Homework 8, Statistical Mechanics: Concepts and applications 2019/20 ICFP Master (first year)

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Please study this homework carefully, as it illustrates essential aspects of mean-field theory. Solutions will be provided shortly

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In lecture 08: "Mean-Field theory (1/2) and its three pillars: Self-consistency, absence of fluctuations, infinite-dimensional limit", we studied different aspects of this important theory, which may describe classical and quantum models, but also systems in computer science (for example graph theory), social interactions, etc. Although mean-field theory thus applies to many situations it is again in the Ising model (where it all began) that we find he theme of this week's homework.

I. SINGLE-SITE SELF-CONSISTENCY

The first aspect of mean-field theory, going back to Pierre-Ernest Weiss (1865-1940), is the famous self-consistency relation for the Ising model:

$$m = \tanh\left[\beta\left(Jqm + h_{\text{ext}}\right)\right] \tag{1}$$

where q is the number of neighbors of a single site ($q = 2d$ for a d-dimensional hypercubic lattice), $J = 1$ the interaction strength and h_{ext} the external magnetic field. In lecture 08, we solved this self-consistency equation around the critical point for the Ising model in zero external magnetic field. For small magnetization, we obtained the critical behavior

$$m(T) = \begin{cases} 0 \quad \text{for } T > T_c = qJ \\ \pm\text{const } \left(\frac{T_c}{T} - 1\right)^{\beta} \quad \text{for } T < T_c \end{cases} \tag{2}$$

where $\beta = 1/2$ is not the inverse temperature but the critical exponent of the spontaneaous magnetization.

1. Familiarize yourself with the expression of eq. (1). How is it derived, and how can it be generalized?

   The energy related to size 0 *is*

$$E_0 = -J\sum_i \sigma_i\sigma_o - h_{ext}\sigma_0$$

Assuming the spin 0 is interacting with a 'mean field', all its neighbour is substitute by the average magnetization m. The energy becomes

$$E_0 = -Jqm\sigma_0 - h_{ext}\sigma_0$$

where q is the number of neighbours. The magnetization of spin 0 is then

$$m_0 = \frac{1}{Z}\sum_{\sigma_0=\pm} \sigma_0 \mathrm{e}^{-\beta(Jqm\sigma_0 + h\sigma_0)\beta} = \tanh\left(\beta(Jqm + h_{ext})\right)$$

The site 0 should not be special compared to the other sites. Thus, there is the self-consistency condition

$$m = m_0 = \tanh\left(\beta(Jqm + h_{ext})\right)$$

2. Review how eq. (1) is solved under the assumption $|m| \ll 1$, so that it yields eq. (2). This was treated in lecture 08.

At critical point, $h_{ext} = 0$. eq. (1) becomes

$$m = \tanh(\beta Jqm)$$

The RHS of eq. (1) could be substitute by its Taylor expansion,

$$m = \beta Jqm - \frac{1}{3}\beta^3(Jqm)^3$$

and leads to

$$m\left(\frac{1}{3}\left(\beta Jq\right)^3 m^2 - (\beta Jq - 1)\right) = 0$$

$m = 0$ is always a solution. If $\beta Jq - 1 > 0$, there are two other solutions. Define $\beta_c = 1/T_c \equiv 1/Jq$, then these solutions are

$$m = \pm\sqrt{3}\left(\frac{T}{T_c}\right)^{3/2}\left(\frac{T_c}{T} - 1\right)^{1/2}$$

Thus, the scaling of m (which is applicable near the critical point), is found by setting $T \sim T_c$:

$$m = \pm const\left(\frac{T_c}{T} - 1\right)^{1/2}$$

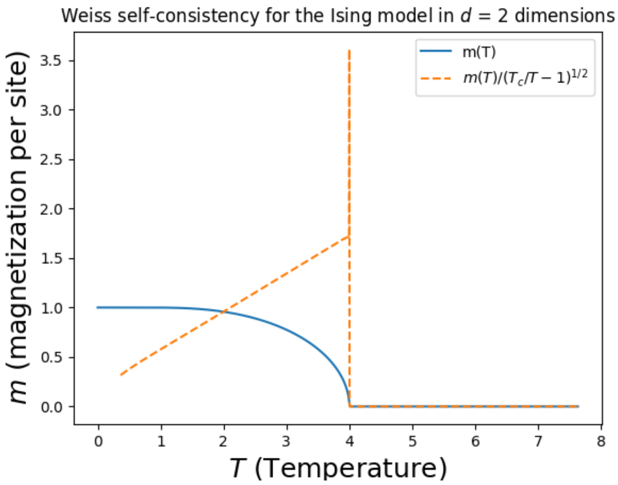

FIG. 1: The solid line is m as a function of T, and the dashed line is $m(T)/(T_c/T-1)^{1/2}$.

