Recipes for metastable states in Spin Glasses

Silvio Franz (1), Giorgio Parisi (2)

(1) NORDITA and CONNECT
Blegdamsvej 17,
DK-2100 Copenhagen Ø
Denmark
e-mail: *franz@nordita.dk*

(2) Dipartimento di Fisica
Università di Roma I, "La Sapienza"
P.le A.Moro 5
00185 Rome
Italy

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Abstract: In this paper we develop a method introduced by one of us to study metastable states in spin glasses. We consider a 'potential function' defined as the free energy of a system at a given temperature T constrained to have a fixed overlap with a reference configuration of equilibrium at temperature T'. We apply the method to the spherical p-spin glass and to some generalization of this model in the range of temperatures between the dynamic and the static transition. The analysis suggests a correspondence among local minima of the potential and metastable states. This correspondence is confirmed studying the relaxation dynamics at temperature T of a system starting from an initial configuration equilibrated at a different temperature T'.

1 Introduction

The off-equilibrium dynamics of glassy system is a fascinating subject. Experimental [1] and numerical [2] evidence show that out of equilibrium phenomena persist in glasses for the largest reachable observation times.

Recently a partial comprehension of these phenomena in mean field has been achieved [3, 4, 5]. The phenomenon of aging is described in the mean field theory as an asymptotic stationary state, where time translation invariance and the fluctuation dissipation relation do not hold. This regime turns out to be closely related to the nature of the static glassy transition. The models studied up to now can be divided in two classes according to their pattern of replica symmetry breaking (RSB) [6]. If the RSB is "continuous", i.e. if the Parisi order parameter function $q(x)$ is continuous, then the static and the dynamic transitions occur at the same temperature. The asymptotic state is such that expected values of quantities which depend only on the configuration of the system at a single time (e.g. the energy or the distribution of the magnetizations) tend to their Boltzmann-Gibbs values. If instead the Parisi function is discontinuous, e.g. a single step function, the dynamic transition occurs at a temperature higer then the static one, and the quantities mentioned above tend to limits different to their canonical averages. However, a careful analysis in the *spherical p-spin model* [3] have shown how this limiting values can be related to the values of the same observables in a particular class of metastable solutions of the TAP equations, with free energy higher than the ones dominating the partition function. It then raises spontaneously the question whether it is in general possible to relate the properties of the asymptotic dynamic state to some static properties of the systems.

This paper constitute a step forward in this direction. Our basic tool of investigation will be a "potential function" introduced in [7], defined as the minimal work needed to keep a system at temperature T at a fixed overlap from a typical equilibrium configuration of the same system at a different temperature T'. The models we choose to study are a family of spherical spin glass models which present a one step RSB. The most studied representant of this class is the spherical p-spin model. This model has the remarkable (and atypical) property that the order in free energy of the solutions of the TAP equations do not vary with the temperature. It is interesting to consider more general models where the order of the solution depends of T, and in the spin glass phase the low-lying states at different temperature are not correlated.

The basic theses of this paper is that the minima of the potential are related to (meta)stable states. To confirm this point we study the dynamics at temperature T starting from a configuration which is perfectly thermalized at a different temperature T' at the initial time.

Work on subjects related to the ones treated in this paper has been very recently achieved by R.Monasson [8]. We thank him to make us aware of some of his results prior to publication. Applications of 'potential' model to Ising spin has also been done by [9].

The organization of the paper is the following: In section 2 we present a short summary of the static and dynamic properties of the model. This chapter is part review and part new elaboration. Then in section 3 we introduce and discuss some basic properties of the potential function. Section 4 is devoted to the study of the potential for the spherical model. In section 5 we present the dynamic theory of the evolution of a system at temperature T starting from an equilibrium configuration at temperature T'. We finally sketch our conclusions.

2 The Model

The spherical p-spin model [10] is defined by the Hamiltonian

$$H_p[\mathbf{s}] = \sum_{i_1<i_2<...<i_p} J_{i_1,...,i_p} s_{i_1}...s_{i_p} \tag{1}$$

where the "spins" s_i, $i = 1, ..., N$ are real variables subjected to the constraint $(1/N)\sum_i s_i^2 = 1$, and the couplings $J_{i_1,...,i_p}$ are independent Gaussian variables with variance: $\overline{J^2_{i_1,...,i_p}} = \frac{p!}{2N^{p-1}}$.

It can be observed that such model is (dynamically and statically) equivalent to a model in which the functional form of the Hamiltonian is not specified explicitly and one just take it as a random Gaussian function of the spin configuration with correlation function given by

$$\overline{H[\mathbf{s}]H[\mathbf{s}']} = N\frac{1}{2}q^p_{\mathbf{s},\mathbf{s}'} \tag{2}$$

$q_{\mathbf{s},\mathbf{s}'} = \mathbf{s}\cdot\mathbf{s}'/N = (1/N)\sum_i s_i s'_i$ is the overlap among the two configurations $\mathbf{s}$ and $\mathbf{s}'$. One can then easily generalize the spherical model to random Hamiltonian [11, 12] with arbitrary correlation functions:

$$\overline{H[\mathbf{s}]H[\mathbf{s}']} = Nf(q_{\mathbf{s},\mathbf{s}'}). \tag{3}$$

Polynomial functions $f(q)$ with positive coefficients correspond to Hamiltonians representable as a sums of independent monomials of the kind (1). Depending on the function f the model can undergo either 'continuous replica symmetry breaking' or 'discontinuous' one. If the function $g(q) = (f''(q))^{-3/2} f'''(q)$ is *monotonically increasing* with q in the interval [0,1], we are in the first case and we find a low temperature phase characterized by a continuous Parisi function $q(x)$[1]. If otherwise the function g *monotonically decreasing* one finds $q(x)$ to be a single step function in the spin glass phase. Throughout this paper, if not stated otherwise, we will consider this second case; we will also always consider functions f such that $f'(0) = 0$. Here the asymptotic off-equilibrium dynamics and the statics lead to different results as far as the expect ed values mentioned in the introduction are concerned. Notably it is found for the energyat temperatures less than a dinamical critical temperature T_D: $\lim_{t\to\infty} E_{Dyn}(t) > E_{Gibbs}$, where $E_{Dyn}(t)$ is the energy computed in the infinite volume limit starting from a random initial configuration .

For further reference we give here the result of standard static and dynamic analysis for the generalized spherical model.

