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A variational approach to Ising spin glasses in finite dimensions

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Abstract. We introduce a hierarchical class of approximations of the random Ising spin glass in d dimensions. The attention is focused on finite clusters of spins where the action of the rest of the system is properly taken into account. At the lowest level (cluster of a single spin) our approximation coincides with the SK model while at the highest level it coincides with the true d-dimensional system. The method is variational and it uses the replica approach to spin glasses and the Parisi ansatz for the order parameter. As a result we have rigorous bounds for the quenched free energy which become more and more precise when larger and larger clusters are considered.

1. Introduction

Research around spin glasses in finite dimensions is very active since it is still unclear if they share all the qualitative features of the mean-field model SK. Since a direct study of these systems is quite complicated, both from a numerical and an analytic point, it could be of some interest to consider corrections to the SK model which partially take the dimensionality into account. Our aim is to find out a systematic and rigorous way to introduce these corrections. As a result, we generate a class of models which interpolate between the mean-field SK model and exact spin glasses in finite dimensions. Our approach uses the replica formalism together with the celebrated Parisi ansatz for the order parameter.

The standard replica approach to the SK model reduces the problem to a single spin whose replicas interact via the variational order parameters $\{q^{ab}\}$ that can be thought as 'coupling fields'. This is the analogue of what one has for the mean-field model of the ordinary ferromagnetic Ising systems. In this second case, in fact, one has a single spin in a magnetic field generated by the rest of the system.

Both models, SK and mean-field Ising model, can be regarded as an approximation of the associated Ising system in finite d dimensions, but in both cases any reference to the dimensionality is lost. The approximation can be improved and a memory of the dimensionality can be maintained if, in spite of considering a single spin in a bath, one focuses the attention on a cluster of interacting spins in a bath generated by the rest of the system. The strategy, which is very successfully applied for ordinary spin systems (Bethe–Peierls approximation [1, 2]), has recently been extended to spin glasses [3, 4]. Actually the approach of [3, 4] turns out not to be very effective, since it does not allow for a study of the replica symmetry breaking. This fact reduces the scope of the method to low-dimensional

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spin glasses, while for $d \geqslant 3$ dimensions it fails to describe the most striking feature of these systems.

In this paper we introduce a new approach which allows for symmetry breaking. The attention is focused on finite clusters of spins where the action of the rest of the system is properly taken into account. The approximations we obtain are organized hierarchically according to the size of the clusters. At the lower level (cluster of a single spin) our approximation coincides with the SK model while at the highest level it coincides with the true d-dimensional system. The method is variational and it uses the replica approach to spin glasses and the Parisi ansatz for the order parameter. As a result we have rigorous bounds for the quenched free energy which become more and more precise when larger and larger clusters are considered.

Let us briefly sum up the contents of the paper. In section 2, we introduce the model and we generalize the standard replica approach in order to take advantage from the cluster partition of the lattice. In section 3, we derive the new variational approach and we find out analytic lower bounds of the free energy of the d-dimensional spin glass. In section 4, we choose the Parisi ansatz in order to obtain a computable solution to the problem. In particular, we write down the free energy in the case of k symmetry breaking. In section 5, we test our method against of the case of a plaquette of four spins in $d = 2$ dimensions; the free energy and the order parameter are obtained at all the temperatures for the replica symmetry and one symmetry breaking solutions. In section 6, we resume the results obtained, and some future developments are discussed.

2. New look at the replica approach

We consider Ising spin-glass models with nearest neighbours interactions on a d-dimensional lattice of N sites. The Hamiltonian is

$$H = -\frac{1}{(2d)^{\frac{1}{2}}} \sum_{(i,j)} J_{i,j}\sigma_i\sigma_j$$

where the $\{\sigma_i = \pm 1\}$ are the N spin variables and the $\{J_{i,j}\}$ are the dN independent normal Gaussian random variables (zero mean and unitary variance). The sum runs on all the dN nearest neighbours sites (i, j).

The partition function reads

$$Z = \sum_{\{\sigma\}} \exp\{-\beta H\}$$

where β is the inverse temperature. The quenched free energy is

$$f_d = -\lim_{N\to\infty} \frac{1}{\beta N} \overline{\ln Z} \tag{2.1}$$

where $\overline{\cdot}$ indicates the average over the disorder variables $\{J_{i,j}\}$. Indeed, almost all the disorder realizations have the same free energy in the thermodynamic limit $N \to \infty$.

Unfortunately, it is not possible to find an explicit expression of (2.1) in terms of simple functions because of the presence of the logarithm in the disorder average. The standard replica approach [5] tries to avoid this difficulty by replacing the above quenched average with the average of the nth power of the partition function Z with an integer n. In fact, if the result can be analytically continued to real n, one has

$$f_d = -\lim_{n\to 0} \lim_{N\to\infty} \frac{1}{\beta N n} \ln \overline{Z^n}. \tag{2.2}$$

The average over the Gaussian disorder variables gives

$$\overline{Z^n} = \exp\left\{\frac{1}{4}\beta^2 Nn\right\} \sum_{\{\sigma\}} \exp\left\{\frac{\beta^2}{2d} \sum_{(i,j)} \sum_{a<b} \sigma_i^a \sigma_i^b \sigma_j^a \sigma_j^b\right\} \tag{2.3}$$

where σ_i^a is the ath replica of the spin in the ith site.

Unfortunately, even in the replica context the free energy can be computed only in the infinite-dimension limit. In this case, in fact, one reverts to the well known SK model [6], and one has

$$f_\infty = -\frac{\beta}{4} + \lim_{n\to 0} \frac{1}{n} \max_{\{q^{ab}\}} \left[\frac{\beta}{2} \sum_{a<b} (q^{ab})^2 - \frac{1}{\beta} \ln \sum_{\{\sigma\}} \exp\left\{\beta^2 \sum_{a<b} q^{ab} \sigma^a \sigma^b\right\}\right] \tag{2.4}$$

where q^{ab} is a real matrix. In the limit $n \to 0$ this maximum is found following the Parisi ansatz [7–9]. When d is finite, no analogous results are available, so it is sensible to look for approximations as in this paper.

