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Barriers between metastable states in the p-spin spherical model

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Abstract

In the context of the p-spin spherical model for generalized spin glasses, we give an estimate of the free energy barriers separating an equilibrium state from the metastable states close to it.

1. Introduction.

The structure of the phase space in the p-spin spherical model below the dynamical transition temperature T_d is characterized by the presence of an exponentially high number of metastable states [1,2]. If we consider corrections to mean field theory when the size N of the system is finite but large, the dynamics is determined essentially by two factors: the mutual disposition of the states and the free energy barriers between them.

The *real replica method* shed some light into the structure of the metastable states of this model [1,3,4] and the same method can be used to estimate the barriers. It is now known that, given an equilibrium state, there are many metastable states of various energies at finite overlaps with it; it is therefore interesting to evaluate the free energy barriers between an equilibrium state and the metastable states close to it.

In [4] we introduced a three replica potential: the first replica is located into an equilibrium state, while the second one is constrained to stay into a metastable state at given overlap with the first one (for particular values of the overlap this second state can be of equilibrium too); we then calculated the free energy of a third replica as a function of its distances from the other two and found two non trivial minima of this free energy, corresponding to replica 3 in equilibrium into the state of replica 1 or into the state of replica 2. In this context, it is reasonable to give an estimate of the barrier between these two states, following the free energy profile of replica 3 when it moves from a minimum to the other. This is the purpose of the present letter.

2. The method.

The p-spin spherical model is defined by the Hamiltonian

$$H(\sigma) = \sum_{i_1<i_2<\ldots<i_p} J_{i_1\ldots i_p}\sigma_{i_1}\ldots\sigma_{i_p} \tag{2.1}$$

where the σ are real variables satisfying the spherical constraint $\frac{1}{N}\sum_i \sigma_i^2 = 1$ and the couplings $J_{i_1 \ldots i_p}$ are Gaussian variables with zero mean and variance $\frac{p!}{2N^{p-1}}$ [5,6,7,8]. We consider the case $p = 3$.

The organization of the states in this model is quite complex [1,2]. In the range of temperature $T_c < T < T_d$ (T_c is the static transition temperature) the equilibrium states coincide with those TAP solutions [9] which optimize the balance between the free energy f and the complexity $\Sigma(f)$, i.e. solutions which minimize the function $\phi = f - T\Sigma(f)$; all other TAP solutions correspond to metastable states.

To inspect the structure of all these states, i.e. their mutual overlaps, we defined in [4] a three replica potential $V_3(q_{12}|q_{13}, q_{23})$, having the following features: replica 1 is an equilibrium configuration of the system, while replica 2 is a typical configuration of a system forced to equilibrate at overlap q_{12} with 1; in other words, replica 2 chooses the most convenient configuration compatibly with the imposed constraint; V_3 is then the free energy of a third replica 3, constrained to have overlaps (q_{13}, q_{23}) with the first two quenched replicas. We studied V_3 in the plane $\pi \equiv (q_{13}, q_{23})$, at fixed value of q_{12}: a minimum of the potential in this plane corresponds to replica 3 having found a state into which it can thermalize.

In the temperature range $T_c < T < T_d$, at given q_{12}, V_3 has two non trivial minima, from here on M_1 and M_2:

- In M_1 replica 3 is located near replica 1, that is in the same equilibrium state; indeed, in M_1 the free energy and the self overlap of replica 3 satisfy the relation of TAP equilibrium solutions.
- On the other hand, M_2 corresponds to replica 3 near replica 2 and its free energy and self overlap satisfy the relation of TAP metastable solutions; this means that replica 3 has thermalized into a metastable state at distance q_{12} from the equilibrium state of replica 1.

Varying q_{12}, M_1 always corresponds to the same equilibrium state, while M_2 identifies with different metastable states, at various distances.

The important thing is then that, fixed q_{12}, we have the possibility of studying the

free energy barrier between two well defined states, via the analysis of the free energy contour around M_1 and M_2 given by V_3. In particular, we are interested in the barrier that has to be crossed to go from the equilibrium state represented by M_1 into the metastable state represented by M_2. Indeed, the computation of this barrier is useful for a comparison with the dynamical situation at finite N, in which a configuration starts at time zero from an equilibrium state and after an exponentially large time jumps to a metastable state.