3. Write a computer program to solve the self-consistency (eq. (1)) at all temperatures (concentrate on the positive branch, that is, suppose $m \geqq 0$). For your convenience (cadeau!), the program is already available (see `mean_field_self_consistency_single_site.py`), but you may add the plot for the exact asymptotic expression near the critical point. In this case, obtain the const in eq. (2) exactly (not by fitting) .

   In Fig. 1, The solid line is m as a function of T, and the dashed line is $m(T)/(T_c/T-1)^{1/2}$. The numerical result shows that, below T_c, the non-zero solution is always preferred. This indicates that there is a phase transition at T_c. Below T_c, there is spontaneous magnetization; however, the magnetization disappears when $T > T_c$. The constant in eq. (2) is y-coordinate of the dashed plot at critical point. (Please ignore the peak at the T_c, since it is purely numerical artifact.) It is roughly $\sqrt{3}$, which is consistent of the analytical result.

II. LATTICE SELF-CONSISTENCY: ABSENCE OF FLUCTUATIONS

In lecture 08, we also treated mean-field theory on a lattice. In this case, one no longer supposes that all sites of the lattice are equivalent (have the same magnetization), but still neglects all fluctuations. In this case, one generalizes

$$m_i = \tanh\left[\beta\left(J\sum_{\text{nn } j} m_j + h_{\text{ext}}\right)\right], \tag{3}$$

where for each site i, the sum goes over the nearest neighbors (nn) j of i.

1. Show that for a d-dimensional lattice of $N = L^d$ sites with periodic boundary conditions, the solution of eq. (3) is the same as the solution of eq. (1), for a proper choice of q.

   The local magnetization is defined as

   $$m_i = \frac{1}{Z} \sum_{\{\sigma\}} \sigma_i \mathrm{e}^{-\beta E(\{\sigma\})}$$

   For simplicity, assuming that this is a 1D system. The expression of energy of the system could be written as

   $$E(\{\sigma\}) = -\sum_{i=1}^{N} \sum_{j=i+1,i-1} J\sigma_i\sigma_j - h_{ext} \sum_i \sigma_i$$

   Thus, massaging the expression of local magnetization,

   $$\begin{aligned} m_k &= \frac{1}{Z} \sum_{\{\sigma\}} \sigma_k \exp\left[\beta \left(\sum_{i=1}^{N} \sum_{j=i+1,i-1} J\sigma_i\sigma_j + h_{ext} \sum_i \sigma_i \right)\right] \\ &= \frac{1}{Z} \sum_{\{\sigma\}} \sigma_{k-1} \exp\left[\beta \left(\sum_{i=0}^{N-1} \sum_{j=i+1,i-1} J\sigma_i\sigma_j + h_{ext} \sum_i \sigma_i \right)\right] \\ &= \frac{1}{Z} \sum_{\{\sigma\}} \sigma_{k-1} \exp\left[\beta \left(\sum_{i=1}^{N} \sum_{j=i+1,i-1} J\sigma_i\sigma_j + h_{ext} \sum_i \sigma_i \right)\right] \\ &= m_{k-1} \end{aligned}$$

   The second line is derived by relabeling and the third line is derived by using periodic boundary condition. Thus, with periodic boundary condition, all the spins are identical from a statistical point of view. With the same trick, it is also possible to prove that all the local magnetizations are the same for a D-dimensional Ising model. Thus, it is possible to substitute the m_i*s in eq. (3) by* m*. eq. (3) then becomes eq. (1) with* $q = 2D$*. For simplicity, all the following calculation will be done in 1D.*

2. Write a computer program to actually solve eq. (3) for a finite lattice. For your convenience, the program is already available (see `mean_field_gen_d_Ising_lattice.py`). Simply download and run this program and check that the overall magnetization is the same as in Section I.

