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LETTER TO THE EDITOR

Dynamics within metastable states in a mean-field spin glass

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Abstract. In this letter we present a dynamical study of the structure of metastable states (corresponding to TAP solutions) in a mean-field spin–glass model. After reviewing known results of the statical approach, we use dynamics: starting from an initial condition thermalized at a temperature between the statical and the dynamical transition temperatures, we are able to study the relaxational dynamics within metastable states and we show that they are characterized by a true breaking of ergodicity and exponential relaxation.

The recent developments in the theory of spin–glass dynamics [1] have made clearer the similarity of behaviour in spin glasses and in glasses [2, 3]. In this context it seems at the moment that a certain category of spin glasses, those which are described by a so-called one-step replica-symmetry breaking (RSB) transition [4], are good candidate models for a mean-field description of the glass phase [5, 6]. In these systems the presence of metastable states generates a purely dynamical transition (which is supposed to be rounded in finite-dimensional systems [5, 6]) at a temperature T_d higher than the one obtained within a theory of static equilibrium, T_s.

The spherical p-spin spin glass introduced in [7, 8] is an interesting example of this category. It is a simple enough system in which the metastable states can be defined and studied by the TAP method [9]. In this paper we want to provide a better understanding of these metastable states, using a dynamical point of view. We shall show the existence of a true ergodicity breaking such that these metastable states, in spite of being excited states with a finite excitation free energy per spin, are actually dynamically stable even at temperatures above T_d. Note that a connection between dynamics and TAP approach was made in [18], for a similar model, but not in the same spirit.

The spherical p-spin spin glass describes N real spins $s_i,\ i \in \{1, \ldots, N\}$ which interact through the Hamiltonian

$$H(s) = -\sum_{1\leqslant i_1<\cdots<i_p\leqslant N} J_{i_1,\ldots,i_p}\, s_{i_1}\ldots s_{i_p} \tag{1}$$

together with the spherical constraint on the spins: $\sum_{i=1}^{N} s_i^2 = N$. The couplings are Gaussian, with zero mean and variance $p!/(2N^{p-1})$. In the $p > 2$ case it shows an interesting spin–glass behaviour, simple enough to allow for detailed analytical treatment.

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In the static approach, one describes the properties of the Boltzmann probability distribution of this system. The replica method shows the existence of a static transition with a one-step RSB at temperature T_s [7]. This transition reflects the fact that, below T_s, the Boltzmann measure is dominated by a few pure states, a scenario which is well known from the random energy model [10].

Staying within a static framework, the TAP approach [11, 12] provides some more insight into the physical nature of this system. The TAP equations can be derived through a variational principle on the local magnetizations $m_i = \langle s_i \rangle$, from a free energy $f(\{m_i\})$ which is best written in terms of radial and angular variables, q and $\hat{s}_i$ (with $m_i = \sqrt{q}\hat{s}_i$), in the form [11]

$$f(\{m_i\}) = q^{p/2} E^0\left(\{\hat{s}_i\}\right) - \frac{T}{2}\ln(1-q) - \frac{1}{4T}[(p-1)q^p - pq^{p-1} + 1] \tag{2}$$

where the angular energy is

$$E^0\left(\{\hat{s}_i\}\right) \equiv - \sum_{1 \leqslant i_1 < \cdots < i_p \leqslant N} J_{i_1,\ldots,i_p}\, \hat{s}_{i_1} \ldots \hat{s}_{i_p} \ . \tag{3}$$

At zero temperature the TAP states are just unit vectors which minimize the angular energy E^0. There actually exist such states for $E^0 \in [E_{min}, E_c = -\sqrt{2(p-1)/p}]$. Denoting by $\hat{s}_i^\alpha$ one zero temperature state, of energy E^0_α, it gives rise at finite temperature T to one TAP state α given by

$$m_i^\alpha = \sqrt{q\left(E^0_\alpha, T\right)}\hat{s}_i^\alpha \tag{4}$$

where $q(E, T)$ is the largest solution of the equation:

$$(1-q)q^{p/2-1} = T\left(\frac{-E - \sqrt{E^2 - E_c^2}}{p-1}\right). \tag{5}$$

The free energy of this state, f_α, at temperature T, is obtained by inserting in the TAP free energy (2) the corresponding values of the angular energy, $E^0 = E^0_\alpha$ and of the self-overlap, $q = q_\alpha \equiv q\left(E^0_\alpha, T\right)$. The corresponding energy is

$$E_\alpha = q_\alpha^{p/2} E^0_\alpha - \frac{1}{2T}[(p-1)q_\alpha^p - pq_\alpha^{p-1} + 1] \, . \tag{6}$$

