NATIONAL UNIVERSITY OF SINGAPORE

PC5202 ADVANCED STATISTICAL MECHANICS

(Semester II: AY 2016-17)

Time Allowed: 2 Hours

INSTRUCTIONS TO STUDENTS

1. Please write your student number only. Do not write your name.
2. This assessment paper contains 4 questions and comprises 3 printed pages.
3. Students are required to answer ALL the questions.
4. Each question carries 25 marks.
5. Students should write the answers for each question on a new page.
6. This is a CLOSED BOOK examination.

1. Answer briefly the following questions:
   a. State the Callen postulate II about entropy.
   b. In a micro-canonical distribution, the probability density ρ is a constant when $E \leq H < E + \Delta$, and 0 outside the energy interval. In the limit $\Delta \to 0$, the system can only stay on the energy surface $H = E$. Explain why the distribution is not uniform on surface, but proportional to $d\sigma/|\nabla H|$, where $d\sigma$ is surface element.
   c. State the scaling assumption for the singular part of the free energy per spin, $f(T, h)$, using the Ising model as an example here. Also, give the Widom scaling law.
   d. Explain the Jarzynski equality, and also elaborate in what way it is consistent with the Clausius inequality $TdS \geq \delta Q$ in thermodynamics.
   e. State the *H*-theorem of Boltzmann.

A.there exits a function called entropy of the extensive parameters of any composite system, defined for all equilibrium states and having the following property: the value assumed by the extensive parameters in the absence of an internal constraint are these that maximize the entropy over the manifold of constrained equilibrium states. B. even when Δ goes to 0, it is the volume that is invariant due to Liouville theorem. So the area times height is invariant. The weight per area is different at different locations in phase space. C. the scaling assumption for free energy per spin is $f(t, h) = b^{-d} f(b^Y t, b^X h)$, and the Widom scaling law is $\beta(\delta - 1) = \gamma$. D. The Jarzynski equality is $< e^{-\beta W} > = e^{-\beta \Delta F}$. Using convexity, this implies $< W > \geq \Delta F$, consistent with Clausius inequality. E: $\frac{dH}{dt} \leq 0$, $H = \int f \ln f \, d\mathbf{r} \, d\mathbf{p}$. The entropy is $S = -k_B H$.

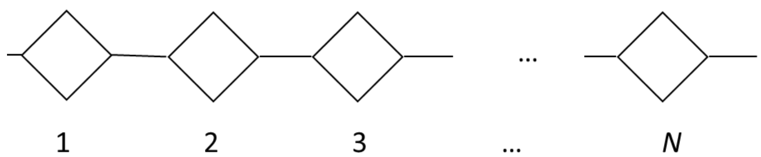
2. Consider the equation of state of a classical monoatomic gas slightly modified from the ideal gas law. We assume a pair-wise interaction potential $v(r)$ between two particles with the distance *r* = |**r**| dependence as

$$v(r) = \begin{cases} \infty, & r < a, \\ -\varepsilon, & a \leq r < b, \\ 0, & r \geq b. \end{cases}$$

   a. Write down the partition function Z_N of *N* particles in canonical ensemble and express it as a product of two factors, a temperature dependent part and a configurational partition function, $Z_N = P_N Q_N$. Evaluate the temperature dependent part, P_N.
   b. Give the expression for the grand partition function Θ of the grand-canonical ensemble, using the result in Part a. Evaluate the configurational partition functions in a box of volume *V* much larger than a^3 and b^3 for zero particle Q_0, one particle Q_1, and two particles Q_2.
   c. Determine the equation of state (pressure P as a function of volume V and temperature T), using the results in Part b above, based on Q_0, Q_1, Q_2, ignoring the higher order terms Q_N for $N > 2$ for the grand partition function Θ.