All the above expressions are so classical that it may seem completely useless to have reproduced them here, indeed, the reason is that we would like to recast them in a more general form by introducing the notion of cluster partition of the set of N spins. The new formulation, which is more general and provides the technical ingredients for our variational approach, reduces to the standard replica trick in the case of clusters of a single spin.

To have an idea of the clusters imagine a plaquette of four nearest-neighbour spins in two dimensions, or a cube of eight spins in three dimensions. In general, we perform a decomposition of the set of the spins into clusters of the same shape, such that each spin belongs to one and only one of them. In the following we indicate with $(i, j)'$ all the couples of nearest-neighbour sites that belong to the same cluster, and with $\overline{\cdot}^{\prime}$ the disorder average over the couplings between them. In the same way $(i, j)''$ denotes all the nearest-neighbour sites of different clusters, and $\overline{\cdot}^{\prime\prime}$ the related disorder average. Finally, $(i)'$ runs only over the boundary sites of all the clusters. Moreover, the following definitions are useful

$$\begin{cases} n_\sigma = \text{number of spins in a cluster} \\ n_b = \text{number of boundary spins in a cluster} \\ n_J = \text{number of bonds in a cluster} \end{cases}$$

which imply that $\frac{N}{n_\sigma}$ is the total number of clusters in the system, and that

$$\begin{cases} \displaystyle\sum_{(i)'} 1 = \frac{n_b}{n_\sigma} N \\ \displaystyle\sum_{(i,j)'} 1 = \frac{n_J}{n_\sigma} N \\ \displaystyle\sum_{(i,j)''} 1 = \left(d - \frac{n_J}{n_\sigma}\right) N. \end{cases}$$

For instance, in figure 1 one has clusters of $n_\sigma = 12$ spins, with $n_b = 8$ boundary spins and $n_J = 16$ internal bonds per cluster.

Then, we again compute the free energy with the replica trick, but this time we perform the average of Z^n only over those bounds that couple different clusters:

$$f_d = -\lim_{N\to\infty} \lim_{n\to 0} \frac{1}{\beta N n} \overline{\ln \overline{Z^n}^{\prime\prime}}^{\prime}. \tag{2.5}$$

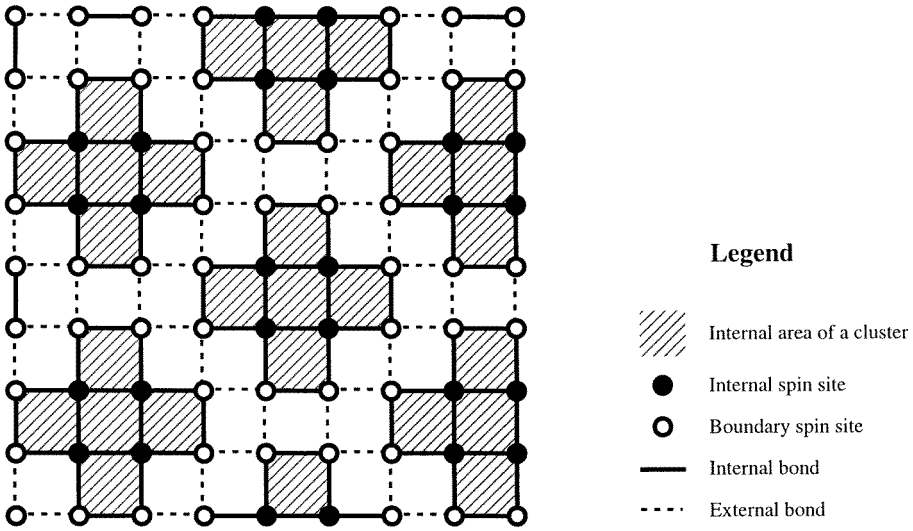

Figure 1. Decomposition of a two-dimensional spin lattice in clusters of $n_\sigma = 12$ spins, with $n_b = 8$ boundary spins (white circles), 4 internal spins (black circles) and $n_J = 16$ internal bonds (full lines) per each cluster. The broken lines represent the bonds between spins belonging to different clusters.

Somehow, this expression interpolates between (2.2) which corresponds to clusters of a single spin (no couplings inside the clusters) and the quenched expression (2.1) which corresponds to a single cluster of size of order N spins.

A simple calculation gives

$$\overline{Z^n}'' = \exp\left\{\frac{1}{4}\beta^2 Nn\left(1 - \frac{n_J}{dn_\sigma}\right)\right\}\sum_{\{\sigma\}}\exp\{-\beta H^{(n)}\} \tag{2.6}$$

where

$$H^{(n)} = -\frac{1}{(2d)^{\frac{1}{2}}}\sum_{(i,j)'} J_{i,j}\sum_{a=1}^{n}\sigma_i^a\sigma_j^a - \frac{\beta}{2d}\sum_{(i,j)''}\sum_{a<b}\sigma_i^a\sigma_i^b\sigma_j^a\sigma_j^b. \tag{2.7}$$

Note that the first sum, which runs on internal couplings, disappears when the clusters are of a single spin. In this case (2.6) and (2.7) reduce to (2.3).

3. The variational approach

Let us start by only considering clusters where all boundary spins are topologically equivalent, as for example a d-dimensional hypercube of 2^d spins, or the crosses shown in figure 1 on a two-dimensional lattice.

