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

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

(2.1)
where the \( \sigma \) 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 \( \frac{p!}{2^{N-p-1}} \) \([5,6,7,8]\). 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 $\pi$ is the image of the phase space $\Gamma$ through the mapping which, fixed $q_{12}$,
maps a configuration $\sigma$ of $\Gamma$ into its distances $(q_{13}, q_{23})$ from configurations 1 and 2. In
this way, a path in $\Gamma$ is mapped into a single path in $\pi$, while, obviously, the opposite
does not hold. Due to this, a path in the plane $\pi$ 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 $\pi$ 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

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

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
\( q_{12} = q^*(T) \), 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 \( q^* \).

We can distinguish three different ranges:

i. \( q_{12} < q^* \): 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

\[
M_1 \rightarrow S_1 \rightarrow S_2 \rightarrow M_2 .
\]  

Since the highest saddle is \( S_1 \), we have

\[
\Delta F \geq V_3(S_1) - V_3(M_1) .
\]  

(3.1)

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

\[
\Delta F \geq V_3(S_2; q_{12}) - V_3(M_1)
\]  

(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).
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

\[
M_1 \rightarrow S \rightarrow M_2
\]  
(3.4)
and

\[
\Delta F \geq V_3(S; q_{12}) - V_3(M_1).
\]

(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 \( \beta=1.64 \), \( q^*=0.295 \) and \( q'=0.362 \).](image)

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

![Figure 4: The free energy barrier \( \Delta F \) as a function of \( q_{12} \).](image)
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 $Q_{ab}^{33}$ 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 $M_1 \rightarrow S \rightarrow M_2$, 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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