NATIONAL UNIVERSITY OF SINGAPORE

PC5202 ADVANCED STATISTICAL MECHANICS

(Semester II: AY 2018-19)

Time Allowed: 2 Hours

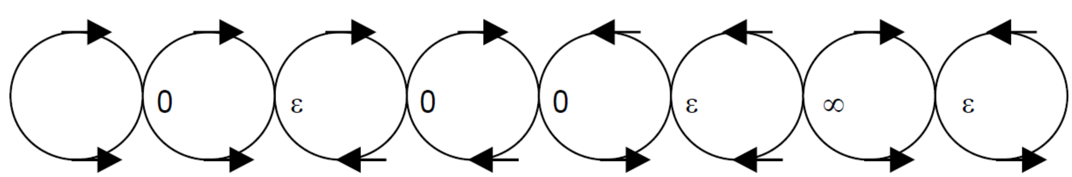
INSTRUCTIONS TO STUDENTS

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. Consider a classical particle of mass m trapped in a parabolic potential in three dimensions, $V(\boldsymbol{r}) = \frac{1}{2}ar^2$, here a is some control constant, and $\boldsymbol{r} = (x, y, z)$ is a three-dimensional position vector. The Hamiltonian of the particle is $H = \frac{\boldsymbol{p}^2}{2m} + V(\boldsymbol{r})$, where $\boldsymbol{p}$ is the momentum vector.
   a. Compute the partition function Z of the single particle system in the canonical ensemble. From it, determine the Helmholtz free energy F.
   b. The particle is assumed initially in thermal equilibrium at temperature $T = 1/(k_B\beta)$. If we drive the system by changing the shape a of the confining potential, from a_i to the final a_f, in some way $a(t)$, what is the expectation value of $e^{-\beta w}$ according to the Jarzynski equality for the nonequilibrium process? Give the definition of the work w.

   a. *The partition function* $Z = \frac{1}{h^3}\int_{-\infty}^{+\infty} dxdydzdp_xdp_ydp_z e^{-\beta[\frac{(P_x^2+p_y^2+p_z^2)}{2m}+\frac{1}{2}a(x^2+y^2+z^2)]}$. *Here we note* $r^2 = x^2 + y^2 + z^2$, *and similarly* $p^2 = p_x^2 + p_y^2 + p_z^2$. *The calculation involves a 6-dimensional integral which can be done for each of the dimensions separately. We need to use the formula for Gaussian integration, which is* $\int_{-\infty}^{+\infty} e^{-\frac{x^2}{2}}dx = \sqrt{2\pi}$. *Using this result, we find* $Z = \left[\frac{1}{\hbar\beta}\sqrt{\frac{m}{a}}\right]^3$. *The free energy is* $F = -\frac{1}{\beta}\ln Z$. *The free energy difference is* $\Delta F = F_f - F_i = \frac{3}{2\beta}\ln\frac{a_f}{a_i}$, *which is needed for part b.*
   b. *The Jarzynski equality is* $\langle e^{-\beta w}\rangle = e^{-\beta(F_f - F_i)} = \left(\frac{a_i}{a_f}\right)^{3/2}$. *The work done w is the difference of the Hamiltonians at the beginning and end of the process,* $w = H(a_f, \boldsymbol{p}_f, \boldsymbol{r}_f) - H(a_i, \boldsymbol{p}_i, r_i)$. *With index i it is the starting phase space point/parameter and index f the final ones. (w can also be expressed as an integral over the path of the differential of the Hamiltonian). [See lecture notes page 124-125].*

2. Consider a 1D ice model illustrated below. The Ising-like discrete degrees of freedom are indicated by the arrows for the orientation of electric dipole moments on the links. Four arrows merge at a vertex. At each vertex, if the number of incoming arrows equals outgoing arrows, the energy is 0; if four of the arrows are all pointing inwards, or all pointing outwards, the energy is $+\infty$; for the rest of cases, the energy is ϵ.
   a. Give the transfer matrix P such that the partition function is $Z = \mathrm{Tr}(P^N)$.
   b. Derive the polynomial equation that the eigenvalues of P must satisfy.
   c. Give the expression for the free energy in the thermodynamic limit, $N \to \infty$.



(a) If we focus on a pair of arrows above and below the circle, we can uniquely specify the states of the system on each circle as four possibilities: RR, RL, LR, LL (right-right, right-left, etc.). Based on the rule of the energy given, if we have RR & RR, we have two in arrows and two out arrows, the energy is 0. If we have RR & LL, the energy is infinite, and so on. Based on this energytic consideration, we have the transfer matrix P as 4x4 matrix: $P = \begin{pmatrix} 1 & x & x & 0 \\ x & 1 & 1 & x \\ x & 1 & 1 & x \\ 0 & x & x & 1 \end{pmatrix}$*. Here we define* $x = e^{-\beta\epsilon}$*. Then the partition function is given as* $Z = \mathrm{Tr}(P^N)$*. (b) The eigenvalues of P is given by the equation* $\det(P - \lambda I) = 0$*, where I is the identity matrix. The determinant equation can be expanded using Laplace expansion, we find* $\lambda(\lambda - 1)(2 - 4x^2 - 3\lambda + \lambda^2) = 0$*. (c) The free energy in the thermodynamic limit is given by the largest eigenvalue. It is* $F = -\frac{1}{\beta}\ln\lambda_{max}$*, here the largest eigenvalue is the solution of the quadratic equation, given* $\lambda_{max} = \frac{1}{2}(3 + \sqrt{1 + 16x^2})$*.*