When changing the temperature, one can follow the metastable states which keep the same angular direction; their order in free energy or energy, at fixed T, is the same as their order in E^0. When raising T, a state disappears at a temperature $T_{\max}(E^0)$ (where equation (5) ceases to have solutions). $T_{\max}(E^0)$ is a decreasing function of E^0; the most excited states, with $E^0 = E_c$, disappear first at $T_{\max}(E_c)$, and the lowest at $T_{\max}(E_{min}) \equiv T_{\mathrm{TAP}}$. Above T_{TAP}, the only remaining state is the paramagnetic one with $q = 0$ and free energy $F_{\mathrm{para}} = -1/(4T)$.

To complete the description of metastable states at any temperature, one only needs the density of states $\rho(E^0)$ with an angular energy E^0. This has been computed in [12]; the multiplicity is exponentially large, giving a finite complexity density $s_c^0(E^0)$, defined as

$$s_c^0(E^0) = \lim_{N\to\infty} \frac{\log \rho(E^0)}{N} \ . \tag{7}$$

The complexity at finite temperature is easily deduced from this s_c^0. We shall denote by $S_c(f, T)$ the logarithm of the number of TAP states at free energy f and temperature T. The Boltzmann partition function can then be approximated as the sum over all TAP solutions:

$$Z = \int \mathrm{d}f \exp\left(-\frac{(f - TS_c(f, T))}{T}\right) \tag{8}$$

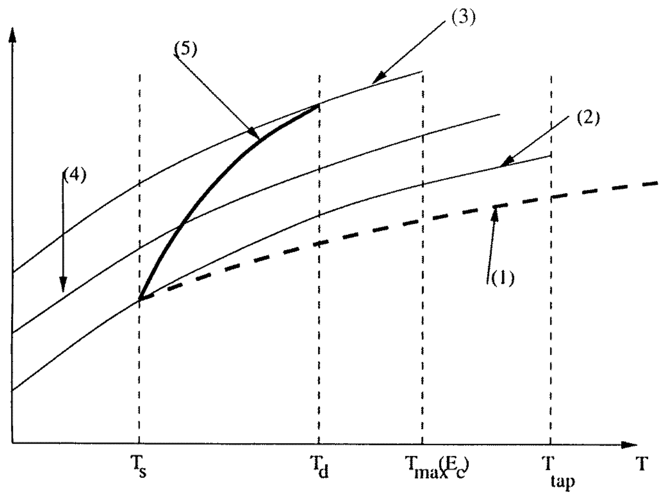

Figure 1. free energy versus temperature; (1) free energy of the paramagnetic solution for $t > t_d$, f_{tot} for $t < t_d$; (2) free energy of the lowest TAP states, with zero temperature energy e_{min}; (3) free energy of the highest TAP states, corresponding to e_c; (4) an intermediate value of e_0 leads to an intermediate value of f at any temperature; (5) $f_{eq}(t)$; the difference between curves (5) and (1) gives the complexity $TS_c(f_{eq}(t), t)$.

which can be evaluated at large N by a saddle-point method. At temperatures $T > T_d$, with $T_d = \sqrt{p(p-2)^{p-2}(p-1)^{1-p}/2}$, the Boltzmann measure is dominated by the paramagnetic state $q = 0$. At any $T \in [T_s, T_d]$, the Boltzmann measure is dominated by a class of TAP solutions, those of free energy $f = f_{eq}(T)$. Because of their extensive complexity, this gives for the total equilibrium free energy:

$$f_{tot} \equiv -T \ln(Z) = f_{eq}(T) - TS_c(f_{eq}(T), T) . \tag{9}$$

The computation of f_{eq} is easily done [7, 14]. One finds that f_{tot} is *equal to* the paramagnetic free energy in this range. Below T_s the lowest lying TAP states dominate the Boltzmann measure, leading to RSB. The situation is summarized in figure 1. Compared to a usual phase transition, the situation is complicated by the existence of a finite complexity. Actually we see that between the two transition temperatures T_s and T_d, the situation is unclear: the total equilibrium free energy seems to get two equal contributions, from the paramagnetic state and from a bunch of TAP solutions with non-zero q. One can wonder if there is a phase coexistence, or simply a problem of double counting in the TAP approach. This issue, which is an important one if one aims at understanding the finite-dimensional behaviour of this type of systems [6], can in fact be clarified within a dynamical approach as we now show. Let us also mention that some purely static approaches also carry relevant information on related issues [13, 19].

