Cluster approximation for Ising spin glasses

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Abstract

We report about a new variational method [9] which approximates in a hierarchical way the random Ising spin glass on lattice in d dimensions. At the lowest level our approximation coincides with the Sherrington-Kirkpatrick model, while at the highest level it coincides with the true d-dimensional system. The attention is focused on finite size clusters of spins where the action of the rest of the system is taken into account by a coupling field, which is the variational parameter of the problem.

The Sherrington-Kirkpatrick (SK) model [1] is a mean field approximation for an Ising spin glass. This fact can be easily seen since the problem can be reduced to a single spin whose replicas interact via the variational order parameter q^{ab} which can be thought as a 'coupling field'. The free energy, in fact, reads

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

where the q^{ab} is a real matrix. In the limit $n \to 0$ this maximum is found following the Parisi ansatz [2]-[4].

This is the analogue of the mean field model for the ordinary ferromagnetic Ising systems. In this 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 ferromagnetic Ising model, can be regarded as an approximation of the associated Ising system on lattice 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 [5] -[6]), has been recently extended to spin glasses [7] -[8]. Actually the approach [7] -[8] 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.

Recently, we have proposed a new approach [9] which allows for symmetry breaking. In spite of a single (replicated) spin as in (1), we consider a finite cluster of replicated spins. The action of the rest of the system is properly taken into account by the interaction with the coupling field q^{ab}. From this point of view there is not difference with [7] -[8], the new fact being that our approach is variational. This fact has two advantages, the first is that we have rigorous bounds for the free energy, the second is that we can look for symmetry breaking solutions of the maximization problem following the Parisi ansatz.

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 on a lattice. The estimations of the quenched free energy become more and more precise when larger and larger clusters are considered.

Following our procedure [9], we start by considering a partition of the lattice in clusters as, for example, d-dimensional hyper-cubes of 2^d spins. Than, we introduce a trial hamiltonian in the replica space where the interactions between spins of the same cluster are left unchanged, while the boundary spins of different clusters do not interact directly, but they are coupled with q^{ab}. Therefore, the trial hamiltonian is the sum of the hamiltonians $\Omega^{(n)}$ of each cluster. The form of $\Omega^{(n)}$ for a representative cluster is

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

where $(i,j)'$ indicates all the couples of nearest-neighbours sites of the cluster and $\overline{\cdot}^{\,\prime}$ the related disorder averages, while $(i)'$ runs only over the boundary sites of the cluster. Moreover, the following definitions are used

$$\begin{aligned} n_\sigma &\equiv \text{number of spins in a cluster} \\ n_b &\equiv \text{number of boundary spins in a cluster} \\ n_J &\equiv \text{number of bonds in a cluster} \end{aligned}$$

The intuitive meaning of our approximation is clear: the coupling field q^{ab} (the variational parameter of the problem) simulates, in the replica space, the action of the rest of the system over the boundary of a cluster. After the variational computation has been performed it turns out that the free energy of the system is

$$\tilde{f}_d \equiv -\frac{\beta}{4}\left(1 - \frac{n_J}{d\, n_\sigma}\right) + \lim_{n\to 0} \frac{1}{n} \max_{\{q^{ab}\}} \left[\frac{\beta}{2}\left(1 - \frac{n_J}{d\, n_\sigma}\right) \sum_{a<b} (q^{ab})^2 - \frac{1}{\beta n_\sigma} \overline{\ln \sum_{\{\sigma\}} \exp\{-\beta \Omega^{(n)}\}}^{\,\prime} \right] \tag{3}$$

and the maximum is reached when

$$q^{ab} = \frac{1}{n_b} \sum_{\{i\}'} \overline{\langle \sigma_i^a \sigma_i^b \rangle}^{\,\prime} \tag{4}$$

Notice that $\tilde{f}_d$ is a generalization of the SK free energy f_∞ (1). In fact, independently of the dimension d, $\tilde{f}_d$ reduces to (1) when one chooses a cluster of a single spin. This fact is quite interesting since it implies that the well-known expression (1) for the SK model free energy represents in our framework 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 always reduces to the SK model. Moreover, $\tilde{f}_d$ turns out to be a lower limit of the quenched free energy of the real d-dimensional spin glass, which is approximated better and better when the size of the cluster increases.

The structure of $\tilde{f}_d$ is essentially the same of (1); the main difference with the SK model is the presence of a coupling term in the hamiltonian $\Omega^{(n)}$, but since it does not mix different replicas, the Parisi ansatz [2] - [4] can be easily adapted to our more general $\tilde{f}_d$.

The replica symmetry solution, (the maximum in (1) with the constraints that all the q^{ab} assume the same value) 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 [2] -[4] to broke the above symmetry. 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

$$q^{ab} = q_s \qquad \text{if} \qquad \left[\frac{a}{m_s}\right] = \left[\frac{b}{m_s}\right] \qquad \text{and} \qquad \left[\frac{a}{m_{s+1}}\right] \neq \left[\frac{b}{m_{s+1}}\right] \tag{5}$$

with $1 \leq a < b \leq n$ and $0 \leq s \leq k$, 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 trouble-free 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, 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

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

which allows for a well-defined overlap probability.

