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 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.

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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 into account of the dimensionality. 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 focus 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 been recently extended to spin glasses [3]-[4]. Actually the approach of [3]-[4] turns out to be not too much effective, since it does not allows for a study of the replica symmetry breaking. This fact reduces the scope of the method to low dimensional spin glasses, while for \(d \geq 3\) dimensions it fails in describing 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 of 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 discuss some aspects of our approach which seems to be useful for improving usual Monte Carlo simulations for spin glasses in finite dimensions.

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

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

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 $\beta$ is the inverse temperature. The quenched free energy is

$$f_d = -\lim_{N \to \infty} \frac{1}{\beta N} \ln Z$$  \hspace{1cm} (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 $N \to \infty$. 

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Unfortunately, it is not possible to find out 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 \cite{5} tries to avoid this difficulty replacing the above quenched average with the annealed average of the \(n\)-th power of the partition function \(Z\) with integer \(n\). In fact, if the result can be analytically continued to real \(n\), one has

\[ f_d = - \lim_{n \to 0} \lim_{N \to \infty} \frac{1}{\beta N n} \ln Z^n \]  

(2.2)

The average over the gaussian disorder variables gives

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

(2.3)

where \(\sigma_i^a\) is the \(a\)-th replica of the spin in the \(i\)-th 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 reduce to the celebrated \(SK\) model \cite{6}, and one has

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

(2.4)

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

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

To have an idea of the clusters we have in mind think to a plaquette of four nearest-neighbours 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-neighbours sites that belong to the same cluster, and with \((-')\) the disorder average over the couplings between them. In the same way \((i,j)''\) denotes
all the nearest-neighbours sites of different clusters, and \( \overline{\cdot}'' \) the related disorder average. Finally, \((i)'\) runs only over the boundary sites of all the clusters. Moreover, the following definitions are useful

\[
\begin{align*}
&\begin{cases}
n_{\sigma} = \text{number of spins in a cluster} \\
n_b = \text{number of boundary spins in a cluster} \\
n_J = \text{number of bonds in a cluster}
\end{cases}
\end{align*}
\]

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

\[
\begin{align*}
&\begin{cases}
\sum_{(i)'} 1 = \frac{n_b}{n_{\sigma}} N \\
\sum_{(i,j)'} 1 = \frac{n_J}{n_{\sigma}} N \\
\sum_{(i,j)''} 1 = \left( d - \frac{n_J}{n_{\sigma}} \right) N
\end{cases}
\end{align*}
\]

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

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

\[
f_d = - \lim_{N \to \infty} \lim_{n \to 0} \frac{1}{\beta N n} \ln \overline{Z^{n''}'}
\]

(2.5)

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

An easy calculation gives

\[
\overline{Z^{n''}} = \exp \left\{ \frac{1}{4} \beta^2 N n \left( 1 - \frac{n_J}{d n_{\sigma}} \right) \right\} \sum_{\{\sigma\}} \exp\{-\beta H^{(n)}\}
\]

(2.6)

where

\[
H^{(n)} = -\frac{1}{(2d)^2} \sum_{(i,j)'} J_{i,j} \sum_{a=1}^{n} \sigma_i^a \sigma_j^a - \frac{\beta}{2d} \sum_{(i,j)''} \sum_{a < b} \sigma_i^a \sigma_b^a \sigma_j^b \sigma_b^b
\]

(2.7)

Remark 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 hyper-cube of $2^d$ spins, or the crosses shown in fig. 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

$$\sigma_i^a \sigma_j^b \sigma_i^a \sigma_j^b \rightarrow q^{ab} \left( \sigma_i^a \sigma_j^a + \sigma_j^a \sigma_i^b \right)$$

(3.1)

where the $\{q^{ab}\}$ are a set of variational parameters of the problem. Let us 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 a the boundary of a cluster in the replica space. Remark that now the spins on the boundary of different cluster 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

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

(3.2)

with

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

(3.3)

where now the sums $\sum_{(i,j)'}^{\text{clust}}$ and $\sum_{(i)'}^{\text{clust}}$ 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 $n > 1$:

$$\ln \sum_{\{\sigma\}} \exp\{-\beta H(n)\}' = \ln \left( e^{-\beta (H(n) - \tilde{H}(n))} \right)' + \ln \sum_{\{\sigma\}} \exp\{-\beta \tilde{H}(n)\}' \geq \max_{\{q^{ab}\}} \left[ -\beta \langle H(n) - \tilde{H}(n) \rangle' + \ln \sum_{\{\sigma\}} \exp\{-\beta \tilde{H}(n)\}' \right]$$

(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

$$
\langle \sigma_i^a \sigma_j^b \rangle' = \langle \sigma_i^a \sigma_j^b \rangle' = \langle \sigma_i^a \sigma_j^b \rangle' \quad (3.5)
$$