2.1 Statics

From the standard study of the equilibrium measure of the model by means of the replica method it is find a free energy functional given (in standard notations) by the one step RSB form

$$\begin{aligned} F &= -\frac{T}{N} \log Z \\ &= -\frac{1}{2} \left\{ \beta [f(1) - (1-x) f(q)] + T \log(1-q) - T \frac{1}{x} \log \left(\frac{1-q}{1-(1-x)q} \right) \right\} \end{aligned} \tag{4}$$

q and x are variational parameters with respect to which F has to be maximized. In the high temperature phase q is equal to zero, and it is discontinuous at the transition point $T = T_S$, where $x = 1$ and q verifies:

$$\beta_S^2 f(q) + \log(1-q) + q = 0 \qquad \beta_S^2 f'(q) - \frac{q}{1-q} = 0. \tag{5}$$

[1]It has been observed in [12] that the model with $f(q) = (1/2)(q^2 + q^4)$ has the same critical behaviour the SK spin-glass.

2.2 Off-equilibrium dynamics

One studies here the Langevin dynamics associated to the model with random initial condition. The system is analyzed supposing that the thermodynamic limit is taken *before* the infinite time limit, so as to prevent full equilibration in presence of a phase transition.

The relevant objects of investigation (order parameters) turn out to be the correlation function $C(t,t') = 1/N \sum_i s_i(t)s_i(t')$, and its associated response function $G(t,t') = 1/N \sum_i \frac{\delta s_i(t)}{\delta h_i(t')}$ (here and in what follows $t \geq t'$). One finds then the set of coupled equations:

$$\frac{\partial G(t,t')}{\partial t} = -\mu(t)G(t,t') + \int_0^t ds\ f''(C(t,s))G(t,s)(G(t,t') - G(s,t'))\ , \quad (6)$$

$$\begin{aligned}
\frac{\partial C(t,t')}{\partial t} &= -\mu C(t,t') + \int_0^{t'} ds\ f'(C(t,s))\ G(t',s) \\
&+ \int_0^t ds\ f''(C(t,s))G(t,s)\ (C(t,t') - C(s,t'))\ , \\
\mu(t) &= \int_0^t ds\ f'(C(t,s))\ G(t,s) \\
&+ \int_0^t ds\ f''(C(t,s))G(t,s)\ (C(t,t) - C(s,t))\ + T.
\end{aligned} \quad (7)$$

Following the analysis of [3] for the p-spin model, one finds that for large times, two regimes are important: a first one in which one takes the limit $t, t' \to \infty$ fixing to a finite value the difference $\tau = t - t'$ and a second one where the limit is taken fixing the ratio $\lambda = h(t')/h(t)$. h is a function that at present the theory is not able to specify.

- In the first regime the correlation function decays with τ from the value one to a finite value q (dynamic Edward-Anderson parameter) and the fluctuation dissipation relation $TG_{as}(\tau) = -\partial C_{as}/\partial\tau$ is satisfied.

- In the second regime one finds a non time homogeneous form $C(t,t') = \mathcal{C}(h(t')/h(t))$, with $\mathcal{C}(\lambda)$ monotonically increasing with λ and $\mathcal{C}(1) = q$ and $\mathcal{C}(0) = 0$. The response function is equal in this regime to $TG(t,t') = x\frac{\partial C(t,t')}{\partial t'}$. The constant x is found to be a number between zero and one in the low temperature phase. The parameters q and x are solution of the equations:

$$x = \frac{1-q}{q}\left[\frac{qf''(q)}{f'(q)} - 1\right]; \qquad \beta^2 f''(q)(1-q)^2 = 1. \quad (8)$$

The dynamical transition is marked by the condition $x = 1$ at $T = T_D$, and one can check that $T_D > T_S$. The first of eq. (8) is equivalent to the variational equation $\partial F/\partial q = 0$ in statics, while the second one coincides with the condition that 'replicon eigenvalue' of the fluctuation matrix in replica space is equal to zero. We will refer to that equation as marginality condition.

2.3 TAP approach

For completeness we mention a third approach that is useful to investigate the system. This is the one of the TAP equations, in which one writes mean field equations for the magnetizations for fixed disorder. Using the diagrammatic approach of [13], based on the skeleton expansion introduced in [14], one easily finds the TAP free energy function:

$$F_{TAP}[\mathbf{m}, q] = \frac{1}{N} H[\mathbf{m}] - \frac{T}{2} \log(1-q) - \frac{\beta}{2}[f(1) - f(q) - (1-q) f'(q)] \tag{9}$$

where the variables m_i represent the average magnetizations, and the self-overlap q is given by $1/N \sum_i m_i^2$. The physical states are solutions of variational equations both with respect to the m's and q.

In the p-spin model it was found useful [15] to rescale the variables to

$$m_i \to \sqrt{q} s_i \quad \frac{1}{N} \sum_i s_i^2 = 1. \tag{10}$$

It then follows from (1) that

$$H[\mathbf{m}] = q^{p/2} H[\mathbf{s}] \tag{11}$$

The points of extreme of F_{TAP} with respect to the s_i, as well as their order in free energy do not depend on temperature [15]. Let us stress here that this is a highly non generic property which depends critically on the homogenity of the Hamiltonian (1). In general we can expect the order of the solutions to depend on temperature. The situation in which this happens for the lowest states is usually called chaotic in the literature [16], and has been recently fully demonstrated in the SK model [17]. A complete analysis of the TAP equations equations is at present missing. In section 4 we will find evidence for chaos with respect to temperature in spherical models with the method we propose in the next section.

3 The Method

We now introduce the "potential", our basic tool of analysis in this paper.

We consider an arbitrary configuration of the spins $\mathbf{s}$, drawn as a typical realization of the canonical probability distribution at temperature T', $P_{Can}[\mathbf{s}] = \exp(-\beta' H[\mathbf{s}])/Z(T')$. WE can then compute the cost in free energy at a temperature T (in general different from T') to keep the system at a fixed overlap $\tilde{p} = q_{s,\sigma}$ with s; namely

$$V = -\frac{T}{N} \log Z[\mathbf{s}; \tilde{p}] - F[T]; \tag{12}$$

$$Z[\sigma; \tilde{p}] = \int \mathrm{d}\sigma \exp\left(-\beta H[\sigma]\right) \delta\left(\tilde{p} - q_{\mathbf{s},\sigma}\right) \tag{13}$$

where $F[T]$ is the free energy without constraint. As Z in (13) is a sum of positive terms, V in (12) is a positive quantity. It is reasonable to suppose that V in addition of being self-averaging with respect to the quenched disorder in the Hamltonian, it is also self-averaging with respect to the probability distribution of the reference configuration $\mathbf{s}$. In this problem the spins s_i are quenched variables on the same foot as the random Hamiltonian itself. In this respect the present method allows to extend and improve the analysis of ref. [18], where there were considered different 'real replicas' coupled in a symmetric way.

