

MATH 585 – TOPICS IN MATHEMATICAL PHYSICS – FALL 2006
MATHEMATICS OF MEAN FIELD SPIN GLASSES AND THE REPLICIA METHOD
LECTURE 3: THE MOLECULAR-FIELD THEORY FOR THE ISING MODEL

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1. INTRODUCTION

In the last lecture we introduced the Sherrington-Kirkpatrick mean-field model of a spin glass, as well as the Edwards-Anderson model. There we stated that Sherrington and Kirkpatrick invented their model, to some extent, to *justify* the “molecular field theory” of Edwards and Anderson. Such a statement may seem mysterious to the mathematician and probabilist unfamiliar with such models and approximations.

In order to give some background, we will now consider the analogous ideas in the context of the Ising spin system. We will also continue this investigation for the next few lectures. In this lecture we will consider the “molecular field theory”, and in the next few lectures we will consider the exactly solvable “mean-field” version of the Ising model: the Curie-Weiss model. By a “mean-field” model we mean a statistical mechanical system on a complete graph. In contradistinction, a “molecular field theory” is not a statistical mechanical model, but is more of a phenomenological model of the thermodynamics.

The molecular field theory of Weiss (following ideas of Curie and Langevin, his student) predated the Ising model by many years. However, the explanation we give here will be historically inaccurate, as we will start with the Ising model. In fact, we will motivate Weiss’s modification of the Langevin equation as deriving from a lower bound to the exact thermodynamic pressure of the d -dimensional Ising model. (It is well-known that the molecular field equations lead to lower bounds on the pressure, i.e. upper bounds on the free energy.)

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In case the reader is more interested in learning about magnetism in general, especially in the context of a historical description, I would highly recommend Chapter 1 of Mattis's textbook [1]. I also found another nice article online, [2].

2. THE ISING MODEL REDUX

Let us start by redefining the Ising model on a d -dimensional lattice. The d -dimensional lattice is $\Lambda_N = \mathbb{Z}_N^d$. See Figure 1 for an example in two-dimensions. At each site $x \in \Lambda_N$,

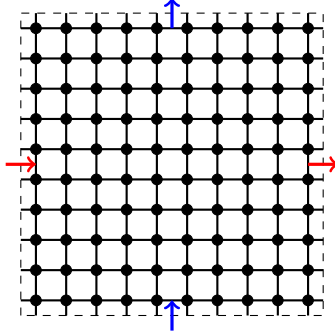


FIGURE 1. A two-dimensional lattice: \mathbb{Z}_{10}^2

there is a spin $\sigma_x \in \{+1, -1\}$. Therefore, a spin configuration on the whole lattice is a collection of spins, $\sigma = (\sigma_x : x \in \Lambda_N)$. The set of all spin configurations is $\Omega_N = \{+1, -1\}^{\Lambda_N}$. The Ising model then assigns the energy

$$H_N(\sigma) := -\frac{J}{2d} \sum_{\langle x,y \rangle} \sigma_x \sigma_y - h \sum_x \sigma_x,$$

to a spin configuration $\sigma \in \Omega_N$. (Recall that the sum with index $\langle x, y \rangle$ means to sum over all pairs $\{x, y\}$ in Λ_N which are nearest-neighbors.) The real number J is the interaction strength between nearest-neighbor spins, and h is the strength of an external magnetic field. Our current normalization is a little different than what we defined in Lecture 1 because we divide by $2d$. But the present normalization is much more convenient, and only amounts to a redefinition of J .

2.1 Thermodynamic Functions.

It is important to know what are the quantities of interest. Of course, the most interesting object is the Boltzmann-Gibbs distribution, $\mu_{N,\beta}$ which is a probability measure on Ω_N , such that

$$\mu_{N,\beta}(\sigma) := \frac{e^{-\beta H_N(\sigma)}}{Z_N(\beta)},$$

where $Z_N(\beta)$ is the normalization

$$Z_N(\beta) := \sum_{\sigma \in \Omega_N} e^{-\beta H_N(\sigma)},$$

known as the “partition function”. From the Boltzmann-Gibbs distribution, one can calculate everything else; for example one can calculate all the so-called correlation functions. But the second most interesting object is the partition function itself, and thermodynamic quantities derivable from it.

