Computation of the zero temperature RSB parameter in Bethe Lattice Spin Glasses

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Abstract

Bethe Lattice Spin Glasses (BLSG) are models with finite connectivity which undergo a Replica Symmetry Breaking (RSB) phase transition in field, even at zero temperature. The order parameter describing this phase is a function related to the non-trivial organization of the states. We compute numerically the spin glass order parameter at zero temperature in BLSG with coordination number $z = 3$ and couplings $J = \pm 1$, near the transition. The method is based on a universal formula which relates the order parameter to the joint probability distribution of the energy gaps of the lowest lying states. Such distribution is derived numerically by introducing a convenient bulk perturbation to the Hamiltonian.

1 Introduction

A spin glass differs from a normal magnet because of the non-trivial structure of the space of its many equilibrium states, when the system is in the low-temperature phase. This scenario is known as Replica Symmetry Breaking (RSB). In this context, the order parameter contains crucial information on the structure of the space of the states and on the inherent level of replica symmetry breaking.

For some models, the order parameter can be obtained analytically by means of a replica computation, provided that the full RSB scheme is known. However, this requirement is met only in very general cases and for a wide class of systems the solutions are approximated to the first RSB steps. In these models determining the order parameter could be crucial to understand to which extent the RSB scenario describes their low-temperature phase.

An alternative approach which does not use the typical replica computation has been proposed for computing the RSB order parameter at zero temperature
The approach is based on a universal formula obtained considering the ultrametric organization of the states typical of systems in the RSB phase\(^1\). The formula relates the order parameter to the joint distribution of the overlaps and energy gaps of the lowest lying states. For a given model, the latter function can be obtained numerically from the probability distribution induced by a convenient coupling between two Hamiltonians which differ by a quantity of order 1.

We used this method to compute the order parameter at zero temperature of the Bethe lattice spin glass (BLSG) with quenched disorder distributed according to a bimodal distribution. The reason why we are interested in this model is twofold.

First, from the theoretical physics point of view, it is a particular case of a model with finite connectivity with a topology which facilitates the analytic approach to its full RSB solution. Nevertheless, an exact solution is yet to be found. The best solution is provided by the cavity method\(^4,5\) with a level of approximation equivalent to the 1RSB step of the replica computation. In this respect, we believe the method we apply in our study to be a valid tool of investigation for either supporting the theoretical advance towards the full RSB solution or for understanding to what extent the system differs from the RSB phase.

Second, from the computational point of view, the BLSG is related to a wide class of optimization problems studied in computer science classified as NP-hard. In this respect, the inquiry into the low-temperature properties of this model provides the ground for testing faster and more reliable algorithms.

In the following the main ideas behind the derivation of the formulas shall be first introduced (section 2), followed by a brief description of the model (section 3). Thus, the results (section 4) and the computational methods (section 5) shall be discussed, followed by some conclusions and perspectives of our work (section 6).

## 2 The RSB order parameter

It is well known that the physical order parameter of a spin glass corresponds to the probability distribution of the overlap between the states, or its cumulative distribution \(x(q)\)\(^6\). In the RSB phase this function has continuous support in an interval \(0 < q_m < q_M < 1\), depending on the temperature and the external field. As the temperature approaches zero, the order parameter can be written as:

\[
x(q, T) = Ty(q) + O(T^2),
\]

where \(y(q)\) is singular at \(q = 1\)\(^7\). In the Sherrington-Kirkpatrick (SK) model \(y(q) \sim (1 - q)^{-1/2}\) for \(q \to 1\).
We are interested in characterizing the cumulative distribution
\[
Y(q) = \int_{-\infty}^{q} dq' y(q)
\]
The first step consists in determining the joint probability distribution of the overlaps and energy gaps of the lowest lying states. This can be done by means of a probabilistic computation over the hierarchical tree of states, starting from two basic assumptions: the space of the states is ultrametric and the energies of the lowest states can be treated like random variables with an exponential distribution [2, 3]. These two hypotheses regarding the physical space of the states can be considered an alternative formulation of the full RSB in the replica space. We skip the details of the computation, which can be found in [1], and describe the general ideas behind the derivation of the formula.