   Fig. 2 and Fig. 3 show that the system is homogeneous, which means it's safe to remove the indices in eq. (3). Then, eq. (3) becomes eq. (1) and their solution has to be the

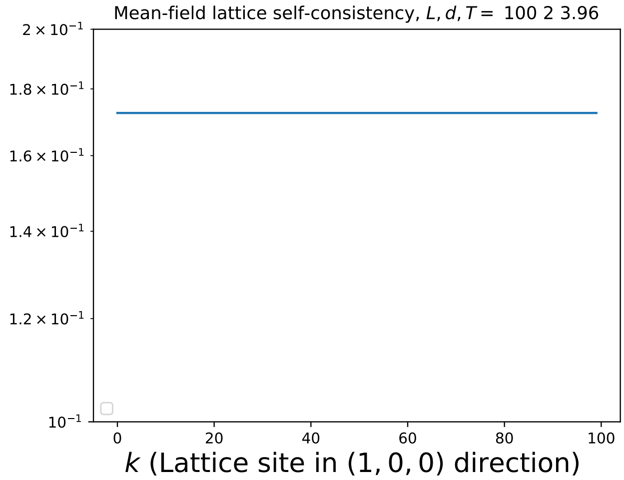

FIG. 2: Magnetization as a function of r at $T = 0.99T_c$

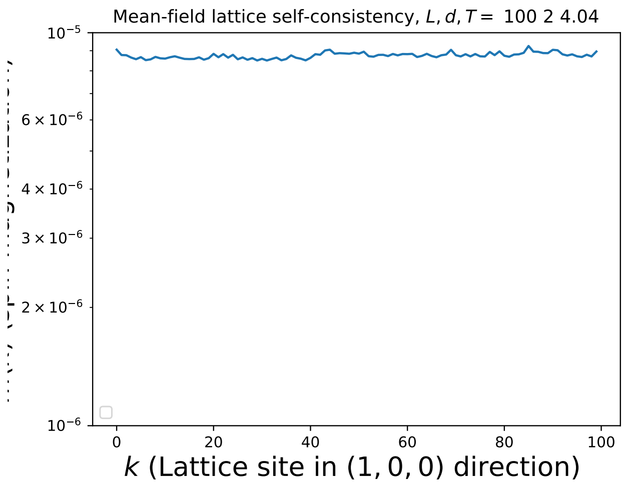

FIG. 3: Magnetization as a function of r at $T = 1.01T_c$

same. It is also possible, after showing that there is almost no fluctuation in the system, plot the magnetization of a specific site (or the average over the system) as a function of T. This plot should be identical to the solid line in Fig. 1, but plotting it is a little time consuming.

3. By changing one single character (sic!) on a single site (sic!), modify the program so that it keeps the magnetization at site 0 equal to 1, while updating all other spins over and over again in order to solve the mean-field equations for all sites. From the converged solution, check that for temperatures above T_c, one can define a *correlation length*: Show that the

correlation of the magnetization decays as:

$$\langle m(0)m(k)\rangle \sim \exp\left[-k/\xi(T)\right] \tag{4}$$

(As $m(0) = 1$, this correlation function is the same as the magnetization at site k). Notice the crucial point: Mean-field theory allows to define a spatial correlation function, and a correlation length.

The character, which needs to be changed, is the beginning position of the array of magnetization when the self-consistency relation is solved recursively. Since $m(0) = 1$ is fixed,

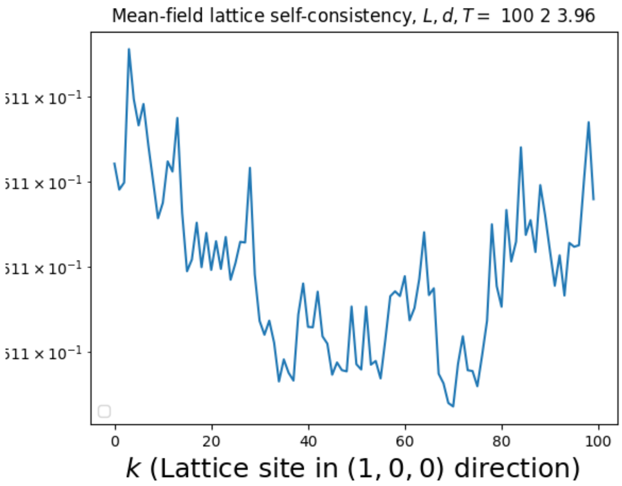

FIG. 4: Magnetization as a function of r at $T = 1.01T_c$. Magnetization at $r = 0$ is set to 1.

