On the number of metastable states in spin glasses

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June 13, 1995

Abstract

In this letter, we show that the formulae of Bray and Moore for the average logarithm of the number of metastable states in spin glasses can be obtained by calculating the partition function with m coupled replicas with the symmetry among these explicitly broken according to a generalization of the 'two-group' ansatz. This equivalence allows us to find solutions of the BM equations where the lower 'band-edge' free energy equals the standard static free energy. We present these results for the Sherrington-Kirkpatrick model, but we expect them to apply to all mean-field spin glasses.

cond-mat/9506049

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There has been recently a renewed interest in the study of metastable states in spin glasses. Current problems range form their potential relevance in spin glass dynamics to the formulation of renormalization group analysis in the presence of many minimas of the action. Nevertheless, it is interesting to use our present knowledge to shed some light old problems and to understand the connection between new and older techniques.

One recent development is the use of coupled real replicas as a way to explicitly break ergodicity revealing the 'complexity' of the system [1, 2]. It was not known up to now whether or not these techniques were equivalent to the now classical computations of the number of TAP solutions of Bray and Moore (BM) [3, 4]. It has been shown to be true for the spherical p-spin model, the Potts glass and for part of the spectrum of the random orthogonal model (ROM) [5, 6, 7]. A much older question that remained partly unanswered is whether the computation of BM for the Sherrington-Kirkpatrick model (SK) using continuous RSB gives at the lower 'band-edge' the same free energy as the static calculation. It was shown in Ref. [4] that they agreed near the transition, at least to the first non-trivial order in the reduced temperature t. The BM computation involves a function $Q(x)$ similar to the usual Parisi function $q(x)$ but in this computation the critical value of x (x_c) is equal to $\frac{1}{2}$ near T_c while its static counterpart only equals $2t$. Finally, a never explained coincidence is the fact that the 'direct average' of BM both for SK and ROM can be obtained by calculating the partition function under the two-group replica symmetry-breaking scheme. If one does not let the number of replicas n go to zero, the two-group partition function gives the Laplace transform of the number of TAP solution with n conjugated to $-\beta f$ [7, 8].

The contribution of this letter is to show that a generalization of the two-group ansatz makes the connection between the 'real replicas' and the BM framework. This connection in turns helps us understand why, in the 'naive' two-group approach, n becomes the Laplace conjugate of the free energy. The two-group model, in its unbroken form, gives us the proper ansatz to look for solutions of the BM saddle point that reduces to the static free energy at the lower band-edge. All these points are illustrated on the SK model but we believe that they should apply to any mean-field spin glass. Unfortunately, a crucial point stills eludes us, that is the physical significance of the two-group ansatz and the difference, if any, between metastable states that break the two-group symmetry and those that don't.

In Ref. [1] it was argued that the number of pure states in a glassy system can be computed by introducing m real replicas of the system. More precisely, for a mean-field model with quenched randomness where one introduces n replicas to average over the disorder, we have the following relation

$$\max_f \left[\langle \log \mathcal{N}(f)\rangle - m\beta f\right] = \lim_{n\to 0} \frac{1}{n} \log \langle Z^{mn} \rangle \,, \tag{1}$$

where $\mathcal{N}(f)$ is the number of metastable states as a function of their free energy and Z^{mn} is the partition function of $n \times m$ copies of the original system with the replica symmetry explicitly broken into n groups of m replicas.

It is useful to consider both f and $\langle \log \mathcal{N}(f) \rangle$ as function of the independent parameter m through the relation $f = f^*(m)$ i.e. the particular f that maximizes the l.h.s. of Eq. (1). Varying m then traces out the $\langle \log \mathcal{N}(f) \rangle$ vs f curve, in general a bell shaped curve (e.g. SK or ROM [3, 7]) or an 'interrupted bell' shape (e.g. p-spin, both spherical and Ising [5, 9]). The maximum of this curve is given by $m = 0$ (white average) while increasing m favors states of lower free energy. In particular $m = 1$ picks out the states that contribute to the Gibbs measure. Finally, we call the lower band-edge the infimum of the free energies for which $\langle \log \mathcal{N}(f) \rangle > 0$.

This formula along with the simplest replica symmetry ansatz gives a very good description of the metastable states for mean-field models with 'first-order RSB' (e.g. spherical p-spin, the Potts glass and ROM). It predicts that at the dynamical transition, a large number of metastable states start to contribute to the free energy (extensive complexity) and that at the RSB transition the complexity ceases to be extensive [1]. In the case of SK, a simple one-step ansatz in Eq. (1) always gives either zero or a negative result for the complexity. As we shall see, the presence of metastable states in SK can be uncovered by a more complex replica symmetry breaking scheme.

