Controlling Mean-Field Theory

Mean field theories of Van der Waals and Weiss provide a decent description of the gross qualitative features describing first and second order phase transitions. In their historic form, however, they have been derived in a rather heuristic and uncontrolled fashion, leaving it unclear precisely how accurate these theories are. After these early successes of theory, refined experiments revealed a number of shortcomings of such approaches, in particular in their descriptions of the critical point. In the following we fist explore a slightly more rigorous formulation of these theories, which also indicate how systematic corrections can be obtained and calculated.

Heuristic derivation revisited

We concentrate on a model of an Ising ferromagnet, with the Hamiltonian

$$H = -\frac{J}{2}\sum_{<ij>} S_i S_j - h\sum_i S_i,$$

where $S_i = \pm 1$, and the lattice sum runs over all pairs of nearest neighbor sites on a given lattice, and h is an external magnetic field. As we have seen, the simplest way to obtain the Weiss theory is to replace

$$h_i = J\sum_{j=1}^{z} S_j \rightarrow h_W = J\left\langle \sum_{j=1}^{z} S_j \right\rangle = Jz\,\langle S_j\rangle = Jz\,m.$$

where z is the coordination number (number of neighbors to any given site), and m is the magnetization per spin. Physically, it is clear what this approximation amounts to. The instantaneous (fluctuating) molecular field h_i acting on the spin S_i is being replaced by its thermal average, the "Weiss field" h_W.

When is this justified? Are the results qualitatively or only quantitatively incorrect? To answer this question precisely, we have to identify some limit where the approximation is exact, and then examine systematic corrections.

Infinite range model

A simple argument clarifies precisely when is the mean field theory exact. At any finite temperature, the instantaneous orientations of spins are random, thus the molecular field h_i is simply a sum of z random numbers. As we know from elementary statistics, any sum of random numbers is increasingly well represented by its algebraic average, provided that the number of terms becomes larger and larger. We this expect mean field theory to be a good approximation for z sufficiently large. But how large? Well...most certainly in the limit of large coordination $z \to \infty$. But isn't this limit pathological? Not necessarily! If we properly *scale* the interaction with the coordination number $J \to J/z$, and then take the $z \to \infty$ limit, then the (free) energy per spin will remain finite, while mean field theory becomes exact. In the following we present a formal calculation to calculate the partition function exactly in the $z \to \infty$ limit.

Gaussian transformation

We concentrate on an infinite range model having N lattice sites, where each spin interacts with each other spin with exactly the same interaction J/N (in this case $z = N - 1 \approx N$ for N large). In this case the Hamiltonian can be written as

$$H = -\frac{J}{2N} S^2; \; S \equiv \sum_{j=1}^{N} S_j.$$

The partition function is

$$Z = \mathrm{Tr} \exp\{-\beta H\} = \sum_{\{S_i = \pm 1\}} \exp\left\{ \frac{\beta J}{2N} S^2 + \beta h S \right\}.$$

To rewrite this in a convenient way, such that we end up in an expression being a simple exponential in S, we use the Gaussian identity

$$\exp\left\{ \frac{\beta J}{2N} S^2 \right\} = \left(\frac{\beta J}{2\pi} \right)^{1/2} \int dt \, \exp\left\{ N \frac{t^2}{2\beta J} + tS \right\}.$$

The partition function takes the form

$$Z = \left(\frac{\beta J}{2\pi} \right)^{1/2} \int dt \, \exp\left\{ N \frac{t^2}{2\beta J} \right\} \sum_{\{S_i = \pm 1\}} \exp\left\{ (\beta h + t) \sum_{j=1}^{N} S_j \right\}$$

We note that the second second exponential looks just like a Boltzmann factor for N independent spins in an external field $h + t/\beta$. The spin sum then factors out and we can write

$$Z = \left(\frac{\beta J}{2\pi}\right)^{1/2} \int dt \, \exp\left\{-N\frac{t^2}{2\beta J}\right\} \left[Z_1(t,h)\right]^N ,$$

where

$$Z_1(t,h) = \sum_{\{S_i=\pm 1\}} \exp\left\{(\beta h + t)S_j\right\} = 2\cosh\left\{\beta h + t\right\} .$$

We get

$$Z = \left(\frac{\beta J}{2\pi}\right)^{1/2} \int dt \, \exp\left\{N\left(-\frac{t^2}{2\beta J} + \ln\cosh\left\{\beta h + t\right\} + \ln 2\right)\right\} .$$

We have thus reduced the calculation of the partition function to a Gaussian integral, which is exact in this infinite range model.

Saddle point solution

At finite N the integral must be computed numerically, but the situation amazingly simplifies in the large N limit! This is easiest to appreciate if we simply use the computer to numerically plot the integrand for some large but finite N. We find (**Problem 2.1**) that for N large, the integrand is strongly peaked at some specific value(s) of $t_{\max}$. In this limit, the integrand essentially looks like one (or several, see below) delta functions, and we can evaluate the integral by a saddle-point method. What's the idea? Simply, if we have a sharply peaked integrand, then we can first identify where the peak is, and then approximate the integrand by a Gaussian centered at the peak.