$\langle m(0)m(k)\rangle = m(k)$. As Fig. 5 shows, the correlation function decays exponentially. Thus, it is possible to measure define $\xi(T)$ in eq. (4).

4. (If you have time): Show that even below the critical temperature, the connected correlation function decays exponentially:

$$\langle m(0)m(k)\rangle_c = \langle m(0)m(k)\rangle - \langle m(0)\rangle \langle m(k=\infty)\rangle \sim \exp\left[-k/\tilde{\xi}(T)\right], \tag{5}$$

that is, although there is long-range order, the correlations also decay exponentially. In eq. (5), $m(k = \infty)$ can be obtained from Section I. It just describes how fast correlations decay towards the spontaneous magnetization of an infinite system.

Again, $m(0) = 1$ and $\langle m(0)m(k)\rangle = m(k)$. As Fig. 5 shows, the correlation function decays exponentially. Like the $T > T_c$ case, the correlation function decays until it

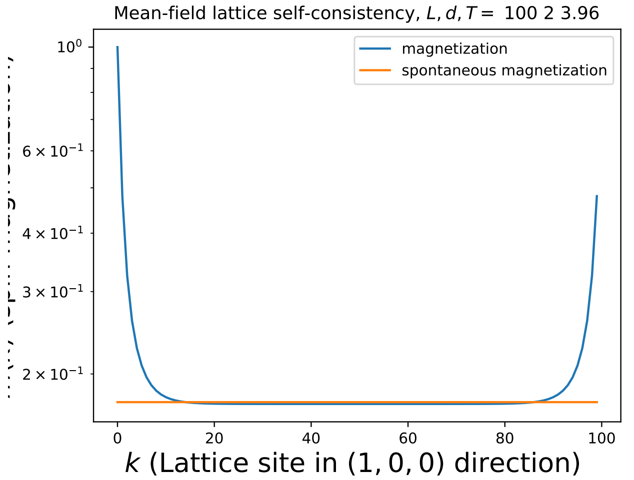

FIG. 5: Magnetization as a function of r at $T = 0.99T_c$. Magnetization at $r = 0$ is set to 1.

reaches the spontaneous magnetization given by the self-consistency relation. However, in this case, it decays much faster than in the $T > T_c$ case.

5. Show (by trying out different values of the temperature) that the correlation length ξ diverges as one approaches the critical temperature, both from above and from below. If you have time, try to extract the exponent ν describing this divergence above the critical temperature, as well as the analogous exponent ν' below. It can be shown easily that $\nu' = \nu$.

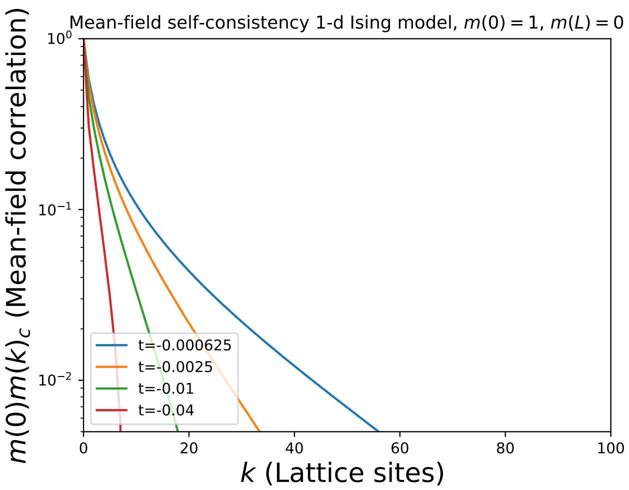

FIG. 6: Correlation function when $t = (T/T_c - 1)^{1/2}$ is negative. Magnetization at $r = 0$ is set to 1.