The partition function of the replicated SK model is given by (see e.g. [10])

$$\langle Z^{mn} \rangle = \operatorname*{Ext}_{\mathbf{Q}} \exp \left\{ N \left[\frac{\beta^2}{4} \left(mn - \mathrm{Tr}\mathbf{Q}^2 \right) + \log \sum_{\{\sigma_a^i\}} \exp \left(\tfrac{1}{2} \beta^2 \sum_{abij} Q_{ab}^{ij} \sigma_a^i \sigma_b^j \right) \right] \right\}, \quad (2)$$

where the extremum is taken over matrices Q_{ab}^{ij} ($1 \leq a, b \leq n$ and $1 \leq i, j \leq m$) with zeros on the diagonal $Q_{aa}^{ii} \equiv 0$.

The point of this letter is to show that the formula for the average logarithm of the number of TAP solution of Ref. [4] can be obtained from Eq. (1) using a direct generalization of the 'two-group' replica symmetry breaking [8]. We will use the following ansatz on each of the n^2 sub-matrices $\mathbf{Q}_{ab}$ of size $m \times m$ (i.e. the matrices Q_{ab}^{ij} with (a, b) fixed and (i, j) varying form 1 to m):

$$\mathbf{Q}_{ab} = \begin{pmatrix} \overbrace{Q_{ab}^{+}}^{y} & \overbrace{Q_{ab}}^{m-y} \\ Q_{ab} & Q_{ab}^{-} \end{pmatrix}, \quad (3)$$

where y is to be taken to infinity. A convenient way to parameterize the matrices Q_{ab}^{+} and Q_{ab}^{-} in order to obtain a finite result as $y \to \infty$ is

$$Q_{ab}^{\pm} = Q_{ab} \pm \frac{A_{ab}}{y} + \frac{B_{ab}}{y^2}. \quad (4)$$

Note that the 'diagonal matrices' $\mathbf{Q}_{aa}$ have the extra constraint that their diagonal elements Q^{ii}_{aa} be zero; their off-diagonal elements, in general non-zero, are also parameterized according to Eq. (4). We do not need to specify the structure of the three matrices Q_{ab}, A_{ab} and B_{ab} in order to make the connection with the BM formulation, but in practice they will be taken to have the usual utrametric structure (see e.g. [10]). Using this ansatz, we can compute the partition function (2) in a manner similar to that of Ref. [7]. We find

$$\begin{aligned} \langle Z^{mn} \rangle &= \operatorname{Ext} \exp \Big\{ nN \left[m \log 2 + \tfrac{1}{4}\beta^2 m (1-Q)^2 - \beta^2 A (1-Q) \right] \\ &\quad - N\beta^2 \left[\sum_{ab} \tfrac{1}{2} A_{ab}^2 + Q_{ab} B_{ab} + m Q_{ab} A_{ab} + \tfrac{1}{4} m^2 Q_{ab}^2 \right] + N \log I \Big\} , \end{aligned} \tag{5}$$

where

$$\begin{aligned} I &= \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \prod_a \frac{dx_a}{2\pi \mathrm{i}} \int_{-1}^{1} \prod_a \frac{dm_a}{(1-m_a^2)} \exp \Big\{ - \sum_a \Big[x_a \tanh^{-1} m_a \\ &\quad + \tfrac{1}{2} m \log(1-m_a^2) \Big] + \beta^2 \sum_{ab} \tfrac{1}{2} Q_{ab} x_a x_b + B_{ab} m_a m_b + A_{ab} m_a x_b \Big\} , \end{aligned} \tag{6}$$

and where A and Q are the diagonal terms A_{aa} and Q_{aa}, note that the sum over (a,b) also includes diagonal terms. If we put this formula in Eq. (1), we find that the average log number of metastable states is identical to the average log number of TAP solutions as computed in Ref. [4]. We recall that in that paper, the number of TAP solutions is written as the integral over all configurations of an appropriate delta function, replicas are introduced to average the logarithm over the disorder. The equivalence between our formula and Eq. (11) of Ref. [4] can be rendered more obvious by the following change of variables,

$$\begin{aligned} &\eta_{ab} = \beta^2 Q_{ab} \,,\ \rho_{ab} = -\beta^2 \left(A_{ab} + \tfrac{1}{2} m Q_{ab} \right) \,,\ \eta^*_{ab} = \beta^2 \left(2B_{ab} + m A_{ab} + \tfrac{1}{4} m^2 Q_{ab} \right) , \\ &q = Q \,,\ \Delta = \beta^2 \left(A + \tfrac{1}{2} m Q \right) \,,\ \lambda = \beta^2 \left(B + \tfrac{1}{2} m A + \tfrac{1}{8} m^2 Q \right) \text{ and } u = -m \,, \end{aligned} \tag{7}$$

and a shift of the integration variable ($x'_a = -x_a + \frac{1}{2} m m_a$).