We now introduce a trial Hamiltonian $\tilde{H}^{(n)}$ instead of $H^{(n)}$, where the first term related to the interactions between spins of the same cluster is left unchanged, while the second is modified with the replacement

$$\sigma_i^a\sigma_i^b\sigma_j^a\sigma_j^b \to q^{ab}(\sigma_i^a\sigma_i^b + \sigma_j^a\sigma_j^b) \tag{3.1}$$

where the $\{q^{ab}\}$ are a set of variational parameters of the problem. Recall that i and j are a couple of boundary sites of different clusters. The intuitive meaning of our approximation is clear: the coupling field $\{q^{ab}\}$ simulates the action of the rest of the system over the

boundary of a cluster in the replica space. Note that now the spins on the boundaries of different clusters do not interact, so that the total Hamiltonian is the sum of the Hamiltonians of each cluster. Therefore, with the replacement (3.1), the new Hamiltonian $\tilde{H}^{(n)}$ has the form

$$\tilde{H}^{(n)} = \sum_{\text{clust}} \Omega_{\text{clust}}{}^{(n)} \tag{3.2}$$

with

$$\Omega_{\text{clust}}{}^{(n)} = -\frac{1}{(2d)^{\frac{1}{2}}} \sum_{(i,j)'}^{\text{clust}} J_{i,j} \sum_{a=1}^{n} \sigma_i^a \sigma_j^a - \frac{\beta}{n_b}\left(n_\sigma - \frac{n_J}{d}\right) \sum_{(i)'}^{\text{clust}} \sum_{a<b} q^{ab} \sigma_i^a \sigma_i^b \tag{3.3}$$

where the sums $\sum_{(i,j)'}^{\text{clust}}$ and $\sum_{(i)'}^{\text{clust}}$ now run over, respectively, the internal nearest neighbours bonds and the boundary sites of a single cluster.

Using the convexity of the exponential, the following inequality holds for any integer $n > 1$:

$$\begin{aligned}\overline{\ln \sum_{\{\sigma\}} \exp\{-\beta H^{(n)}\}}' &= \overline{\ln \langle \mathrm{e}^{-\beta(H^{(n)} - \tilde{H}^{(n)})}\rangle}' + \overline{\ln \sum_{\{\sigma\}} \exp\{-\beta \tilde{H}^{(n)}\}}' \\ &\geqslant \max_{\{q^{ab}\}} \left[-\beta \overline{\langle H^{(n)} - \tilde{H}^{(n)}\rangle}' + \overline{\ln \sum_{\{\sigma\}} \exp\{-\beta \tilde{H}^{(n)}\}}' \right]\end{aligned} \tag{3.4}$$

where the $\langle\cdot\rangle$ indicates the average over the Gibbs measure induced by the Hamiltonian $\tilde{H}^{(n)}$. Since the sites i and j belong to different clusters, one has

$$\overline{\langle \sigma_i^a \sigma_i^b \sigma_j^a \sigma_j^b\rangle}' = \overline{\langle \sigma_i^a \sigma_i^b\rangle}' \overline{\langle \sigma_j^a \sigma_j^b\rangle}' = \overline{\langle \sigma^a \sigma^b\rangle}'^2 \tag{3.5}$$

where the indices have been suppressed because of the equivalence of boundary spins. As a consequence one can write the simple expression

$$-\beta \overline{\langle H^{(n)} - \tilde{H}^{(n)}\rangle}' = \frac{1}{2}\beta^2 N \left(1 - \frac{n_J}{d n_\sigma}\right) \sum_{a<b} \left(\overline{\langle \sigma^a \sigma^b\rangle}'^2 - 2 q^{ab} \overline{\langle \sigma^a \sigma^b\rangle}' \right). \tag{3.6}$$

The maximum in the right-hand side of (3.4) can be found by deriving it with respect to each q^{ab}, so that after some trivial algebra one has the following system of $\frac{1}{2}n(n-1)$ self-consistent equations

$$q^{ab} = \overline{\langle \sigma^a \sigma^b\rangle}' \qquad 1 \leqslant a < b \leqslant n. \tag{3.7}$$

The right-hand side of (3.4) is the maximum of an expression containing averages with respect to the Gibbs measure which are quite complicated. Fortunately, it can be replaced by the more simple and compact expression

$$\max_{\{q^{ab}\}} \left[-\frac{1}{2}\beta^2 N \left(1 - \frac{n_J}{d n_\sigma}\right) \sum_{a<b} (q^{ab})^2 + \overline{\ln \sum_{\{\sigma\}} \exp\{-\beta \tilde{H}^{(n)}\}}' \right] \tag{3.8}$$

which not only has the same value but also leads to the same self-consistent equations (3.7), as shown in appendix A. Then, bearing in mind that $\tilde{H}^{(n)}$ is a Hamiltonian fully decomposed into the Hamiltonians $\Omega_{\text{clust}}{}^{(n)}$ corresponding to the $\frac{N}{n_\sigma}$ different clusters, it is possible to perform the thermodynamic limit and then the limit $n \to 0$. In doing this second limit one has to be careful since the inequality (3.4) has been established for integer $n > 1$ and it changes direction when we perform the analytic continuation to real $n < 1$. In conclusion, one has

$$f_d \geqslant \tilde{f}_d \tag{3.9}$$

with

$$\tilde{f}_d \equiv -\frac{\beta}{4}\left(1-\frac{n_J}{dn_\sigma}\right)+\lim_{n\to 0}\frac{1}{n}\max_{\{q^{ab}\}}\left[\frac{\beta}{2}\left(1-\frac{n_J}{dn_\sigma}\right)\sum_{a<b}(q^{ab})^2 - \frac{1}{\beta n_\sigma}\overline{\ln\sum_{\{\sigma\}}\exp\{-\beta\Omega^{(n)}\}}'\right] \tag{3.10}$$

where $\Omega^{(n)}$ is a representative Hamiltonian of a single cluster.

