Advanced Statistical Physics

TD — The mean-field approach

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1 Mean-field approximation(s) for the Ising model

The Ising model is defined as follows. On each node $i = 1, \ldots, N$ of a d-dimensional Euclidean lattice of N nodes one places a classical spin-1/2 variable, $s_i = \pm 1$. The Hamiltonian of the model is given by

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i \, , \tag{1}$$

where $J > 0$ is the strength of the ferromagnetic coupling, h is an external magnetic field, and $\langle i,j \rangle$ denotes the sum over all *pairs* of nearest-neighbor nodes of the lattice. The convetion is such that each of them counted only once.

1.1 Preliminary questions

a) What is(are) the ground state(s) of the model for $h \neq 0$ and for $h = 0$?

b) Show that for $h = 0$ the Hamiltonian is symmetric under global spin inversion and hence at finite N the average magnetization $M = \langle \sum_{i=1}^{N} s_i \rangle = 0$ at any temperature.

c) Under which condition you expect a phase transition?

d) Consider the case $J = 0$. Compute the partition function of the model, the free-energy, and the average magnetization as a function of βh (with $\beta \equiv (k_B T)^{-1}$).

1.2 The "fully-connected" mean-field approximation

In the "fully connected" limit the underlying d-dimensional lattice is replaced by a complete graph in which each node is connected to all other nodes. The Hamiltonian becomes

$$H = -\frac{J}{2N} \sum_{i \neq j} s_i s_j - h \sum_i s_i \, . \tag{2}$$

The coupling constant is divided by N in order to ensure the extensivity of the energy for J of $O(1)$.

a) Show that in the large N limit, up to leading order, the Hamiltonian can be rewritten as a function of the magnetization only: $H[\{s_i\}] \approx H[M]$.

b) Using the following Hubbard-Stratonovich identity for Gaussian decoupling:

$$e^{\frac{x^2}{2\sigma^2}} = \int \frac{\mathrm{d}z}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{z^2}{2\sigma^2}+\frac{zx}{\sigma^2}}\,, \tag{3}$$

show that the partition function at leading order in N takes the form:

$$Z \simeq \int \mathrm{d}z\, e^{-N\beta f(z)}\,, \tag{4}$$

and give the expression of the Ginzburg-Landau free-energy $f(z)$.

c) Using the fact that $M = \partial \ln Z/\partial(\beta h)$, show that in the $N \to \infty$ limit the saddle-point value of z gives the intensive mangetization $m = M/N$.

d) Consider the case $h = 0$. Find the self-consistent equation for the intensive magnetization, determine the critical temperature T_c, and the critical exponent β governing the critical behavior of the magnetization close to T_c as $m \propto (T_c - T)^{\beta}$.

e) Compare the results found with this method to the ones derived in the Lectures.

f) Perform a Taylor expansion of the free-energy around $z = 0$ up to the fourth order. Compute the magnetic susceptibility $\chi = \partial m/\partial h|_{h=0}$ above and below T_c and determine the critical exponent γ governing its critical behavior as $\chi \approx A_{\pm}|T - T_c|^{\gamma}$.

g) Compute the specific heat and determine the critical exponent γ governing its critical behavior close to T_c as $C \propto |T - T_c|^{\alpha}$. Do these critical exponents verify the scaling relation?

2 The Bethe approximation

In the Bethe approximation, the underlying Euclidean lattice is replaced by a tree with a fixed branching ratio. The spins are then arranged at the nodes of a tree, as shown in the figure on the left. This tree is a hierarchical lattice, which can be constructed iteratively: each site of a given generation is connected to one site of the previous generation and to k sites of the next generation. The number k is called the branching ratio of the lattice. The coordination number of the lattice is therefore fixed and equal to $k + 1$. We call this structure a *Bethe lattice*.

a) Starting from an origin node, that we label 0, what is the number $S(n)$ of nodes in the n-th ($n \geq 1$) generation of the lattice?

b) Deduce the total number N of nodes in a tree with R generations (i.e., inside a sphere of radius R).

c) In an Euclidean lattice, the dimension d of space is defined by $d = \lim_{R\to\infty} \frac{\ln N}{\ln R}$. Deduce the dimension of the Cayley tree.

On a tree, the partition function of the Ising model can be calculated recursively. To do this, we assume that after exact integration of all spins belonging to the successive generations of the branch, we know the probability P that a spin of the (n+1)-th generation is equal to $+1$ when the spins of the n-th generation are not (yet) present. By adding the spins of the n-th generation, we thus find an exact recurrence formula for Z.