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

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

The maximum in the right hand side of (3.4) can be found deriving it 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

$$
q^{ab} = \langle \sigma^a \sigma^b \rangle' \quad 1 \leq a < b \leq n \quad (3.6)
$$

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, a more simple and compact expression exists which has the same maximum in the same point corresponding to the solution of (3.6). This expression is

$$
-\frac{1}{2} \beta^2 N \left( 1 - \frac{nJ}{d \ n_\sigma} \right) \sum_{a < b} (q^{ab})^2 + \ln \sum_{\{\sigma\}} \exp \{-\beta \tilde{H}(n)\}' (3.7)
$$

Therefore, (3.7) can be used to replace the one into the square parenthesis in the right hand side of (3.4). Then, taking in mind that $\tilde{H}(n)$ is an 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

$$
f_d \geq \tilde{f}_d \quad (3.8)
$$

with

$$
\tilde{f}_d \equiv -\frac{\beta}{4} \left( 1 - \frac{nJ}{d \ n_\sigma} \right) +
\lim_{n \to 0} \frac{1}{n} \max_{\{q^{ab}\}} \left[ \frac{\beta}{2} \left( 1 - \frac{nJ}{d \ n_\sigma} \right) \sum_{a < b} (q^{ab})^2 - \frac{1}{\beta n_\sigma} \ln \sum_{\{\sigma\}} \exp \{-\beta \Omega^{(n)}\}' \right] \quad (3.9)
$$
where $\Omega^{(n)}$ is a representative hamiltonian of a single cluster.

Before ending this section we would like to stress that (3.9), derived for clusters where the boundary spins are topologically equivalent, can be easily extended to a generic cluster decomposition of the lattice (see Appendix). In this case to every boundary spin $\sigma_i$ is associated a different $q^a_{ib}$ and the maximization can become very complicated. Nevertheless, (3.8) and (3.9) with a single $q^a_{ib}$ still hold although $\tilde{f}_d$ is not anymore the optimal approximation. The maximum is reached when

$$q^a_{ib} = \frac{1}{n_b} \sum_{\{i\}'} \langle \sigma^a_i \sigma^b_i \rangle'$$

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 free energies $\tilde{f}_d$ approximate better and better the $f_d$ when 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 $n \to 0$.

Notice that $\tilde{f}_d$ turns out to be a generalization of the expression (2.4) for the SK model free energy $f_\infty$. 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 $q^a_{ib}$ assume the same value

$$q^a_{ib} = q_0 \quad 1 \leq a < b \leq n$$  (4.1)

with $q_0 \geq 0$. 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 replicas. His choice is at the first stage 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 repeating the same procedure for each group and all its subgroups, so that the \( k \)-th order breaking can be written as

\[
q^{ab} = q_s \quad \text{if} \quad \begin{cases} \left[ \frac{a}{m_s} \right] = \left[ \frac{b}{m_{s+1}} \right] \quad \text{with} \quad 1 \leq a < b \leq n \\ \left[ \frac{a}{m_{s+1}} \right] \neq \left[ \frac{b}{m_{s+1}} \right] \quad \text{with} \quad 0 \leq s \leq k \end{cases}
\]  

(4.2)

where \( [\cdot] \) means integer part. All the \( \{q_s - q_{s-1}\} \) are assumed to be non-negative and it also assumed \( m_0 \equiv n \) 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

\[
0 \leq \ldots \leq m_s \leq m_{s+1} \leq \ldots \leq m_{k+1} \equiv 1
\]

This constraint allows for a well-defined overlap probability. We recall that it is sufficient to use few symmetry replica 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 \( k \geq 0 \) breaking can be written as

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

(4.3)

with

\[
f_k = -\frac{1}{\beta n_\sigma m_1} \ln \left[ \ldots \left[ \frac{Z_k}{m_1} \right]^{h_{(k)}} \left[ \frac{m_{k-1}}{m_k} \right]^{h_{(k-1)}} \ldots \right],
\]  

(4.4)
\[ Z_k = \sum_{\{\sigma\}} \exp\{-\beta H_k\} \quad (4.5) \]

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

Each of the \( k + 1 \) averages \( \{ \cdot h_s^{(s)} \} \) \((0 \leq s \leq k)\) 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 \( \cdot J,h^{(0)} \) together with the \( n_j \) random couplings \( \{ J_{i,j} \} \) internal of the cluster. Notice that in the hamiltonian \( (4.6) \) we have replicated only the \( n_{\sigma} \) 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 only can 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 interesting 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 plays only the role of a parameter.