We need then, in order to compute V, to perform the average over the Hamiltonian and the reference configuration $\mathbf{s}$.

$$NV = \overline{\frac{1}{Z[\beta']} \int \mathrm{d}\mathbf{s} \exp\left(-\beta' H[\mathbf{s}]\right) \left[-T \log Z[\mathbf{s}; \tilde{p}] - F[T]\right]}. \tag{14}$$

This average can be done with the aid of replica method. We found two strategies which consistently lead to the same results. The first one is based on the formula

$$NV = -T \lim_{n\to 0} \lim_{R\to 1} \overline{\frac{\partial}{\partial R} \left\{ \sum_s \exp\left(-\beta' H[\mathbf{s}]\right) Z[\mathbf{s}; \tilde{p}]^{R-1} \right\}^n}. \tag{15}$$

One then evaluates the average for integer R and n and obtains V by analytic continuation.

The starting point of the second strategy is the formula

$$NV = -T \lim_{n\to 0} \lim_{m\to 0} \overline{\sum_s \exp\left(-\beta' H[\mathbf{s}]\right) Z[\beta']^{n-1} \left(\frac{Z[\mathbf{s}; \tilde{p}]^m - 1}{m}\right)} \tag{16}$$

and again one performs an analytic continuation from integer n and m. The use of one procedure instead of the other is mainly a matter of taste. We will sketch the first stages of the formal manipulations for both the procedures, and we will treat our model with the second one.

Let us start with the first procedure. The replicated partition function is:

$$Z_1^{(n,R)} = \overline{\int \mathrm{d}\mathbf{s}^{a,r} \exp\left[\beta' \sum_{a=1}^{n} H[\mathbf{s}^{\mathbf{1},\mathbf{a}}] + \beta \sum_{a=1}^{n}\sum_{r=2}^{R} H[\mathbf{s}^{\mathbf{r},\mathbf{a}}]\right] \prod_{a=1}^{n}\prod_{r=2}^{R} \delta\left(\sum_i s_i^{1,a} s_i^{r,a} - N\tilde{p}\right)}. \tag{17}$$

One can then perform the average over the distribution of the Hamiltonian, and introduce the order parameters:

$$\mathbf{Q}_{(a,r),(b,s)} = \frac{1}{N}\sum_i s_i^{r,a} s_i^{s,b}. \tag{18}$$

The logarithm of $Z_1^{n,R}$ divided by N is then found to be equal to the saddle point over the Q's of

$$\frac{1}{2}\sum_{r,s}^{1,R}\sum_{a,b}^{1,n} \beta^r \beta^s f(\mathbf{Q}_{(a,r),(b,s)}) + \frac{1}{2}\mathrm{Tr}\log\mathbf{Q} \tag{19}$$

where $\beta^r = \beta'$ for $r = 1$, $\beta^r = \beta$ for $r = 2, ..., n$. As usual one needs a scheme to perform the analytic continuation in the number of replicas.

With the second procedure, one has

$$Z_2^{(n,m)} = \overline{\int \mathrm{d}\mathbf{s}^a \int \mathrm{d}\sigma^\alpha \exp\left[\beta' \sum_{a=1}^{n} H[\mathbf{s}^{\mathbf{a}}] + \beta \sum_{\alpha=1}^{m} H[\sigma^\alpha]\right] \prod_{\alpha=1}^{m} \delta\left(\sum_i s_i^1 \sigma_i^\alpha - N\tilde{p}\right)}. \tag{20}$$

After the average over the distribution of the Hamiltonian is performed, one introduce the order parameter matrices:

$$Q_{ab} = \frac{1}{N}\sum_i s_i^a s_i^b \tag{21}$$

$$R_{\alpha\beta} = \frac{1}{N}\sum_i \sigma_i^\alpha \sigma_i^\beta \tag{22}$$

$$P_{a\alpha} = \frac{1}{N}\sum_i s_i^a \sigma_i^\alpha \tag{23}$$

with $a, b = 1, ..., n$ and $\alpha, \beta = 1, ..., m$. Combining the order parameters in the single $(n + m) \times (n + m)$ matrix

$$\mathbf{Q} = \begin{pmatrix} Q & P \\ P^T & R \end{pmatrix} \tag{24}$$

one finds

$$\frac{1}{N}\log Z_2^{(n,m)}=\frac{1}{2}\left[\sum_{a,b}^{1,n}\beta'^2 f(Q_{a,b})+\sum_{\alpha,\beta}^{1,n}\beta^2 f(R_{\alpha,\beta})+2\sum_{a,\alpha}^{1,n}\beta\beta' f(P_{a,\alpha})\right]+\frac{1}{2}\mathrm{Tr}\log\mathbf{Q}. \tag{25}$$

Observing that the constraint implies $P_{1,\alpha}=\tilde{p}$ for any $\alpha=1,...,m$, a sensible ansatz is to assume that the matrix P has elements $P_{a,\alpha}\equiv P_a$ independent of α for any a. A simple computation based on the formula $\mathrm{Tr}\log(\mathbf{Q})\sim\log\left(\int \mathrm{d}\mathbf{x}\exp(-\mathbf{x}\mathbf{Q}\mathbf{x})\right)$ reveals then the identity:

$$\mathrm{Tr}\log[\mathbf{Q}]=\mathrm{Tr}\log[Q]+\mathrm{Tr}\log[R-A] \tag{26}$$

where A is a $m\times m$ matrix with all the elements equal to $A_{\alpha,\beta}=\sum_{a,b}P_a(Q^{-1})_{ab}P_b$.

Note that with this ansatz for P, $\mathrm{Tr}\log[Q]$ is of order n, while $\mathrm{Tr}\log[R-A]$ is of order m. So, neglecting terms of order m one finds that the equation specifying the matrix Q is just

$$\beta'^2 f'(Q_{ab})+(Q^{-1})_{ab}=0 \tag{27}$$

which is independent of P and R and is just the saddle point equation for a system at equilibrium at temperature T'. This is a good consistency check for the ansatz: the $\mathbf{s}$ system, which is at equilibrium, should not be affected by the σ system. The variational equations for P and R are respectively written as

$$-2\beta\frac{\partial V}{\partial P_a} = \beta\beta' f'(P_a)+\sum_b (Q^{-1})_{ab}P_b\sum_{\alpha,\beta}\left((R-A)^{-1}\right)_{\alpha\beta}=0 \tag{28}$$

$$-2\beta\frac{\partial V}{\partial R_{\alpha\beta}} = \beta\beta' f'(R_{\alpha\beta})+\left((R-A)^{-1}\right)_{\alpha\beta}=0 \tag{29}$$

For $a=1$ the l.h.s. of equation (28) represents the derivative of V with respect to $\tilde{p}$ and has not to be equated to zero. We note that for $\tilde{p}=0$ the solution to (28) is simply $P_a=0$ for any a. One has then $\frac{\partial V}{\partial\tilde{p}}=0$ and the potential takes its minimal value $V=0$.