It is straightforward to write in this ansatz the free energy $\tilde{f}_d^{(k)}$ with $k \geq 0$ breakings. It is important to remark that since the method is variational, we have rigorous bounds for the quenched free energy. The free energy of our cluster approximation delimits from below the free energy of the random Ising spin glass in d dimensions and it becomes more and more precise when larger and larger clusters are considered.

We check our method in $d = 2$ dimensions choosing the elementary plaquette of four nearest neighbours spins as the cluster, so that $n_\sigma = n_b = n_J = 4$.

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

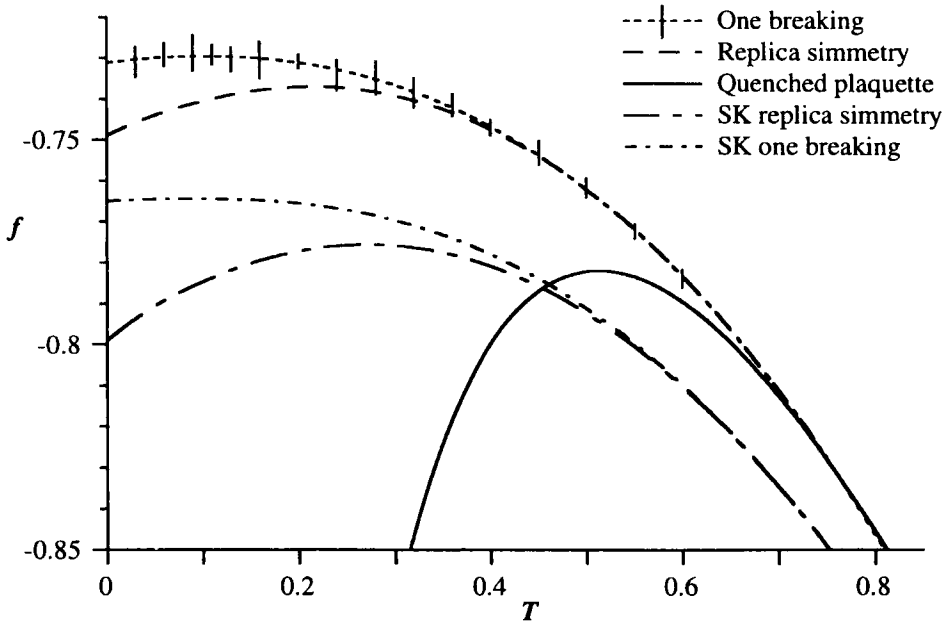

Figure 1: Free energy as function of the temperature T in $d = 2$ dimensions: replica symmetry and one breaking solutions for the four spins plaquette (dashed lines), SK replica symmetry and SK one breaking (dot-dashed lines), single plaquette (full line) with no boundary field ($q^{ab} = 0$). The vertical bars represent the numerical error on the one breaking solution for the plaquette.

In fig.1 we plot the free energies of the replica symmetry solution $\tilde{f}^{(0)}$ and of the solution with one breaking $\tilde{f}^{(1)}$ 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 field. Our free energies show a certain improvement respect to the SK ones from