In Ref. [8] it was shown that the original two-group partition function (with n in general non-zero) gives the Laplace transform of the annealed averaged number of metastable states with n conjugated to $-\beta f$. We recover this annealed result by setting the 'off-diagonal' matrices $\mathbf{Q}_{ab}$ to zero, leaving us only with n diagonal blocks of $m \times m$ two-group matrices. This explains the strange scaling with n, i.e. the size of the total matrix Q^{ij}_{ab} has to be taken to zero, while the ij block size m remains finite and becomes the Laplace conjugate of the free energy. Similarly, using an ij-two-group over an RS Q_{ab}, we recover the 'innocent replica' treatment, in this case, the full matrix Q^{ij}_{ab} can be viewed as a one-step matrix with blocks of size m within which lies a two-group structure.

Our formulation of the BM problem allows us to find a class of simple solutions to the saddle point equations, i.e. the 'unbroken two-group'. Indeed one can show that $A_{ab} = B_{ab} = 0$ forms self-consistent solution of these equations. The problem is then reduced to finding the extremum with respect to a single matrix Q_{ab} with a diagonal term Q. The computation with a k-step RSB ansatz on the matrix Q_{ab} is equivalent to the usual computation of the partition function with $k+1$-steps with RSB parameters $0 \leq mx_1 \leq \ldots \leq mx_k \leq m \leq 1$. In particular, since Eq. (1) implies

$$\log \langle \mathcal{N}(f) \rangle = -m^2 \frac{dF(m)}{dm} \text{ when } \beta f = \frac{d}{dm}(mF(m)), \tag{8}$$

where

$$F(m) = \lim_{n \to 0} \frac{1}{mn} \log \langle Z^{mn} \rangle, \tag{9}$$

the condition for the lower band-edge is just the usual minimization with respect to the last RSB parameter m.

In the simplest case, the 'innocent replicas' admit a solution that is equivalent to the one-step partition function. We have explicitly checked that the expansion of (5) near T_c (Eqs. (12,13)[1] of Ref. [4]) admits a saddle point of the form (7) with $\mathbf{A} = \mathbf{B} = 0$, we find, for the lower band-edge

$$q = t + \tfrac{25}{27}t^2 + \mathrm{O}(t^3), \; q_\circ = \tfrac{1}{3}t + \mathrm{O}(t^2), \; m = \tfrac{4}{3}t + \mathrm{O}(t^2),$$

and

$$\beta f/N = -\log 2 - \tfrac{1}{4}\beta^2 + \tfrac{1}{6}t^3 + \tfrac{11}{24}t^4 + (5099/7290)t^5 + \mathrm{O}(t^6). \tag{10}$$

This solution should be compared with that of Ref. [3], where it was found $q_\circ = 0.3471t + \mathrm{O}(t^2)$. Our solution can be followed to other values of the parameter m, but we find it to be only valid at the lower band-edge. As expected, for $m > \frac{4}{3}t$, it gives a negative log-number of TAP solutions. Whereas for $m < \frac{4}{3}t$, f decreases with decreasing m indicating that we are on an unphysical branch. The correct solution for $m < \frac{4}{3}t$ must therefore include two-group symmetry breaking.

The same 'unbroken two-group solution' can be found for continuous RSB near T_c. We find a solution very similar to that of Ref. [4], except for the value of m which in turns changes the value of all other parameters. We find

$$q = t + t^2 + \mathrm{O}(t^3), \; q(x) = tx \, (x \leq x_c = 1), \; m = 2t + \mathrm{O}(t^2),$$

and

$$\beta f/N = -\log 2 - \tfrac{1}{4}\beta^2 + \tfrac{1}{6}t^3 + \tfrac{11}{24}t^4 + \tfrac{7}{10}t^5 + \mathrm{O}(t^6) \tag{11}$$

The apparent discrepancy between the value of $x_c = 1$ and that of the usual static solution ($x_c = 2t$) is understood by realizing that it is not the matrix Q_{ab} which

[1] We think that the factor $(1-4Q)$ in that second equation should read $(1-5Q)$.

should equal the static one but rather the full matrix Q^{ij}_{ab}. When n goes to 0, the full matrix can be parameterized by a function $q_{\rm full}(x)$,

$$q_{\rm full}(x) = q(x/m)\,,\ 0 \le x \le m\,;\ \ q_{\rm full}(x) = Q\,,\ m < x \le 1\,, \qquad (12)$$

in perfect agreement with the static solution.

Acknowledgments

We wish to thank M. Ferrero and R. Monasson for useful discussions.

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