

Dynamics within metastable states in a mean-field spin glass

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1996 J. Phys. A: Math. Gen. 29 L81

(<http://iopscience.iop.org/0305-4470/29/5/001>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.71

The article was downloaded on 02/06/2010 at 04:08

Please note that [terms and conditions apply](#).

LETTER TO THE EDITOR

Dynamics within metastable states in a mean-field spin glass

A Barrat, R Burioni and M Mézard

Laboratoire de Physique Théorique de l'Ecole Normale Supérieure†, 24 rue Lhomond, 75231 Paris Cedex 05, France

Received 6 December 1995

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 static approach, we use dynamics: starting from an initial condition thermalized at a temperature between the static 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 , $i \in \{1, \dots, N\}$ which interact through the Hamiltonian

$$H(s) = - \sum_{1 \leq i_1 < \dots < i_p \leq N} J_{i_1, \dots, i_p} s_{i_1} \dots s_{i_p} \quad (1)$$

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.

† Unité propre du CNRS, associée à l'Ecole Normale Supérieure et à l'Université de Paris Sud, Paris, France.

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]

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

where the angular energy is

$$E^0(\{\hat{s}_i\}) \equiv - \sum_{1 \leq i_1 < \dots < i_p \leq N} J_{i_1, \dots, i_p} \hat{s}_{i_1} \dots \hat{s}_{i_p}. \quad (3)$$

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^α one zero temperature state, of energy E_α^0 , it gives rise at finite temperature T to one TAP state α given by

$$m_i^\alpha = \sqrt{q(E_\alpha^0, T)} \hat{s}_i^\alpha \quad (4)$$

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

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

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, $E^0 = E_\alpha^0$ and of the self-overlap, $q = q_\alpha \equiv q(E_\alpha^0, T)$. The corresponding energy is

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

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 $T_{\max}(E_{min}) \equiv T_{\text{TAP}}$. Above T_{TAP} , the only remaining state is the paramagnetic one with $q = 0$ and free energy $F_{\text{para}} = -1/(4T)$.

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

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

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:

$$Z = \int df \exp\left(-\frac{(f - T S_c(f, T))}{T}\right) \quad (8)$$

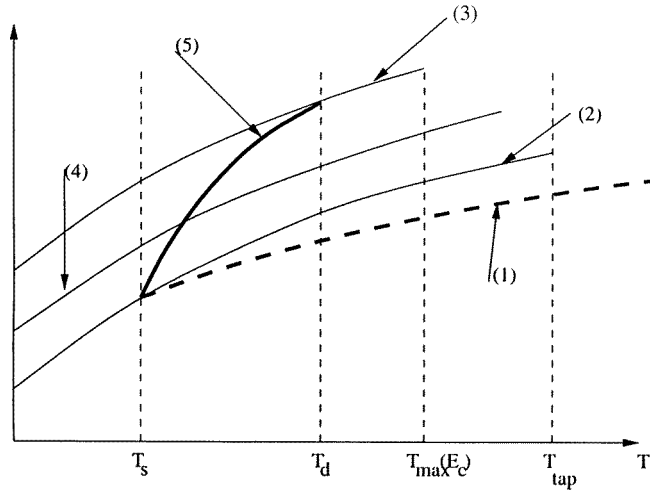


Figure 1. free energy versus temperature; (1) free energy of the paramagnetic solution for $t > t_d$, f_{tot} for $t < t_d$; (2) free energy of the lowest tap states, with zero temperature energy e_{min} ; (3) free energy of the highest tap states, corresponding to e_c ; (4) an intermediate value of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

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 $f = f_{\text{eq}}(T)$. Because of their extensive complexity, this gives for the total equilibrium free energy:

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

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 $f_{\text{eq}}(T')$. 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:

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

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

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

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 $t > t'$:

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

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): $C(t, t') =$

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

$$\frac{\partial C_{\text{eq}}(\tau)}{\partial \tau} = -\mu_{\infty} C_{\text{eq}}(\tau) - \frac{p}{2T} \int_0^{\tau} du C_{\text{eq}}^{p-1}(\tau - u) \frac{\partial C_{\text{eq}}(u)}{\partial u} \quad (13)$$

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

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

(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 $f_{\text{eq}}(T)$. 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 $T > T_d$). We can also exclude the possibility of a coexistence, which would lead to some intermediate value: the paramagnetic state has disappeared at T_d , and the Gibbs state is formed by the bunch of TAP solutions having the suitable free energy $f_{\text{eq}}(T)$, and a finite complexity density.

To get further insight, always starting from a thermalized configuration at temperature $T' \in [T_s, T_d]$, 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].