The TAP structure of states is usually not explored dynamically: indeed, the usually studied out of equilibrium dynamics of the spherical p-spin model starts from a random configuration, and never goes below the threshold corresponding to the upper TAP solutions. This process has been studied in [15]: an interesting aging behaviour has been found at temperatures $T < T_d$, but the energy density of the system only goes asymptotically to one of the highest TAP states (the threshold states with angular energy $E^0 = E_c$). Hence, it is impossible to explore TAP states via this kind of dynamics.

Here we will use a different approach for the dynamics [18, 19], where we start from a spin configuration which is picked up from a Boltzmann distribution at temperature T', and then let the system relax at temperature T. We shall concentrate on the case where $T' \in [T_s, T_d]$, which means that our initial configuration will belong to the TAP states with free energy $f_{eq}(T')$. This will lead to the study of the relaxation *inside* one TAP state.

The relaxational dynamics at temperature T is given by the Langevin equation:

$$\frac{ds_i(t)}{dt} = -\frac{\partial H}{\partial s_i} - \mu(t)s_i(t) + \eta_i(t) \tag{10}$$

where H is the Hamiltonian (1), μ is the Lagrange multiplier implementing the spherical constraint, and η_i is a Gaussian white noise with zero mean and variance $2T$. The dynamics is described by the behaviour of two-times correlation and response functions defined by

$$C(t,t') = \frac{1}{N}\sum_{i=1}^{N} \overline{\langle s_i(t)s_i(t')\rangle} \qquad r(t,t') = \frac{1}{N}\sum_{i=1}^{N} \frac{\partial \overline{\langle s_i(t)\rangle}}{\partial h_i(t')} \tag{11}$$

where $\langle\cdot\rangle$ is a mean over the thermal noise, and an overline denotes a mean over the coupling constants.

Using the usual field-theoretical techniques for out of equilibrium dynamics [16], in the large-N limit, it is possible to study the dynamics at temperature T, starting from a Boltzmann measure at temperature T'. In order to implement this initial sample dependent-measure, it is necessary to introduce replicas [17–19] and to write dynamical equations for two-times overlaps between replicas $C^{ab}(t,t') = \overline{\langle s^a(t)s^b(t')\rangle}$, a and b being replica indices. The equations obtained differ from the usual out of equilibrium ones (corresponding to $T' = \infty$ [15]) by terms involving a coupling to the initial configuration, i.e. $C^{ab}(t,0)$. Besides, as noted in [19], the time evolution respects the initial replica-symmetric or RSB structure of the C^{ab}, i.e. the static replica structure describing equilibrium at T'.

For the p-spin model with $T' > T_s$ the initial condition is replica symmetric, with $C^{ab}(0,0) = \delta_{ab}$. Therefore, at all times we can write $C^{ab}(t,t') = C(t,t')\delta_{ab}$. The obtained equations for the correlation and response functions read[19], for any $T' > T_s$, and $t > t'$:

$$\begin{aligned}
\mu(t) &= \int_0^t ds\, \left[\frac{p^2}{2}C^{p-1}(t,s) - \frac{p(p-1)}{2}C^{p-2}(t,s)\right] r(t,s) + T \\
&\quad - \frac{p}{2T'}C^{p-1}(t,0)\,(1-C(t,0)) \\
\frac{\partial r(t,t')}{\partial t} &= -\mu(t)r(t,t') - \frac{p}{2T'}C^{p-1}(t,0)\, r(t,t') \\
&\quad - \frac{p(p-1)}{2}\int_0^t ds\, C^{p-2}(t,s)r(t,s)(r(t,t') - r(s,t')) \\
\frac{\partial C(t,t')}{\partial t} &= -\mu(t)C(t,t') + \frac{p}{2}\int_0^{t'} ds\, C^{p-1}(t,s)r(t',s) \\
&\quad - \frac{p(p-1)}{2}\int_0^t ds\, C^{p-2}(t,s)r(t,s)(C(t,t') - C(s,t')) \\
&\quad - \frac{p}{2T'}C^{p-1}(t,0)\, C(t,t') + \frac{p}{2T'}C^{p-1}(t,0)\, C(t',0)\,.
\end{aligned} \tag{12}$$

