Lesson 5 & 6 by Baiesi

For systems in equilibrium at a temperature T (and $\beta = 1/T$, with Boltzmann constant $k_B = 1$), average quantities in the canonical ensemble are obtained by running weighted sums over all possible configurations S,

$$\langle X \rangle = \frac{\sum_S X[S] e^{-\beta H[S]}}{\sum_S e^{-\beta H[S]}} \tag{1}$$

The denominator is the partition function

$$Z = \sum_S e^{-\beta H[S]} \tag{2}$$

and $H[S]$ is the Hamiltonian, or energy function of the system. The free energy is $F = -T \log Z$. If we have X coupled to a parameter α in $H' = H + \alpha X$, we see from the structure of (1) that $\langle X \rangle = \frac{1}{\beta} \partial F / \partial \alpha |_{\alpha=0}$ derives from a suitable derivative of the free energy, which acts as a generating function. Hence, the knowledge of F allows to predict the mean behavior of the system.

One of the standard theoretical models of condensed matter is the Ising model for ferromagnets, which is the paradigm of a system displaying a phase transition by varying the temperature. In the following we use this model to show how the free energy should be evaluated in systems with some quenched disorder. To emphasize the similarities and the differences from the non-disordered system, we start by recalling the solution of the mean field Ising model.

0.1 Ising Model (mean field)

A standard Ising model, with spins $S_i \in \{-1, 1\}$ for $i = 1...N$ and Hamiltonian

$$H = -\frac{J}{N} \sum_{i \neq j} S_i S_j - h \sum_i S_i \tag{3}$$

is in a "mean-field" version if the sum runs over all possible pairs of $1 \leq i \leq N$ and $1 \leq j \leq N$ with $i \neq j$ (in the next section also the (i, i) pair will be included for simplifying the calculations; such constant energy shift is irrelevant thermodynamically). The system is ferromagnetic if $J > 0$ and hence $-J < 0$ favors the alignment of the spins. The external field h is the same for all spins.

We are interested in the thermodynamic limit $N \to \infty$. From the point of view of a given spin j, a myriad of other spins should contribute with an average effect due to the central limit theorem. The average magnetization

$$m = \frac{1}{N} \sum_i \langle S_i \rangle \tag{4}$$

should thus play a relevant role. Indeed, it enters in the calculation of the typical energetic contribution from j,

$$\begin{aligned} H_j &= S_j \left[-\frac{2J}{N} \sum_i S_i - h \right] && (5) \\ &\simeq S_j \left[-\frac{2J}{N} \sum_i \langle S_i \rangle - h \right] \qquad \text{(for large } N\text{)} && (6) \\ &\equiv -h_m S_j \qquad \text{with average field} \quad h_m = 2Jm + h && (7) \end{aligned}$$

(we would have had J and not $2J$ if pairs $i < j$ were considered).

The mean field approximation yields a non-interacting system of a single spin S_j in a field h_m. Its two possible states at inverse temperature $\beta = 1/T$ thus appear with probability given by Boltzmann weights normalized by the partition function Z,

$$P(S_j) = \frac{e^{\beta H_j}}{Z} = \frac{e^{\beta h_m S_j}}{e^{\beta h_m} + e^{-\beta h_m}} \tag{8}$$

There is still a self-consistency condition to impose on h_m and thus on the magnetization m:

$$\begin{aligned} m &= \sum_{S_j = \pm 1} P(S_j) S_j && (9) \\ &= \frac{e^{\beta h_m} - e^{\beta h_m}}{e^{\beta h_m} + e^{-\beta h_m}} && (10) \\ &= \tanh(\beta h_m) && (11) \end{aligned}$$

