Basins of attraction of metastable states of the spherical p-spin model

LETTER TO THE EDITOR

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Abstract. We study the basins of attraction of metastable states in the spherical p-spin spin-glass model, starting the relaxation dynamics at a given distance from a thermalized condition. Weighting the initial condition with the Boltzmann distribution we find a finite size for the basins. In contrast, a white weighting of the initial condition implies vanishing basins of attraction. We correspond our results to those of a recently constructed effective potential.

The so-called spherical p-spin spin-glass model has been the subject of many studies: indeed, being mean-field, it allows for a detailed analytic study, while still displaying very rich static and dynamical behaviours. In particular in recent papers [1, 2, 3], it has been shown that the structure of its metastable states, which dominate the Gibbs measure between two temperatures noted T_s and T_d (where the static and dynamic transitions respectively occur [4]), is very rich and complex. The existence of these states is revealed using the approach of Thouless *et al* [5] and they are therefore often called 'TAP states' [6, 7]. These recent works make use of the real replicas method: copies of the system are considered, at various distances from each other, and the free energy cost (called 'effective potential' function) to keep them at given distances is computed. The minima of the potential can then be associated with the fact that the replicas lie in metastable states, thus giving information on the distances between states.

This method is therefore purely static; indeed, the dynamics after a quench do not see all the metastable states, instead giving rise to the phenomenon known as ageing [8]: quenched below T_d, the system remains out of equilibrium for all times with an energy higher than the thermodynamic one. On the other hand, it was shown in [1, 9, 10] that particular initial conditions for the dynamics (namely, taking the system thermalized at a certain temperature between T_s and T_d, and then letting it evolve to another temperature) could allow a dynamical exploration of the metastable states finding results consistent with the picture coming from the two-replica potential.

In this letter we address the problem of determining the size of the basins of attraction of the TAP states. This will be done by studying the Langevin relaxation of a system starting at an initial time at a given fixed overlap (q_{12} in the following) from an equilibrium configuration. This, of course, does not specify completely the initial conditions. In the following we will consider two families of them (for fixed q_{12}), weighting the initial conditions with the Boltzmann distribution and with the uniform one.

As we will see, the case of Boltzmann weighting can be related to the results found for a three-replica potential [2] recently introduced. Therefore, for future use, we briefly recall the results of the two-and three-replicas potentials, V_2 and V_3, for the p-spin model†: indeed, the results of the study of V_2 will be used to determine the initial conditions of the dynamics, and those of the study of V_3 will be compared with the outcome of the dynamics.

The two-replicas potential V_2 is defined [1] as the free energy cost to keep a configuration τ at a fixed overlap q_{12} with an equilibrium configuration σ. While in general the two replicas can be at different temperatures, we will here limit ourselves to the case of equal temperature T for replicas 1 (σ) and 2 (τ). The overlap between the replicas is denoted q_{12}, while the use of the replica trick leads to a description of the second replica by a one-step replica-symmetry breaking (RSB) matrix Q^{22} of parameters (r_1, r_0, x), determined variationally. The absolute minimum of the potential is always for $q_{12} = 0$: then the second replica is at equilibrium, with no constraint, so the free-energy cost is zero. For $T < T_d$, σ lies in one of the metastable states that dominate the statics (of Edwards–Anderson parameter q_{EA}) and a relative minimum appears for a non-zero value of q_{12}: it corresponds to having the second replica in the same TAP state as the first.

In order to study the organization of the metastable states in the phase space, the construction was generalized to three replicas in [2]. There, a first replica ρ is free to thermalize at T; a second replica σ is constrained to thermalize at T with a fixed overlap q_{12} with ρ, and the potential V_3 is defined as the free-energy cost to keep a third replica τ (at the same temperature T) at overlaps q_{13} from ρ and q_{23} from σ. We will take $T_s < T < T_d$: then the first replica is in a certain TAP state of equilibrium at T.

Since the two first replicas are independent of the third, the overlap matrices that describe them are identical to those used for V_2. The third replica is described by a one-step RSB matrix. In the minima of the potential, this matrix is in fact replica symmetric, with only one parameter q_{33}.

The analysis of [2] showed that, depending on the value of q_{12}, the potential can have one or two nontrivial minima (apart from the minimum at $q_{13} = q_{23} = 0$ corresponding to the third replica in an unspecified equilibrium state at T, different from those of replicas 1 and 2). The first minimum, called M_1, exists for any value of q_{12}, and has $q_{13} = q_{EA}$ and $q_{23} \approx q_{12}$. Its interpretation is that the third replica lies in the same state as the first one. It therefore exists independently of the value of q_{12}. The second, more interesting minimum, called M_2 in [2], corresponds to the third replica close to the second one ($q_{23} \approx q_{EA}$, $q_{13} \approx q_{12} < q_{EA}$). Its interpretation is that the second replica lies in the basin of attracion of a metastable state at nonzero overlap q_{12} from the first replica, while the third replica is at equilibrium in this state. This solution exists only for values of q_{12} lower than a certain $\bar{q}$ (which depends on the temperature), with $\bar{q} < q_{EA}$ (see figure 1). This $\bar{q}$ gives therefore the minimum distance (or maximum overlap), from an equilibrium state at T, at which can be found another metastable state.