5. An application in \( d = 2 \) dimensions

We check our method in \( d = 2 \) dimensions 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:

\[
\tilde{f}_0 = \max_{q_0} \left[ -\beta \frac{(1 - q_0)^2}{8} - \frac{1}{4\beta} \ln \sum_{\{\sigma\}} \exp\{-\beta H_0\} \right] \quad (5.1) \]

with
\[
H_0 = -\frac{1}{2} \sum_{i=1}^{4} J_i \sigma_i \sigma_{i+1} - \frac{1}{2\pi} q_0 \sum_{i=1}^{4} h_i^{(0)} \sigma_i
\]
while the solution with one replica breaking \((k = 1)\) is:

\[
\tilde{f}_1 = \max_{\{q_0, q_1, m\}} \left[-\frac{\beta}{8} ((1 - q_1)^2 + m(q_0^2 - q_1^2)) - \frac{1}{4\beta m} \ln \left(\sum_{\{\sigma\}} \exp\{-\beta H_1\}\right)\right]^{m h^{(1)} h^{(0)}}
\]

with

\[
H_1 = -\frac{1}{2} \sum_{i=1}^{4} J_i \sigma_i \sigma_{i+1} - \frac{1}{2\beta} \sum_{i=1}^{4} \sigma_i \left(\frac{1}{4} h_i^{(0)} + (q_1 - q_0)^2 h_i^{(1)}\right)
\]

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 out using 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 \(T_{cr} \sim 0.86\), that is sensibly lower of the corresponding one of the SK model \((T_{cr} = 1)\).

In fig. 2 we plot the free energies \(\tilde{f}_0\) and \(\tilde{f}_1\) as a function of the temperature \(T\) in the range \(0 < T < T_{cr}\). 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 respect to the SK ones from a quantitatively point of view, while the isolated plaquette badly describes the systems below the temperature \(T = 0.7\).

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

6. Conclusions

Let us start this paragraph by 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 has to compute first a quenched average over \(n_J + n_b\) Gaussian variables (the \(J\)'s and the \(h^{(0)}\)'s); then an average over other \(n_b\) variables (the \(h^{(1)}\)'s), and so on. Using MonteCarlo algorithms this leads to a computing time \(t\) for \(f^{(k)}_{\text{clust}}\) proportional to

\[
t \sim (n_J + n_b) n_b^k
\]
so that a unitary growth of the breaking number corresponds to a big growth of \( t \) which is amplified of a factor \( n_b \). On the contrary \( t \) 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 significative, since the complexity of the algorithm does not depend on \( d \).

A second remark is that the hamiltonian (4.6) and the free energy (4.3) in case of replica symmetry correspond to a single replica spin glass of finite size with gaussian magnetic fields at the boundary. The variance has to be 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 Suzuzi ([10]-[11]), where the variance is fixed by a self-consistent equation).

For these two reasons we believe that our approach could be used to improve the numerical simulations of spin glasses. In fact, the numerical approach tries to understand the properties of spin glasses in thermodynamical limit using finite size systems, i.e. finite clusters with periodic boundary or open conditions. In our replica symmetry context we save this scheme but we can take into account more carefully of the action of the rest of the system without increasing too much the computing time. The ordinary numerical study chooses zero variance of magnetic field at the boundary, 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 \( \frac{1}{n_b} \sum_{\{i\}'} \langle \sigma^a_i \sigma^b_i \rangle' \) (notice that \( q_0 = 0 \) would correspond to the standard numerical study with open boundaries).

Investigations about this numerical strategy are actually in progress.

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Appendix A.

In this appendix we derive a generalization of formulae (3.8) and (3.9) for the more
general case of a full decomposition of the lattice in equal clusters with no topological
equivalence of boundary sites.

For instance, think to 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 determine the strength of the interaction with external spins. For these reasons, in
general, the averaged overlap $\langle \sigma_a^i \sigma_b^i \rangle'$ 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 in $n_b$ classes; each class consists of $\frac{N}{n_b}$ 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 to be the representative elements of each
class. Then, we introduce the function $k(i)$ which associate the generic boundary site $i$
to 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
($\tilde{k} \rightarrow k$) indicates all the adjoint nearest neighbours $\tilde{k}$ of the site $k$.