Before ending this section we would like to stress that (3.10), derived for clusters where the boundary spins are topologically equivalent, can be easily extended to a generic cluster decomposition of the lattice (see appendix B). In this case to every boundary spin σ_i is associated a different q_i^{ab} and the maximization can become very complicated. Nevertheless, (3.9) and (3.10) with a single q^{ab} still hold although $\tilde{f}_d$ is no longer the optimal approximation. The maximum is reached when

$$q^{ab}=\frac{1}{n_b}\sum_{\{i\}'}\overline{\langle\sigma_i^a\sigma_i^b\rangle}'.$$

Let us briefly sum up the results of this section. We have found lower limits $\tilde{f}_d$ for the quenched free energy f_d of a spin glass in d dimensions via the replica formalism. The approximations of the f_d by the free energies $\tilde{f}_d$ improve as the size of the cluster increases. The structure of the solution is familiar, since we have to compute a maximum of a function which depends on a set of $\frac{1}{2}n(n-1)$ variational parameters in the limit $n\to 0$.

Note that $\tilde{f}_d$ turns out to be a generalization of the expression (2.4) for the SK model free energy f_∞. In fact, independently of the dimension d, $\tilde{f}_d$ reduces to (2.4) when one chooses a cluster of a single spin. The proof is trivial since in this case one has $n_\sigma=1$, $n_b=1$ and $n_J=0$ so that the first term in the Hamiltonian $\tilde{H}^{(n)}$ vanishes. This fact is quite interesting since it implies that the well known expression (2.4) for the SK model free energy represents in our scheme, so to speak, the zero-order approximation of the random Ising spin glass in finite dimensions.

It also should be remarked that in the limit $d\to\infty$, independently on the size of the clusters, one reduces to the SK model.

4. Replica symmetry breaking with the Parisi ansatz

It is quite simple to show that in the SK model, for any integer $n>1$, the maximum in (2.4) is reached when all the q^{ab} assume the same value

$$q^{ab}=q_0 \qquad 1\leqslant a<b\leqslant n \tag{4.1}$$

with $q_0\geqslant 0$. This is the replica symmetry solution, but unfortunately it turns out to be unstable and unphysical in the limit $n\to 0$ (for example, it has a negative zero temperature entropy).

Parisi has proposed a simple way [7–9] to break the above symmetry between the n replicas. He chooses to organize them in $\frac{n}{m_1}$ groups of m_1 replicas, and to assume a q^{ab} with two different values. The larger value corresponds to a and b belonging to the same group, and the smaller one to a and b in different groups. This strategy can be iterated by repeating the same procedure for each group and all its subgroups, so that the kth order

breaking can be written as

$$q^{ab} = q_s \qquad \text{if} \begin{cases} \left[\dfrac{a}{m_s}\right] = \left[\dfrac{b}{m_s}\right] \\ \left[\dfrac{a}{m_{s+1}}\right] \neq \left[\dfrac{b}{m_{s+1}}\right] \end{cases} \qquad \text{with} \begin{cases} 1 \leqslant a < b \leqslant n \\ 0 \leqslant s \leqslant k \end{cases} \tag{4.2}$$

where $[\cdot]$ means an integer part. All the $\{q_s - q_{s-1}\}$ are assumed to be non-negative and it is also assumed that $m_0 \equiv n$ and $m_{k+1} \equiv 1$.

The above Parisi ansatz is straightforward for integer n if all the $\{m_s\}$ and the $\{\frac{m_s}{m_{s+1}}\}$ can be chosen as integers. The intriguing point is that, after the analytic continuation to real n in the limit $n \to 0$, the $\{q_s, m_s\}$ are treated as a set of $2k+1$ real variational parameters with the constraint

$$0 \leqslant \cdots \leqslant m_s \leqslant m_{s+1} \leqslant \cdots \leqslant m_{k+1} \equiv 1.$$

This constraint allows for a well-defined overlap probability. Recall that it is sufficient to use few replica symmetry breaking (say $k = 2$) to achieve a solution of the SK model with realistic behaviours (such as, $T = 0$ free energy consistent with numerical simulations, or $T = 0$ non-negative entropy).

The ansatz (4.2) can be easily adapted to our more general $\tilde{f}_d$. The main difference with the SK model is the presence of the coupling terms in the Hamiltonian $\Omega^{(n)}$, but they do not mix different replicas, so that the usual steps used for solving the SK model can be repeated. Recalling the well known trick of the Gaussian integral, the solution of $\tilde{f}_d$ with $k \geqslant 0$ breaking can be written as

$$\tilde{f}_{d,k} = \max_{\{q_s, m_s\}} \left[-\frac{\beta}{4}\left(1 - \frac{n_J}{d n_\sigma}\right)\left((1-q_k)^2 + \sum_{s=1}^{k} m_s (q_{s-1}^2 - q_s^2)\right) + f_k \right] \tag{4.3}$$

with

$$f_k = -\frac{1}{\beta n_\sigma m_1} \ln \overline{\overline{\left[\cdots \overline{\left[\overline{[Z_k]^{m_k}}^{h^{(k)}}\right]^{\frac{m_{k-1}}{m_k}}}^{h^{(k-1)}} \cdots \right]^{\frac{m_1}{m_2}}}^{h^{(1)}}}^{J,h^{(0)}} \tag{4.4}$$

$$Z_k = \sum_{\{\sigma\}} \exp\{-\beta H_k\} \tag{4.5}$$

and

$$H_k = -\frac{1}{(2d)^{\frac{1}{2}}} \sum_{(i,j)'}^{\text{clust}} J_{i,j}\sigma_i\sigma_j - \frac{1}{n_b^{\frac{1}{2}}}\left(n_\sigma - \frac{n_J}{d}\right)^{\frac{1}{2}} \sum_{(i)'}^{\text{clust}} \sigma_i \left(q_0^{\frac{1}{2}} h_i^{(0)} + \sum_{s=1}^{k} (q_s - q_{s-1})^{\frac{1}{2}} h_i^{(s)} \right). \tag{4.6}$$

Each of the $k+1$ averages $\{\overline{\cdot}^{h^{(s)}}\}$ $(0 \leqslant s \leqslant k)$ contains n_b independent normalized Gaussian fields $\{h_i^{(s)}\}$ acting only on the boundary spins of the cluster. The set $\{h_i^{(0)}\}$ is the only one to appear in a quenched average $\overline{\cdot}^{J,h^{(0)}}$ together with the n_j random couplings $\{J_{i,j}\}$ internal of the cluster. Note that in the Hamiltonian (4.6) we have replicated only the n_σ spin variables of the cluster.