and by recalling what is h_m, the self-consistent equation becomes

$$m = \tanh(\beta 2Jm + \beta h) \tag{12}$$

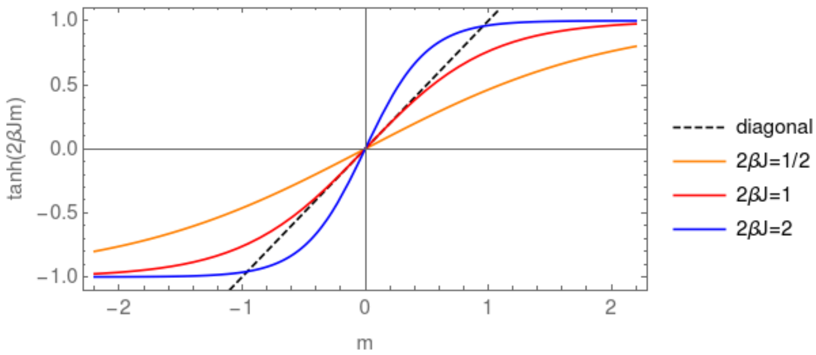

Figure 1: The graphical solution of (12) is obtained by finding the intersections of the $\tanh(2\beta Jm)$ function with the function m. The three curves are for low, critical, and large β.

Even for the simplest case $h = 0$ without external field, one should find the solution graphically as shown in Figure 1. At low β (high temperature) the function $\tanh(\beta 2Jm)$ is quite flat and stays below the function m, hence there is only one solution at $m = 0$. At a critical β_c three solutions merge at $m = 0$ and they split above β_c into $m = -m^*, 0, +m^*$ because $\tanh(\beta Jm)$ is steep enough to cross the diagonal m three times. The critical β_c is found by requiring that the tangent of $\tanh(\beta 2Jm)$ is equal to 1 at $m = 0$, which yields $\beta_c = 1/(2J)$.

0.2 Random Field Ising Model (RFIM)

We aim at understanding what changes from the standard Ising model if the field h_i is now randomly assigned to each site i. To stress that this random field is a fixed feature of each system, we call it *quenched disorder*. We may expect that this disorder added to the thermal randomness is a crucial factor when much stronger than the total ferromagnetic coupling with the other spins. In this sense, we could have a paramagnetic phase also if the temperature is very low because the spins prefer to follow their own local h_i rather than the global trend given by the magnetization.

We thus study a Random Field Ising Model (RFIM): the ferromagnetic coupling between spins $S_i \in \{-1, 1\}$ (in a configuration denoted by $S = (S_1, \ldots, S_N)$) is as in the standard Ising model and the interaction is again not limited to nearest neighbor but runs over all pairs i, j,

$$H_h[S] = -\frac{J}{N} \sum_{i,j} S_i S_j - \sum_i h_i S_i \tag{13}$$

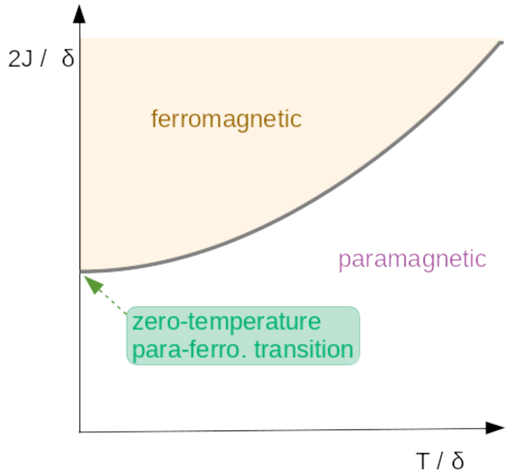

Figure 2: Phase diagram of the RFIM.