The plane π is the image of the phase space Γ through the mapping which, fixed q_{12}, maps a configuration σ of Γ into its distances (q_{13}, q_{23}) from configurations 1 and 2. In this way, a path in Γ is mapped into a single path in π, while, obviously, the opposite does not hold. Due to this, a path in the plane π could correspond to no continuous path in the phase space and for this reason we can only give a lower bound for the free energy barrier between the two states.

The proposal is to find in π the path linking M_1 to M_2 which minimizes the variation of V_3 and to consider this variation as a lower bound for the free energy barrier between the two corresponding states. To this aim it is clearly important to consider not only the minima of V_3 but also its saddles; indeed, as can be seen from next figures, the problem of finding the best path from M_1 to M_2 reduces to single out the chain of saddles which minimizes the variation of V_3; the estimate of the barrier is then given by

$$\Delta F \geq \; V_3(S_{max}) - V_3(M_1) \tag{2.2}$$

where S_{max} is the highest saddle crossed along the path.

3. The results.

Before analyzing the structure of minima and saddles of V_3 at various values of q_{12}, we remind that the minimum M_2 exists only in the range $0 \leq q_{12} \leq \bar{q}(T)$, and that for

$q_{12} = q^\star(T)$, the state associated to M_2 is an equilibrium one [4]. This means that, given an equilibrium state, the nearest metastable state that can be seen with this method is at overlap $\bar{q}$ with it and the nearest equilibrium state is at overlap $q^\star$.

We can distinguish three different ranges:

i. $q_{12} < q^\star$: from Figure 1 we can see that in this range there are only two saddles, S_1 and S_2, and the path which links the two minima is then

$$M_1 \to S_1 \to S_2 \to M_2 \ . \tag{3.1}$$

Since the highest saddle is S_1, we have

$$\Delta F \geq \ V_3(S_1) - V_3(M_1) \ . \tag{3.2}$$

It is worth to note that the value of V_3 in M_1 and S_1 does not depend on q_{12} and therefore in this range the barrier is constant. In [3] it has been introduced a two replica potential V_2, function of the distance q_{12} of replica 2 from the equilibrium state of replica 1. V_2 has two minima corresponding to equilibrium states with zero mutual overlap: the most natural hypothesis is then that the maximum separating these minima represents a first estimate of the free energy barrier between remote equilibrium states. It turns out that this estimate coincides with (3.2), in agreement with the small value of q_{12} in this range.

ii. $q^\star < q_{12} < q'$: at $q^\star$ S_2 becomes higher than S_1 (see Figure 2) and so now the path is the same as in (3.1), but the barrier is

$$\Delta F \geq \ V_3(S_2\,; q_{12}) - V_3(M_1) \tag{3.3}$$

that depends on q_{12}. We note from Figure 2 that in this range there is a value of q_{12} at which a new saddle S appears together with a maximum; however, since for $q_{12} < q'$ we have $V_3(S) > V_3(S_2)$, the path that minimizes the variation of V_3 still is (3.1).