Equations (4.3)–(4.6) have the same structure of the Parisi solution of the SK model with k replica symmetry breaking, except for a more general form of H_k. In particular, the Parisi solution for the SK model can be recovered, independently on the dimension d, choosing a cluster of a single spin. For a larger cluster the Parisi solution can only be

recovered when $d \to \infty$. In both cases, in fact, the first sum in (4.6) disappears, and the factor in front of the second sum equals one.

It is worth noting that the dependence of the solution from the number of dimensions d is purely algebraic, once the shape of the cluster is fixed, so that the same algorithm holds for every dimension d, which only plays the role of a parameter.

5. An application in $d = 2$ dimensions

We check our method in $d = 2$ dimensions by choosing the elementary plaquette of four nearest neighbours spins as the cluster, so that $n_\sigma = n_b = n_J = 4$. With this choice the replica symmetry solution ((4.3)–(4.6) with $k = 0$) reads

$$\tilde{f_0} = \max_{q_0} \left[-\frac{\beta}{8}(1-q_0)^2 - \frac{1}{4\beta} \overline{\ln \sum_{\{\sigma\}} \exp\{-\beta H_0\}}^{J,h^{(0)}} \right] \tag{5.1}$$

with

$$H_0 = -\frac{1}{2}\sum_{i=1}^{4} J_i \sigma_i \sigma_{i+1} - \frac{1}{2^{\frac{1}{2}}} q_0^{\frac{1}{2}} \sum_{i=1}^{4} h_i^{(0)} \sigma_i$$

while the solution with one replica breaking ($k = 1$) is

$$\tilde{f_1} = \max_{\{q_0, q_1, m\}} \left[-\frac{\beta}{8}((1-q_1)^2 + m(q_0^2 - q_1^2)) - \frac{1}{4\beta m} \overline{\ln \overline{\left[\sum_{\{\sigma\}} \exp\{-\beta H_1\} \right]^m}^{h^{(1)}}}^{J,h^{(0)}} \right] \tag{5.2}$$

with

$$H_1 = -\frac{1}{2}\sum_{i=1}^{4} J_i \sigma_i \sigma_{i+1} - \frac{1}{2^{\frac{1}{2}}} \sum_{i=1}^{4} \sigma_i (q_0^{\frac{1}{2}} h_i^{(0)} + (q_1 - q_0)^{\frac{1}{2}} h_i^{(1)}).$$

It is obvious that (5.2) reduces to (5.1) when $q_1 = q_0$ and $m = 0$. The maximum in (5.1) and (5.2) can be found through standard numerical methods. For instance, deriving (5.2) with respect to $\{q_0, q_1, m\}$, one can write down a set of self-consistent equations which can be solved numerically.

The result is that the order parameters differ from 0 below a critical temperature $T_{\rm cr} \sim 0.86$, that is sensibly lower than the corresponding one of the SK model ($T_{\rm cr} = 1$).

In figure 2 we plot the free energies $\tilde{f_0}$ and $\tilde{f_1}$ as a function of the temperature T in the range $0 < T < T_{\rm cr}$. They are compared with the SK results and with the free energy of an isolated plaquette with Gaussian couplings and no boundary fields. Our free energies show a certain improvement with respect to the SK ones from a quantitative point of view, while the isolated plaquette badly describes the systems below the temperature $T = 0.7$.

In figures 3(a) and (b) the q_0, q_1 and the m order parameters of the one breaking solutions are plotted, respectively, as a function of the reduced temperature $T/T_{\rm cr}$. The qualitative behaviours are very similar to the SK corresponding parameters.

Let us finish this paragraph with a technical remark about the implementation of an algorithm able to find the maximum in (4.3). The expression (4.4) for f_k suggests that the number of breaking k is the main source for the algorithmic complexity. In fact, one must first compute a quenched average over $n_J + n_b$ Gaussian variables (the J and the $h^{(0)}$); then an average over other n_b variables (the $h^{(1)}$), and so on. Using Monte Carlo algorithms this leads to a computing time t for $f_{\rm clust}^{(k)}$ proportional to