including the i, i interaction, for later convenience. Here, as a novelty, the disorder is realized by picking each local field h_i from the same Gaussian distribution with variance δ^2,

$$p(h_i) = \frac{1}{\sqrt{2\pi\delta^2}} e^{-h_i^2/2\delta^2} \qquad \forall i \leq N \tag{14}$$

and fixing it. Thus, every system is characterized by a given quenched disorder $h = \{h_i | i = 1, \ldots, N\}$ (of i.i.d. random variables) with full probability

$$p(h) = \prod_{i=1}^{N} p(h_i) \tag{15}$$

We would like to prove that the phase diagram of the RFIM is as that shown in Figure 2, where two phases (ferromagnetic with a macroscopic magnetization, and paramagnetic) appear. The diagram is as a function of the ratios T/δ and J/δ. The value T/δ quantifies how thermal energy is relevant with respect to the disorder. The value J/δ quantifies the relevance of the ferromagnetic coupling with respect to the disorder, and obviously the ferromagnetic phase appears where J/δ is sufficiently large, where "sufficiently" is quantified by the dense line separating the phases (note its monotonic increase with T: why?). The phase diagram also shows that, for given values of J and T, there is always a value of δ that can randomize the system enough to make it paramagnetic. Even for $T = 0$ we may see a para-ferromagnetic phase transition by varying δ.

The new issue is to find the typical behavior of a system by averaging its behavior over the realizations of the disorder. As discussed later, this centers around averaging the free energy

$$F_h = -T \log Z_h \tag{16}$$

over the disorder, rather than averaging the partition function

$$Z_h = \sum_S e^{-\beta H_h[s]} \tag{17}$$

An average over the disorder is denoted by an overline in the following. For example,

$$\overline{F} = -T\overline{\log Z_h} = -T \int \prod_i dh_i \, p(h) \log Z_h \tag{18}$$

The average of a nonlinear function as the log is problematic and it turns out to be simpler to average the n-th power $(Z_h)^n$. Because of this, it is useful to follow the *replica trick*. In its various forms, it reads

$$\begin{aligned} \overline{\log Z_h} &= \lim_{n\to 0} \frac{\overline{Z^n} - 1}{n} && (19) \\ &= \lim_{n\to 0} \frac{1}{n} \log \overline{Z^n} && (20) \\ &= \frac{\partial}{\partial n} \overline{Z^n} \Big|_{n=0} && (21) \end{aligned}$$

This is a useful mathematical step that, however, comes at the price of performing a weird limit of $n \to 0$ replicas. Each replica is one of the n copies of the system, all sharing the same disorder h.

We label each replica by an index $a = 1, \ldots, n$, and we let it understood that $Z = Z_h$ and $H_h[S] = H[S]$ depend on a quenched h. The n-th power of the partition function is then

$$\begin{aligned} \overline{Z^n} &= \overline{\sum_{\{S^a\}} \exp\left(\frac{\beta J}{N} \sum_a \sum_{ij} S_i^a S_j^a \right) \exp\left(\beta \sum_i \sum_a S_i^a h_i \right)} \\ &= \sum_{\{S^a\}} \exp\left(\frac{\beta J}{N} \sum_a \sum_{ij} S_i^a S_j^a \right) \underbrace{\overline{\exp\left(\beta \sum_i \sum_a S_i^a h_i \right)}}_{\equiv \overline{e^{\lambda_i \sum_i h_i}}} \end{aligned} \tag{22}$$

where $\sum_{\{S^a\}}$ means sum over all possible configurations of all replicas and

$$\lambda_i = \beta \sum_a S_i^a \tag{23}$$

Since the average over disorder is limited to the last term with h_i's, and since each term yields its own average via a Gauss integral,

$$\overline{e^{\lambda_i h_i}} = \int dh_i p(h_i) e^{\lambda_i h_i} = e^{\delta^2 \lambda_i^2/2}, \tag{24}$$

we may rewrite

$$\overline{Z^n} = \sum_{\{S^a\}} \exp\left[\frac{\beta J}{N}\sum_a \sum_{ij} S_i^a S_j^a + \frac{\beta^2\delta^2}{2}\sum_i \left(\sum_a S_i^a\right)^2\right] \tag{25}$$

$$= \sum_{\{S^a\}} \exp\left[\frac{\beta J}{N}\sum_a \left(\sum_i S_i^a\right)^2 + \frac{\beta^2\delta^2}{2}\sum_i \left(\sum_a S_i^a\right)^2\right] \tag{26}$$

where we noted that the first term in the exponential is just the square of $\sum_i S_i^a$. This is possible thanks to the choice of running the interactions also over the (i,i) pairs.

