

NATIONAL UNIVERSITY OF SINGAPORE

PC5202 ADVANCED STATISTICAL MECHANICS

(Semester II: AY 2019-20)

Time Allowed: 3 Hours (1:00-4:00pm, Tuesday 30 April 2020)

INSTRUCTIONS TO STUDENTS

1. This assessment paper contains 4 questions and comprises 3 printed pages (including this cover page).
2. Students are required to answer ALL the questions.
3. Each question carries 25 marks.
4. This is an OPEN BOOK examination. Students may consult any references but discussion with anyone is not allowed. If you like to ask question, use the private chat function in zoom.
5. Email a scanned soft copy in PDF to phywjs@nus.edu.sg before 4:00pm

1. Classically, we can think of a magnet as a point particle moving on a surface of a sphere of some radius with a moment of inertia I . The particle position is specified by the polar angle θ and azimuthal angle ϕ , here $0 \leq \theta < \pi$ and $0 \leq \phi < 2\pi$. The Lagrangian of the system is given by

$$L = \frac{1}{2} I(\dot{\theta}^2 + \dot{\phi}^2 \sin^2 \theta) + B\mu \cos \theta.$$

Here B is the magnetic field and μ is the magnetic moment.

- Determine the Hamiltonian H .
- Give the expression of the single particle partition function Z and evaluate the multi-dimensional integral. You may need the Gaussian integral which is

$$\int_{-\infty}^{+\infty} e^{-x^2/2} dx = \sqrt{2\pi}.$$

- Determine the magnetization m (conjugate to the magnetic field B).
- Determine the magnetic susceptibility χ at the $B \rightarrow 0$ limit.
- Determine the heat capacity C at constant B .

(a) *The general formula for going from Lagrangian to Hamiltonian is $H = \sum p\dot{q} - L$. Here we choose θ and ϕ as coordinates; it is a two degrees of freedom system and no radial r . And the associated conjugate momenta are $p_\theta = \frac{\partial L}{\partial \dot{\theta}} = I \dot{\theta}$, and $p_\phi = \frac{\partial L}{\partial \dot{\phi}} = I \dot{\phi} \sin^2 \theta$. To be called a Hamiltonian, we must eliminate the velocities and express the Hamiltonian in terms of the conjugate pairs, so $H = p_\theta \dot{\theta} + p_\phi \dot{\phi} - L = \frac{p_\theta^2}{2I} + \frac{p_\phi^2}{2I \sin^2 \theta} - B \mu \cos \theta$.*

(b) *The classical statistical mechanics is formulated in generalized coordinates and their conjugate momenta we called q and p . We need to know what are these conjugate momenta for this specific problem. The answer is given in part (a). The usual classical integration measure $d\Gamma = dq dp$ is $d\theta dp_\theta d\phi dp_\phi$ in calculating the partition function Z for integration over the phase space. Note that there is no extra \sin factor, since it is not the surface area of the sphere that play a role but the phase space volume, which is a canonical invariant. Performing the elementary integration we find $Z = 8\pi^2 I \sinh(\beta B \mu) / [(\hbar\beta)^2 B \mu]$. And the Helmholtz free energy $F = -\left(\frac{1}{\beta}\right) \ln Z$. If you get the partition function wrong, the rest of (c) to (e) cannot be calculated correctly.*

(c) *The magnetization is calculated by taking derivative with respect to B , obtain $m = -\frac{\partial F}{\partial B} = \mu / \tanh(\beta B \mu) - \frac{1}{\beta B}$. This is due to $dF = -SdT - m dB$, notice the minus sign there.*

(d) *The susceptibility is $\chi = \partial m / \partial B$, and then take the $B \rightarrow 0$, we get $\chi = \beta \mu^2 / 3$. Notice the extra $1/3$ factor. We can get this result by Taylor expanding the m result and take the linear coefficient in B . You have to make the Taylor expansion with enough accuracy to get the correct factor.*

(e) *Finally, the heat capacity can be computed by take the derivative of the internal energy respect to temperature T . The internal energy is $U = \langle H \rangle = -\frac{\partial \ln Z}{\partial \beta} = 2k_B T - B \mu / \tanh(\beta B \mu)$. This gives the heat capacity at constant B as $C = 2k_B - k_B (\beta B \mu)^2 / \sinh^2(\beta B \mu)$. Alternatively, you can also start with entropy S .*