Let us examine the situation first for $T = T'$ (this case was studied in [18]; supposing *a priori* equilibrium dynamics, they were able to connect it with the TAP approach): since we start at equilibrium, we expect equilibrium dynamics satisfying both time translation invariance (TTI) and the fluctuation dissipation theorem (FDT): $C(t,t') =$

$C_{\rm eq}(t-t')$, $r(t,t')=r_{\rm eq}(t-t')$ with $r_{\rm eq}(\tau)=-\frac{1}{T}\frac{\partial C_{\rm eq}}{\partial\tau}$. Equations (12) reduce, with this ansatz, to a single equation for the evolution of $C_{\rm eq}(\tau)$:

$$\frac{\partial C_{\rm eq}(\tau)}{\partial\tau}=-\mu_\infty C_{\rm eq}(\tau)-\frac{p}{2T}\int_0^\tau {\rm d}u\, C_{\rm eq}^{p-1}(\tau-u)\ \frac{\partial C_{\rm eq}(u)}{\partial u} \tag{13}$$

where $\mu_\infty=T$, and $C_{\rm eq}(0)=1$. Above $T_{\rm d}$, this equation describes the relaxation within the paramagnetic state, with $\lim_{\tau\to\infty}C_{\rm eq}(\tau)=0$. Below $T_{\rm d}$, the condition of dynamical stability $\frac{\partial C_{\rm eq}(\tau)}{\partial\tau}\leqslant 0$ leads to a non zero limit C_∞ for $C_{\rm eq}(\tau)$ [8]; this limit is given by the largest solution of

$$\frac{p}{2T^2}C_\infty^{p-2}(1-C_\infty)=1 \tag{14}$$

(the other non-zero solution is unstable with respect to the dynamics (13)). This value is precisely the self-overlap q of the TAP states reflecting the statics at T, i.e. with free energy $f_{\rm eq}(T)$. This means that, for temperatures between the statical and the dynamical transition temperatures, the thermalized system is trapped inside a TAP state, and not in a paramagnetic state, for which C_∞ would be zero (as for $T>T_{\rm d}$). We can also exclude the possibility of a coexistence, which would lead to some intermediate value: the paramagnetic state has disappeared at $T_{\rm d}$, and the Gibbs state is formed by the bunch of TAP solutions having the suitable free energy $f_{\rm eq}(T)$, and a finite complexity density.

To get further insight, always starting from a thermalized configuration at temperature $T'\in[T_{\rm s},T_{\rm d}]$, we now study the dynamics at a temperature T different from T'. In our study of the dynamical equations (12), we have found numerically (using the type of algorithm developed in [20]) and analytically that after a short transient the system reaches a stationary regime where TTI and FDT hold (see figure 2). The possibility of such a situation has already been conjectured in [19], together with an interesting connection to the static approaches developed in [13, 19].

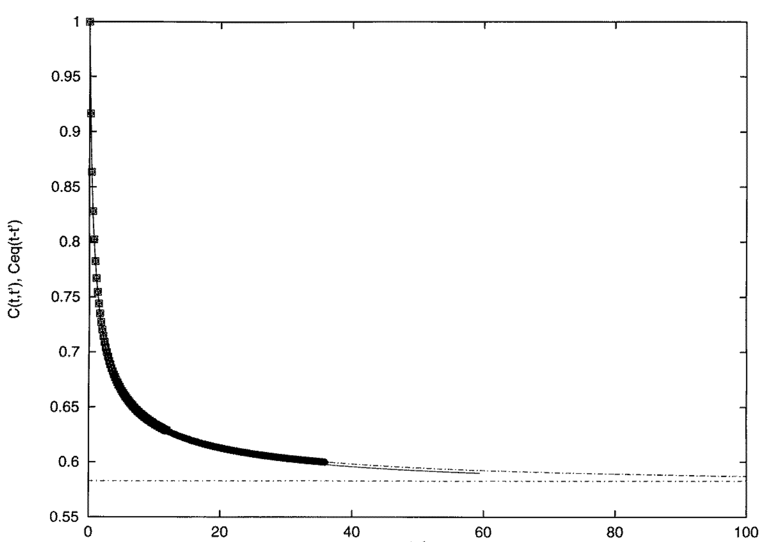

Figure 2. $p=3$ model, with $T_{\rm s}\approx 0.586$, $T_{\rm d}\approx 0.612$; numerical integration of equations (12) for $T'=0.605$, $T=0.6$; we plot $C(t,0)$ versus t (full curve), and $C(t,t')$ versus $t-t'$ for $t'=6, 12, 18, 24$ (symbols); the dotted curve is the numerical integration of (15), and the dotted curve is the value of C_∞ obtained by (16).

