Theoretische Physik IV: Statistische Mechanik, Exercise 12

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1. 1D classical Ising Model: Part 1 (Written)

Consider a chain of N classical, binary magnetic moments $s_i \in \{-1, +1\}$. The physics is defined by the *1D Ising* Hamiltonian

$$\mathcal{H}_{\mathrm{1D}}(\{s_j\}) = -J \sum_{i=1}^{N-1} s_i s_{i+1} \tag{1}$$

with coupling constant $J \in \mathbb{R}$. In the following we consider open boundary conditions (OBC), i.e. the term $s_{N+1}s_1$ is missing.

(a) Explain pictorially why for $J > 0$ ($J < 0$) the system is called *ferromagnetic* (*antiferromagnetic*).

(b) Calculate the canonical partition function

$$Z_N(T) = \sum_{\{s_j\}} e^{-\beta \mathcal{H}_{\mathrm{1D}}(\{s_j\})} \tag{2}$$

with inverse temperature $\beta \equiv \frac{1}{k_B T}$. Here $\sum_{\{s_j\}}$ denotes the sum over all configurations $\{s_j\}$.
Derive an expression for the free energy per site in the thermodynamic limit, $f(T) = -\lim_{N\to\infty} \frac{1}{\beta N} \ln Z_N(T)$.

(c) Calculate the two-point correlation function

$$\langle s_i s_{i+k} \rangle = Z_N(T)^{-1} \sum_{\{s_j\}} s_i s_{i+k}\, e^{-\beta \mathcal{H}_{\mathrm{1D}}(\{s_j\})} \tag{3}$$

for $i = 1, \ldots, N$ and $k \leq N - i$ and conclude that there is no phase transition for $T > 0$. Hint: Show that $\langle s_i s_{i+k} \rangle \to 0$ for $k, N \to \infty$ and fixed i. That is, there is no long-range order for finite T in the thermodynamic limit.
What happens for $T = 0$?

2. 1D classical Ising Model: Part 2 (Oral)

Let us go one step further and switch on a magnetic field h which contributes the energy $-hs_i$ for each magnetic moment s_i. Therefore the new Hamiltonian reads

$$\mathcal{H}_{\mathrm{1D}}(\{s_j\}) = -J \sum_{i=1}^{N} s_i s_{i+1} - h \sum_{i=1}^{N} s_i \tag{4}$$

where we now impose periodic boundary conditions (PBC), i.e. the term $s_{N+1}s_1$ is present and we identify $s_{N+1} \equiv s_1$.

(a) Again calculate the canonical partition function $Z_N(T, h)$. To this end, show that the partition function can be cast in the form

$$Z_N(T, h) = \mathrm{Tr}\left[\mathbb{T}^N\right] \tag{5}$$

where $\mathbb{T} \in \mathbb{R}^{2\times 2}$ is a symmetric 2×2-matrix and $\mathrm{Tr}[\bullet]$ denotes the trace ($\mathbb{T}$ is called *transfer matrix*).

Recall that for any diagonalisable matrix $M \in \mathbb{R}^{n\times n}$ with eigenvalues $\lambda_1, \ldots, \lambda_n$ it holds 1) M^N has eigenvalues λ_i^N and 2) $\mathrm{Tr}[M] = \sum_{i=1}^N \lambda_i$. Thereby derive an expression for $Z_N(T, h)$.

(b) Show that the free energy per site in the thermodynamic limit reads

$$f(T, h) = -\frac{1}{\beta} \ln\left[e^{\beta J} \cosh \beta h + \sqrt{e^{2\beta J} \sinh^2 \beta h + e^{-2\beta J}}\right]. \tag{6}$$

(c) Derive an expression for the magnetization $m(T, h)$ and the susceptibility $\chi(T, h = 0)$. To this end, show that the ensemble average of the magnetic moment per spin can be calculated (in the thermodynamic limit) as

$$m \equiv \lim_{N\to\infty} \frac{1}{N} \left\langle \sum_i s_i \right\rangle = \lim_{N\to\infty} \frac{1}{N} \frac{\partial(\ln Z_N)}{\partial(\beta h)} \tag{7}$$

and use the free energy $f(T, h)$ to evaluate this expression. Is there now a phase transition, meaning a finite magnetization for vanishing magnetic field h and finite T? Explain the behaviour of $\chi(T, h = 0)$ for $T \to 0$.

(d) Compare the results in (c) with the corresponding results of problem 4 on exercise sheet 11 for the non-interacting magnetic moments.

Remark: In contrast to the one-dimensional Ising *chain* which we considered here, there *is* a phase transition at a finite temperature $T_c > 0$ in *two* dimensions. The analytical solution due to Onsager is considered a milestone of theoretical physics.

3. Repetition of Quantum Mechanics: Density operators (Oral)

This exercise sets up some crucial concepts of *quantum* statistical mechanics. Some (if not all) of them should already be known from your quantum mechanics lecture.

