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Advanced Statistical Physics
Problem Class 6
Tübingen 2022

24/05/2022

Please encircle the questions you have solved and are able to present/discuss in class.

6.1(a)	6.1(b)	6.1(c)	6.1(d)	6.2(a)	6.2(b)

Problem 6.1: Landau theory of the infinite-range Ising model (5 points + 3 bonus points)

Consider the Ising model where all the spins interact with each other. Its Hamiltonian is given by

$$H = -\frac{\epsilon}{N}\frac{1}{2}\sum_{i,k=1}^{N} s_i s_k - h\sum_{i=1}^{N} s_i. \tag{1}$$

The ferromagnetic coupling constant $J = \epsilon/N$, with $\epsilon > 0$, is rescaled by the number of spins N so that the total energy remains an extensive quantity. Also, note that the factor $1/2$ compensates the fact that in the sum each index i and k runs independently from 1 to N, and therefore each pair of spins (i, k) is counted twice. Furthermore, in Eq. (1), h denotes the strength of an applied magnetic field. In the following we set the constant $\epsilon = 1$ to simplify the calculations.
In this exercise we are going to show that the mean-field approximation is exact for this model in the thermodynamic limit $N \to \infty$. We will further discuss, within the Landau theory of phase transitions, the first and the second order phase transition that the model defined by Eq. (1) displays.

(a) In order to calculate the partition function of the Hamiltonian (1) we will introduce an auxiliary field, which is denoted by λ. Show that the Boltzmann weight, which appears in the partition function, can be written as an integral over λ as follows:

$$e^{-\beta H} = \sqrt{\frac{N\beta}{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}\lambda \exp\left(-\frac{N\beta\lambda^2}{2} + \sum_{i=1}^{N}\beta(\lambda + h)s_i\right). \tag{2}$$

Hint: Remember the Gaussian integral $\int \mathrm{d}x e^{-ax^2} = \sqrt{\frac{\pi}{a}}$ and complete the square in the integrand on the right hand side of Eq. (2). (**1 point**)

(b) Show that the partition function Z can be written as

$$Z = \sqrt{\frac{N\beta}{2\pi}}\int_{-\infty}^{\infty} \mathrm{d}\lambda\, e^{-N\beta A(\lambda)}, \quad \text{with} \quad A(\lambda) = \frac{\lambda^2}{2} - \frac{1}{\beta}\ln[2\cosh(\beta(\lambda + h))]. \tag{3}$$

(**1 point**)

We compute the integral over the auxiliary field λ in the thermodynamic limit $N \to \infty$. In this limit the integral of the exponential is dominated by the minimum of the function $A(\lambda)$ in the exponential. The integral is then computed by expanding the function $A(\lambda)$ in the exponent to second order around its minimum, and neglecting higher order terms in the expansion. This approximation is called saddle-point/Laplace/steepest descent method.

(c) Determine the particular value λ_0 of λ which minimizes the function $A(\lambda)$. Which equation must λ_0 satisfy in order to minimize the function $A(\lambda)$? Derive the equation for λ_0. Show that the partition function Z in Eq. (3) can be written, as $N \to \infty$, as

$$Z = e^{-\beta N f}, \quad \text{with} \quad f(\lambda_0) = A(\lambda_0) + \frac{1}{2N\beta}\ln A''(\lambda_0) \simeq A(\lambda_0), \tag{4}$$

with $f = \lim_{N\to\infty} F/N$ the free energy density and $A''(\lambda_0)$ denoting the second derivative of $A(\lambda)$ with respect to λ evaluated at the value λ_0. Remember, that λ_0 is the particular value of λ which minimizes the function $A(\lambda)$, as stated above. Henceforth in the calculations we will neglect the second term appearing on the right hand side of the equation for f in the second equation in (2). This is possible because this terms is subleading (subextensive) with respect to the leading (extensive) term $A(\lambda_0)$, which is of order $\mathcal{O}(1)$ with respect to the number of spins N. (**1 point**)