To solve the equations (28,29) for $n,m\to 0$, it is of course needed a continuation scheme for the various order parameter matrices. For Q the usual hierarchical ansatz [6] has to be employed. A sensible choice is to take also the matrix R of the hierarchical form (with associated Parisi function $r(x)$), and the vector with components P_a, as the first line of a hierarchical matrix P^*_{ab} associated to the diagonal element $\tilde{p}$ and to a function $p(x)$. Although this general form can be of interest for many probems, notably whenever RSB is necessary to find the free energy, we will see later that a replica symmetric ansatz will be enough for the problem addressed in this paper, at least for the class of models we consider.

In the next section we will devote a lot of attention to the points of minimum of the potential $V(\tilde{p})$. The basic theses of this paper is that the minima of the potential correspond to metastable states.

Before leaving this section we just comment on the fact that in the case of continuous RSB transition where the probability distribution $P(q)$ is different from zero in a whole interval $q_{min} \le q \le q_{max}$, we checked that as it has to be expected, the potential is flat and equal to zero in the whole interval $[q_{min}, q_{max}]$.

4 The potential in the intermediate regime.

We study in this section the properties of the potential when the system $\mathbf{s}$ is in the high temperature phase, and the order parameter matrix is replica symmetric and given by $Q_{a,b} = \delta_{a,b}$. According to the picture proposed in [19, 15, 13] for $T_D \le T$ this replica symmetric phase does not describe an ergodic phase, but a situation in which there are an exponentially large number of states, with zero overlap among each other [19]. The triviality of the Parisi probability function $P(q) = \delta(q)$, implied by the replica symmetric solution, is just due to entropic reasons. It is then natural to suppose for P and R a replica symmetric structure with

$$\begin{aligned} P_a &= \delta_{a,1}\tilde{p} \\ R_{a,b} &= \delta_{a,b} + (1-\delta_{a,b})r. \end{aligned} \tag{30}$$

The insertion in (25) gives for the potential

$$V = -\frac{1}{2\beta}\left\{2\beta\beta' f(\tilde{p}) - \beta^2 f(r) + \log(1-r) + \frac{r-\tilde{p}^2}{1-r}\right\} \tag{31}$$

where r is the only parameter with respect to which the potential has to be maximized. The maximization equations (28,29) reduce to the single equation

$$\beta^2 f'(r) = \frac{r-\tilde{p}^2}{(1-r)^2}. \tag{32}$$

It turns out that for any concrete form of the function f that we have analyzed that this equation admits a unique solution in the range of β' where the replica symmetry is not broken. As we stressed in the previous sections the points of extremum of V with respect to $\tilde{p}$ are of particular importance in our analysis, the minima correspond to stable or metastable states in which the system can be trapped. Let us then write the equation that specifies the points of extremum:

$$\beta\beta' f'(\tilde{p}) = \frac{\tilde{p}}{1-r} \tag{33}$$

We stress again that the point $r = \tilde{p} = 0$ is always a solution of (33,32), and is always an absolute minimum with $V = 0$.

Let us start our analysis considering the case of equal temperatures $T' = T$. In this case the qualitative features of the potential are largely model independent. In figure 1 we show the picture of the potential for four different temperatures in the case $f(q) = q^3/2$, similar plots are obtained for arbitrary functions. From top to bottom, they represent the potential at temperature higher then T_D, equal to T_D between T_D and T_S, and right at T_S. We can see from the figure that for $T > T_D$ the potential is monotonically increasing, and the only extremum of the potential is the minimum at $\tilde{p} = 0$. At the temperature T_D where the dynamical transition happens, the potential develops for the first time a minimum with $\tilde{p} = r$. It is interesting to observe that the energy in this flex point [2] is equal to the asymptotic value of the energy in the off equilibrium dynamics. The same is true for the parameter r which turns out to be equal to the dynamical Edward-Anderson parameter.

The condition for the potential of having a flex coincides with the marginality condition. Indeed the flex implies a zero eigenvalue in the longitudinal sector and at $x = 1$ the replicon and the longitudinal eigenvalues are degenerate (see for example the formulae in ref. [20]). This marginality condition is well known to give exact results for the transition temperatures in p-spin spherical models. It also give accurate results, compared with the Monte Carlo, in the case of the Ising model with random orthogonal matrix [20] (ROM model).

We have observed that in general more then one minimum can be present in the potential. In the p-spin model it happens that two minima develop at the same point. The rightmost one, that we will call primary is the one with $\tilde{p} = r$, while the other, secondary, has $\tilde{p} < r$. For temperatures smaller than T_D the minima have a finite depth, i.e. are separated by extensive barriers from the absolute minimum.

The primary minimum is easily interpreted. There the system denoted by s is in the same pure state as the system σ. In the region $T_S < T < T_D$ the number of

[2] See the following for the definition.

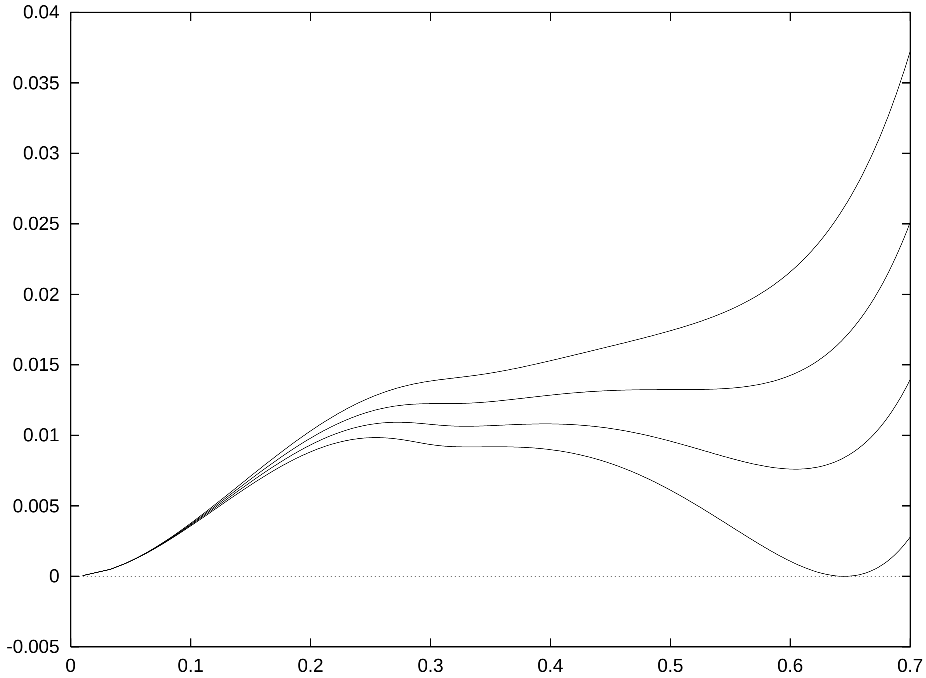

Figure 1: The potential function in the $p = 3$-spin model for $T = T'$ and various temperatures. From top to bottom $\beta = 1.59, \beta = \beta_D = 1.63, \beta = 1.66, \beta = \beta_S = 1.70$,. Observe that a minimum is first present at the dynamical temperature, and the value of the minimum of potential at the statical temperature is zero.