2. This question concerns the duality relation for the two-dimensional Potts model.
- Given a lattice, define the dual lattice. When this concept of dual lattice is meaningful and when it cannot be defined? Given the honeycomb lattice consisting of hexagons filling the plane, determine its dual lattice.
 - The q -state Potts model is similar to the Ising model except that the values of the spins σ_i take integers $1, 2, \dots, q$. When $q = 2$ it is equivalent to the Ising model. The Hamiltonian is given by

$$H = -J \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j}.$$
 The energy of the nearest neighbor interaction is $-J$ if the values of spins at site i and j are the same, and 0 otherwise. Consider a high temperature expansion of the partition function Z on a square lattice with appropriate expansion variable x , give the first three nonzero terms of the result.
 - Develop a low temperature expansion of Z for the same square lattice, starting from the ground state (which is q -fold degenerate), also obtain the first three nontrivial terms.
 - Use the duality argument to determine the transition temperature T_c .

(a) *To get a dual lattice from the original lattice, we put a dual site on each face of the original lattice, and connect the dual sites by dual links. The dual link always crosses the original link. This can be done only for planar graphs; not possible for 3D lattices. The hexagonal lattice has a dual lattice which is the triangular lattice.*

(b) *This is trickier than one thinks. The most obvious expansion variable is to use $e^{K\delta_{\sigma\sigma'}} = 1 + x\delta_{\sigma\sigma'}$, with $x = e^K - 1$. But this expansion doesn't have the Ising-like property in the sense averaging over spins produce 0, and the duality relation between high and low temperature expansion of the partition function cannot be established. But most students did it this way. Then when we expand, we get no delta factor (no bonds), one delta factor (one bond), and two delta factors (two bonds). Not that for the two delta factor case, the bond can be disconnected or connected, this gives two possible terms, thus the partition function is $Z = q^N + 2Nxq^{N-1} + N(2N-1)x^2q^{N-2} + O(x^3)$. Alternative to the delta expansion above is to use $q\delta_{\sigma\sigma'} - 1$. This has the property that a single term average to zero, so to get a nonzero value we must form a loop (as in the Ising case). We can write $e^{K\delta_{\sigma\sigma'}} = \frac{e^{K+q-1}}{q} [1 + y(q\delta_{\sigma\sigma'} - 1)]$, here $y = \frac{e^K - 1}{e^{K+q-1}} = \frac{x}{x+q}$ replacing x . With variable y we can form loops of 4 sided and 6 sides, the first three terms are $Z = q^N \left(\frac{e^{K+q-1}}{q}\right)^{2N} (1 + N(q-1)y^4 + 2N(q-1)y^6 + O(y^8))$. [But the trouble seems to be why the coefficient has the $q-1$ factor and not other expressions? Note the curious mathematical fact: if we define a $q \times q$ matrix P with elements $q\delta_{\sigma\sigma'} - 1$, we have $\text{Tr}(P^k) = q^k(q-1)$.]*

- (c) *The low temperature expansion is straightforward, the ground state is q -fold degenerate with energy $-J2N$, and first excited states change one site, with energy higher by $4J$ and it is $Nq(q-1)$ fold degenerate, and next higher states flip two spin side-by-side, having energy higher than ground state by $6J$. So partition function is $Z = qe^{2NK} + q(q-1)Ne^{(2N-4)K} + 2Nq(q-1)e^{(2N-6)K} + \dots$.*
- (d) *We see the coefficients in part (b) and (c) are the same. This means duality is also true for Potts model and we can identify T_c by the equation $y = \frac{e^K - 1}{e^K + q - 1} = e^{-K}$. Solving the equation for K , we find $K_c = \frac{J}{k_B T_c} = \ln(1 + \sqrt{q})$.*

3. The Jarzynski equality relates the equilibrium free energy to a nonequilibrium process.

- State the Jarzynski equality, explain your symbols used.
- Consider a classical Hamiltonian of the form

$$H(t) = \frac{p^2}{2m} + \frac{1}{2}k(x - vt\theta(t))^2$$

which represents a harmonic oscillator with the center of the force moving with velocity v when $t > 0$. Here the step function $\theta(t) = 0$ if $t < 0$ and 1 when $t \geq 0$. Determine the free energy difference $F(t) - F(0)$ associated with the Hamiltonian $H(t)$ and $H(0)$. Here t is a fixed time.