By inspecting the structure of (26) we note that we arrived at a system with interacting replicas! At the same time, the disorder has disappeared from the formulas. This trade of complications will finally lead to a solution of the RFIM.

Next we use the Hubbard-Stratonovich (HS) transformation,

$$e^{\frac{b}{2}z^2} = \frac{1}{\sqrt{2\pi b}} \int dx\, e^{-\frac{x^2}{2b} \pm zx} \tag{27}$$

(for negative exponent it becomes $e^{-\frac{b}{2}z^2} = \frac{1}{\sqrt{2\pi b}} \int dx e^{-\frac{x^2}{2b} \pm izx}$) which is useful for transforming squares in exponentials. In physical terms, this is translated to a replacement of interactions between degrees of freedom (z^2) by interactions with a mediating field x (the term zx) which follows a Gaussian statistics (x^2). The left-hand side of the HS formula can be seen in (26) if we identify

$$z_a = \sqrt{2J\beta}\sum_i S_i^a \tag{28}$$

$$b = \frac{1}{N} \tag{29}$$

$$e^{\frac{b}{2}z_a^2} = \frac{1}{\sqrt{2\pi b}} \int dx_a e^{-\frac{x_a^2}{2b} + z_a x_a} \tag{30}$$

By performing the HS transformation we get a version of $\overline{Z^n}$ in which spins S_i appear decoupled from the others,

$$\overline{Z^n} = \left(\frac{N}{2\pi}\right)^{n/2} \sum_{\{S^a\}} \int \prod_a dx_a \exp\Bigg[-\frac{N}{2}\sum_a x_a^2 \\ + \underbrace{\sqrt{2J\beta}\sum_i\sum_a S_i^a x_a + \frac{\beta^2\delta^2}{2}\sum_i\left(\sum_a S_i^a\right)^2}_{\sum_i \dots \text{ gives } N \text{ times the same object } \log Z_1}\Bigg] \tag{31}$$

$$= \left(\frac{N}{2\pi}\right)^{n/2} \int \prod_a dx_a \exp\left[N\left(-\frac{1}{2}\sum_a x_a^2 + \log Z_1(x_a)\right)\right] \tag{32}$$

with

$$Z_1(x_a) = \sum_{\{S^a=\pm 1\}} \exp\left(\sqrt{2\beta J}\sum_a x_a S^a + \frac{\beta^2\delta^2}{2}\left(\sum_a S^a\right)^2\right) \tag{33}$$

where we set $S_i^a \to S^a$ due to the independence of Z_1 on the index i.

The exponent $\sim N$ in (32) shows that we can now use the saddle point approximation for large N. In doing this, we also assume that all replicas share the same $x_a = x$ (like in a replica symmetric solution), hence $\sum_a x_a = nx$, and $\sum_a x_a^2 = nx^2$. The saddle point, denoted by x_m, solves the equation

$$\frac{\partial}{\partial x}\left[-\frac{1}{2}nx^2 + \log Z_1(x)\right] = 0 \quad \rightarrow \quad nx = \frac{\partial}{\partial x}\log Z_1(x) \tag{34}$$

hence

$$nx_m = \sqrt{2\beta J}\frac{\sum_{\{S^a=\pm1\}}\left(\sum_a S^a\right) e^{A[S,x_m]}}{\sum_{\{S^a=\pm1\}} e^{A[S,x_m]}} \tag{35}$$

where

$$A[S,x] = \sqrt{2\beta J}x\sum_a S^a + \frac{\beta^2\delta^2}{2}\left(\sum_a S^a\right)^2 \tag{36}$$

The structure of (35) reveals that x_m is proportional to the average over the replicas of the spins, i.e. the magnetization m, in an ensemble where the Boltzmann weight e^A determines averages $\langle \dots \rangle$,

$$\frac{x_m}{\sqrt{2\beta J}} = \left\langle \frac{1}{n}\sum_a S^a \right\rangle \equiv m \tag{37}$$