In practice, the integrand has a sharp peak, wherever the expression

$$f(t,h) = -\frac{t^2}{2\beta J} + \ln\cosh\left\{\beta h + t\right\} + \ln 2$$

has a maximum, i.e. $f'(t_{\max} = \beta J m) = 0$ (we have called the position of the peak $t_{\max} = \beta J m$. We get

$$m = \tanh\left(\beta h + \beta J m\right) ,$$

precisely the Weiss self-consistency condition. We have already seen how this equation can be solved, and how nontrivial $m \neq 0$ (for $h = 0$) solution emerges at $T < T_c = J$ (remember that the coordination number $z = N$ is absorbed in our definition of the interaction J).

But is this justified. In the following we will see how the procedure is valid only in the thermodynamic limit $N \to \infty$.

Spontaneous symmetry breaking in the thermodynamic limit

Where are the saddle-point solutions (maxima of the integrand). We have seen that they are determined by the solution of the Weiss equation. Thus, there is only one solution, thus only one sharp peak of the integrand for $T > T_c$. For $h = 0$ the peak is precisely at $t = 0$, and for h finite it shifts left or right. However, since the integrand is symmetric, we can immediately see that the resulting expression for the partition function $Z(h)$ is an **even** function of the external field h. Thus the zero-field magnetization per spin

$$m = \lim_{h\to 0} \frac{1}{N} \frac{\partial}{\partial \beta h} \ln Z(h) = 0.$$

(This is because for even function the first derivative vanishes at the origin). At $T > T_c$ this is what we expect anyway. But what happens at $T < T_c$?

At $T < T_c$ we can see easily see that the Weiss equation now has two nontrivial solutions, and one trivial solutions. At $h = 0$ these correspond to two sharp maxima at $t_{\max} = \pm\beta J m$ and one very shallow minimum at $t = 0$. Within our saddle-point scheme, and if we have more then one sharp maximum of the integrand, the proper evaluation is obtained only if we sum over all these saddle-point solutions. Now comes the confusing part!!! At $h = 0$ these peaks are completely symmetrically distributed around zero, and just as before, we conclude that $Z(h)$ is an **even** function of the external field h!!!. Does this mean that there is no spontaneous magnetization??!! Well...it depends. At any finite N, the argument is perfectly correct, in agreement with our previous qualitative analysis suggesting no spontaneous symmetry breaking for any finite size system. But how could the result be possibly different in the thermodynamic limit $N \to \infty$?

Well...it can! And to see this, let us turn on a small but finite external field h and carefully evaluate the two saddle-point contributions to the integral. To leading order (when the peaks are very sharp), the contribution to the integral from each saddle point can simply be estimated by replacing the integral by the integrand evaluated at the saddle point:

$$Z(h) \sim \exp\{N f_+(h)\} + \exp\{N f_-(h)\}.$$

Here, $t_\pm \approx \pm\beta J m$, and

$$f_\pm(h) = f(t_\pm, h) = -\frac{t_\pm^2}{2\beta J} + \ln\cosh\{\beta h + t_\pm\} + \ln 2.$$

Since $f(t, h = 0)$ is an even function of t,

$$f_+(0) = f_-(0) = f(0) = -\frac{\beta J m^2}{2} + \ln\cosh\{\beta J m\} + \ln 2,$$

and they differ very little for h small, where we find by expanding in h

$$f_\pm(h) \approx f(0) \pm \beta h \tanh\{\beta J m\} = f(0) \pm \beta h m.$$

We can therefore write

$$Z(h) \sim \exp\{N f(0)\}\left[\exp\{N\beta h m\} + \exp\{-N\beta h m\}\right].$$

Now comes the interesting part! Consider first N finite and let $h \to 0$. As we can see, the partition function is still an **even** function of h, thus no ferromagnetism emerges! In contrast, consider a small but finite field $h > 0$. The let us approach the thermodynamic limit $N \to \infty$. As we can see, one of the exponents in this limits blows up, while the other vanishes **exponentially** fast in N! In the thermodynamic limit we can thus drop one of the contributions, and the partition function now reads

$$Z(h) \sim \exp\{N f(0) + N\beta h m\}.$$

Using the formula for the magnetization, we immediately see that now $m \neq 0$ and ferromagnetism emerges!

This example is very instructive, since it makes it clear on an exactly solvable model how the limits $h \to 0$ and $N \to \infty$ do not commute, so that qualitatively new physics emerges in the thermodynamic limit.

Large coordination limit generalized

As we can seen, the limit of large coordination (or equivalently large dimensions; $z = 2d$ on hypercubic lattices) offers a situation where the many-body problem can be systematically yet exactly solved, yet preserving a number of nontrivial features of the exact solution. The example we explored it the simplest one that comes to mind. The method is general, and it

has been used a great deal to explore the phase transitions is many classical and quantum systems. For example, we can use it for a clasical Heisenberg antiferromagnet in a uniform external field (**Problem 2.2**), to show how the susceptibility has a cusp at T_N, the specific heat jumps (in this mean-field limit), and many other features.

A veritable industry using this general approach has emerged in the last ten years to study the Mott-Hubbard transition and other examples of strongly correlated electrons (see "*The Local Impurity Self Consistent Approximation (LISA) to Strongly Correlated Fermion Systems and the Limit of Infinite Dimensions*" by A. Georges, G. Kotliar, W. Krauth, M. Rozenberg, Rev. Mod. Phys. **68,** 13 (1996)). Another line of work using similar approaches combined with the "replica symmetry breaking" methods has been applied to glassy systems by Parisi and his followers since 1980. An application to the glassy behavior of electrons has been presented in the following paper: "*Nonlinear screening theory of the Coulomb glass*", by S. Pankov, V. Dobrosavljevic, Phys. Rev. Letters **94**, 046402 (2005).