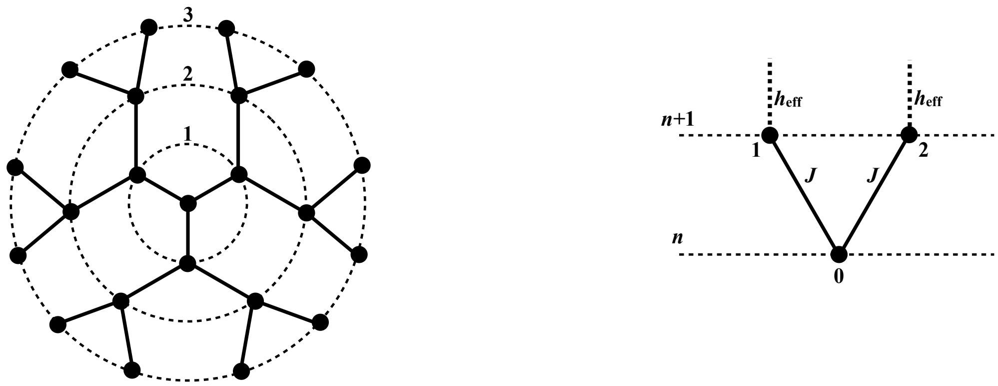

FIG. 1 – *Left: The Bethe lattice with 3 generations and branching ratio* $k = 2$. *Right: Recursion process: We sum over all configurations of the k spins* $\{s_1, \ldots, s_k\}$ *of the* $(n+1)$*-th generation in the presence of an effective field* h_{eff} *to find the effective field acting on the spin* s_0 *of the n-th generation.*

As shown in the figure on the right, we are therefore interested in a subsystem consisting of a branch of the tree starting from an arbitrary site 0 of the n-th generation. We call s_0 the spin on node 0 and $\{s_1, \ldots, s_k\}$ the nearest neighbor spins of s_0 from the $(n+1)$-th generation. Suppose that we have already integrated over all spins belonging to successive generations of the branch, and that we know the probability P that a spin of the $(n+1)$-th generation is equal to $+1$ when the spin s_0 is not (yet) present.

d) To begin, consider a single isolated spin s in a magnetic field h_{eff}. Express the probability P that $s = +1$ as a function of h_{eff}. Also, express the average magnetization $m = \langle s \rangle$ of this spin as a function of h_{eff}.

We now add the spin of the n-th generation (i.e., the spin s_0 in our case, see the figure). The subsystem is therefore reduced to $k+1$ spins: the spin s_0, and its k neighbors from the $n+1$-th generation who are subject to the effective field h_{eff} due to the contribution of spins from successive generations. The energy of this subsystem is therefore:

$$H = -Js_0 \sum_{j=1}^{k} s_j - hs_0 - h_{\text{eff}} \sum_{j=1}^{k} s_j \,.$$

e) Write the partition function of the system without trying to calculate it for now.

f) Show that

$$\sum_{s=\pm 1} e^{\beta J s_0 s + \beta h_{\text{eff}} s} = c(J,h_{\text{eff}})\, e^{\beta u(J,h_{\text{eff}}) s_0} \quad ,$$

by providing the expressions for the functions of the control parameters $u(J,h_{\text{eff}})$ and $c(J,h_{\text{eff}})$.

g) In an infinite tree, it is expected that h_{eff} does not depend on the generation n. Using the answer to the previous question, and summing over the spins $\{s_1, \ldots, s_k\}$

(but not over s_0) in the partition function, show that the partition function becomes $Z = C \sum_{s_0=\pm 1} e^{\beta h_{\text{eff}} s_0}$, where C is a constant that can be determined. Find the self-consistent equation for h_{eff}.

h) Using the answer to question d), write this equation as a self-consistent equation for the average magnetization m.

i) First, consider the case of zero magnetic field, $h = 0$. Show that this equation admits a non-trivial (non-zero) solution only below a certain critical temperature T_c, which we will calculate. Compare T_c found in the Bethe approximation with the Curie-Weiss critical temperature $T_c = J/(k+1)$.

j) If the coordination number of the network is $k + 1 = 2d$, as in Euclidean networks in d dimensions, is there a phase transition for $d = 1$?

k) Write a Taylor expansion of the self-consistent equation near the critical point (where h_{eff} and m are close to 0) and show that $m \sim (T_c - T)^\beta$ for $T \lesssim T_c$, where β is a critical exponent that we will determine.

l) Calculate the partial derivative $\partial m/\partial h|_{h=0}$ as a function of m, T, and h using the self-consistent equation, and deduce the magnetic susceptibility at zero field χ as a function of T. Show that near the critical point $\chi \sim |T - T_c|^\gamma$, where γ is a critical exponent that we will determine.

3 Optional exercise: The Blume-Capel model

The Blume-Capel model is intended to reproduce the relevant features of superfluidity in He^3-He^4 mixtures [1, 2, 3]. In this study, we will consider infinite range, mean-field like interactions between the relevant variables. With this choice, the phase diagram can be obtained analytically both within the canonical and the microcanonical ensembles [4, 5] and the analysis enables one to get a better understanding of the effect of the non-additivity on the thermodynamic behaviour of the model.

