Homework 9, Statistical Mechanics: Concepts and applications
2016/17 ICFP Master (first year)

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This homework will not count for your grade (and it will not be graded). Please study it nevertheless carefully, as it illustrates essential aspects of mean-field theory.

(Dated: November 8, 2016)

In lecture 09: "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 09, 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?

2. Review how eq. (1) is solved under the assumption $|m| \ll 1$, so that it yields eq. (2). This was treated in lecture 09.

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) .

II. LATTICE SELF-CONSISTENCY: ABSENCE OF FLUCTUATIONS

In lecture 09, 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.

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.

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.

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.

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 $\nu' = \nu$.

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

Please revise the last part of lecture 09, 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 10, next week.