A: The temperature part is the momentum integrals, configuration partition function is the position integrals, so if $Z_N = P_N Q_N$, $P_N = \left(\frac{2\pi m}{\beta h^2}\right)^{3N/2} \frac{1}{N!}$. B. $\Theta = \sum_{N=0}^{\infty} e^{\beta\mu N} Z_N = Q_0 + \alpha Q_1 + \frac{\alpha^2 Q_2}{2} + \cdots$, where $\alpha = e^{\beta\mu}\left(\frac{2\pi m}{\beta h^2}\right)^{3/2}$. $Q_0 = 1$, $Q_1 = V$, $Q_2 = V\left[e^{\beta\epsilon}\frac{4\pi}{3}(b^3 - a^3) + V - \frac{4\pi}{3}b^3\right]$.
C. In grand canonical ensemble, $\frac{PV}{k_B T} = \ln \Theta$, and $N = \frac{1}{\beta}\frac{\partial \ln \Theta}{\partial \mu}$. Equation of state is obtained after eliminating α from these two equations.

3. Consider a quasi-one-dimensional chain of Ising spins formed by connected rhombuses as shown below. Each site has a spin without a magnetic field, with a ferromagnetic coupling constant J between the sites connected by a line. We assume the units are repeated exactly N times with the periodic boundary condition. Determine the partition function Z in two ways:
   a. Use the transfer matrix method.
   b. Based on high-temperature expansion.



A. Sum over the two spins at the outer vertices of the square, we can write the transfer matrix as PQ, here $P = \begin{pmatrix} z^4 + \frac{1}{z^4} + 2 & 4 \\ 4 & z^4 + \frac{1}{z^4} + 2 \end{pmatrix}$ and $Q = \begin{pmatrix} z & 1/z \\ 1/z & z \end{pmatrix}$, where $z = e^K = e^{\beta J}$. B. There are two types of loops, loop over the squares with various combinatorial choices; the zigzag pathes going from 1 to N and back to 1 again. This gives $Z = 2^{4N}\cosh^{5N}(K)\,[(1 + x^4)^N + (2x^3)^N]$, where $x = \tanh(K)$.

4. A particle moving under gravity in a fluid (sedimentation) or a charged particle in a field follows the Langevin equation with a constant force f, as
$$m\frac{dv}{dt} = -m\gamma v + f + R(t), \qquad \frac{dx}{dt} = v,$$
where $R(t)$ is the random white noise with zero mean and the correlation $\langle R(t)R(t')\rangle = 2m\gamma k_B T\delta(t - t')$.
   a. Determine the mobility μ of the particle, which is defined as the proportionality constant of the average velocity to the force, $\langle v\rangle = \mu f$.
   b. Present the associated Fokker-Planck equation for the Langevin equation for the joint probability density $P(v, x, t)$ of velocity v and position x. You may use without a proof the more general result: if the Langevin equation is $\dot{X} = G(X) + \xi$, then the associated

Fokker-Planck equation is $\frac{\partial P}{\partial t} = -\left(\frac{\partial}{\partial X}\right)^T GP + \left(\frac{\partial}{\partial X}\right)^T D \frac{\partial}{\partial X} P$, where $\langle \xi(t)\xi(t')^T \rangle = 2D\delta(t-t')$.

c. What is the steady state distribution of the velocity and position, $P(v,x)$?

A.$\mu = 1/(m\gamma)$, *B.* $\frac{\partial P}{\partial t} = -\frac{\partial}{\partial v}\left[\left(-\gamma v + \frac{f}{m}\right)P\right] - \frac{\partial (vP)}{\partial x} + \frac{\gamma k_B T}{m}\frac{\partial^2 P}{\partial v^2}$. $P = P(t,x,v)$ *is a function of three variables, t, x, v. C. set left hand side to 0, we can solve the (ordinary) different equation, given* $P(x,v) \propto e^{-\beta(\frac{1}{2}mv^2 - xf)}$. *Proportionality constant is fixed by normalization.*

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