For example, we call the quantity,

$$p_N(\beta) := \frac{1}{|\Lambda_N|} \log(Z_N(\beta)),$$

the “pressure”. In principle, one would like to know

$$p(\beta) := \lim_{N \rightarrow \infty} p_N(\beta),$$

if it exists. One can also define some other quantities. The magnetization is

$$\bar{m}(\beta) := \frac{1}{\beta} \cdot \frac{\partial}{\partial h} p(\beta, J, h).$$

When it exists, this is the limit of the finite-volume magnetizations

$$\bar{m}_N(\beta) := \frac{1}{\beta} \cdot \frac{\partial}{\partial h} p_N(\beta, J, h).$$

The fact that one can commute the derivative through the limit is just because, by definition, $p_N(\beta, J, h)$ is convex in h , and such a result holds for limits of convex functions. (For a review of elementary properties of convex functions, see for example Section I.3 of [3].) Of course the most interesting points are where the magnetization does not exist, because it has a jump discontinuity. The reason for calling this the magnetization is just that

$$\bar{m}_N = \mathbf{E}^{\mu_{N,\beta}}[m_N(\sigma)] \quad \text{where} \quad m_N(\sigma) = \frac{1}{|\Lambda_N|} \sum_x \sigma_x.$$

This is an identity that the reader should check as an exercise. Another quantity of interest is the following

$$\chi(\beta) := \beta^{-1} \frac{\partial}{\partial h} \bar{m}(\beta, J, h).$$

We will call this the isothermal susceptibility, although we may be off by a factor of β .

3. MOLECULAR FIELD THEORY

Let us consider one approach to the molecular field theory, which is somewhat systematic. We return our attention to the actual Ising Hamiltonian H_N , and its Boltzmann-Gibbs measure $\mu_{N,\beta}$. We will recall the Gibbs variational principle. Let $\mu_{N,0}$ be the uniform probability measure on Ω_N . Then relative entropy of $\nu \in \mathcal{M}_1(\Omega_N)$, relative to $\mu \in \mathcal{M}_1(\Omega_N)$, is defined as

$$S_N(\nu|\mu) := \int_{\Omega_N} u \left(\frac{d\nu}{d\mu} \right) d\mu = \sum_{\sigma \in \Omega_\Lambda} u \left(\frac{\nu(\{\sigma\})}{\mu(\{\sigma\})} \right) \mu(\{\sigma\}),$$

where

$$u(x) = \begin{cases} -x \log(x) & \text{for } x \in (0, \infty]; \\ 0 & \text{for } x = 0. \end{cases}$$

(We interpret $u(\nu(\sigma)/\mu(\sigma))\mu(\sigma) = \infty$ if $\mu(\sigma) = 0$ and $\nu(\sigma) \neq 0$.) Then the Gibbs variational principle says that

$$p_N(\beta) = \max_{\nu \in \mathcal{M}_1(\Omega_N)} |\Lambda_N|^{-1} \left(S_\Lambda(\nu|\mu_{N,0}) - \mathbf{E}^\nu[\beta H_N(\sigma)] + \log(|\Omega_N|) \right). \quad (3.1)$$

Here $\mathcal{M}_1(\Omega_N)$ is the set of all probability measures on Ω_N . Moreover, the unique optimizing ν is $\nu = \mu_{N,\beta}$, the Boltzmann-Gibbs measure.

This is very easy to prove. One first notes that u is strictly concave. Therefore, $S_N(\nu|\mu)$ is strictly concave in ν , for each μ . But the Gibbs functional on the right hand side of equation (3.1) is actually just $p_N(\beta) + S_N(\nu|\mu_{N,\beta})$, as a calculation shows. Therefore, if it has any local maximizer, then it that is the unique maximizer. On the other hand, $S_N(\nu|\mu)$ is always bounded above by 0, because of Jensen's inequality applied to the concave function u .

Therefore, if we want to know $p_N(\beta)$ exactly, we only have to maximize the right hand side of equation (3.1) over all measures $\nu \in \mathcal{M}_1(\Omega_N)$. Now the approximation that brings us back to the molecular field equations is to maximize, but only over i.i.d. product measures. Thus we will not get the actual pressure $p_N(\beta)$, but only a lower bound. Every i.i.d. product measure is characterized by an external field. I.e., given $\eta \in \mathbb{R}$, let $\nu_{N,\beta\eta}$ be the measure such that

$$\nu_{N,\beta\eta}(\sigma) = \frac{e^{\beta\eta|\Lambda_N|m_N(\sigma)}}{[2 \cosh(\beta\eta)]^{|\Lambda_N|}}.$$