At this point is straightforward to replace $q_{ab}$ with a set of $n_b$ parameters \{q_{k}^{ab}\}, one
per each 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 be now generalized as
follows:

$$\sigma_a^i \sigma_b^i \sigma_a^j \sigma_b^j \rightarrow q_{k(j)}^{ab} \sigma_a^i \sigma_b^i + q_{k(i)}^{ab} \sigma_a^j \sigma_b^j \quad \text{(A.1)}$$

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

With the replacement (A.1) the hamiltonian of a cluster reads

$$\Omega^{(n)} = -\frac{1}{(2d)^{\frac{1}{2}}} \sum_{(i,j)'}^\text{clust} J_{i,j} \sum_{a=1}^n \sigma_a^i \sigma_a^j - \frac{\beta}{2d} \sum_{a<b}^\text{clust} \sum_{(i)'}^\text{clust} \sigma_a^i \sigma_b^j \sum_{(\tilde{k} \rightarrow k(i))} q_{\tilde{k}}^{ab} \quad \text{(A.2)}$$

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

$$\langle \sigma_a^i \sigma_b^i \sigma_a^j \sigma_b^j \rangle' = \langle \sigma_a^i \sigma_b^i \rangle' \langle \sigma_a^j \sigma_b^j \rangle' = \langle \sigma_{k(i)}^a \sigma_{k(i)}^b \rangle' \langle \sigma_{k(j)}^a \sigma_{k(j)}^b \rangle'$$

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Formula (3.4) still holds for any integer $n > 1$, so that
\[
\ln \sum_{\{\sigma\}} \exp\{-\beta H^{(n)}\}' \geq \max_{\{q_{a}^{b}\}'} \left[ -\beta \langle H^{(n)} - \tilde{H}^{(n)} \rangle' + \ln \sum_{\{\sigma\}} \exp\{-\beta \tilde{H}^{(n)}\}' \right]
\] (A.3)

where
\[
-\beta \langle H^{(n)} - \tilde{H}^{(n)} \rangle' = \frac{\beta^2}{4d} \frac{N}{n_{\sigma}} \sum_{a<b} \sum_{(k)'} (\sigma_{a_{k}}^{c} \sigma_{b_{k}}^{c})' \sum_{(k)} \left( \langle \sigma_{a_{k}}^{c} \sigma_{b_{k}}^{c} \rangle' - 2 q_{a_{k}}^{b} \right)
\]

The maximum in the right hand side of (A.3) can be found by solving the following system of $\frac{1}{2} n(n-1)$ self-consistent equations
\[
\sum_{(k \rightarrow k)} q_{a_{k}}^{b} = \sum_{(k \rightarrow k)} (\sigma_{a_{k}}^{c} \sigma_{b_{k}}^{c})' \quad \left\{ \begin{array}{l}
1 \leq k \leq n_{b} \\
1 \leq a < b \leq n
\end{array} \right.
\] (A.4)

and the expression to be maximized in (A.3) can be replaced by the following expression which has the same maximum in the same point:
\[
-\beta^2 \frac{N}{4d n_{\sigma}} \sum_{a<b} \sum_{(k)'} q_{a_{k}}^{b} \sum_{(k \rightarrow k)} q_{a_{k}}^{b} + \ln \sum_{\{\sigma\}} \exp\{-\beta \tilde{H}^{(n)}\}'
\]

Finally, the analytic continuation to real $n \to 0$ gives
\[
f_{d} \geq \tilde{f}_{d}
\] (A.5)

with
\[
\tilde{f}_{d} \equiv -\frac{1}{4} \beta \left( 1 - \frac{n_{J}}{d n_{\sigma}} \right) + \ln \lim_{n \to 0} \frac{1}{n} \max_{\{q_{k}^{ab}\}} \left[ \frac{\beta}{4d n_{\sigma}} \sum_{a<b} \sum_{(k)'} q_{a_{k}}^{b} \sum_{(k \rightarrow k)} q_{a_{k}}^{b} - \frac{1}{\beta n_{\sigma}} \ln \sum_{\{\sigma\}} \exp\{-\beta \Omega^{(n)}\}' \right]
\] (A.6)

Notice 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 (A.6) with the constraint
\[
q_{k}^{ab} = q^{ab} \quad \forall \ k = 1, \ldots, n_{b}
\]
we reduces to formula (3.9). Therefore, in this context, (3.9) is a worse approximation, except all the boundary sites of the cluster are topologically equivalent.
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**Figure Captions**

Fig. 1. Decomposition of a two-dimensional spin lattice in clusters of \( n_x = 12 \) 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 dashed lines represent the bonds between spins belonging to different clusters.

Fig. 2. Free energy as function of the temperature \( T \) in \( d = 2 \) dimensions: replica symmetry and one breaking solutions for the four spins plaquette (dashed lines), SK replica symmetry and SK one breaking (dot-dashed lines), 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.

Fig. 3. Order parameters for the four spins plaquette in \( d = 2 \) dimensions, as function of the reduced temperature \( T/T_{cr} \): a) replica symmetry \( q_0 \) and one breaking \( q_1 \); b) one breaking \( m \).
Fig. 1

Legend

- Internal area of a cluster
- Internal spin site
- Boundary spin site
- Internal bond
- External bond
Fig. 2
Free energy
Fig. 3a

Order parameters

$q_1$

$q_0$

$T / T_c$
Fig. 3b