$$t \sim (n_J + n_b) n_b^k$$

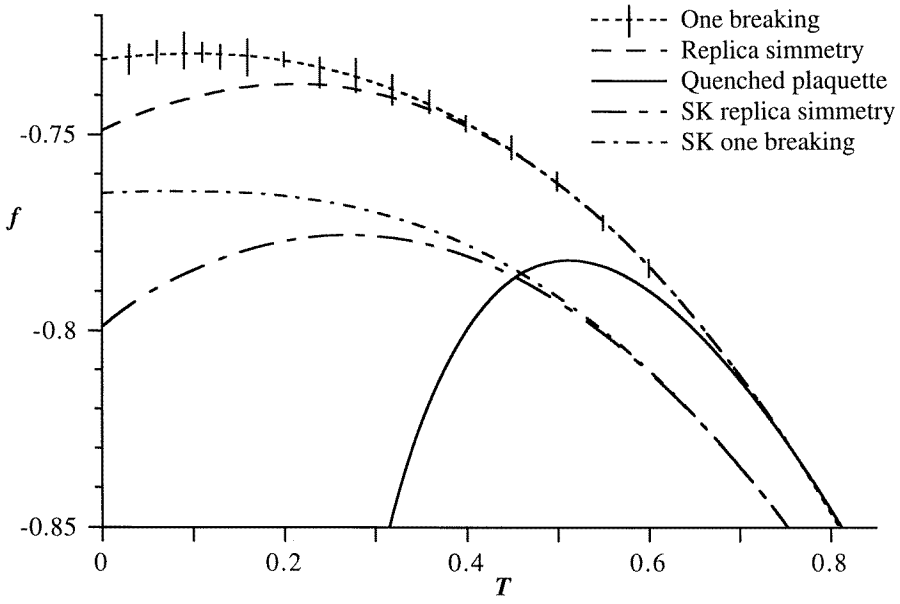

Figure 2. Free energy as a function of the temperature T in $d = 2$ dimensions: replica symmetry and one breaking solutions for the four spins plaquette (broken curves), SK replica symmetry and SK one breaking (chain curves), single plaquette (full line) with no boundary fields ($q^{ab} = 0$). The vertical bars represent the numerical error on the one breaking solution for the plaquette.

so that a unitary growth of the breaking number corresponds to a large growth of t which is amplified of a factor n_b. In contrast t only has a polynomial dependence on n_J and n_b, so that it is less difficult to increase the size of the cluster. Finally, the dimension d is not significant, since the complexity of the algorithm does not depend on d.

6. Conclusion

In this paper we have presented a new method which approximates in a hierarchical way the random Ising spin glass in d dimensions. At the lowest level our approximation coincides with the SK model while at the highest level it coincides with the true d-dimensional system. The attention is focused on finite clusters of spins where the action of the rest of the system is taken into account and it turns out that the larger the cluster, the better the approximation. Since the method is variational, we have rigorous bounds for the quenched free energy which become more and more precise when larger and larger clusters are considered.

Our approach uses the replica trick and the Parisi ansatz for the order parameter. We have explicitly written the solution for both the replica symmetric and replica breaking case. In the case of replica symmetry the Hamiltonian (4.6) reduces to the case of a spin glass of finite size with Gaussian magnetic fields of variance q_0 at the boundary. This variance is than chosen in order to feign at the best the action of the rest of the system (a similar approach has been proposed by Hatano and Suzuki [10, 11], where the variance is fixed by a self-consistent equation).

We have explicitly computed the free energy for a four-spins plaquette in two dimensions both in the replica symmetric and in the replica breaking context. In principle, in this second case we should have considered an infinite breaking number, in practice, we only consider

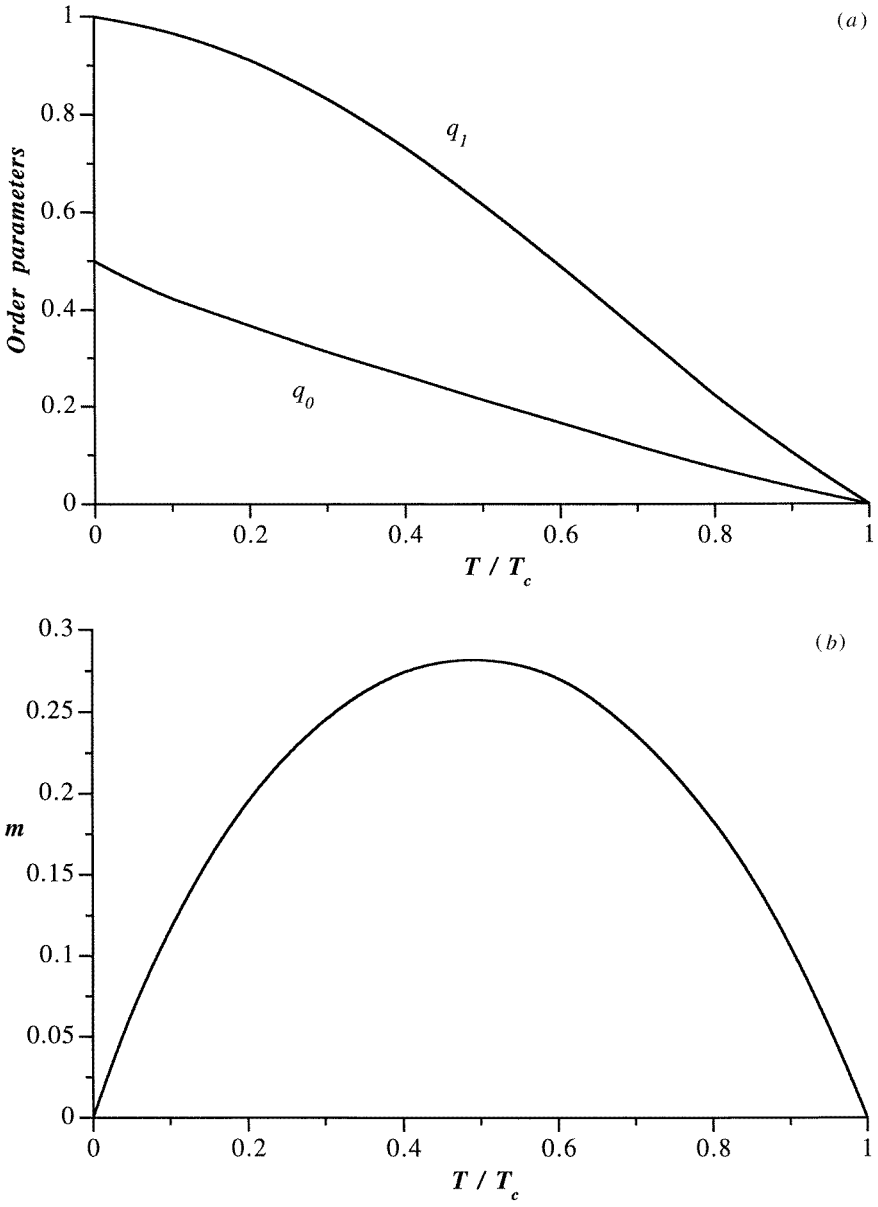

Figure 3. Order parameters for the four-spins plaquette in $d = 2$ dimensions, as a function of the reduced temperature T/T_{cr} : (a) replica symmetry q_0 and one breaking q_1; (b) one breaking m.

a single breaking since the amount of computational work increases enormously when one consider a larger breaking number while the value of the thermodynamical quantities changes very little.