- Solve the equation of motion of the oscillator to determine $x(t)$ and $p(t)$ in terms of the initial values of position x_0 and momentum p_0 , as well as time t .
- Give the expression for the work W done going from microscopic state (x_0, p_0) to the state $(x(t), p(t))$, according to Jarzynski. Express the work W as a function of the initial state only.
- Assuming that the initial distribution of (x_0, p_0) follows the canonical distribution determined by the initial Hamiltonian $H(0)$, show that the exponential average of the work, $\langle e^{-\beta W} \rangle_0$, by explicit calculation of the average, is given by the Jarzynski equality. Here $\beta = 1/(k_B T)$, k_B is the Boltzmann constant and T is temperature.

(a) *The Jarzynski equality takes the form $\langle e^{-\beta w} \rangle = e^{-\beta(F_B - F_A)}$, here $\beta = \frac{1}{k_B T}$, and F_A is the free energy of the initial state and F_B is the free energy of the final state, $w = H_B - H_A$ is the microscopic work, and the average is over the initial canonical distribution $\rho_A = e^{-\beta H_A} / Z_A$. Although the expression for w looks simple, we must note that H_A is evaluated at the initial state (x_0, p_0) while H_B is evaluated at the final state $(x(t), p(t))$ which depends on the initial state and time t .*

(b) *The partition function at a fixed time t is $Z(t) = \frac{1}{h} \iint dx dp e^{-\beta(\frac{p^2}{2m} + \frac{1}{2}k(x-vt)^2)}$. This is just a product of two gaussians one for p centered around 0 and another x centered around vt . The integral has the similar form, thus we obtain $Z(t) = 1/(\beta \hbar \omega)$, here we have defined the angular frequency as $\omega =$*

$\sqrt{\frac{k}{m}}$. Since the result is independent of time t , this means the free energy difference $F(t) - F(0) = 0$.

(c) Applying the Hamilton equations of motion, we can eliminate the momentum, then the coordinate satisfies the equation $m\ddot{x} = -m\omega^2x + vkt$. We can take care of the extra time dependent term if we use $x(t) = vt$. The full solution is a sum of sin and cos function together with the vt term. We can fix the initial condition by x_0 and p_0 of initial position and momentum. We find $x(t) = x_0 \cos \omega t + \frac{p_0 - mv}{m\omega} \sin \omega t + vt$. The momentum is obtained by differentiation, $p(t) = m\dot{x}(t)$.

(d) The microscopic work w is completely determined by the initial position x_0 , initial momentum p_0 , and the time t , that is $w(x_0, p_0, t) = H(x(t), p(t), t) - H(x_0, p_0, 0)$. This expression can be simplified to find $w = -2v \sin(\frac{\omega t}{2}) \left[m\omega x_0 \cos(\frac{\omega t}{2}) + (p_0 - mv) \sin(\frac{\omega t}{2}) \right]$. As far as the initial position and momentum is concerned, it is a linear function in them and t is just a fixed parameter. This expression is put into the Jarzynski exponential average of the work.

(e) To evaluate the exponential work explicitly (not evoking the Jarzynski theorem), we note the canonical distribution for the harmonic oscillator is just gaussian, and adding the extra $-\beta w$ term only shifts the center of the gaussian, after completing the squares we find it is just one, $\langle e^{-\beta w} \rangle = \int dx_0 dp_0 \frac{1}{h Z(0)} e^{-\beta \left(\frac{p_0^2}{2m} + \frac{1}{2} k x_0^2 \right) - \beta w} = 1$. (Steps omitted here). $Z(0) = \frac{1}{\beta \hbar \omega}$ is the partition function.