The Blume-Capel model is defined as follows [1, 2, 3]. On each site of a complete graph one places a spin-1 variable, $s_i = \pm 1, 0$. Each spin is coupled to all others with the same strength $J_0 > 0$. The Hamiltonian is given by

$$H = -\frac{J_0}{2} \sum_{i \neq j} s_i s_j + \Delta \sum_i s_i^2 \tag{5}$$

with $\Delta > 0$. Let us start by analysing the parameter dependence in the Hamiltonian.

3.1 Energetic analysis

Consider the case $\Delta = 0$.

a) Which kind of order favours the exchange J_0? What is the model obtained and what does it describe?

b) How does one need to scale J_0 to ensure a reasonable thermodynamic, $N \to \infty$, limit and the extensivity of the energy? Call the new relevant coupling parameter J.

c) What is the nature of the phase transition expected in this case? (We will derive it below.)

Consider now $\Delta \neq 0$.

d) What is the role played by this parameter?
e) Which are the two states that you may expect to be ground states, in the canonical ensemble, at zero temperature? Find the relation between the parameters Δ, J where the preferred one changes. Discuss the result.

3.2 The canonical ensemble

a) Write the partition function.
b) Think about introducing the auxiliary variable $x = N^{-1} \sum_i s_i$, as it is usually done in the study of the fully-connect Ising model. In this case, in which the spins take values ± 1,0, which is the difficulty encountered?
c) Use an alternative method, the Hubbard-Stratonovich identity or Gaussian decoupling, to render the expression in the exponential of the partition sum, local in the spin variable. Perform the sum over the spin variables explicitly.
d) Identify the "Ginzburg-Landau" free-energy density as a function of x and call it $\tilde{f}(x)$.
e) Show, in the $N \to \infty$ limit, that the saddle-point value of x is equal to the spontaneous magnetisation per spin m.
f) Identify the extrema of the Ginzburg-Landau free-energy function and study their stability.
g) Set up the Taylor expansion of the Ginzburg-Landau free-energy function around $x = 0$ and find the critical line on which the coefficient of the quadratic term vanishes and the one of the quartic term remains larger than zero. This is the *second order phase transition* ending at a tricritrical point $(\Delta/J, T/J)_c$ where the two coefficients vanish. Prove that the canonical tricritical point is located at $J/(2\Delta) = 3/\ln 16 \simeq 1.0820$, $\beta J = 3$.
h) The *first order phase transition* corresponds to the parameters $(\Delta/J, T/J)$ on which $\tilde{f}(\beta J, \beta\Delta, x \neq 0) = \tilde{f}(\beta J, \beta\Delta, x = 0)$. Find the line with a numerical solution of the corresponding equation.
i) Use a graphical facility to plot the Ginzburg-Landau free-energy function as a function of x for various values of the control parameters βJ and $\beta\Delta$. Confirm the results found in the previous two items for the critical lines from the visual inspection of the evolution of $\tilde{f}(x)$.
j) Draw the *canonical phase diagram* in the $(\Delta/J, T/J)$ plane.

3.3 The microcanonical ensemble

A microscopic configuration is determined by the number of spins taking value $+1$, that we call N_+, number of spins taking value -1, that we call N_-, and the number of spins taking value 0, that we call N_0. We will now study the macroscopic observables as functions of these number.

a) Write a constraint that relates N_+, N_-, N_0 to the total number of spins N.

b) Write the total magnetisation, $M = \sum_i s_i$, the quadrupole moment $Q = \sum_i s_i^2$, the total energy as functions of N_+, N_-, N_0.

c) Calculate the number of microscopic configurations, Ω, that are compatible with the macroscopic occupation numbers N_+, N_-, N_0.

d) Using Stirling's approximation, compute the entropy $S = k_B \ln \Omega$ and write it as a function of $m = M/N$, $q = Q/N$ and $e = E/N$. Note that one of this intensive parameters is absent from $s = S/N$.

e) We will fix the energy and look for the equilibrium magnetisation density values that render the entropy maximal.

   In the paramagnetic phase $m = 0$ and the Taylor expansion of $s(m{,}e)$ around this value has negative quadratic and quartic coefficients. The second order phase transition occurs when the coefficient of the quadratic term vanishes while the one of the quartic term remains negative.

   The tricritical point is located at the parameters such that the two coefficients vanish. The microcanonical tricritical point is located at $J/(2\Delta) \simeq 1.0813$, $\beta J = 3.0272$. This has to be compared with the canonical tricritical point located at $J/(2\Delta) \simeq 1.0820$, $\beta J = 3$.

In conclusion the microcanonical critical line extends beyond the canonical one.

Références

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