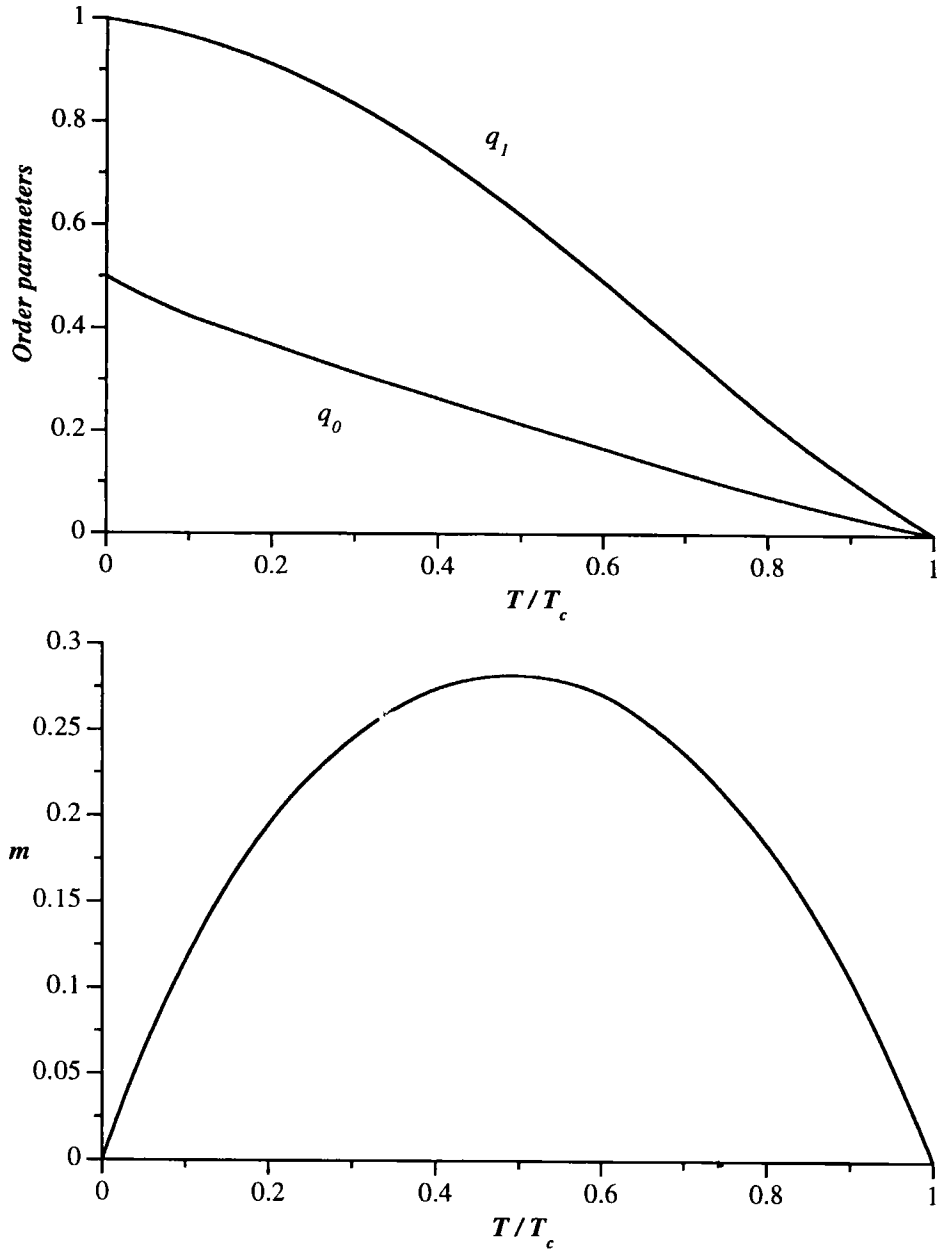

Figure 2: Order parameters for the four spins plaquette in $d = 2$ dimensions, as function of the reduced temperature T/T_{cr} : a) replica symmetry q_0 and one breaking q_1; b) one breaking m.

a quantitatively point of view, while the isolated plaquette badly describes the systems below the temperature $T = 0.7$.

In fig.2a and fig.2b 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.

The result shown in the figures concerns the simple case of a four spin plaquette, larger clusters can bee considered at the price of a longer computational work. Nevertheless, 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. This is very important since in the replica symmetry case one can reduce to a spin glass of finite size with gaussian magnetic fields of variance q_0 at the boundary (see [9]). 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). The conclusion is that 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 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 the action of the rest of the system without increasing too much the computing time. The ordinary numerical study chooses zero variance magnetic field at the boundary ($q_0 = 0$), while we have a variance which can be optimized. We propose to consider the finite size system and apply gaussian fields of variance q_0 at the boundary for various values of q_0 and choose the parameter in order that it equals the overlap $\frac{1}{n_b} \sum_{\{i\}'} \overline{\langle \sigma_i^a \sigma_i^b \rangle}'$. Then compute numerically the free energy at this value of q_0. Investigations about this numerical strategy represents the first natural development and are actually in progress.

We think that our approach will also be useful to study the most striking feature of spin glasses, i.e. the phase transition to a glassy phase at finite temperature for high dimensionality ($d \geq 3$). Once again, our hope lies on 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 respect to other approaches to the problem (for instance, [7] - [8]). Therefore, the second natural development of the present work could consist in performing a wide numerical analysis of the $d \geq 3$ case, with larger and larger spin clusters, in order to deeply investigate the glassy phase transition.

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References

[1] D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35** (1975) 1792

[2] G. Parisi, Phys. Lett. A **73** (1979) 203

[3] G. Parisi, J. Phys. A **13** (1980) L115

[4] G. Parisi, J. Phys. A **13** (1980) 1101

[5] H. Bethe, Proc. R. Soc. London **150** (1935) 552

[6] R. Peierls, Proc. R. Soc. London **154** (1936) 207

[7] G. Paladin and M. Serva, J. Phys. A **29** (1996) 1381

[8] M. Serva and G. Paladin, Phys. Rev. E **54** (1996) 1

[9] R. Baviera, M. Pasquini and M. Serva, J. Phys. A (to be published)

[10] N. Hatano and M. Suzuki, J. Stat. Phys. **63** (1991) 25

[11] N. Hatano and M. Suzuki, J. Stat. Phys. **66** (1991) 897