We would like to remark, that in spite of the fact that the replica broken solution is always better than the unbroken one (given a finite-size cluster), both of them converge to the real d-dimensional spin glass when the size of the cluster is increased. Therefore, our

approach can be used to improve the numerical simulations of spin glasses. In fact, the numerical approach tries to understand the properties of spin glasses in the thermodynamical limit using finite-size systems, i.e. finite clusters with periodic boundary or open conditions. In our replica symmetry context we retain this scheme but we can take into account the action of the rest of the system without increasing too much computing time. The ordinary numerical study chooses a zero-variance magnetic field at the boundary ($q_0 = 0$), while we have a variance which can be optimized. In conclusion, one should:

(1) consider the finite-size system and apply Gaussian fields of variance q_0 at the boundary;

(2) compute numerically the free energy and the overlap for various values of q_0;

(3) choose q_0 in order that it equals the overlap $\frac{1}{n_b}\sum_{\{i\}'}\overline{\langle\sigma_i^a\sigma_i^b\rangle}'$ (we stress once more that $q_0 = 0$ would correspond to the standard numerical study with open boundaries).

Investigations concerning this numerical strategy represents the first natural development and are actually in progress.

We think that our approach will also be useful in studying the most striking feature of spin glasses, i.e. the phase transition to a glassy phase at finite temperature for high dimensionality ($d \geqslant 3$). We also think that one should be able to find out eventual specific characteristic of the finite-dimension spin-glass phase. Once again, our hope lies in the fact that, in principle, we are able to interpolate between the SK model (cluster of a single spin) and the finite d-spin glass (cluster of infinite spins). This is a clear improvement with respect to other approaches to the problem (for instance, [3, 4]). In particular, the advantages with respect to the formulation of [3, 4] are two: first, we can write inequalities concerning the free energy; second, we are able to include the replica symmetry breaking. Indeed, the initial motivation of this research was precisely to extend the results of [3, 4] to the broken symmetry case.

Actually, this fundamental key point will be the second natural development of this work. In particular, the next step will consist of performing a wide numerical analysis of the two- and three-dimensional cases, with larger and larger spin clusters, in order to deeply investigate the glassy phase transition.

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Appendix A

In order to compute

$$\max_{\{q^{ab}\}}\left[-\beta\overline{\langle H^{(n)}-\tilde{H}^{(n)}\rangle}'+\overline{\ln\sum_{\{\sigma\}}\exp\{-\beta\tilde{H}^{(n)}\}}'\right] \tag{A.1}$$

we derive the expression to be maximized with respect to q^{ab}. Taking into account (3.6), one has that this derivative vanishes when

$$\beta^2 N\left(1-\frac{n_J}{dn_\sigma}\right)\sum_{a'<b'}\frac{\partial\overline{\langle\sigma^{a'}\sigma^{b'}\rangle}'}{\partial q^{ab}}\left(\overline{\langle\sigma^{a'}\sigma^{b'}\rangle}'-q^{a'b'}\right)-\beta^2 N\left(1-\frac{n_J}{dn_\sigma}\right)\overline{\langle\sigma^a\sigma^b\rangle}'$$

$$+\frac{\beta^2}{n_b}\left(n_\sigma - \frac{n_J}{d}\right)\sum_{(i)'}\overline{\langle\sigma^a\sigma^b\rangle}' = 0. \tag{A.2}$$

Since $\sum_{(i)'} 1 = \frac{n_b}{n_\sigma}N$, the sum of the last two terms identically vanishes and one immediately obtains the self-consistency equations

$$q^{ab} = \overline{\langle\sigma^a\sigma^b\rangle}' \qquad 1 \leqslant a < b \leqslant n. \tag{A.3}$$

On the other hand, let us consider the simpler expression (3.8)

$$\max_{\{q^{ab}\}}\left[-\frac{1}{2}\beta^2 N\left(1 - \frac{n_J}{dn_\sigma}\right)\sum_{a<b}(q^{ab})^2 + \overline{\ln\sum_{\{\sigma\}}\exp\{-\beta\tilde{H}^{(n)}\}}'\right]. \tag{A.4}$$

The derivative with respect to q^{ab} vanishes when

$$-\beta^2 N\left(1 - \frac{n_J}{dn_\sigma}\right)q^{ab} + \frac{\beta^2}{n_b}\left(n_\sigma - \frac{n_J}{d}\right)\sum_{(i)'}\overline{\langle\sigma^a\sigma^b\rangle}'$$
$$= \beta^2 N\left(1 - \frac{n_J}{dn_\sigma}\right)\left(\overline{\langle\sigma^a\sigma^b\rangle}' - q^{ab}\right) = 0 \tag{A.5}$$

which again leads to the self-consistency equations (A.3).

Finally, it is easy to check that (A.1) and (A.4) assume the same value when $\overline{\langle\sigma^a\sigma^b\rangle}' = q^{ab}$.

Appendix B

In this appendix we derive a generalization of formulae (3.9) and (3.10) for the more general case of a full decomposition of the lattice in equal clusters with no topological equivalence of boundary sites.

For instance, imagine a square cluster of L^2 sites in $d = 2$ dimensions. First of all, the corner sites have two external bonds at variance with the unique external bond of the other boundary sites. Furthermore, the external location of the site along the boundary also determines the strength of the interaction with external spins. For these reasons, in general, the averaged overlap $\overline{\langle\sigma_i^a\sigma_i^b\rangle}'$ depends on the boundary site i, and (3.5) does not hold anymore. It follows that we have to modify the replacement rule (3.1) in order to take into account the topological differences between the various boundary spins.