The following step is considering an arbitrary ultrametric tree with \( k \) levels. At every level \( l \) of the tree is assigned an energy \( E_l \) in a way such that the number of nodes with energy between \( E_l \) and \( E_l + dE \) branching from a node of energy \( E_{l-1} \) is a Poisson variable with average \( \exp(y_l(E_l - E_{l-1}))dE_{l-1} \). In order to ensure the convergence of the integrals the coefficients must verify: \( y_0 = 0 < y_1 < \ldots < y_l \). It can be proved that the joint probability of the energy gaps is:
\[
P(\Delta_{k}, \ldots, \Delta_0) = \prod_{i=1}^{k} (y_i - y_{i-1})e^{(y_i - y_{i-1})\Delta_i}
\]
Performing the limit of continuous branching, the coefficients become a continuous variable \( y(q) \), and the joint distribution becomes:
\[
P(\{\Delta_q\}) = e^{-\int_{0}^{1} dq y'(q)\Delta(q)} \prod y'(q) dq
\]
The \( \Delta(q) \) distribution for a given model can be obtained by studying the excitations induced on a large number of samples by a \( q \)-dependent perturbation, acting on the unperturbed Hamiltonian \( \mathcal{H}_0 \). For a given sample the new Hamiltonian is
\[
\mathcal{H}_\epsilon(\sigma) = \mathcal{H}_0(\sigma) + \epsilon q(\sigma)
\]
where \( q(\sigma) = 1/N \sum_i \sigma_i \sigma_i^0 \) is the overlap of the configuration \( \sigma \) with the unperturbed ground state \( \sigma_0 \). The effect of the perturbation is to induce a transition from the original ground state to a nearby excited state whose energy is:
\[
E_{GS}(\epsilon) = E_{GS}(0) + \min_{0 \leq q \leq 1} \{\Delta(q) + \epsilon q\}
\]
Let \( q \) be the value which minimizes the rhs of the previous formula, and let \( \Delta \) be the relative energy difference. In order to have a transition \( (q < 1) \) the inequality \( \Delta < \epsilon (1 - q) \) must be verified, so that \( \Delta(1) \) is always zero. Using these conditions it can be proved that the joint distribution depends on \( q, \Delta \) only in the combination
\[
w = \Delta/\epsilon + q
\]
Thus, this final formula is recovered:

$$Y(w) = -\frac{\ln Q(w)}{\epsilon}$$

(3)

where

$$Q(w) = \int_w^1 P(w') \, dq =$$

$$= \exp \left( -\epsilon \int_{q}^{w} dq (y(q) - y(0)) \right) =$$

$$= \exp \left( -\epsilon Y(w) \right)$$

(4)

3 The model

There are different kinds of Bethe lattices. The spin glass version of the model is typically represented on a random regular graph (RRG), a random lattice with constant connectivity $z$. Loops occur only on large scale in these graphs, as their size is usually of order $\log N$. Such property results in a homogeneous locally tree-structure with rare small loops, whose number remains finite in the thermodynamic limit, therefore providing a well-defined realization of a Bethe lattice. Spins are located at the vertices of the graph and interact with neighboring spins with exchange couplings. For each edge $<i,j>$, the $J_{ij}$ coupling is an independent quenched random variable with probability distribution $P(J)$.

The Hamiltonian of the model is:

$$\mathcal{H} = -\sum J_{ik} \sigma_i \sigma_k - \sum h_i \sigma_i$$

where $\sigma_i$ are Ising variables. We consider the $J\pm$ model, in which the $J$ coefficients are extracted from a bimodal distribution with $J = \pm 1$ and zero mean. Moreover, we consider the action of an external random magnetic field with gaussian distribution, characterized by zero mean and variance $H$.