pure states is exponentially large in N: $\mathcal{N} = e^{N\Sigma(T)}$. Consequently the probability of finding two system in the same state is exponentially small and proportional to $e^{-N\Sigma(T)}$. The free energy cost to constrain two systems to be in the same state is then proportional to the logarithm of this probability, namely we have

$$V_{primary} = T\Sigma(T). \tag{34}$$

Coherently at the statical transition temperature $T = T_S$ one finds $V_{primary} = 0$. The quantity Σ has been computed for the p-spin model in ref. [13] as the number of solution of the TAP equation with given free energy and coincides with our calculation. The secondary minima, could aso be associated to metastable states, but at present we do not have an interpretation for them. This conclusion on the equivalence of the potential with the number of solution of the TAP equation hold also in the ROM [21], and it has been argued by in ref. [8] on general grounds.

The study of the potential for temperatures smaller than T_S would require to take into account RSB effects, which would complicate a bit the analysis. However it is physically clear that the shape of the potential in that region it is not different qualitatively from the one at $T = T_S$. It has a minimum where $r = \tilde{p}$ are equal to the Edwards Anderson parameter and the value of potential is zero.

In the case of different temperatures $T \neq T'$ the properties of the potential depend on the presence or absence of chaos with respect to temperature changes. The primary minimum of the potential if it exists, reflects the properties of the states which are of equilibrium at temperature T' when they are followed at temperature T. In the p-spin model, where the order of the levels do not depend on the temperature, and each level has temperature independent complexity, the value of the potential in the primary minimum can be related to the properties of the solutions to the TAP equations when they are followed in temperature. Denoting by $F_{TAP}(T, E')$ the free energy of the TAP states that dominate at temperature T' when they are followed at temperature T, we find:

$$V_{primary} = -T\Sigma(T') + F_{TAP}(T, E') - F(T) \tag{35}$$

where $F(T)$ is the free energy at temperature T and $F_{TAP}(T, E')$ is the TAP free energy at temperature T of the states which are of equilibrium at temperature T'. We also note that q is equal to the EA parameter of the aforementioned TAP solution. Of particular interest is the case $T' = T_D$ where the primary minimum is marginally stable for any value of T, and has energy, defined as $E_{primary} = (\partial/\partial\beta)\beta[V_{primary} - F(T)]$

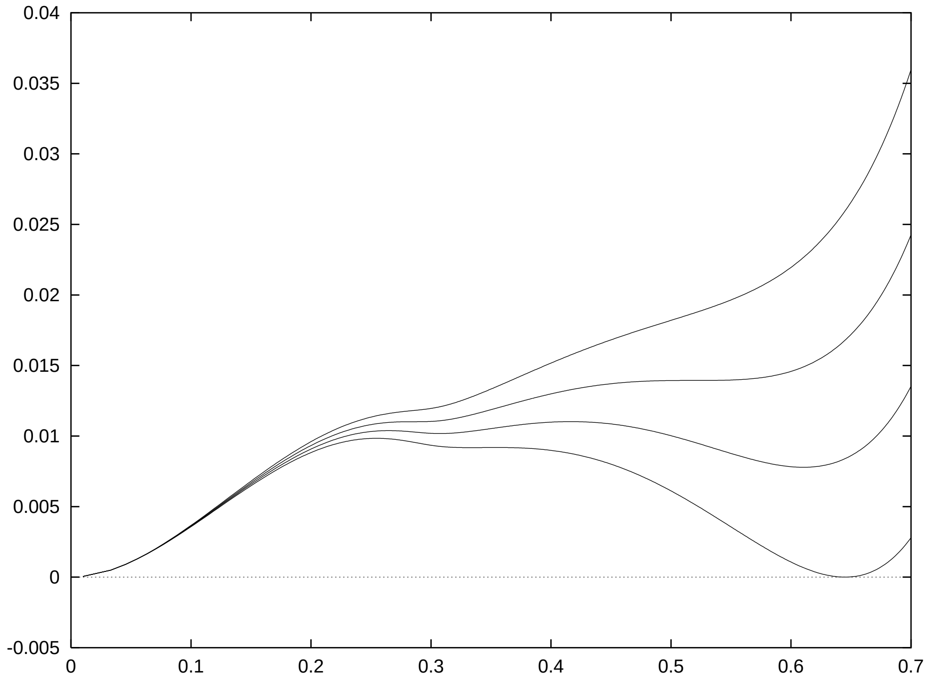

Figure 2: The potential for the $p = 3$-spin model and different temperature. The curves are drown for $\beta = \beta_s$ and, from top to bottom, $\beta' = 1.59$, $\beta' = \beta_D = 1.63$, $\beta' = 1.66$, $\beta' = \beta_S = 1.70$.

and EA parameter equal to the these of the off-equilibrium asymptotic state. In figure 2 we show the potential for $p = 3$ at fixed $\beta = (\beta_D + \beta_S)/2$, and various values β'. For a given T' the minimum exists in the range of temperatures for which the corresponding solutions to the TAP equations exist.

In the case models with inhomogeneous Hamiltonian the situation for $T \neq T'$ is different. We did not try a systematic study of this case and we concentrated on the case of a $3+4$ spin model with $f(q) = (1/2)(q^3 + \epsilon q^4)$. The first thing that we note in this case is that the horizontal flex present for $T = T' = T_D$ disappears as soon as, for $T' = T_D$ we take $T \neq T_D$. For $T' < T_D$ it exists an interval of values of T around T' in which the minimum exists. In figure 3 we display the potential of the 3+4 model for fixed $T' < T_D$ and various values of T.

