

Theorie der Wärme – Statistical Physics
 (Prof. E. Frey)

Problem set 11

Problem 11.1 *Ising model* (6 pts)

Use Bogoliubov's inequality (Problem 6.6) to find an upper bound for the free energy of the Ising model on a d -dimensional cubic lattice

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i, \quad \sigma_i = \pm 1, \quad i = 1, \dots, N = L^d$$

where the first sum is restricted to nearest neighbors, in terms of the solvable model

$$\mathcal{H}_0 = -H_0 \sum_i \sigma_i, \quad \sigma_i = \pm 1, \quad i = 1, \dots, N = L^d$$

Determine the effective field H_0 that minimizes the bound.

Problem 11.2 *Ising model in one dimension* (6 pts)

Evaluate the partition sum $Z(T, N; \{J_i\})$ for a one dimensional Ising chain with N spins:

$$\mathcal{H}_N = - \sum_{i=1}^{N-1} J_i \sigma_i \sigma_{i+1}, \quad \sigma_i = \pm 1.$$

Here the couplings J_i are fixed numbers dependent on the site i . It is favorable to sum over the bond variables $\tau_i = \sigma_i \sigma_{i+1}$ instead over the spin variables σ_i . Convince yourself that each configuration is characterized by one end spin and the sequence of bonds. An important quantity is the spatial correlation function $G_{i,n} = \langle \sigma_i \sigma_{i+n} \rangle$ that characterizes the decay of spin correlation as a function of distance n . Show that one can also write

$$G_{i,n} = \left\langle \prod_{k=i}^{i+n-1} \tau_k \right\rangle = Z(T, N; \{J_i\})^{-1} \left[\prod_{k=i}^{i+n-1} \frac{\partial}{\partial (J_k / k_B T)} \right] Z(T, N; \{J_i\})$$

and evaluate $G_{i,n}$. For the case of equal couplings $J_i \equiv J$, demonstrate that the spatial correlation function decreases exponentially with increasing distance $G_{i,n} = \exp(-n/\xi)$. Determine the correlation length ξ and derive its leading low-temperature behavior. Also for equal couplings, calculate the extensive part of the susceptibility

$$\chi = \frac{1}{k_B T} \sum_{i,j=1}^N \langle \sigma_i \sigma_j \rangle$$

and discuss χ as a function of temperature.

Problem 11.3 *critical properties of the van-der Waals fluid* (6 pts)

The empirical equation of state of a van-der Waals fluid reads

$$\left(P + \frac{N^2 a}{V^2} \right) (V - Nb) = N k_B T,$$

where $P, V = Nv, T$ and N denote the pressure, volume, temperature, and the number of particles, respectively, and a, b are some non-universal constants. Show that by introducing reduced variables $\hat{P} = P/P_c, \hat{v} = v/v_c, \hat{T} = T/T_c$ with $P_c = a/27b^2, v_c = 3b, k_B T_c = 8a/27b$ one obtains a parameter-free form

$$\left(\hat{P} + \frac{3}{\hat{v}^2} \right) (3\hat{v} - 1) = 8\hat{T}.$$

Demonstrate that $\hat{P} = \hat{v} = \hat{T} = 1$ corresponds to a critical point, i.e. $(\partial P/\partial v)_T = (\partial^2 P/\partial v^2)_T = 0$. Expand the reduced pressure for small $t = \hat{T} - 1, \phi = \hat{v} - 1$ [Answer: $\hat{P} = 1 + 4t - 6t\phi - 3\phi^3/2 + \mathcal{O}(\phi^4, t\phi^2)$]. Derive the free energy per particle. Convince yourself that one has to use a Maxwell construction for $t < 0$ and discuss the shape of the coexistence curve in a P - v diagram. Evaluate the specific heat per particle $c_V = C_V/N$ above and below T_c at $v = v_c$. Calculate the isothermal compressibility κ_T

- (a) at $v = v_c$ for temperatures $T > T_c$.
- (b) at the coexistence boundary for $T < T_c$.

Termine für Übungsgruppen:

Do 12-14 in T3, 1.3.48 (Franosch)

Do 16-18 in T1, 1.3.21 (Parmeggiani, Lattanzi) in englischer Sprache

Fr 12-14 in E2, 1.1.53 (Falcke)

Abgabe: In der Vorlesung vom 10.7.02