Fig. 6 and Fig. 7 show how the correlation function behaves when $t \approx 0$. The correlation length is proportional to the x-coordinate when the correlation function intersect with

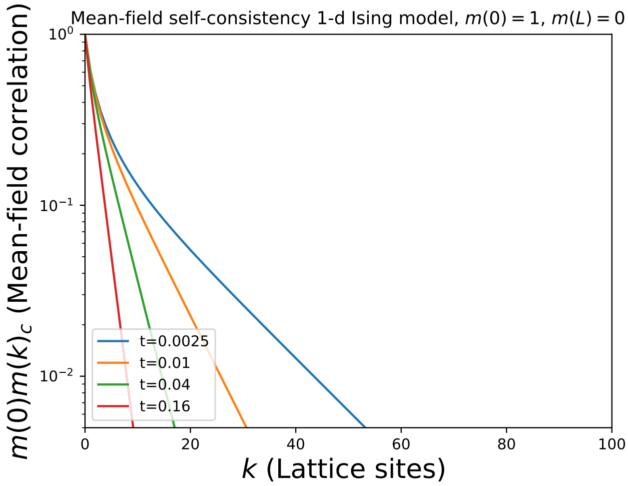

FIG. 7: Correlation function when $t = (T/T_c - 1)^{1/2}$ is positive. Magnetization at $r = 0$ is set to 1.

the x axis. No matter $t \to 0^+$ or $t \to 0^-$, the correlation length become larger when $t \to 0$. And these figures also indicates $\nu' = \nu = 0.5$.

III. COMPLETE GRAPH OF N SITES WITH $N \to \infty$

Please revise the last part of lecture 08, where we showed that the self-consistency condition of eq. (1) is exact for the complete graph on N sites with $N \to \infty$. Three points are crucial:

1. The complete-graph system is an exact physical model, although it is unrealistic. Furthermore, it is described exactly by the mean-field self-consistency, putting it (the self-consistency) on a much stronger base. This physical model (Ising on a complete graph) must have consistent thermodynamics, that is, positive entropy, and a free energy that satisfies $F = U - TS$, etc.

2. The free energy of the mean-field model can be expressed as a function of m, T, and h_{ext}.

3. We may then expand the free energy as a power of the order parameter. This is the beginning of Landau theory (1937), the subject of lecture 09, the next lecture.

In a fully connected model, the total field acting on spin i is

$$h_{ext} + (N-1)^{-1} qJ \sum_{j \neq i} \sigma_j$$

where the sum is over all of the sites except for site i. The strength of the interaction is $qJ/(N-1)$. The production of q and J is effectively one number, and the factor $(N_1)^{-1}$ preserves the relation $E \sim N$. The total energy of the mean-field model is thus

$$E(\{\sigma\}) = -\frac{qJ}{N-1}\sum_{(i,j)}\sigma_i\sigma_j - h_{ext}\sum_i \sigma_i$$

where the first sum is over $N(N-1)/2$ possible pairs. The total magnetization of the system is

$$M = \sum_i \sigma_i$$

Using the relation

$$M^2 = \sum_{i,j}\sigma_i\sigma_j = 2\sum_{(i,j)}\sigma_i\sigma_j + \sum_i \sigma_i^2$$

the total energy of the system could be written in terms of M as

$$E(\{\sigma\}) = \frac{qJ}{2(N-1)}(M^2 - N) - h_{ext}M$$

When r spins are down and $N-r$ spins are up, $M = N-2r$. Combining with the fact that there are $\binom{N}{r}$ configurations for $M = N-2r$, the partition function of the system could be expressed as

$$Z = \sum_r c_r$$

where

$$c_r = \binom{N}{r}\exp\left\{-\beta\left[-\frac{qJ}{2(N-1)}\left((N-2r)^2 - N\right) - h_{ext}\left(N-2r\right)\right]\right\}$$

In order to find which r dominates, define

$$d_r = \frac{c_{r+1}}{c_r} = \frac{N-r}{r+1}\exp\left\{-\beta\left[2\frac{qJ}{(N-1)}(N-2r-1) - 2h_{ext}\right]\right\}$$

The mean magnetization of each site is

$$m = \frac{1}{N}M = 1 - \frac{2r}{N}$$

which means d_r could also be expressed by

$$d_m \approx \frac{1+m}{1-m}\exp\left[-2\beta(qJm + h_{ext})\right]$$

If c_r reach its extreme value at r_0, r_0 has to satisfy

$$d_{r_0} = 1$$

It is possible to derive, from this equation, the relation that $m_0 = 1 - \frac{2r_0}{N}$ satisfies. It is

$$m_0 = \tanh\left[(qJm_0 + h_{ext})/kT\right]$$

The fluctuation of m could be ignored when compared with m. Thus the configurations, in which $m \neq m_0$, could be ignored. Thus

$$m = \tanh\left[(qJm + h_{ext})/kT\right]$$

which is the self-consistency relation and is identical to the one in the first section.