It is easy to calculate

$$|\Lambda_N|^{-1} S_\Lambda(\nu_{N,\beta\eta}|\mu_{N,0}) = \log(\cosh(\beta\eta)) - \beta\eta \tanh(\beta\eta),$$

as well as

$$-\mathbf{E}^{\nu_{N,\beta\eta}}[\beta H_N(\sigma)] = \frac{\beta J}{2} \tanh^2(\beta\eta) + \beta h \tanh(\beta\eta).$$

Therefore, the molecular field approximation to the pressure, which is now independent of N , is

$$\tilde{p}(\beta) = \max_{\eta \in \mathbb{R}} \left[\log(2 \cosh(\beta\eta)) - \beta\eta \tanh(\beta\eta) + \frac{\beta J}{2} \tanh^2(\beta\eta) + \beta h \tanh(\beta\eta) \right]. \quad (3.2)$$

Let us call the left hand side $G(\eta)$, where G stands for Gibbs functional. Then we easily find,

$$G'(\eta) = [\beta(h - \eta) + \beta J \tanh(\beta\eta)] \operatorname{sech}^2(\beta\eta).$$

In order to have a critical point, one should require

$$\frac{\eta - h}{J} = \tanh(\beta\eta),$$

and that is the main equation of molecular field theory. We will call this the self-consistent molecular field equation, although in the present framework, we have derived it from a variational approach, not a self-consistent one.

3.1 Graphical analysis.

Let us define a few new variables. Let $x^* = \beta\eta$, let $x = \beta h$ and let $t = \beta J$. Then the

self-consistent molecular field equation

$$\tanh(x^*) = \frac{x^* - x}{t}.$$

Also, let $m = (\eta - h)/J = (x^* - x)/t$, which is the average magnetization. This is hard to solve explicitly analytically, but easy to solve graphically. One simply graphs $y = \tanh(x^*)$

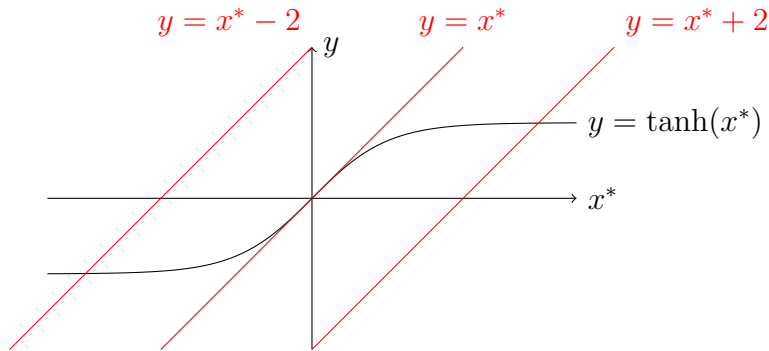


FIGURE 2. Plot of $y = \tanh(x^*)$ and three lines. This corresponds to $t = \beta J = 1$ and $x = \beta h = -2, 0, 2$. One would look for the x^* -coordinate of the intersection point.

and then graphs the line $y = (x^* - x)/t$, where x and t are constants determined by β , J and h . Then the points of intersection give the solution to the molecular field equation.

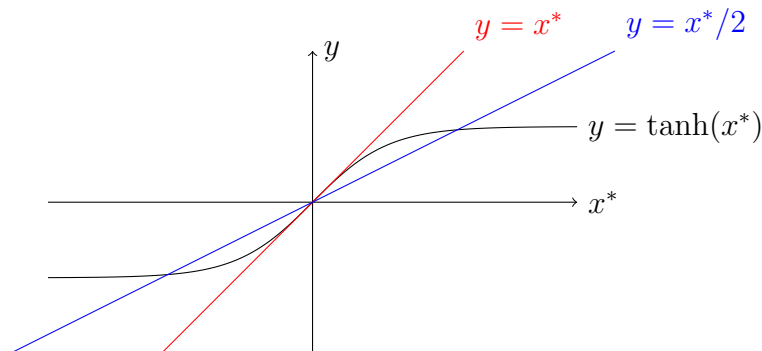


FIGURE 3. Plot of $\tanh(x)$ and the corresponding lines for $\beta h = 0$ and two values of βJ : 1 and 2. At $\beta J = 1$ the unique intersection point is $(0, 0)$, but at $\beta J = 2$, there are three points of intersections. One needs an external criterion for deciding which of these solutions is/are correct.