One might wonder if the point of horizontal flex of the potential are associated to the dynamical state as it happens in the p-spin model. To do that we have looked at values of T and T' such that the marginality condition $\beta^2(1-r)^2 f''(r) = 0$ was verified in the minimum of the potential. In that points we found that the minimum has a finite depth and the energy does not coincide with that of the dynamical

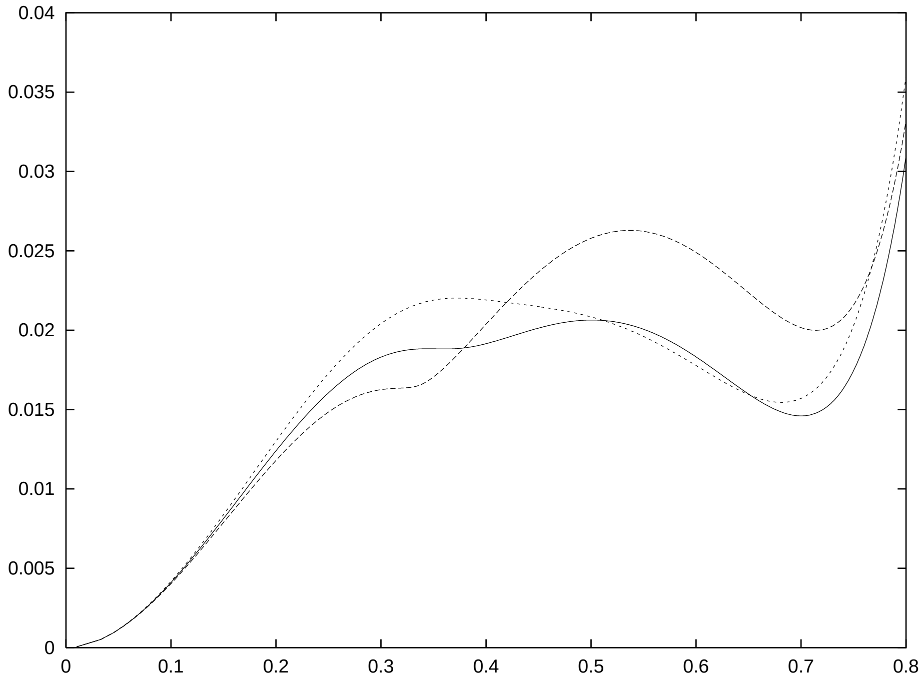

Figure 3: The potential for $f(q) = 1/2(q^3 + q^4)$ for $\beta' = (\beta_D + \beta_s)/2 = 1.27$ and $\beta = 1.21$ (dots) $\beta = 1.31$ (full line) and $\beta = 1.41$ (dashes).

states.

It is tempting to interpret the minima of the potential as the properties of equilibrium TAP solutions at temperature T' when followed at temperature T, we are however very cautious on this point due to the possibility of crossing of the solutions in free-energy. Let us just mention that this should be valid below the static transition ($T' < T_S$) where the lowest TAP states dominates the partition sum, and where there can not be crossing. Chaos with respect to temperature implies that the free energy of these solutions at temperature T will be typically higher then that of the equilibrium solution. One could expect that the minimum of the potential has a value higher then zero for any $T \neq T'$. We aspect then that $V_{primary}(T, T') \approx (T - T')^{2k}$, with integer k.

5 Dynamics

We study now the relaxation dynamics at temperature T of a system starting its evolution at time zero from an equilibrium configuration at temperature T'. We start from the usual Langevin equation for the model

$$\begin{aligned}
\frac{\mathrm{d}s_i(t)}{\mathrm{d}t} &= -\mu(t)s_i(t) - \frac{\partial H}{\partial s_i} + \eta_i(t) \\
\langle \eta_i(t)\eta_j(t')\rangle &= 2T\delta_{ij}\delta(t-t')
\end{aligned} \tag{36}$$

As usual the time dependence of $\mu(t)$ is chosen to enforce the spherical constraint $|\mathbf{s}|^2 = N$ at any time. The dynamical generator of the correlation function [22], averaged over the initial condition is

$$Z_{Dyn} = 1 = \overline{\begin{array}{l} \int \mathcal{D}\eta \mathcal{D}s \mathcal{D}\hat{s} \frac{1}{Z(T')} \exp\{-\beta' H[s(0)]\} \cdot \\ \exp\left[\int_0^t \mathrm{d}t' \sum_i i\hat{s}_i(t')[\dot{s}_i(t') + \frac{\partial H}{\partial s_i} + \mu(t)s_i(t') + Ti\dot{s}_i(t')]\right] \end{array}} \tag{37}$$

The term $1/Z(T')$ obliges us to introduce replicas to perform the quenched average. One possible way is to start from the average of the logarithm of Z_{Dyn} and replicate the system at each time [23]. We follow here a different route, using the relation $1/Z = \lim_{n\to 0} Z^{n-1}$ and replicating only the system at time zero. So, "replica number 1" will be present at all times, while replicas 2 to n will only be present at time zero. We will denote as $s_i^a(0)$ the spins of the a-th replica at time zero. Coherence would require the notation $s_i^1(t)$ for the value of the spins at time t; we will use instead $s_i(t)$. Using standard manipulations to average over the disorder we find

$$\begin{aligned}
Z_{Dyn} = \quad & \int \mathcal{D}s\mathcal{D}\hat{s} \exp\left[\sum_{a,b}^{1,n} \beta'^2 f(\mathbf{s}_a(0)\cdot \mathbf{s}_b(0)/N) - \frac{\mu}{2}\sum_{a,i} s_i^a(0)^2\right] \\
& \exp\left[\int_0^t \mathrm{d}t' \sum_i \hat{s}_i(t')[i\dot{s}_i(t') + Ti\dot{s}_i(t')]\right] \\
& \exp\left[\int_0^t \mathrm{d}t'\mathrm{d}t'' f'(\mathbf{s}(t')\cdot\mathbf{s}(t'')/N) \sum_i i\hat{s}_i(t') i\hat{s}_i(t'') + \right. \\
& \left. f''(\mathbf{s}(t')\cdot\mathbf{s}(t'')/N)\mathbf{s}(t')\cdot i\hat{\mathbf{s}}(t'')/N \sum_i i\hat{s}_i(t')s_i(t'')\right] \\
& \exp\left[\beta' \sum_a \int_0^t \mathrm{d}t' f'(\mathbf{s}(t')\cdot\mathbf{s}_a(0)/N)\sum_i i\hat{s}_i(t')s_i^a(0)\right]
\end{aligned} \tag{38}$$

Introducing the correlation function $C(t',t'') = \mathbf{s}(t')\cdot\mathbf{s}(t'')/N$, the response $G(t',t'') = \mathbf{s}(t')\cdot i\vec{\hat{s}}(t'')/N$ $(t' > t'')$ and the correlation with the initial condition $C_a(t') =$

$\mathbf{s}(t') \cdot \mathbf{s}_a(0)/N$, and observing that they are non-fluctuating quantities for $N \to \infty$, we recognize in (38) the dynamical generator functional of a system of N independent spins subject to the Langevin equation

$$\begin{aligned}
\frac{\mathrm{d}s_i(t)}{\mathrm{d}t} &= -\mu(t)s_i(t) + \int_0^t f''(C(t,t'))G(t,t')s_i(t') + \beta' \sum_{a=1}^{n} f'(C_a(t))s_i^a(0) + B_i(t) \\
\langle B_i(t)B_j(t')\rangle &= 2T\delta_{ij}\delta(t-t') + \delta_{i,j}f'(C(t,t'))
\end{aligned} \tag{39}$$

satisfying the self consistency equations:

$$\begin{aligned}
C(t,t') &= \mathbf{s}(t)\cdot\mathbf{s}(t')/N \\
G(t,t') &= \mathbf{s}(t)\cdot i\hat{\mathbf{s}}(t')/N \quad t > t' \\
C_a(t) &= \mathbf{s}(t)\cdot\mathbf{s}_a(0)/N.
\end{aligned} \tag{40}$$