In order to study this solution analytically, we introduce as previously $C_{\rm eq}(\tau)$, $r_{\rm eq}(\tau)$, $C_\infty = \lim_{\tau\to\infty} C_{\rm eq}(\tau)$, $\mu_\infty = \lim_{t\to\infty}\mu(t)$, and $l = \lim_{t\to\infty} C(t,0)$, and obtain the equation:

$$\frac{\partial C_{\rm eq}(\tau)}{\partial\tau} = -\left(\mu_\infty - \frac{p}{2T}C_\infty^{p-1} + \frac{p}{2T'}l^{p-1}\right)C_{\rm eq}(\tau) + \frac{p}{2}\int_0^\tau {\rm d}u\; C_{\rm eq}^{p-1}(u)\; r_{\rm eq}(\tau-u) - \frac{p}{2T}C_\infty^p + \frac{p}{2T'}l^p\,. \qquad (15)$$

Besides, μ_∞, C_∞ and l satisfy the following set of equations, obtained by taking $t' = 0$, $t\to\infty$ in (12), and $\tau\to\infty$ in (15):

$$\begin{aligned} \mu_\infty &= T + \frac{p}{2T}C_\infty^{p-1}(1-C_\infty) - \frac{p}{2T'}l^{p-1}(1-l) \\ l^{p-2} &= \frac{2TT'}{p(1-C_\infty)} \\ TC_\infty &= \frac{p}{2T'}l^p(1-C_\infty) + \frac{p}{2T}C_\infty^{p-1}(1-C_\infty)^2 \end{aligned} \qquad (16)$$

and the energy reached dynamically at large times is $E_\infty = \frac{1}{2T}(C_\infty^p - 1) - \frac{l^p}{2T'}$.

It is then straightforward to check that the overlap C_∞ and the energy E_∞ are identical to the values characteristic of certain TAP states at the temperature T. These states are precisely those obtained by following the equilibrium TAP states at temperature T' (which pick up a certain value $E^0_{T'}$ of the angular energy) to temperature T, by keeping the same direction in $\hat{s}$ space, but changing the overlap from $q(E^0_{T'}, T')$ to $q(E^0_{T'}, T)$.

From equation (15), it is possible to show that the relaxation of $C_{\rm eq}(\tau)$ is of the form $\tau^{-3/2}\exp(-\tau/\tau_0)$. The relaxation time τ_0 can also be computed, and has a quite complicated expression that we do not reproduce here. It diverges for the highest TAP states (corresponding to $E^0 = E_{\rm c}$). Of course, this exponential relaxation can only happen as long as the followed TAP solution still exists at temperature T: if T becomes larger than $T_{\max}(E^0_{T'})$, we observe a fast relaxation to the paramagnetic state, with $C_\infty = l = 0$.

We have thus shown that the TAP solutions are real states, corresponding to a full breaking of ergodicity: starting within a TAP state (which can be achieved by our trick of using thermalized initial conditions at a temperature T'), one relaxes within this state with a finite relaxation rate, and one can even follow this state when changing the temperature. Besides, the Gibbs measure below the dynamical transition is made of a superposition of TAP states, which are different ergodic components, totally separated from each other in the dynamical evolution. The paramagnetic solution, valid above $T_{\rm d}$, disappears at $T_{\rm d}$. Note that the way in which this occurs is not clear, and we leave this open question, which is crucial for a better understanding of aging dynamics, for future work. Some TAP states exist as independent ergodic components even at temperatures $T \in [T_{\rm d}, T_{\rm TAP}]$. They are not seen in the usual dynamics because they are difficult to find: starting from random initial conditions one stays in the big paramagnetic ergodic component. If one succeeds in starting within a TAP state, one stays within this state even by rising the temperature above $T_{\rm d}$ (but below the $T_{\max}$ of this state). One should notice that the usual dynamics at a temperature below $T_{\rm d}$, starting from a random configuration, only leads to a 'weak ergodicity breaking' [21, 15], where the self-overlap vanishes at very large time differences (much larger than the waiting time). This is explained [15, 22] by the fact that the system, which was initially in the (infinite temperature) paramagnetic state, does not find any TAP state in a finite time, but stays at energy density O(1) (going to zero as t goes to infinity) above the threshold. In contrast, there is no sign of aging when one starts within a TAP state. This is in agreement with some recent intuitive scenarios for aging [22, 23].

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