If one is willing to accept the self-consistent molecular field equation, then one still faces an obstacle: for certain values of x and t there are multiple solutions of x^* . For example, while in Figure 1 there are three values of x and t which lead to unique solutions of x^* , in Figure 2 there is one value $(t, x) = (2, 0)$ that has multiple solutions of x^* . Hence, one needs an external method of determining which is (are) the right solution(s). Let us illustrate this in another way. One can easily parametrize the solutions of m as a function of x , for a fixed

value of t , if one is willing to accept parametric solutions of both x and m . Namely, let s be the parametric variable, and

$$x = s - t \tanh(s) \quad \text{and} \quad m = \tanh(s).$$

Then, since $x^* = x + tm$, this gives $x^* = s$, and of course

$$x = s - t \tanh(s) \Rightarrow \tanh(s) = \frac{s - x}{t},$$

which is the right equation upon substitution $s = x^*$. Plotting such functions, one again sees

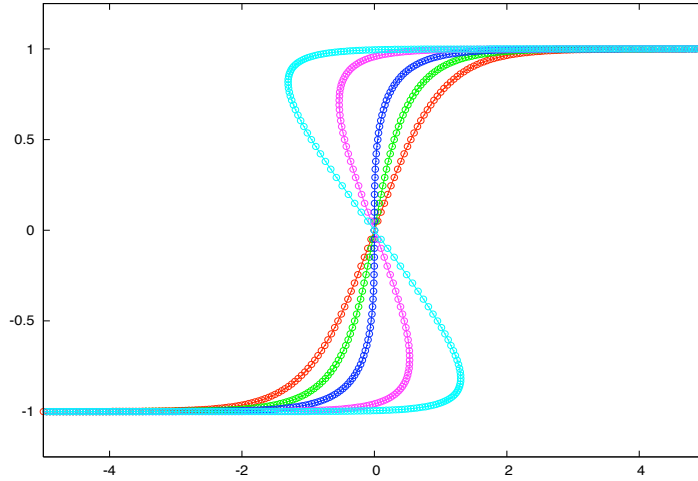


FIGURE 4. One can easily plot m as a function of x , using the parametric equation explained above. Here we have plotted $m(x)$ for fixed t : red, $t = 0$; green, $t = 0.5$; blue, $t = 1$ (which is the critical time when a shock first occurs); maroon, $t = 2$; and cyan, $t = 3$. The problem is that after $t = 1$, the waveforms obtained this way are multi-valued. I.e., they have overhangs.

that for some values of t and x , there are multiple solutions for m . In the present plots, this shows up as overhangs. This starts to be a problem at $t = 1$. For example see Figure 4.

There is a standard resolution of this problem called the Maxwell construction. By spin-flip symmetry, one has $H_N(\sigma) = H_N(-\sigma)$ for all $\sigma \in \Omega_N$. This implies that $p_N(1, t, x) = p_N(1, t, -x)$. In particular, this means that

$$\int_{-R}^R \bar{m}_N(1, t, x) dx = 0,$$

independent of t . Therefore, if we are going to make a vertical cut in the multivalued profiles, in order to make them single valued (everywhere except at the vertical cut where it is undefined), then it should be done so as to chop off equal areas in the overhangs to the left and right of the cut. Otherwise the integral above would begin to have a t -dependence. In this problem, that means that the cut must be made at $x = 0$, which is also the most symmetric choice. See Figure 5. This construction holds in greater generality than what we used here. But now we know what we are aiming for.

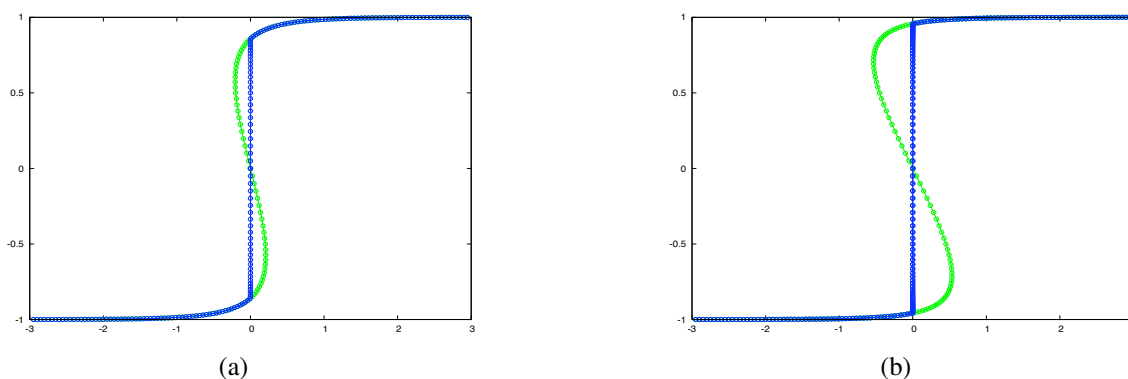


FIGURE 5. Here we make a cut-off satisfying the Maxwell construction, equal area rule. The green curve is the one obtained by the parametric, multivalued curves, and the blue curve is the correct one with a single jump discontinuity at $x = 0$. (a) “Time” $t = 1.5$. (b) “Time” $t = 2$.

