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Advanced Statistical Physics
Wintersemester 2022/23

Problem sheet 2, handed out: Friday 4th November, 2022
due: **Sunday 13th November, 2022 (via email/ studip)**

1 Phase transition and large deviations in the infinite range Ising model (20 pts. + 6 bonus pts.)

The Hamiltonian for the infinite range Ising model (in zero field) is

$$H = -\frac{1}{2N}\sum_{i,j=1}^{N} J\,\sigma_i\sigma_j$$

with Ising spins $\sigma_i = \pm 1$. The aim of this question is to analyse the (equilibrium) fluctuations of the magnetization $M = \sum_{i=1}^{N}\sigma_i$ in this system, as a function of temperature $T = 1/\beta$.

a) Show that the probability of observing magnetization M is

$$P(M) = \frac{1}{Z}\frac{N!}{((N+M)/2)!((N-M)/2)!}\,e^{\beta J M^2/(2N)}$$

(Hint: Count how many spin configurations have a given M.) (3 pts.)

b) Use the Stirling approximation to show from (a) that the rate function for the magnetization is, with $m = M/N$,

$$I(m) = -\beta J m^2/2 + \frac{1+m}{2}\ln\frac{1+m}{2} + \frac{1-m}{2}\ln\frac{1-m}{2} + \text{const}$$

and sketch $I(m)$ for $\beta J < 1$ and $\beta J > 1$. Why does the form in the latter case indicate a phase transition? (6 pts.)

c) Derive the "Hubbard-Stratonovich" transformation

$$e^{\beta J M^2/(2N)} = \int \frac{dx}{\sqrt{2\pi\beta J/N}}\,e^{-Nx^2/(2\beta J)+Mx}$$

which is used to factorize the sum defining the partition function $Z = \operatorname{Tr} e^{-\beta(H-hM)}$ in a field h into independent sums over individual spins. Carry out these sums to express Z as an integral over x, and deduce that the free energy per spin becomes for $N \to \infty$

$$f(h) = \min_x \left[\frac{x^2}{2\beta^2 J} - \frac{1}{\beta} \ln(2\cosh(\beta h + x)) \right]$$

Find the condition for the position $x^*(h)$ of the minimum. Sketch function to be minimized for $\beta J < 1$ and > 1 and a few h? (5 pts.)

d) Find the average magnetization $m = -f'(h)$ and show that it obeys $m = \tanh(\beta(Jm + h))$. (Hint: $f(h)$ depends on h both explicitly and via $x^*(h)$; show using the chain rule that only the explicit dependence is needed to calculate $f'(h)$.) (3 pts.)

e) Discuss qualitatively, and sketch, how the rate function $I^*(m)$ that is obtained by applying the Gärtner-Ellis-Theorem to $f(h)$ differs from the result of (b). (3 pts.)

f) (bonus) Verify explicitly that $I^*(m)$ agrees with $I(m)$ in the appropriate range of m. (2 pts.)

g) (bonus) Explain how the rate function $I(m)$ for $\beta = 0$ can be used to write down the rate function for the fluctuations of the end-to-end distance of a one-dimensional polymer, consisting of N chain segments of fixed length l that can randomly point left or right. (4 pts.)

2 Properties of equilibrium correlation functions (10 pts.)

Correlation functions are important for describing time-dependent fluctuations of a system and can be used e.g. to deduce transport properties. In this exercise, we want to prove some general properties of correlation functions, defined as in the lectures as $C_{AB}(t,t') = \operatorname{Tr} A(t)B(t')\rho(0)$ where $A(t)$, $B(t')$ are time-dependent phase space observables (classically) or Hermitian operators.

a) In the classical case one has $C_{BA}(t',t) = C_{AB}(t,t')$. Prove that in the quantum case, $C^*_{BA}(t',t) = C_{AB}(t,t')$. (Hint: Use that $(\operatorname{Tr} M)^* = \operatorname{Tr}(M^\dagger)$ where $\ldots^\dagger$ indicates Hermitian conjugation.) (2 pts.)

b) From now on, consider equilibrium correlators, which can be expressed as $C_{AB}(t,t') = (A(t), B(t'))$ in terms of the product $(A,B) = \operatorname{Tr} AB\rho^{\text{eq}}$.