(d) Perform the mean-field approximation on the Hamiltonian in Eq. (1) by writing

$$s_i = m + \delta_i, \tag{5}$$

and expanding the Hamiltonian H up to the first order in δ_i (we have performed a similar calculation in one of the previous problem sheets). You should get the following mean-field approximation, H_{MF}, of the Hamiltonian H:

$$H_{MF} = \frac{Nm^2}{2} - (m+h)\sum_{i=1}^{N} s_i, \tag{6}$$

where m is magnetization density

$$m = \frac{1}{N}\sum_{i=1}^{N} s_i, \tag{7}$$

i.e., the order parameter. Compute the mean-field free energy density $f_{MF} = \lim_{N\to\infty} F_{MF}/N$ associated with the Hamiltonian H_{MF}. You should get the following result

$$f_{MF}(m) = \frac{m^2}{2} - \frac{1}{\beta}\ln[2\cosh(\beta(m+h))]. \tag{8}$$

Which is the self-consistency equation that m in Eq. (8) has to satisfy? On the basis of this, show that λ_0 in Eq. (4) is precisely equal to m in Eq. (8): $\lambda_0 = m$. This shows that the mean-field free energy density f_{MF} is equal to the free energy density $f_{MF} = f$ of the model in the thermodynamic limit, $N \to \infty$. Therefore the mean-field approximation is, in this case, exact (in the thermodynamic limit).
Hint: The mean-field Hamiltonian H_{MF} in Eq. (5) is the Hamiltonian of a non-interacting paramagnet in a "magnetic field" $m + h$. **(2 points)**

This is a "**bonus question**", i.e., you can gain 3 extra points from this beyond the points given in the previous (and in the following) questions. You can then use these 3 extra points to fill some points that you could have missed in the previous (or in the following) sheets.

(e) Expand f_{MF} in Eq. (8) for small m and small h: $m \to 0$ and $h \to 0$. Perform the expansion up to the order m^4 in the order parameter and up to the (leading) order mh in the coupling between the order parameter m and the magnetic field h. You should get the following Landau expansion

$$f(m) = a + \frac{1}{2}r(T)m^2 + s\,mh + u\,m^4. \tag{9}$$

Identify the coefficients a, $r(T)$, s and u. Note that a is just an additive constant, which is not important for the following discussion. The coefficient $r(T)$ depends on the temperature T and on the critical temperature T_c at which the model in Eq. (1) exhibits a second order phase transition for zero magnetic field $h = 0$. Identify the critical temperature T_c. Is the expression that you obtain for T_c related to the critical temperature that you would get from the mean-field equation of state?
Furthermore:
(i): Plot qualitatively $f_{MF}(m)$ vs. m for $h = 0$ for different values of T, above $T > T_c$ and below $T < T_c$ as well as at the critical point $T = T_c$. Discuss why there is a (continuous) second-order phase transition and how this transition can be understood from the plot of $f_{MF}(m)$.
(ii): Plot qualitatively $f_{MF}(m)$ vs m for $T < T_c$ for different values of h, both positive $h > 0$ and negative $h < 0$, as well as for zero $h = 0$. Discuss why there is a (discontinuous) first-order phase transition and how this transition can be understood from the plot of $f_{MF}(m)$. **(3 bonus points)**

Problem 6.2: Landau theory of first-order phase transitions (5 points)

Consider a mean-field theory with a cubic term in the Landau free energy,

$$f(m) = \frac{1}{2}rm^2 + s\,m^3 + um^4, \tag{10}$$

where m is the magnetization density/order parameter and s, r and u are parameters, with a notation analogous to the one used in Eq. (9) of the previous exercise. The coefficient u has to be positive, otherwise the free energy $f(m)$ would be unbounded from below and there would be no equilibrium state. The coefficient s can be assumed positive, without loss of generality, in this exercise. The coefficient r, instead, is a real parameter which can be positive or negative or zero. As we have seen in the previous exercise, the equilibrium configuration is given by looking for the value $\bar{m}$ which minimizes the free energy $f(m)$. In the following we denote with $\bar{m}$ the global minimum of $f(m)$, which corresponds to the equilibrium configuration of the system.

(a) Discuss how the absolute minimum $\bar{m}$ of $f(m)$ in Eq. (10) changes as a function of the parameter r. Plot the function $f(m)$ for different values of r to show how the minimum $\bar{m}$ depends on r.
Hint: When studying the minima of the function $f(m)$ in Eq. (10), you are naturally lead to define the particular value r_0 of r:

$$r_0 = \frac{9s^2}{16u}. \tag{11}$$

It is then useful to consider the cases $r > r_0$, $r = r_0$ and $r < r_0$. (**2 points**)

(b) Show that there is a first-order phase transition for a certain critical value r_c, with $r_c < r_0$. Identify the critical value r_c and the corresponding discontinuity $\bar{m}(r_c)$ of the global minimum of $f(m)$ at the transition point r_c as a function of the other parameters s and u. Discuss this first-order transition graphically from the plot of $f(m)$. In particular, plot $f(m)$ for $r = r_c$. (**3 points**)
Hint: The critical point is reached when the function $f(m)$ develops two degenerate minima at positions m_1 and m_2, with $f(m_1) = f(m_2)$.