The BLSG has widely been studied analytically, both at finite and zero temperature [4,5]. The mean field approach, known as cavity method, shows the presence of an RSB instability in the spin glass phase, providing a solution that is equivalent to the 1-step RSB. At this level of approximation, many thermodynamic quantities show a good agreement with the numerical experiments. However, a further inspection into the nature of the RSB phase is not possible without pushing the calculation to further orders.

The critical temperature $T_C$ which characterizes the continuous spin glass transition depends both on the connectivity and the external field. Due to the finite value of $z$, the critical de Almeida-Thouless (AT) line in the $T,H$ plane converges to a finite value $H_C$ in the zero temperature limit. This value can be obtained by studying the stability of the RS solution in the region above the AT line [8,9]. It follows that, differently from the SK model where the critical line
diverges when $T \to 0$, the BLSG undergoes a RSB transition in field even at zero temperature. For the BLSG with connectivity $z = 3$ and $J \pm$ interactions the critical value is $h_C \sim 1.037$ [10].

Our numerical approach consists in generating a large number of samples and computing the corresponding ground states by means of an optimization algorithm, as described in section 5. Several numerical results on BLSG have been published on this topic [11-13], mostly focusing on the behavior in zero external magnetic field. They report that, despite the BLSG model should tend to the SK model in the large $z$ limit, the behavior at finite $z$ depends on the particular choice of the $P(J)$. For instance, while in the $J \pm$ model the finite-size corrections to the energy scale as $N^{-\omega}$ with $\omega = 2/3$, like in the SK model, in the gaussian model they seem to scale with a different value of the exponent $\omega = 4/5$, unless higher order corrections are taken into account. [13].

Besides obtaining the RSB order parameter at zero temperature, our aim is also to study the finite-size corrections to the energy in the presence of a finite magnetic field.

4 Results
We have considered a large number of samples ($10^4 - 10^5$) with $J = \pm 1$, $z = 3$, for several values of size $N = \{200, 400, 800, 1600, 3200\}$ and variance of the external gaussian field $H = \{0.6, 0.8, 1.0, 1.2\}$. The method consists in computing for each sample first the ground state $\sigma^0$ relative to the unperturbed Hamiltonian $H_0$, and second the ground state relative to the perturbed Hamiltonian $H_\epsilon$, defined in (1). In order to verify that the final $Y(w)$ distribution does not depend on the entity of the perturbation, as long as it is small, the procedure has been repeated for two values of $\epsilon = 1, 2$. From the values of $\Delta(\epsilon) = E_{GS}(\epsilon) - E_{GS}(0)$ and $q$, using (2), we obtained the distributions $Y_{H,N}(w)$ (fig. 1).

In general the $Y_{H,N}(w)$ are weakly dependent on $\epsilon$ and are singular in $w = 1$. When $H$ is fixed, as the size of the systems increases, the left tail of the functions decreases quickly, while in the region close to the singularity the decreasing is slower. This might suggest that under a critical value $w_c(H)$ the scaling is exponential, while for larger values $w_c(H) < w < 1$ the scaling follows a power law. We would like to characterize such limit assuming a power law scaling behavior:

$$Y_{H,N}(w) = Y_H(w) + g_H(w)N^{-\alpha} \tag{5}$$

In order to determine $Y_H(w)$ we fit the data to the asymptotic form (5) for fixed values of $w$. There is a good agreement between the fits and the data using $\alpha = 0.5$, in a region not too close to the singularity(fig. 2). We extrapolated the values $w_c(H)$ as the x-intercept. From the results it appears that $w_c(H)$ tends to 1 as $H \to H_C$.