The boundary sites can be grouped into n_b classes; each class consists of $\frac{N}{n_\sigma}$ topologically equivalent sites, one per cluster. We focus the attention on a given cluster (the reference cluster), so that its n_b boundary sites $(k)'$ are the representative elements of each class. Then, we introduce the function $k(i)$ which associate the generic boundary site i with its representative of the reference cluster. Two sites of the reference cluster, say $k(i)$ and $k(j)$, are 'adjoint nearest neighbours' if the couple i, j belongs to the set $(i, j)''$, and $(\tilde{k} \to k)$ indicates all the adjoint nearest neighbours $\tilde{k}$ of the site k.

At this point, it is straightforward to replace q^{ab} with a set of n_b parameters $\{q_k^{ab}\}$, one per representative k site. The total number of variational parameters is, therefore, $\frac{n_b}{2}n(n-1)$.

The replacement rule (3.1) for a couple of boundary sites can now be generalized as follows:

$$\sigma_i^a\sigma_i^b\sigma_j^a\sigma_j^b \to q_{k(j)}^{ab}\sigma_i^a\sigma_i^b + q_{k(i)}^{ab}\sigma_j^a\sigma_j^b. \tag{B.1}$$

In other words, each replaced external interaction leaves a different memory.

With the replacement (B.1) the Hamiltonian of a cluster reads

$$\Omega^{(n)} = -\frac{1}{(2d)^{\frac{1}{2}}} \sum_{(i,j)'}^{\text{clust}} J_{i,j} \sum_{a=1}^{n} \sigma_i^a \sigma_j^a - \frac{\beta}{2d} \sum_{a<b} \sum_{(i)'}^{\text{clust}} \sigma_i^a \sigma_i^b \sum_{(\tilde{k}\to k(i))} q_{\tilde{k}}^{ab} \tag{B.2}$$

and the averaged overlaps of two boundary sites of different clusters are

$$\overline{\langle \sigma_i^a \sigma_i^b \sigma_j^a \sigma_j^b \rangle}' = \overline{\langle \sigma_i^a \sigma_i^b \rangle}' \, \overline{\langle \sigma_j^a \sigma_j^b \rangle}' = \overline{\langle \sigma_{k(i)}^a \sigma_{k(i)}^b \rangle}' \, \overline{\langle \sigma_{k(j)}^a \sigma_{k(j)}^b \rangle}'.$$

Formula (3.4) still holds for any integer $n > 1$, so that

$$\overline{\ln \sum_{\{\sigma\}} \exp\{-\beta H^{(n)}\}}' \geqslant \max_{\{q_k^{ab}\}} \left[-\beta \overline{\langle H^{(n)} - \tilde{H}^{(n)} \rangle}' + \overline{\ln \sum_{\{\sigma\}} \exp\{-\beta \tilde{H}^{(n)}\}}' \right] \tag{B.3}$$

where

$$-\beta \overline{\langle H^{(n)} - \tilde{H}^{(n)} \rangle}' = \frac{\beta^2}{4d} \frac{N}{n_\sigma} \sum_{a<b} \sum_{(k)'} \overline{\langle \sigma_k^a \sigma_k^b \rangle}' \sum_{(\tilde{k}\to k)} \left(\overline{\langle \sigma_{\tilde{k}}^a \sigma_{\tilde{k}}^b \rangle}' - 2q_{\tilde{k}}^{ab} \right).$$

The maximum in the right-hand side of (B.3) can be found by solving the following system of $\frac{n_b}{2} n(n-1)$ self-consistent equations

$$\sum_{(\tilde{k}\to k)} q_{\tilde{k}}^{ab} = \sum_{(\tilde{k}\to k)} \overline{\langle \sigma_{\tilde{k}}^a \sigma_{\tilde{k}}^b \rangle}' \qquad \begin{cases} 1 \leqslant k \leqslant n_b \\ 1 \leqslant a < b \leqslant n \end{cases} \tag{B.4}$$

and the expression to be maximized in (B.3) can be replaced by the following expression which has the same maximum at the same point:

$$-\frac{\beta^2}{4d} \frac{N}{n_\sigma} \sum_{a<b} \sum_{(k)'} q_k^{ab} \sum_{(\tilde{k}\to k)} q_{\tilde{k}}^{ab} + \overline{\ln \sum_{\{\sigma\}} \exp\{-\beta \tilde{H}^{(n)}\}}'.$$

Finally, the analytic continuation to real $n \to 0$ gives

$$f_d \geqslant \tilde{f}_d \tag{B.5}$$

with

$$\tilde{f}_d \equiv -\frac{1}{4}\beta \left(1 - \frac{n_J}{dn_\sigma}\right) + \lim_{n\to 0} \frac{1}{n} \max_{\{q_k^{ab}\}} \left[\frac{\beta}{4dn_\sigma} \sum_{a<b} \sum_{(k)'} q_k^{ab} \sum_{(\tilde{k}\to k)} q_{\tilde{k}}^{ab} - \frac{1}{\beta n_\sigma} \overline{\ln \sum_{\{\sigma\}} \exp\{-\beta \Omega^{(n)}\}}' \right]. \tag{B.6}$$

Note that the $\{q_k^{ab}\}$ are not all different if there are symmetric sites in the clusters. For example, the sites on the four corners of a square plaquette in $d = 2$ dimensions will share the same overlaps.

Finally, if we look for the maximum of (B.6) with the constraint

$$q_k^{ab} = q^{ab} \qquad \forall k = 1, \ldots, n_b$$

we are left with formula (3.10). Therefore, in this context, (3.10) is a worse approximation, except all the boundary sites of the cluster are topologically equivalent.

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