4. Consider a harmonic oscillator simultaneously experiencing two thermal baths of temperature T_L and T_R modelled by a Langevin equation:

$$m \frac{dv}{dt} = -kx - m\gamma_L v + \xi_L - m\gamma_R v + \xi_R.$$

The position and velocity are related by $\frac{dx}{dt} = v$. Here m is the mass, k is the force constant, ξ_L and ξ_R are the noises of the left and right bath, which follow the fluctuation-dissipation theorem, relating to the damping coefficients γ_L, γ_R by,

$$\langle \xi_\alpha(t) \xi_\beta(t') \rangle = 2m\gamma_\alpha k_B T_\alpha \delta(t - t') \delta_{\alpha\beta}, \quad \alpha, \beta = L \text{ or } R.$$

k_B is the Boltzmann constant. The first δ is the Dirac delta function and the second is the discrete Kronecker delta.

- Derive the associated Fokker-Planck equation for the joint probability of velocity v and position, $P(x, v, t)$.
- Show that the steady state solution, when the probability distribution becomes independent of the time t at long time, can be written in the Gibbsian form, $P(x, v) = \exp(-\beta H)/Z$, here $H = \frac{1}{2}mv^2 + \frac{1}{2}kx^2$ is the total energy of the oscillator. The choice of Z normalizes the total probability to 1. Determine β in terms of the model parameters given.

- c. The average work done by the left bath to the oscillator per unit time is $J = \langle v(-m\gamma_L v + \xi_L) \rangle$. Show that it is given by $J = \frac{\gamma_L \gamma_R}{\gamma_L + \gamma_R} k_B (T_L - T_R)$.

- (a) We can derive the Fokker-Planck equation following the Zwanzig method, or we can just use the formal result in the textbook. The key point to note is that we have two independent variables x , and v , in addition to time t , since we are asking to find the joint probability of v and x . So, the equation of motion must be viewed as two-coupled equation for x and v . Skip the math detail, the final Fokker-Planck equation is $\frac{\partial P}{\partial t} + \frac{\partial(vP)}{\partial x} + \frac{\partial[(-\omega^2 x - \gamma v)P]}{\partial v} = D \frac{\partial^2 P}{\partial v^2}$. Here I have defined $\omega^2 = \frac{k}{m}$, $\gamma = \gamma_L + \gamma_R$, and $D = \frac{k_B}{m} (\gamma_L T_L + \gamma_R T_R)$.
- (b) We assume that the Gibbs form is the solution, we are asked to determine the single parameter β . Setting the time derivative $\frac{\partial P}{\partial t} = 0$, and plugging in the trial form into the Fokker-Planck equation, we find the equation is satisfied provided that $\beta = \frac{\gamma}{mD}$, or stated differently, the effective temperature of the system to be a weighted average $T = \frac{\gamma_L T_L + \gamma_R T_R}{\gamma_L + \gamma_R}$ by the bath couplings.
- (c) To find the energy current, since we know in the steady state the probability distribution is Gibbsian with an effective temperature T , we can easily compute the velocity squared by applying equipartition theorem, but the velocity-noise correlation need some thinking. So we can get quickly $J = \langle v(-m\gamma_L v + \xi_L) \rangle = -\gamma_L k_B T + \langle v \xi_L \rangle$. To find the later term, we need to go back to the Langevin equation to solve position or velocity (since $v = dx/dt$), we can focus on the position x . It is given by the Green's function of the system. The velocity at time t can be expressed as $v(t) = -\frac{1}{m} \int_{-\infty}^t \frac{\partial}{\partial t} G(t - t') \xi(t') dt'$, where the Green's function in frequency domain is given by $\tilde{G}(\omega) = \left[(\omega + i\eta)^2 - \frac{k}{m} + i\gamma\omega \right]^{-1}$. Using this result, the velocity and noise correlation can be computed, applying the noise correlation as delta function, we get $\langle v(0) \xi_L(0) \rangle = -2\gamma_L k_B T_L G'(0)$. Here the last term is the derivative of the Green's function at time $t \rightarrow 0^+$, which can be calculated using inverse Fourier transform and residue theorem, given $-\frac{1}{2}$. Thus, we have $\langle v \xi_L \rangle = \gamma_L k_B T_L$. Putting the two terms together, after some simplification, one obtains the desired result. It is possible to obtain the same result based solely on Fokker-Planck equation, see textbook in the supplementary reading.