We can thus rewrite everything by using $m = x_m/\sqrt{2\beta J}$:

$$\overline{Z^n} \propto e^{N\left[-n\beta J m^2 + \log Z_1(m)\right]} \tag{38}$$

$$Z_1(m) = \sum_{\{S^a=\pm 1\}} e^{A[S,m]} \tag{39}$$

$$A[S,m] = 2\beta J m \sum_a S^a + \frac{\beta^2\delta^2}{2}\left(\sum_a S^a\right)^2 \tag{40}$$

$$m = \frac{1}{Z_1(m)} \sum_{\{S^a=\pm 1\}} \left(\frac{1}{n}\sum_a S^a\right) e^{A[S,m]} \tag{41}$$

where $A[S,m]$ still couples the statistics of the replicas.

We recall that we are looking for a self-consistent equation for the magnetization, in analogy to the solution of the standard mean field Ising model. The square $(\sum_a S^a)^2$ that resisted so far in the exponent is removed by means of another HS transformation,

$$e^{A[S,m]} = \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2 + (2\beta J m + \beta\delta\nu)\sum_a S^a} \tag{42}$$

This brings the advantage of finally decoupling the replicas. With this HS transformation, $Z_1(m)$ becomes

$$\begin{aligned} Z_1(m) &= \sum_{\{S^a=\pm 1\}} e^{A[S,m]} \\ &= \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2} \prod_a \sum_{S^a=\pm 1} e^{(2\beta J m + \beta\delta\nu)S^a} \qquad (n \text{ decoupled replicas}) \\ &= \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2} [2\cosh(2\beta J m + \beta\delta\nu)]^n \\ &= \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2 + n\log[2\cosh(2\beta J m + \beta\delta\nu)]} \end{aligned} \tag{43}$$

We are finally able to perform the limit $n \to 0$ dictated by the replica trick, for which $Z_1 \to 1$.

In analogy, we can prove that also the formula for m can be rewritten without any explicit reference to each replica but with just the number n of replicas appearing (exercise). It turns out that

$$m = \frac{1}{Z_1(m)} \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2 + n\log[2\cosh(2\beta J m + \beta\delta\nu)]} \tanh(2\beta J m + \beta\delta\nu) \tag{44}$$

which, for $n \to 0$, gives

$$m = \int \frac{d\nu}{\sqrt{2\pi}} e^{-\frac{1}{2}\nu^2} \tanh\left(2\beta J m + \beta\delta\nu\right) \tag{45}$$

This further appearence of a Gaussian distribution for ν (unit variance) is welcome as one can convert it to a Gaussian distribution for $h = \delta\nu$ and translate the formula to an average over disorder [see (15)],

$$\begin{aligned} m &= \int \frac{dh}{\sqrt{2\pi\delta^2}} e^{-\frac{h^2}{2\delta^2}} \tanh\left(2\beta J m + \beta h\right) \\ &= \overline{\tanh\left(\beta\left(2Jm + h\right)\right)} \end{aligned} \tag{46}$$

This self-consistent equation for $m = m_{sc}(m)$ with $m_{sc}(m)$ given by the right-hand side of (46) is solved graphically, as shown for the Ising model. The critical line in the phase diagram of Figure 2 corresponds to the points where $\partial m_{sc}/\partial m = 1$, that the values of (T, δ, J) for which the curve is tangent to the diagonal line $m = m$. One can prove (exercise) that this condition turns into the equation

$$2\beta J \int dh\, p(h) \frac{1}{[\cosh(\beta h)]^2} \;=\; 1 \tag{47}$$

which can be recast in several forms; for example, by using reduced variables $J' = J/\delta$, $\beta' = \beta\delta$, $\tilde{h} = \beta h$ related to those in the axis of the phase diagram of Figure 2, we get

$$2\beta' J' \int \frac{d\tilde{h}}{\sqrt{2\pi}} e^{-\frac{\tilde{h}^2}{2\beta'^2}} \frac{1}{\left[\cosh \tilde{h}\right]^2} \;=\; 1 \tag{48}$$

Using this condition, one can show that even for zero temperature one has a para-ferromagnetic transition by varying the ratio $2J/\delta = 2J'$. The transition takes place (exercise) at $2J/\delta = \sqrt{\pi/2}$. Note that the self-consistent equation of the mean field Ising model is recovered from (46) for $\delta \to 0$. In Figure 3 there is an example of ferromagnetic phase disappearing by increasing δ.