3. For a magnetic system, the Widom scaling hypothesis states a certain scaling behavior for the free energy per degree of freedom, f, when the two parameters of the problem, the reduced temperature $t = (T - T_c)/T_c$ and the magnetic field h, are changed by some power of factor b. The free energy per spin of the original one and the scaled one are related by a factor of b^{-d}, where d is the dimension.
    a. State the Widom scaling hypothesis for free energy involving the critical exponents X and Y.
    b. Use the Widom scaling hypothesis to derive relations between α, β, γ and exponents X and Y. Here α is the critical exponent for heat capacity, β is for the magnetization, and γ for the magnetic susceptibility. State clearly the assumptions used in your derivation.
    c. Use the results in b to prove the Rushbrooke relation, $\alpha + 2\beta + \gamma = 2$.

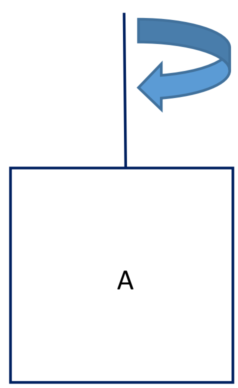
    The Widom scaling is $f(t,h) = b^{-d} f(tb^Y, hb^X)$*. To obtain the order parameter exponent* β*, one set* $tb^Y = 1$*, and then take the first derivative of the free energy with respect to the field h, given* $\beta = \frac{d-X}{Y}$*. The susceptibility exponent is obtained by continuing to second derivative, given* $\gamma = \frac{2X-d}{Y}$*. Lastly, for heat capacity, one need to take the second derivative with respect to t, given* $\alpha = 2 - d/Y$*. Adding up, we find the Rushbrooke value of 2. This question is discussed in class, and the answer can be found in my notes: section 7.2, page 81-83.*

4. An optical mirror suspended in some gas media can be described by the Langevin equation of the overdamped form, $0 = -I\gamma\dot{\theta} + R(t)$. Here I is the moment of inertia of the mirror system, θ is the angle of the mirror, assuming centered around 0, γ is a damping parameter and has the units of inverse time. R is random torque (force times distance) applied to the mirror, with the statistical property that $\langle R(t)\rangle = 0$, $\langle R(t)R(t')\rangle = C\delta(t - t')$.

a. Derive the Fokker-Planck equation associated with the Langevin equation.
b. We assume the mirror is a square of area A, suspended at midpoint, immersed in an ideal gas of particle density $n = N/V$ θ temperature T. Give an estimate of the constant C for the random torque correlation, in terms of the ideal gas parameters and geometry of the mirror. [Hint. If there are N molecules hitting the mirror, the fluctuation will be proportional to $\sqrt{N}$].

One can obtain the Fokker-Planck equation in two ways, compare with the standard form, or derive directly from first principles. I will use the comparison method. We can write the stochastic Langevin equation as $I\gamma \frac{d\theta}{dt} = R(t)$. *Compare with standard form of* $m\frac{dv}{dt} = -m\gamma v + R(t)$, *we have m is* $I\gamma$, *damping term* $-m\gamma v$ *is 0, R is R, and v is* θ. *From the standard Fokker-Planck equation,* $\frac{\partial P}{\partial t} = \frac{\partial(\gamma v P)}{\partial v} + \frac{C}{2m^2}\frac{\partial^2 P}{\partial v^2}$, *we find for the angle problem,* $\frac{\partial P}{\partial t} = \frac{C}{2I^2\gamma^2}\frac{\partial^2 P}{\partial \theta^2}$. *This is just a pure diffusion equation for the angle.*

The second part we first note we should work with a finite time internal t, and define $B = \int_0^t R(t')dt'$. *B is the angular moment transferred during time t from the environment (ideal gas) to the mirror. Then we have* $\langle B^2 \rangle = Ct$, *which is the variance of the angular momentum transfer. Clearly, when a single molecule impacts the mirror, it contributes to the mirror a random torque with random sign (plus or minus). Each impact causes momentum transfer of* $2mv$, *and angular momentum transfer of* $2mvx$, *here x is the distance from the center. We give just an order of magnitude estimates so we take* $x \approx \sqrt{A}$. *We estimate now many molecules hint the mirror in time t, this is given by* $N = nAvt$, *n =* $P/(k_B T)$ *is the particle density and v is the average velocity of the molecule. Apply the law of law numbers, the fluctuation of B is then,* $\sqrt{\langle B^2 \rangle} = \sqrt{Ct} = 2mv\sqrt{A}\sqrt{N}$, *we find* $C \sim m^2 v^3 A^2 n$. *We can replace the velocity by temperature using the equal-partition theorem,* $mv^2 = k_B T$.



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