3.2 Thermodynamic functions at the critical point.

The real purpose of molecular field theory is to allow calculation of various thermodynamic functions. We will make some calculations near the critical points.

In order to proceed further, let us make the substitution $m = \tanh(\beta\eta)$ in equation (3.2). Note that this gives

$$\beta\eta = \frac{1}{2} \log \left(\frac{1+m}{2} \right) - \frac{1}{2} \log \left(\frac{1-m}{2} \right),$$

and

$$\log(2 \cosh(\beta\eta)) = -\frac{1}{2} \log \left(\frac{1+m}{2} \right) - \frac{1}{2} \log \left(\frac{1-m}{2} \right).$$

Thus, the Gibbs variational principle, restricted to i.i.d. product measures becomes

$$\tilde{p}(\beta, J, h) = \max_{m \in [-1, 1]} \left[-\frac{1+m}{2} \log \left(\frac{1+m}{2} \right) - \frac{1-m}{2} \log \left(\frac{1-m}{2} \right) + \frac{m^2 t}{2} + mx \right].$$

We will try to solve this, to find $m(t, x)$. Defining the left-hand-side as $g(m)$ we see that

$$g'(m) = \frac{1}{2} \log \left(\frac{1-m}{1+m} \right) + mt + x,$$

and

$$g''(m) = -\frac{1}{1-m^2} + t.$$

Particularly, when $m = 0$, this is negative only for $t < 1$. For $t > 1$, the critical point $m = 0$ is no longer a minimizer of $g(m)$, it is a maximizer. That is why the critical value of $t = \beta J$ is 1.

Supposing t is greater than 1, and supposing x is equal to 0, there are two solutions: $m_+(t)$ and $m_-(t)$. One can calculate these asymptotically for $t - 1$ positive, but small. The critical

point equation becomes

$$\frac{1}{2} \log \left(\frac{1-m}{1+m} \right) + tm = 0.$$

Expanding the logarithm to third-order gives

$$tm = m + \frac{1}{3}m^3 + O(m^5).$$

Therefore, one has

$$m_{\pm}(t) = \pm \sqrt{3(t-1)}(1 + o(1))$$

for $t > 1$, where $o(1)$ is a quantity vanishing as $t - 1$ approaches 0.

Actually, what the equations are telling us is that $m(t, 0)$ does not exist for $t > 1$. But the limits $m_{\pm}(t) = \lim_{x \rightarrow 0^{\pm}} m(t, x)$ do exist. These are called the spontaneous magnetizations, because, at least within the framework of molecular field theory, the system magnetizes even for a vanishingly small amount of external field. I.e., it magnetizes *spontaneously*.

At $t = 1$ and $x \neq 0$, but small, the same expansion of the logarithm gives

$$x = \frac{1}{3}m^3 + O(m^5).$$

Therefore

$$m(1, x) = (3x)^{1/3}(1 + o(1)),$$

asymptotically, for small x . Finally, by implicit differentiation of the critical point equation

$$\frac{1}{2} \log \left(\frac{1-m}{1+m} \right) + mt + x = 0,$$

one obtains

$$\frac{\partial m}{\partial x} = \frac{1-m^2}{1-t(1-m^2)}.$$

In particular, for $t < 1$ and $x = 0$, we know that $m(t, x) = 0$. Therefore, this leads to

$$\chi(t, 0) = (1-t)^{-1},$$

(exactly) for $t < 1$.

For each of these quantities, near the critical point there is a power-law behavior. The various exponents are called critical exponents. Critical exponents are generally dimension dependent, as well as dependent on some features of the microscopic model, such as the symmetries of the lattice. Here one would expect that as the dimension d approaches ∞ , the critical exponents approach the values listed above. This is because, in some sense, the molecular field theory is supposed to become exact in “infinite dimensions”. We will explain this more in the next lectures after we introduce the Curie-Weiss model.

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