. Aristotelian physics says that the velocity of a particle is proportional to the force applied to it. We consider such a particle connected to a spring to form an oscillator experiencing a random force (white noise) with the equation

$$m\gamma\frac{dx}{dt} = -kx + R(t),$$
$$\langle R(t)\rangle = 0, \quad \langle R(t)R(t')\rangle = 2m\gamma k_B T\delta(t-t'),$$

where γ is the damping parameter, m is mass, k is force constant, x is the position of the particle which is a function of time t. The random force $R(t)$ is the standard white noise.

a. Derive a formal solution $x(t)$ expressed in terms of the random force $R(t)$.
b. Derive the associated Fokker-Planck equation for the average probability distribution $\langle P(x,t)\rangle$ of the position variable x.
c. Show that in the long-time limit when equilibrium is reached, the distribution is given by the Gibbs distribution proportional to $\exp[-(1/2)kx^2/(k_B T)]$.

a) *The solution $x(t)$ is obtained by the method of variation of a constant, where we first let $R(t)=0$, then $x(t)=Ae^{-ct}$ where $c = k/(m\gamma)$. Then we let A -> $A(t)$ and substitute back into the equation to obtain equation for $A(t)$. After integration we get*

$$x(t) = A_0 e^{-ct} + \int_0^t \frac{R(s)}{m\gamma} e^{-c(t-s)} ds.$$

b) *We can follow the standard derivation of Zwanzig, but the equation is identical to the standard one treated in class if we identify x as velocity v, and some change of variables. So the Fokker-Planck equation is the same (skip the derivation)*

$$\frac{\partial\langle P\rangle}{\partial t}=\frac{k}{m\gamma}\frac{\partial\left(x\langle P\rangle\right)}{\partial x}+\frac{k_BT}{m\gamma}\frac{\partial^2\langle P\rangle}{\partial x^2}.$$

c) *We can do it in two ways, either to verify that* exp*(-(1/2)*$kx^2/(k_BT)$*) satisfies the Fokker-Planck equation with* $\partial\langle P\rangle/\partial t = 0$*, or solve the equation* $kx\langle P\rangle + k_BT\,\partial\langle P\rangle/\partial x = const = 0$ *(the constant has to be 0 in order for* $\int_{-\infty}^{+\infty} x\langle P(x)\rangle dx$ *finite.)*

5. A quantum harmonic oscillator in thermal equilibrium with the Hamiltonian, $H_0=\frac{\mathrm{p}^2}{2m}+\frac{1}{2}k\mathrm{x}^2$, is driven by an external time-dependent force $f(t)$ when $t > 0$, so that the total Hamiltonian is explicitly time-dependent, $H(t) = H_0 - f(t)\,\mathrm{x}$. Note that p and x are operators satisfying the canonical commutation relation, $[\mathrm{x}, \mathrm{p}] = i\hbar$, and the mass m, the force constant k, and the external force $f(t)$ are c-numbers.
   a. Give the definitions of the $\mathrm{p}^{\mathrm{I}}(t)$ and $\mathrm{x}^{\mathrm{I}}(t)$, the interaction picture momentum and position operator with respect to H_0, and find explicitly the time-dependence in terms of the original Schrödinger picture operator p and x.
   b. State the equation that the interaction picture density matrix $\rho^{\mathrm{I}}(t)$ must satisfy. Solve this equation perturbatively to the lowest order (i.e. first order) in $f(t)$.
   c. Based on the result of part b, derive the quantum expectation value of the position $\langle \mathrm{x}(t)\rangle$ as

$$\langle \mathrm{x}(t)\rangle=\mathrm{Tr}\left[\rho^{\mathrm{I}}(t)\mathrm{x}^{I}(t)\right]=-\int_0^t G(t,t')\,f(t').$$

   Give the explicit form of the Green's function $G(t,t')$.

a) *The interaction picture operators are* $p^I(t)=e^{\frac{i}{\hbar}H_0t}\,\mathrm{p}\,e^{-\frac{i}{\hbar}H_0t}$*, and* $x^I(t)=e^{\frac{i}{\hbar}H_0t}\,\mathrm{x}\,e^{-\frac{i}{\hbar}H_0t}$.

The associated Heisenberg equations are $\frac{dx^I(t)}{dt}=\frac{1}{i\hbar}[x^I(t),H_0]=\frac{p^I(t)}{m}$*, and*

$\frac{dp^I(t)}{dt}=\frac{1}{i\hbar}[p^I(t),H_0]=-kx^I(t)$. *We have used the fact* $H_0=H_0^I(t)$*. Since the equations are identical to the classical version of a harmonic oscillator, we have the solution (explicit time dependences) as* $x^I(t)=\mathrm{x}\cos(\omega t)+\frac{\mathrm{p}}{\omega m}\sin(\omega t)$*, and*

$p^I(t) = -\mathrm{x}m\omega\cos(\omega t) + \mathrm{p}\cos(\omega t)$, *where* x *and* p *are Schrödinger operators satisfying [*x,p*]=iħ.*

b) *The density matrix in interaction picture satisfies* $i\hbar\frac{d\rho^I(t)}{dt} = [V^I(t), \rho^I(t)]$. *The lowest order solution is* $\rho^I(t) = \rho^I(0) - \frac{i}{\hbar}\int_0^t [V^I(t'), \rho^I(0)]dt' + O(V^2)$ *where* $V^I(t) = -f(t)x^I(t)$.

c) *Compute the average of x(t) using the result of part c and part a in the interaction picture, using the cyclic property of trace, we get*
$$G(t,t') = -\frac{i}{\hbar}\theta(t-t')\left\langle [x^I(t), x^I(t')]\right\rangle = -\frac{\sin\left[\omega(t-t')\right]}{\omega m}.$$

-- End of Paper --

[WJS]