It is easy to check that the "equilibrium part" in the action, involving the parameters $Q_{ab} = \mathbf{s}_a(0)\cdot\mathbf{s}_b(0)/N$ is not affected by the dynamics and, as it should, describes correctly the equilibrium at temperature T'. From the Langevin equation one derives the closed system:

$$\begin{aligned}
\frac{\partial G(t,t')}{\partial t} &= -\mu(t)G(t,t') + \int_0^t ds\ f''(C(t,s))G(t,s)(G(t,t')-G(s,t'))\ , \\
\frac{\partial C(t,t')}{\partial t} &= -\mu(t)C(t,t') + \int_0^{t'} ds\ f'(C(t,s))\ G(t',s) \\
&\quad + \int_0^t ds\ f''(C(t,s))G(t,s)\ (C(t,t')-C(s,t'))\ + \beta' \sum_a f'(C_a(t))C_a(t'), \\
\frac{\partial C_a(t)}{\partial t} &= -\mu(t)C_a(t) + \int_0^t ds\ f''(C(t,s))G(t,s)C_a(s) + \beta' \sum_b f'(C_b(t))Q_{a,b} \\
\mu(t) &= \int_0^t ds\ f'(C(t,s))\ G(t,s) + \int_0^t ds\ f''(C(t,s))G(t,s)\ (C(t,t)-C(s,t)) \\
&\quad +T\ + \beta' \sum_a f'(C_a(t))C_a(t),
\end{aligned} \tag{41}$$

with the conditions:

$$C_1(t) = C(t,0) \quad C_a(0) = Q_{1,a} \tag{42}$$

These equations differ from the usual off-equilibrium equations for the presence of terms which couple with the configuration at time zero. The matrix $Q_{a,b}$ has the usual hierarchical form, and $C_a(0)$ is its first row. It is then natural to assume that $C_a(t)$ continues at any time to have the structure of the first row of a hierarchical matrix. Once this ansatz is plugged in (41) we get a system of equations which admits for any time a unique solution.

The basic question that can be answered with the aid of these equations is whether starting from equilibrium at temperature T' the system equilibrates in a metastable state, or it ends up in an aging state. In this paper we will only consider non-aging solutions to the equations (41). We leave to future work the investigation of possible aging solutions.

We look then for solution where no aging appears, the correlation functions $C(t,t')$ tends for infinite times to the homogeneous function $C_{as}(t-t')$, and the response function is related to C_{as} via the fluctuation dissipation relation: $G_{as}(\tau) = -\beta \frac{\partial C_{as}(\tau)}{\partial \tau}$. In the high temperature regime $C_a(0) = 0$ and the equations coincide with the off equilibrium ones. Interesting phenomena appear for temperature $T' \leq T_D$. Let us study the case $T_S \leq T' \leq T_D$. Here we have $Q_{a,b} = \delta_{a,b}$, a bit of reflection on the equation for $C_a(t)$ reveals. that the replica structure of $C_a(t)$ is at any time of the kind

$$C_a(t) = \delta_{1,a} C(t,0). \tag{43}$$

Using then the notations:

$$\begin{aligned}\tilde{p} &= \lim_{t\to\infty} C(t,0) \\ r &= \lim_{\tau\to\infty} C_{as}(\tau) \\ \mu_\infty &= \lim_{t\to\infty} \mu(t)\end{aligned} \tag{44}$$

one finds for $C_{as}(\tau)$ the equation

$$\frac{\partial C_{as}(\tau)}{\partial \tau} = -\mu_\infty C_{as}(\tau) + \beta[f'(1)C_{as}(\tau) - f'(r)r] - \beta \int_0^\tau f'(C_{as}(\tau+\tau')) \frac{\partial C_{as}(\tau')}{\partial \tau'} + \beta' \tilde{p} f'(\tilde{p}). \tag{45}$$

While $\tilde{p}, r, \mu_\infty$ are solution of the following system

$$\begin{aligned}&-\mu_\infty \tilde{p} + \beta \tilde{p} \mu_\infty \beta' f'(\tilde{p}) = 0 \\ &-\mu_\infty r + \beta q[f'(1) - f'(r)] + \beta(1-r) f'(r) + \beta' \tilde{p} f'(\tilde{p}) = 0 \\ &-\mu_\infty + T + \beta[f'(1) - f'(r)r] + \beta' \tilde{p} f'(\tilde{p}) = 0.\end{aligned} \tag{46}$$

Eliminating μ_∞ we find the remarkable result that the equations specifying r coincide with the equations (32,33) of section 4 for the points of extremum of the potential.

We have seen in section 4 that depending on the form of f and on the temperatures T, T' solutions to (46) can exist or not. In the case in which such solutions

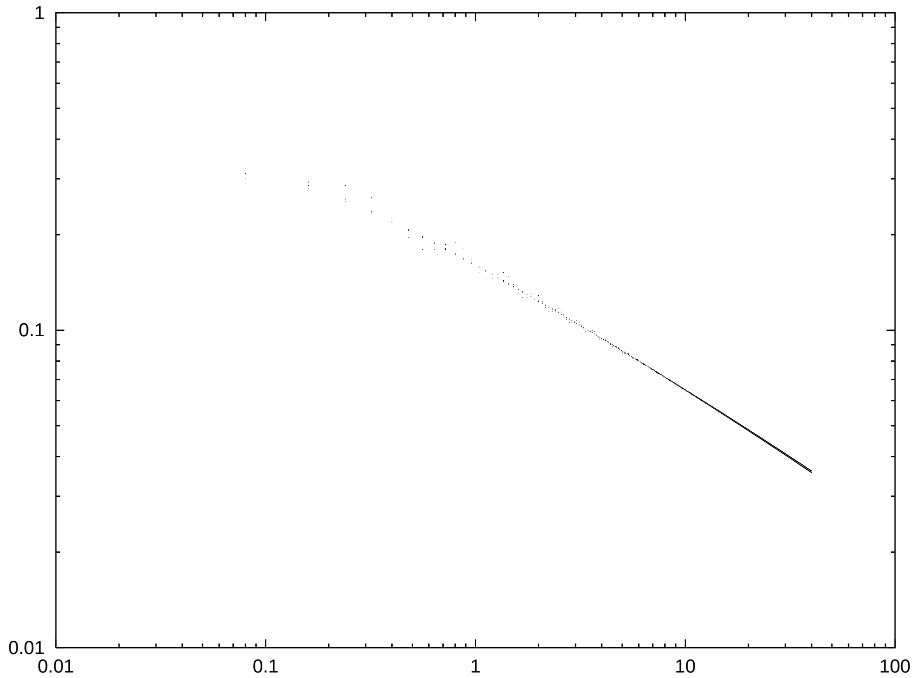

Figure 4: The convergence of $C(t,0)$ to $\tilde{p}$ for the 3+4 model in the case $T = 0.673$, $T' = 0.804$. We plot $C(t,0) - \tilde{p}$ as a function of t in a log-log scale, for $\tilde{p}$ we take the value in the primary minimum of the potential $\tilde{p} = .646$. $C(t,0) - \tilde{p}$ seems to approach zero as a power law. A similar plot is found for the energy as a function of time.