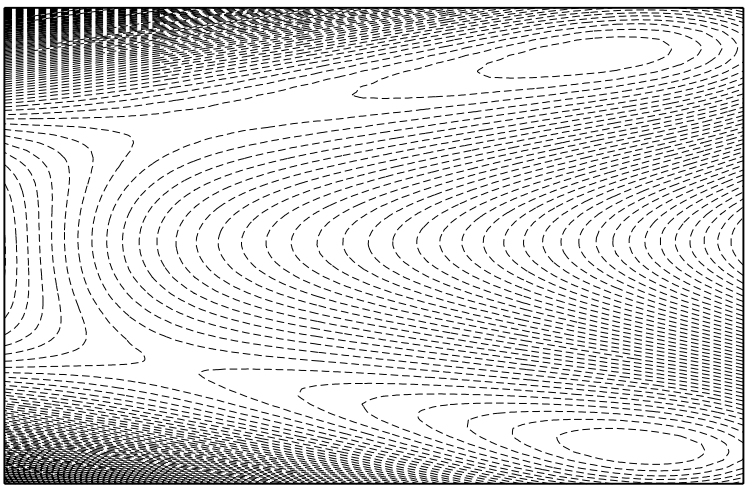

Figure 1: The contour lines of V_3 for q_{12}=0.25 and β=1.64. The axis are $x=\frac{1}{\sqrt{2}}(q_{13}+q_{23})$ in the range [0.25:0.6], and $y=\frac{1}{\sqrt{2}}(q_{13}-q_{23})$ in the range [−0.3,0.3]. The two minima are visible on the right: M_1 (up) and M_2 (down); on the left the two saddles: S_1 (up) and S_2 (down).

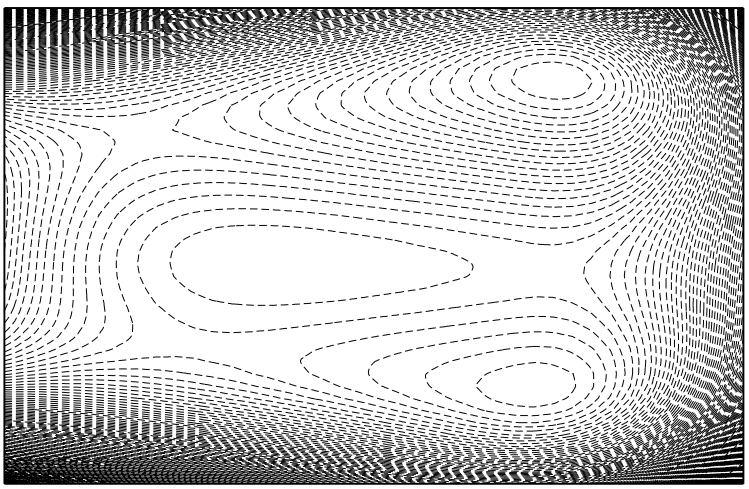

Figure 2: The contour lines of V_3 for q_{12}=0.36. The axis are the same as in Figure 1, with ranges $x\in$[0.35,0.75] and $y\in$[−0.2,0.2]. The new saddle S is clearly visible on the right, in the middle between the two minima.

iii. $q' < q_{12} < \bar{q}$: at q' the path that minimizes the variation of V_3 suddenly changes because S becomes lower than S_2; so we have

$$M_1 \to S \to M_2 \tag{3.4}$$

and

$$\Delta F \geq \; V_3(S;q_{12}) - V_3(M_1) \; . \tag{3.5}$$

This situation holds up to $q_{12} = \bar{q}$, when M_2 disappears merging with S.

The whole behaviour of V_3 in the saddles is shown in Figure 3.

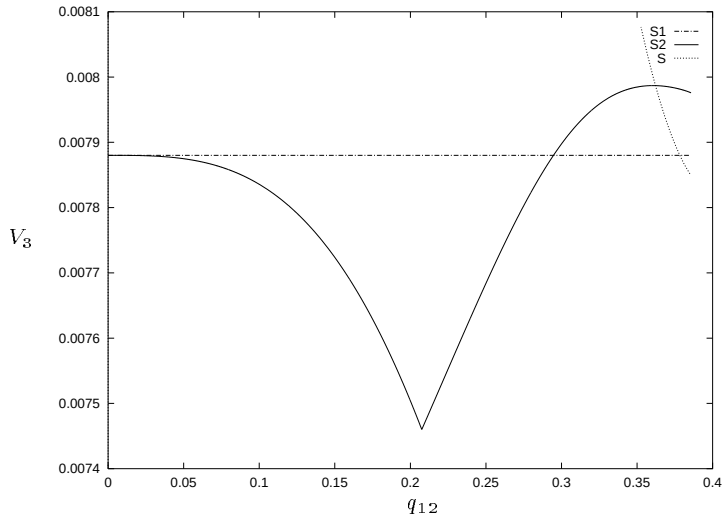

Figure 3: V_3 evaluated in the three saddles S_1, S_2 and S as a function of q_{12}. For β=1.64, $q^\star$=0.295 and q'=0.362.