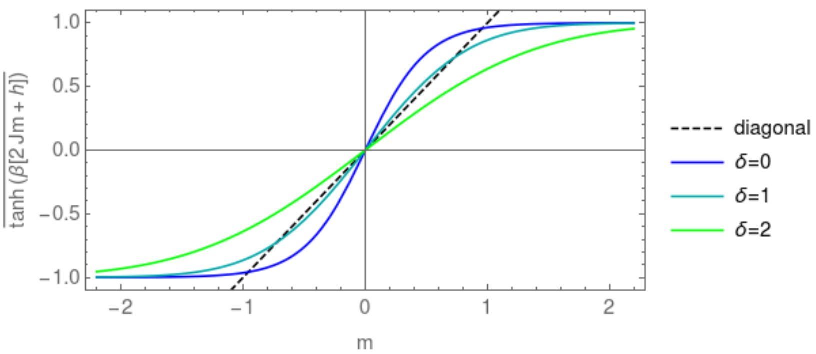

Figure 3: Plot of the self-consistent magnetization (46) vs m, for $\beta = J = 1$. The three curves are for different noise strengths: $\delta = 0$ (standard Ising), $\delta = 1$ and $\delta = 2$. Note that the system without disorder is ferromagnetic for these parameters but becomes paramagnetic at sufficiently high δ.

The free energy averaged over the disorder in the end is

$$\begin{aligned}
\overline{F} &= -T\overline{\log Z} \\
&= -T\left.\frac{\partial}{\partial n}\overline{Z^n}\right|_{n=0} \\
&\simeq -T\frac{\partial}{\partial n}\left[e^{N(-n\beta Jm^2+\log Z_1)}\right]_{n=0} \\
&= -TN\left[-\beta Jm^2 + \frac{\partial}{\partial n}\log Z_1\right]_{n=0} \\
&= N\left[Jm^2 - \frac{T}{Z_1}\frac{\partial}{\partial n}Z_1\right]_{n=0} \\
&= N\left[Jm^2 - T\int\frac{d\nu}{\sqrt{2\pi}}e^{-\frac{1}{2}\nu^2}\log[2\cosh(2\beta Jm+\beta\delta\nu)]\right] \\
&= N\left[Jm^2 - T\int\frac{dh}{\sqrt{2\pi\delta^2}}e^{-\frac{h^2}{2\delta^2}}\log[2\cosh(\beta(2Jm+h))]\right] \qquad (49)
\end{aligned}$$

To wrap up, after deciding that the correct quantity to average is the free energy, one uses the replica trick to convert the computation to that of a system of interacting replicas without disorder. By some massage including two Hubbard-Stratonovich steps (to get rid of quadratic forms in the exponent till we get the right quadratic form, i.e. the disorder average) and by the identification of some quantities with others having physical meaning (magnetization, average over disorder), one finds a self-consistent equation for the magnetization that represents the generalization to a system with quenched disorder of its version for the Ising model. This magnetization enters in the solution for the free energy. The phase diagram of the RFIM follows from these equations, with boundary between phases given by the points where the self-consistent function of the magnetization has derivative 1.

As a final point, let us hightlight that the limits $\lim_{N\to\infty}\lim_{n\to 0}$ have been inverted in the above calculations, becoming $\lim_{n\to 0}\lim_{N\to\infty}$. Performing the thermodynamic limit before the limit to zero replicas is fine for the RFIM.