do not exist, we easily conclude that for long times an asymptotic aging regime sets in the system. To understand if this regime is correlated with the initial condition would require a more complete ansatz then the one we are using here and we leave it f or future work. In the case solutions with $\tilde{p} \neq 0$ exist, we need to show that the solution to (41) converge to one of the solution of (46) and to know to which one. The problem is easily solved for equal temperatures $T = T'$. If we start at equilibrium we stay there. We explicitly verified that the solution to the equations (41) is time translation invariant from the start. We belive that it a general fact that the dynamics tends toward the primary minimum of the potential. To verify that, we performed the numerical integration of the system (41) for $f(q) = 1/2(q^3 + q^4)$ with the method employed in [4]. Figure 4 shows the approach of $C(t,0)$ to $\tilde{p} = .646$ in the case $T = 0.673$, $T' = 0.804$. In the same way it is possible to see that the energy tends to the value predicted by the potential theory.

6 Conclusions

In this paper we have investigated the free-energy landscape of a spherical spin-glass model, in the vicinity of equilibrium states.

The model is chosen in a way to have a low-temperature glassy phase characterized by a single step Parisi function $q(x)$. The study is performed introducing the 'potential function' defined as the minimal work needed to keep a system to a given distance from an equilibrium configuration. In this way we could identify the dynamical transition temperature as the point where first appear a minimum in the potential function at equal temperatures.

In the p-spin model, where the Hamiltonian is an homogeneous function and there is not chaos with respect to temperature changes, the dynamical states for $T < T_D$ can be associated to the points where the potential has a flex. This property is not true any longer whenever chaos is present in the model. In that case, we do not have a recipe to associate properties of the dynamic asymptotic state to some particular point in the phase space of our coupled system.

The minima of the potential have been associated to metastable states. The life of the metastable states can be estimated arguing that the free-energy barrier is just given by the maximum to minimum difference in the potential [7], which is then proportional to the size of the system N. It is interesting to remind here the result of the analysis in [7] in finite dimension. In that case the order parameter is space dependent. The free energy barrier can be estimated with instantonic techniques (see e.g. ref. [24]), introduced in the the contest of spin glass models in [25]. It turns out that in three dimensions the relaxation time of the metastable states scales as $\tau_{max} \sim \mathrm{e}^{\frac{const}{(T-T_s)^2}}$, to be compared with the Vogel-Fulcher law $\tau_{max} \sim \mathrm{e}^{\frac{const}{(T-T_s)}}$, often used to fit the temperature dependence of the viscosity near the glassy transition in structural glasses.

Let us conclude the paper noting that simple generalizations of the potential method would allow to gain further insight on the free-energy landscape of spin-glass models. For example one can consider the free energy cost of a situation where there is a first replica at equilibrium at a given temperature, a second one, at another temperature, is kept at a fixed distance from the first one, and a third replica, at a third temperature kept at fixed distances from the first two.

Also, it would be very interesting to generalize our calculation to models with continuous RSB, to study the property of chaos with respect to temperature changes in that case.

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References

[1] A review on experiments on off equilibrium dynamics of spin glasses can be found in: E. Vincent, J. Hammann and M. Ocio, chapter 7 (p. 207–236) of *Recent Progress in Random Magnets*, D. H. Ryan editor, World Scient., Singapore 1992.

[2] A review on numerical simulations on off equilibrium dynamics in spin glass models can be found in: H. Rieger, in *Annual Reviews of Comp. Phys. II*, ed. D. Stauffer, World Scientific, Singapore (1995).

[3] L.F. Cugliandolo and J. Kurchan, Phys.Rev.Lett.**71** (1993) 173;

[4] S. Franz, M. Mézard, Europhys. Lett. **26** (1994) 209; Physica **A210** (1994) 48

[5] L.F. Cugliandolo and J. Kurchan, J.Phys A **27**, 5749 (1994)

[6] M. Mézard, G. Parisi, and M.A. Virasoro, "Spin glass theory and beyond", World Scientific (Singapore 1987);

[7] G.Parisi preprints cond-mat/9411115, cond-mat/9412004

[8] R.Monasson, preprint *The structural glass transition and the entropy of the metastable states* (March 1995).

[9] E. Marinari, G. Parisi and F. Ritort, work in progress.

[10] T.R. Kirkpatrick, D. Thirumalai, Phys. Rev. **B36**, (1987) 5388; A. Crisanti, H.J.Sommers, Z. Phys. B **87** (1992) 341.

[11] M. Mézard and G. Parisi, *J.Phys.A* **23**, L1229 (1990); *J. Physique. I* **1**, 809 (1991);

[12] Th.M. Nieuwenhuizen preprint cond-mat/9408056

[13] A.Crisanti, H.Sommers, preprint cond-mat/9406051

[14] C. DeDominicis, J. Math. Phys. **4** (1963) 255;

[15] J.Kurchan, G.Parisi, M.A. Virasoro, J.Physique I **3** (1993) 1819

[16] I.Kondor, J.Phys. A **22** (1989) L163, I.Kondor, A. Végsö, J.Phys. A **26** (1993) L641

[17] S.Franz, M.Ney-Nifle preprint cond-mat/9412083

[18] S.Franz, G.Parisi, M.A. Virasoro, J.Physique I **2** (1992) 1969, Europhys.Lett. **22** (1993) 405

[19] T.R. Kirkpatrick and D. Thirumalai, Phys.Rev.Lett. **58** (1987) 2091, Phys.Rev. **B38** (1987) 5388;

[20] E. Marinari, G. Parisi and F. Ritort, J. Phys. A **27** 7647 (1994).

[21] G. Parisi and M. Potters, cond-mat 9503009.

[22] P.C.Martin, E.D.Siggia, H.A. Rose, Phys.Rev. **A8** (1978) 423.

[23] A.Houghton, S.Jain, P.Young, Phys. Rev. **B28** (1983) 2630.

[24] G.Parisi, *Statistical Field Theory* Addison Wesley 1988

[25] S.Franz, G.Parisi, M.A. Virasoro, J.Physique I **4** (1994) 1657