   Prove in the classical case that $(A, \mathcal{L}B) = -(\mathcal{L}A, B)$. Deduce that $(A, e^{\mathcal{L}t'}B) = (e^{-\mathcal{L}t'A}, B)$ and therefore that equilibrium correlation functions are time-translation invariant. (5 pts.)

c) Show that in the classical case, $C_{AA}(\Delta t) \le C_{AA}(0)$, i.e. the autocorrelation function is bounded from above by its equal-time value. (Hint: Start from the average of $[A(\Delta t) - A(0)]^2$.) (3 pts.)

3 Liouville operator for the harmonic oscillator (20 pts. + 5 bonus pts.)

Consider a simple harmonic oscillator in one-dimension. The Hamiltonian of the system is given by

$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{1}$$

a) Write down the Liouville operator $\mathcal{L}$ as defined in the lectures. (2 pts.)

b) Consider the coordinate transformation

$$x = \sqrt{\frac{2J}{m\omega}}\cos\phi, \qquad \text{and} \quad p = \sqrt{2Jm\omega}\sin\phi$$

Show that in these coordinates, the Liouvillian becomes simply

$$\mathcal{L} = -\omega\frac{\partial}{\partial\phi}$$

Hint: Use the chain rule to transform from $(\partial/\partial x, \partial/\partial p)$ to $(\partial/\partial\phi, \partial/\partial J)$; it is convenient to express the Jacobian via the inverse function relation

$$\begin{pmatrix} \frac{\partial\phi}{\partial x} & \frac{\partial J}{\partial x} \\ \frac{\partial\phi}{\partial p} & \frac{\partial J}{\partial p} \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial\phi} & \frac{\partial p}{\partial\phi} \\ \frac{\partial x}{\partial J} & \frac{\partial p}{\partial J} \end{pmatrix}^{-1}$$

(10 pts.)

c) Consider the eigenvalue problem $\mathcal{L}f = \lambda f$. Show that the eigenvalues are of the form $\lambda = -in\omega$ with n an integer, and find the corresponding eigenfunctions f. (8 pts.)

d) (bonus) Show that the eigenvalues of $\mathcal{L}$ are always imaginary in deterministic dynamics, given the anti-self-adjointness of $\mathcal{L}$. (Hint: Anti-self-adjointness for a matrix $\boldsymbol{L}$ and the conventional scalar product would be the property that $\boldsymbol{a}^{\mathrm{T}}\boldsymbol{L}\boldsymbol{b} = -(\boldsymbol{L}\boldsymbol{a})^{\mathrm{T}}\boldsymbol{b}$ for arbitrary vectors $\boldsymbol{a}$, $\boldsymbol{b}$. Deduce that $\boldsymbol{L}$ is antisymmetric (also called skew-symmetric). What does this imply for the eigenvalues?) (5 pts.)

4 Rate function in nonzero field (bonus) (15 pts.)

Consider an extensive observable A with conjugate field h. We discussed in the lectures the Gärtner-Ellis theorem that gives the rate function for the distribution of A at zero field.

a) Generalize the derivation from the lectures to show that the rate function for the distribution of A in a nonzero field h_0 is given by

$$I_{h_0}(a) = \sup_h \beta[ha + f(h_0+h) - f(h_0)]$$

(5 pts.)

b) By shifting h appropriately, show that this result can be rewritten as

$$I_{h_0}(a) = I_0(a) - \beta h_0 a + \beta[f(0) - f(h_0)]$$

where $I_0(a)$ is the zero field rate function derived in the lectures. Interpret this result graphically. (5 pts.)

c) Show that for arbitrary observables,

$$P_{h_0}(A) \propto P_0(A) e^{\beta h_0 A}$$

Find the proportionality constant. Explain how the relation between $P_{h_0}(A)$ and $P_0(A)$ can be used to give an alternative derivation of the result of (b). (5 pts.)