To describe the state of a quantum mechanical system as a vector $|\Psi\rangle \in \mathcal{H}$ in some Hilbert space $\mathcal{H}$, it is essential for the state to be known completely (e.g. by measuring a CSCO, a complete set of commuting observables).

In real setups this is usually not possible which motivates a more general notion of quantum mechanical "states". Such a generalized state is described by the statement that the considered system is with *classical* probability p_i in some state $|\Psi_i\rangle$ for $i = 1, \ldots, n$ (where $\{|\Psi_i\rangle\}$ is a not neccessarily orthogonal set of states). We expect that measuring an observable $\hat{A}$ yields the expectation value

$$\langle \hat{A} \rangle = \sum_{i=1}^{n} p_i \langle \Psi_i | \hat{A} | \Psi_i \rangle \tag{8}$$

where $\langle \Psi_i | \Psi_i \rangle = 1$, $0 \le p_i \le 1$ and $\sum_i p_i = 1$.

The state of the system is now described by the *density operator*

$$\hat{\rho} = \sum_{i=1}^{n} p_i \, |\Psi_i\rangle\langle\Psi_i| \tag{9}$$

(often sloppily called *density matrix*).

A density operator $\hat{\rho}$ is called *pure* if there is a state vector $|\Psi\rangle \in \mathcal{H}$ such that $\hat{\rho} = |\Psi\rangle\langle\Psi|$ and *mixed* otherwise. A mixed state $\hat{\rho}$ therefore encodes a *classical mixture* of quantum states (in contrast to a coherent superposition).

(a) Explain why $\hat{\rho}$ indeed encodes our knowledge of the system completely by showing that the expectation value of an observable $\hat{A}$ can be expressed as $\langle\hat{A}\rangle = \mathrm{Tr}[\hat{\rho}\hat{A}] = \mathrm{Tr}[\hat{A}\hat{\rho}]$ where $\mathrm{Tr}[\bullet]$ denotes the trace of an operator.

(b) Prove the following characterizing properties of any density operator:

  (i) $\hat{\rho} = \hat{\rho}^\dagger$ (self-adjoint)

  (ii) $\langle\phi|\,\hat{\rho}\,|\phi\rangle \geq 0$ for all $|\phi\rangle \in \mathcal{H}$ (positive semi-definite)

  (iii) $\mathrm{Tr}[\hat{\rho}] = 1$ (normalized trace-class)

  Mathematically speaking, a density operator is a (bounded) positive semi-definite and Hermitian trace-class operator with trace one.

In the common perception of quantum mechanics it is perfectly valid to (coherently) superimpose two states $|\Psi_1\rangle, |\Psi_2\rangle \in \mathcal{H}$ to obtain a new *physical* quantum state $|\Psi'\rangle = \alpha\,|\Psi_1\rangle + \beta\,|\Psi_2\rangle$ (up to a normalizing factor). The state space $\mathcal{H}$ (i.e. the Hilbert space) therefore exhibits a vector space structure.

(c) Let $\mathcal{B}(\mathcal{H})$ be the vector space of bounded operators on $\mathcal{H}$ (”matrices”) and denote by $\mathcal{D}(\mathcal{H}) \subseteq \mathcal{B}(\mathcal{H})$ the set of density operators (characterized by the properties in (b)).

  Give an example to show that $\mathcal{D}(\mathcal{H})$ is *not* a vector space. That is, density operators cannot be linearly combined in general to form a new valid density operator. Yet $\mathcal{D}(\mathcal{H})$ features an interesting property: Show that $\mathcal{D}(\mathcal{H})$ is a *convex space*, i. e. show that for two density operators $\hat{\rho}_1, \hat{\rho}_2 \in \mathcal{D}(\mathcal{H})$ it follows

$$t \cdot \hat{\rho}_1 + (1-t) \cdot \hat{\rho}_2 \in \mathcal{D}(\mathcal{H}) \quad \text{for} \quad 0 \leq t \leq 1\,. \tag{10}$$

  This is called a *convex combination* of density operators.

To conclude this short review of density operators, let us focus on the following two important statements:

(d) Show that for any Hermitian operator $\hat{H}$ and $\beta \in \mathbb{R}_0^+$ the operator $\hat{\rho} := e^{-\beta\hat{H}} / \mathrm{Tr}[e^{-\beta\hat{H}}]$ is a density operator.

  Hint: Recall that a Hermitian matrix is positive semi-definite if and only if all eigenvalues are non-negative.

(e) The quantity $\gamma[\hat{\rho}] := \mathrm{Tr}[\hat{\rho}^2]$ is called *purity*. Show that $\gamma[\hat{\rho}] = 1$ if $\hat{\rho}$ is pure and $\gamma[\hat{\rho}] < 1$ if $\hat{\rho}$ is mixed. We conclude that γ can be employed to check whether a given state is a pure quantum state or a classical mixture of quantum states.