Theoretische Physik IV: Statistische Physik und Thermodynamik
Übungsblatt 11

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Aufgabe 1: Mean field treatment of 2D Ising model (*38+10* Punkte*)

Consider a system of N spins σ_i each pointing either up or down. Magnetic field h is applied to the system. Hence a spin pointing in the direction of the field ($\sigma_i = 1$) has energy $-h$. A spin pointing in the opposite direction ($\sigma_i = -1$) gains energy h. To avoid clutter, spin magnetic moment was set $\mu \equiv 1$.
First suppose the spins do not interact.

a) Write out the system Hamiltonian H_0. (*1 Punkt*)

b) Calculate the partition function of the spins. (*3 Punkte*)

Now we treat the interactions. Suppose the spins are located at the nodes of a translation-invariant square lattice. The interaction part of the Hamiltonian is

$$H_{\text{int}} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j,$$

where $\langle ij \rangle$ signifies that i and j are neigbours. Each spin interacts with four neigbours. Each pair is counted once in the summation.

c) Represent each spin i as a sum of average magnetization $\langle \sigma \rangle$ and fluctuating part $\sigma_i - \langle \sigma \rangle$. Show that the system Hamiltonian can be approximated as

$$H = H_0 + H_{\text{int}} \approx -2JN\langle \sigma \rangle^2 - \sum_i h_{\text{eff}} \sigma_i, \quad h_{\text{eff}} = h + 4J\langle \sigma \rangle. \tag{1}$$

Expressions (1) constitute the mean-field Hamiltonian. Give the criterium of applicability of the approximation. (*5 Punkte*)

c') BONUS for doing d)–e) with the proper Hamiltonian (1) including the $\langle \sigma \rangle^2$ term. (*4* Punkte*)

d) Write out the partition function in the mean-field approximation. Calculate the free energy F. (*3 Punkte*)

e) Calculate the average magnetization $\langle \sigma \rangle$. With your result, the self-consistency equation should read

$$\langle \sigma \rangle = \tanh \frac{h_{\text{eff}}}{k_{\text{B}} T}, \tag{2}$$

where T is the temperature of the system. (*4 Punkte*)

f) Consider Eq. (2) on $\langle \sigma \rangle$. Find the critical temperature T_{c} below which the equation has three solutions. Why the mean-field $k_{\text{B}} T_{\text{c}}$ overestimates the precise one, $k_{\text{B}} T = 2J / \ln\big(1 + \sqrt{2}\big)$? (*5 Punkte*)

g) Find $\langle\sigma\rangle$ for $T = 0$. (*3 Punkte*)

h) For $h = 0$, show that

$$\langle\sigma\rangle = \pm\sqrt{-3t}, \quad t = (T - T_\mathrm{c})/T_\mathrm{c} < 0$$

in the vicinity of T_c. To do this, you can start with expanding tanh in Eq. (2). (*6 Punkte*)

i) (BONUS) Approximate F in the vicinity of T_c by expanding it up to $\langle\sigma\rangle^4$ and h^1. This yields

$$F/N + k_\mathrm{B}T\ln 2 \approx h\langle\sigma\rangle + a(T - T_\mathrm{c})\langle\sigma\rangle^2 + b\langle\sigma\rangle^4, \quad a, b > 0. \tag{3}$$

Based on the expression, explain what happens when the system passes $T = T_\mathrm{c}$. (*6* Punkte*)

j) Consider F as a function of $\langle\sigma\rangle$. Sketch F at $h = 0$ for $T < T_\mathrm{c}$ and $T > T_\mathrm{c}$. Sketch F for $h > 0$ and $T < T_\mathrm{c}$. Elucidate on the stability of solutions for $\langle\sigma\rangle$. (*4 Punkte*)

k) Numerically solve Eq. (2) for $h = 0$ and plot $\langle\sigma\rangle$ as function of T. You should plot only the stable solutions. (*4 Punkte*)

Aufgabe 2: Critical point in the van der Waals model (*16 Punkte*)

a) Derive a condition

$$\left(\frac{dp}{dV}\right)_T < 0$$

for a *homogeneous* body to be in equilibrium state. That is, under the condition a state can be either stable or metastable. If the condition does not hold, the state is not thermodynamically possible. In your derivation, use the condition for F to be minimal. (*4 Punkte*)

Consider van der Waals matter of N particles. It obeys the equation

$$p = \frac{Nk_\mathrm{B}T}{V - Nb} - \frac{N^2a}{V^2}, \tag{4}$$

where p, V, and T are pressure, volume, and temperature of the matter, respectively; a and b are positive constants.

b) Sketch the isotherms, which can cross a $p = \text{const}$ line once and three times. Also sketch the boundary isotherm between those two types. There are states on the van der Waals isoterms, which are thermodynamically impossible for a homogeneous body. Mark them with dashed lines. (*3 Punkte*)

Consider the isotherms that can cross a $p = \text{const}$ line three times. On them, liquid and gas can coexist in equilibrium. There exists a temperature T_c and a pressure p_c above which this is not possible. The respective point is called critical point.

c) Write out the conditions on the critical point. They involve $(dp/dV)_T$ and $(d^2p/dV^2)_T$. (*3 Punkte*)

d) Obtain temperature $T_\mathrm{c} = 8a/27b$, volume $V_\mathrm{c} = 3Nb$, and pressure $p_\mathrm{c} = a/27b^2$ in the critical point. (*3 Punkte*)

e) Rewrite Eq. (4) in terms of the reduced values: $T' = T/T_\mathrm{c}$, $V' = V/V_\mathrm{c}$, and $p' = p/p_\mathrm{c}$. The resulting equation should read

$$(p' + 3/V'^2)(3V' - 1) = 8T'.$$

(*3 Punkte*)