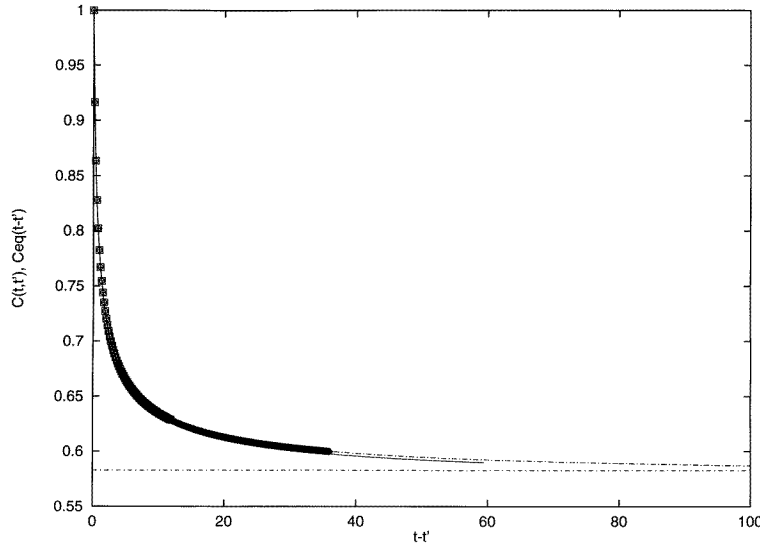


Figure 2. $p = 3$ model, with $T_s \approx 0.586$, $T_d \approx 0.612$; numerical integration of equations (12) for $T' = 0.605$, $T = 0.6$; we plot $C(t, 0)$ versus t (full curve), and $C(t, t')$ versus $t - t'$ for $t' = 6, 12, 18, 24$ (symbols); the dotted curve is the numerical integration of (15),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

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

$$\begin{aligned} \frac{\partial C_{\text{eq}}(\tau)}{\partial \tau} = & - \left(\mu_\infty - \frac{P}{2T} C_\infty^{p-1} + \frac{P}{2T'} l^{p-1} \right) C_{\text{eq}}(\tau) \\ & + \frac{P}{2} \int_0^\tau du C_{\text{eq}}^{p-1}(u) r_{\text{eq}}(\tau - u) - \frac{P}{2T} C_\infty^p + \frac{P}{2T'} l^p. \end{aligned} \quad (15)$$

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

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

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 $E_{T'}^0$ of the angular energy) to temperature T , by keeping the same direction in \hat{s} space, but changing the overlap from $q(E_{T'}^0, T')$ to $q(E_{T'}^0, T)$.

From equation (15), it is possible to show that the relaxation of $C_{\text{eq}}(\tau)$ 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 $E^0 = E_c$). 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 $T_{\text{max}}(E_{T'}^0)$, 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_d , disappears at T_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 $T \in [T_d, T_{\text{TAP}}]$. 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_d (but below the T_{max} of this state). One should notice that the usual dynamics at a temperature below T_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].

It is a pleasure to thank J Kurchan and R Monasson for some very useful discussions and suggestions.

References

- [1] For a short introduction and references, see Mézard M Lecture at Statphys 19 Glassy dynamics *Preprint* LPTENS 95/35
- [2] Franz S and Hertz J 1995 *Phys. Rev. Lett.* **74** 2114
- [3] Bouchaud J P, Cugliandolo L, Kurchan J and Mézard M Mode-coupling approximations, glass theory and disordered systems *Preprint* LPTENS 95/47, condmat 9511042
- [4] Mézard M, Parisi G and Virasoro M A 1987 *Spin-Glass Theory and Beyond* (Singapore: World Scientific)
- [5] Kirkpatrick T R and Thirumalai D 1987 *Phys. Rev. B* **36** 5388
Kirkpatrick T R, Thirumalai D and Wolynes P G 1989 *Phys. Rev. A* **40** 1045 and references therein
- [6] Parisi G Slow dynamics in glasses *Preprint* condmat-9412034
- [7] Crisanti A and Sommers H-J 1992 *Z. Phys. B* **87** 341
- [8] Crisanti A, Horner H and Sommers H-J 1993 *Z. Phys. B* **92** 257
- [9] Thouless D J, Anderson P W and Palmer R G 1977 *Phil. Mag.* **35** 597
- [10] Derrida B 1980 *Phys. Rev. Lett.* **45** 79
Gross D and Mézard M 1984 *Nucl. Phys. B* **240** 431
- [11] Kurchan J, Parisi G and Virasoro M A 1993 *J. Physique I* **3** 1819
- [12] Crisanti A and Sommers H-J 1995 *J. Physique I* **5** 805
- [13] Monasson R 1995 *Phys. Rev. Lett.* **75** 2847
- [14] Monasson R in preparation
- [15] Cugliandolo L F and Kurchan J 1993 *Phys. Rev. Lett.* **71** 173
- [16] Sompolinsky H and Zippelius A 1981 *Phys. Rev. Lett.* **47** 359; 1982 *Phys. Rev. B* **25** 6860
- [17] Houghton A, Jain S and Young A P 1983 *Phys. Rev. B* **28** 290
- [18] Thirumalai D and Kirkpatrick T R 1988 *Phys. Rev. B* **38** 4881
Kirkpatrick T R and Thirumalai D 1989 *J. Phys. A: Math. Gen.* **22** L149
- [19] Franz S and Parisi G 1995 *J. Physique I* **5** 1401
- [20] Franz S and Mézard M 1994 *Physica* **210** A 48
- [21] Bouchaud J P 1992 *J. Physique I* **2** 1705
- [22] Kurchan J and Laloux L 1995 Phase space geometry and slow dynamics *Preprint* condmat 9510079
- [23] Barrat A and Mézard M 1995 *J. Physique I* **5** 941