We studied the finite size corrections to the energy, fitting the data to the
With an exponent  \( \omega = 2/3 \) we obtained a good quantitative agreement with the data. This value is the same found for the SK model and \( J\pm \) model of BLSG in the case of zero external field. The fits are shown in fig.4. The asymptotic values for the ground state energy are reported in tab.1.

\[
E_{GS}(N) = E_{\infty} + AN^\omega
\]  

\( \text{(6)} \)

| \( H \) | \( E_{\infty} \)  | \( \pm \)   | \( \text{0.00004} \) |
|-------|---------|------|------------------|
| 0.6   | -1.37215|      | 0.00004          |
| 0.8   | -1.44046|      | 0.00003          |
| 1.0   | -1.52265|      | 0.00002          |
| 1.2   | -1.61635|      | 0.00002          |

Table 1: Asymptotic values for the ground state energy in the large \( N \) limit, extrapolated using the form (6)

5 Computational methods

The algorithm used to obtain the ground states is known as Cluster Exact Approximation (CEA) \([14,16]\). The CEA is a MINCUT based, zero temperature algorithm which converges to the solution by iteratively optimizing non-frustrated subgraphs, or clusters, extracted randomly from the whole graph. In absence of frustration, like in a Random Field Ising Model, any random cluster coincides with the whole graph, and the algorithm provides the exact solution in just one step. In presence of frustration more steps are needed to reach a minimum. At each step a new cluster is created starting from a random root, adding iteratively new nodes only if their related bonds do not introduce frustrated loops in the subgraph. The cluster is thus optimized by means of a MINCUT algorithm \([17,18]\). In other words, the values assigned to the spin variables of the subgraph are the ones which minimize its energy with respect to the rest of the graph, which acts as boundary. The energy during the process is a monotonically decreasing function and a minimum is eventually reached after a fixed number of steps.

In order to obtain a global minimum, despite the ability of the CEA to avoid local traps that would invalidate a standard zero temperature Monte-Carlo algorithm based on Metropolis dynamics, the procedure must be repeated several times. In our simulations we repeat the optimization starting from random configurations until the same solution is found a fixed number of times.
Figure 1: The $Y_{H,N}(w)$ functions are here represented for different values of the variance of the gaussian field $H$. In each box the different lines represent systems of different size: $N = 200, 400, 800, 1600, 3200$ (from top to bottom). Different values of $\epsilon$ are also represented: $\epsilon = 1$ (solid lines) and $\epsilon = 2$ (dashed lines).

Figure 2: Linear fit to the form $[\beta]$ with $\alpha = 0.5$, at fixed values of $w$
Figure 3: $Y_H(w)$ functions obtained by using $\alpha = 0.5$, for each value of the variance of the external field. The dashed line represents the function relative to the SK model $Y_{SK}(w) = 1 - \sqrt{1 - w^2}$, at zero field.

Figure 4: Fit of the energies to the form $E_H(N) = E_\infty + fN^{-2/3}$.
6 Conclusions

We have computed the RSB order parameter at zero temperature of the BLSG with the lowest coordination number, using a formula which assumes that the system is in full RSB phase. It would be interesting to compare our results with some approach based on weaker assumptions.

The limit to our approach is mostly a computational one. The CEA algorithm is particularly effective on systems with tree-like topology, which allows to optimize large clusters at each step. The ratio between the average size of the clusters and the graph size is $\sim 0.8$ and it seems to be independent of $N$. The computational time required for a complete optimization increases as $O(N^\alpha)$, with $\alpha \sim 3$. The most of the time spent for optimizing large systems is due to the rapidly increasing number of times the algorithm must be applied for finding the same solution a fixed number of times. In order to reduce the time complexity, it might be interesting to use faster algorithms than the MINCUT. For instance, a similar Monte-Carlo algorithm based on Belief Propagation (BP) is described in [19] for optimizing spin glasses at finite temperature. However, due to the requirements of BP algorithms, the selected sub-graphs are trees whose size is $\sim 0.7$ of the entire system. In our simulations we find that using larger clusters which include loops is a more effective technique, as a lower number of steps is required for converging to the solution.

It would be interesting to extend our study to diluted models with spatial structure. A possible development is the lattices in finite dimensions with random regular dilution, where every site interacts with a fixed number of neighbors $z < 2D$. Such analysis might give a perspective on the role of the space dimension on the thermodynamic properties when the number of neighbors is kept constant.

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