STATISTICAL MECHANICS

PRACTICE EXAM 2005

Time allotted: 3 hours for 5 questions.

1. (i) Give a definition of the (Helmholtz) free energy density $f(v,T)$ and show that it is convex as a function of the specific volume v, and concave as a function of the temperature T.
   (ii) Define what is meant by the thermodynamic limit, and give the basic expression of $f(v,T)$ in terms of the partition function $Z_{N,V}(T)$ in the thermodynamic limit.
   (iii) Derive the expression

$$f(v,T) = -k_B T \ln\left(2\cosh\frac{H}{k_B T}\right)$$

   for the free energy density of a system of independent spins $s_i = \pm 1$ with energy levels given by

$$E(s_1, \ldots, s_N) = -H\sum_{i=1}^{N} s_i.$$

2. (i) Derive the expression

$$f(\beta) = -\frac{1}{\beta}\ln\left(e^{\beta J}\cosh\beta H + \sqrt{e^{2\beta J}\sinh^2\beta H + e^{-2\beta J}}\right)$$

   for the free energy density of the 1-dimensional Ising model with periodic boundary conditions, given by the energy levels

$$E(\{s_i\}_{i=1}^{N}) = -J\sum_{i=1}^{N} s_i s_{i+1} - H\sum_{i=1}^{N} s_i.$$

   (ii) Compute the magnetisation $m(\beta, J, H)$ for this model and show that there is no spontaneous magnetisation at any $\beta > 0$.

3. (i) Define the concept of (mixed) state on an algebra of operators $\mathcal{A}$.
(ii) If $\mathcal{A} = \mathcal{B}(\mathcal{H})$ for a Hilbert space $\mathcal{H}$, show that for any $\phi \in \mathcal{H}$, $\rho_\phi(A) = \langle \phi \,|\, A\phi \rangle$ defines a state on $\mathcal{A}$. Give also an example of a state which is not such a vector state.
(iii) Given a finite-dimensional Hilbert space $\mathcal{H}$, define a scalar product on $\mathcal{B}(\mathcal{H})$ and use Riesz' theorem to prove that every mixed state on $\mathcal{B}(\mathcal{H})$ is given by a density matrix.

4. (i) Given a state ρ with density matrix $\underline{\rho}$ on a finite-dimensional matrix algebra $\mathcal{M}$, give the definition of the von Neumann entropy $S(\rho)$ of ρ.
(ii) Given two positive-definite $n \times n$ matrices A and B, prove the inequality

$$\mathrm{Trace}(A \ln A) - \mathrm{Trace}(A \ln B) \geq \mathrm{Trace}(A - B).$$

Hence derive the bounds

$$0 \leq S(\rho) \leq k_B \ln n.$$

(iii) Formulate and prove the variational principle for the free energy $F(\beta, H)$ of a finite spin system with Hamiltonian H.

5. (i) Define the algebra of local observables for a quantum spin system on the lattice $\mathbb{Z}^d$ in dimension d.
(ii) Explain why there does not exist a Hamiltonian for a quantum lattice system on the infinite lattice $\mathbb{Z}^d$. Define the concept of a potential Φ and express the Hamiltonian for a finite subset $\Lambda \subset \mathbb{Z}^d$ in terms of the potential.
(iii) Give the definition of the space of finite-range potentials.
(iv) The nearest-neighbour XY-model on $\mathbb{Z}^d$ is defined by the potentials

$$\Phi(X) = \begin{cases} -Hs_x^1 & \text{if } X = \{x\}; \\ -J(s_x^1 s_y^1 + s_x^2 s_y^2) & \text{if } X = \{x, y\},\ |x - y| = 1; \\ 0 & \text{otherwise.} \end{cases}$$

Here $H \in \mathbb{R}$ is the external magnetic field and $J > 0$ is a coupling constant. s_x^1, s_x^2, s_x^3 are the components of a vector with 2×2 matrix components: $\vec{s}_x = \frac{1}{2}\vec{\sigma}$, where $\sigma^1, \sigma^2, \sigma^3$ are Pauli's σ-matrices. Show that the corresponding finite-volume Hamiltonians can be written as

$$H_\Lambda = -J \sum_{x,y \in \Lambda, \text{n.n.}} R_{xy} - H \sum_{x \in \Lambda} s_x^1,$$

where R_{xy} is the exchange operator given by

$$R\,|s,s'\rangle = \begin{cases} 0 & \text{if } s = s'; \\ |s',s\rangle & \text{if } s \neq s'. \end{cases} \; .$$

Show also that Φ is a translation-invariant, finite-range potential.

(iv) Prove that the finite-range potentials are dense in the Banach space $\mathcal{B}_1$ of translation-invariant potentials Φ satisfying

$$||\Phi||_1 = \sum_{X \subset \mathbb{Z}^d \text{finite}:0 \in X} \frac{||\Phi(X)||}{|X|} < +\infty.$$

Compute the 1-norm of the above potential.

6. (i) Give the definition of the free energy density of a quantum lattice system with potential Φ at inverse temperature $\beta > 0$.

   (ii) Formulate Peierls' inequality for a hermitian $n \times n$-matrix A and use it to derive the inequality

   $$|\ln \mathrm{Trace}\, e^A - \ln \mathrm{Trace}\, e^B| \leq ||A - B||$$

   for hermitian $n \times n$-matrices A and B.

   (iii) Use this inequality to prove that the free energy density is a continuous function of Φ w.r.t. the 1-norm defined under question 5.

7. Assuming that the thermodynamic limit of the free energy density $f(\Phi, \beta)$, the mean internal energy $\rho(e_\Phi)$ and the entropy density $s(\rho)$ for any translation-invariant state exist, formulate and prove the variational theorem for the free energy density of a quantum spin system. [You may assume that the variational principle holds for finite quantum spin systems.]

8. (i) Let ρ be a state on a finite-dimensional matrix algebra $\mathcal{M}$, with density matrix $\underline{\rho} = \frac{1}{z(\beta)} e^{-\beta h}$, where $h \in \mathcal{M}$ is a hermitian matrix and $z(\beta)$ is a normalisation constant. Define $H_N = h_1 + \ldots + h_N$, where h_i is a copy of h in the i-th factor of $\mathcal{A}_N = \otimes_{i=1}^N \mathcal{M}$. Given a polynomial $g : \mathbb{R} \to \mathbb{R}$ and a hermitian matrix $x \in \mathcal{M}$ define finite-volume Hamiltonians $\tilde{H}_N$ by

   $$\tilde{H}_N = H_N + N g(\overline{x}_N),$$

   where $\overline{x}_N = \frac{1}{N}(x_1 + \ldots + x_N)$. Express the corresponding free energy density in the thermodynamic limit by the variational formula

   $$f(\beta) = \inf_{u \in \mathbb{R}} [g(u) + \beta^{-1} I(u)].$$

   Give a general expression for $I(u)$.

   (ii) Apply this formula to the special case of the mean-field Ising model to derive the result on page 18 of the notes.