Finally, Figure 4 shows the behaviour of our estimate of the free energy barrier.

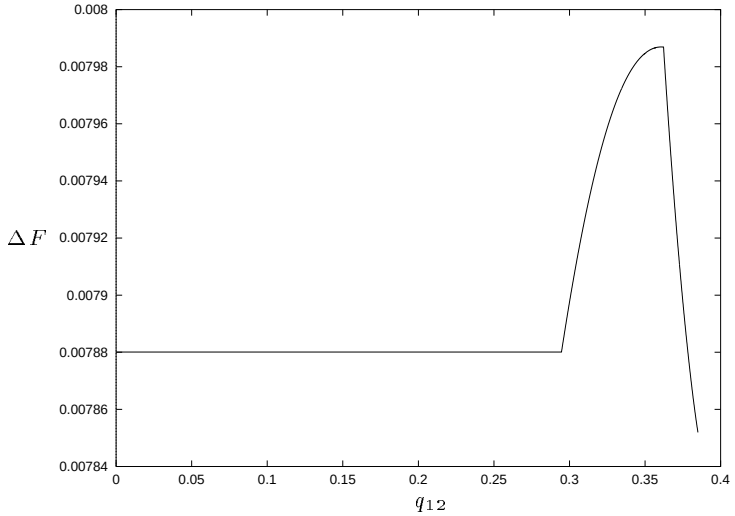

Figure 4: The free energy barrier ΔF as a function of q_{12}.

4. Conclusions.

Before analyzing these results it is useful to consider some properties of the potential in the stationary points.

In the computation of V_3 we introduced the overlap matrix Q^{33}_{ab} of replica 3, and assumed for it a one step RSB form, with parameters (x_s, s_1, s_0), where x_s is the breaking point and $s_1 \geq s_0$ are the overlaps.

The physical meaning of breaking or not the replica symmetry is the usual one adapted to this context. An RS form of the overlap matrix can be associated to two very different situations: the first one corresponds to a system which finds an exponentially high number of states (as in the p-spin model for $T_c < T < T_d$), while in the second one the phase space consists of just one state (as in the paramagnetic case). On the other side, an RSB form means that the phase space is dominated by a number of order N of states (as in the p-spin model for $T < T_c$).

It can be shown that in the minima of the potential it holds $s_1 = s_0$, i.e. Q^{33} turns out to be replica symmetric. This is what we expect: in M_2, for example, q_{23} is big enough to constrain replica 3 to see just one state, the one of replica 2, and for this reason Q^{33} is symmetric, $s_1 = s_0$ representing the self overlap of the state.

This symmetry is a very special feature of this kind of situation; indeed, in the saddles S_1 and S_2 the matrix Q^{33} is actually broken, meaning that the number of states accessible to replica 3 is in this case of order N and that replica 3 does not thermalize into any of them.

Surprisingly enough, in the saddle S the matrix Q^{33} is symmetric again; moreover, in this saddle the free energy f_3 of replica 3 and the overlap $s_1 = s_0$ satisfy the relation between free energy and self overlap of TAP solutions and fulfil the stability condition with respect to fluctuations of the overlap (longitudinal stability condition) of [1,8]. These facts suggest that S corresponds to a well defined TAP solution, but that, despite of the longitudinal stability condition, this solution does not identify a stable state, i.e. it is not a minimum of the TAP free energy. We can then make the hypothesis that S

represents a *real* saddle in the phase space and that it is just the saddle which links the two states corresponding to M_1 and M_2; this conjecture is supported by the geometrical position of S right between M_1 and M_2 (see Figure 2). If this were true, in the range in which the path is $M_1 \to S \to M_2$, expression (3.5) would give the exact free energy barrier, not only a lower bound.

We note that the existence among TAP solutions of saddles which satisfy the longitudinal stability condition of [1,8] requires a more complete analysis of the stability of TAP equations for this model. Moreover, it would be interesting to make a computation of the complexity of these saddles, to single out their contribution to the dynamics of the system.

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