In order to study the basins of attraction of the metastable states, we study the relaxation of a system with the following initial condition. We consider a reference configuration at equilibrium at temperature T. Then the system evolves from a configuration thermalized at temperature T, but with the constraint that its overlap with the reference configuration is equal to q_{12}. At positive time the spins evolve according to an (unconstrained) Langevin dynamics at temperature T:

$$\frac{d\sigma_i(t)}{dt} = -\frac{\partial H}{\partial \sigma_i} - \mu(t)\sigma_i(t) + \eta_i(t) \tag{1}$$

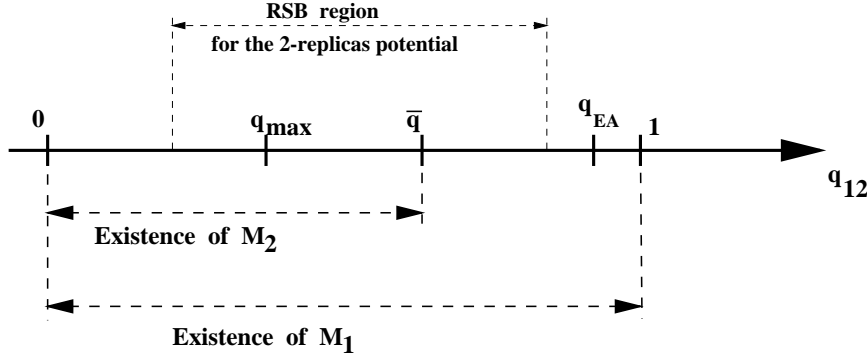† We will not recall the details of the computations, which can be found in [2].

Figure 1. Domains of existence of the minima M_1 and M_2 of the potential V_3.

where the η_i are Gaussian thermal noises with $\langle \eta_i(t)\eta_j(t') \rangle = 2T\delta_{ij}\delta(t - t')$, and $\mu(t)$ is a multiplier that implements the spherical constraint $\sum_i \sigma_i^2 = N$ at all times.

The aim will be to see how the system evolves dynamically, depending on the value of the initial overlap with an equilibrium configuration.

In order to implement the initial conditions, we have to use the replica trick to describe the systems: the first will be described by ρ^a with $a = 1, \ldots, n$; the initial conditions are σ^α, $\alpha = 1, \ldots, m$ and only σ^1 is evolving with time, so we use $\sigma(t)$ instead of $\sigma^1(t)$, with $\sigma(0) = \sigma^1(0)$. The limits $m \to 0$, $n \to 0$ are taken, with a one-step replica symmetric breaking Ansatz. In the infinite N limit, we can obtain, in the same way as in [11, 12, 1, 9], a set of coupled self-consistent dynamical equations for the following quantities (the equations are written in the appendix):

$$C(t,t') = \frac{1}{N}\sum_{i=1}^{N}\overline{\langle \sigma_i(t)\sigma_i(t') \rangle} \qquad R(t,t') = \frac{1}{N}\sum_{i}\overline{\langle \frac{\partial \sigma_i(t)}{\partial \eta_i(t')} \rangle}$$

$$C_\alpha(t) = \frac{1}{N}\sum_{i=1}^{N}\overline{\langle \sigma_i^\alpha \sigma_i(t) \rangle}(\alpha > 1; \text{case } \alpha = 1 : C_1(t) = C(t,0)) \tag{2}$$

$$Q_a(t) = \frac{1}{N}\sum_{i=1}^{N}\overline{\langle \sigma_i(t)\rho_i^a \rangle}.$$

While $C(t,t')$ and $R(t,t')$ are the usual correlation and response functions of the system, the evolution of the C_α and Q_a will give informations on how the system departs from its initial conditions and how close it goes to the equilibrium state of the first real replica ρ.

The initial conditions can be obtained from the study of the two-replicas potential: we first impose $Q_a(0) = Q_{a,1}^{12} = \delta_{a,1}q_{12}$. Since the structure of the equations respect the replica symmetric character or the breaking of replica symmetry of the C_α and Q_a, at all times $Q_a(t) = \delta_{a,1}Q(t)$, with $Q(t) = \frac{1}{N}\sum_{i=1}^{N}\rho_i\sigma_i(t)$. Then, from the value of q_{12}, we use the two-replicas potential to deduct the values for $C_\alpha(0)$. According to the value of q_{12}, it can be replica symmetric or have one step of replica symmetry breaking. Since the replica-symmetric case can be recovered in a simple way from the equations of the RSB case, we will consider only the one-step case. Then the initial conditions for C_α has parameters (r_1, r_0, x); therefore at all times the $C_\alpha(t)$ will have the form

$$C_\alpha(t) = (C(t,0), C_1(t), C_0(t)) \tag{3}$$

with the same breaking parameter x†, and $C_1(0) = r_1$, $C_0(0) = r_0$‡. We define the following limiting values:

$$\lim_{t \to \infty} Q(t) = q_0 \qquad \lim_{t \to \infty} C(t, 0) = \tilde{p}$$

$$\lim_{t \to \infty} C_1(t) = c_1 \qquad \lim_{t \to \infty} C_0(t) = c_0 \qquad \lim_{t \to \infty} \mu(t) = \mu. \qquad (4)$$

A simple check is to look at what happens in two extreme cases: (i) $q_{12} = 1$: the system starts at equilibrium at T; then $r_1 = r_0 = 1$, and obviously we obtain $C(t, 0) = Q(t) = C_1(t) = C_0(t)$, $q_0 = \tilde{p} = c_1 = c_0 = q_{EA}$: the system thermalizes in the particular equilibrium state at T chosen by ρ; (ii) $q_{12} = 0$: the system is not constrained, so clearly we obtain $Q(t) = C_1(t) = C_0(t) = 0$, $C(t, t') = C(t - t') = C(\tau)$: the system thermalizes in an unspecified TAP state of equilibrium at T [1, 9].

For other values of q_{12}, the numerical integration of the dynamical equations shows that the system, after a transient, reaches a certain equilibrium behaviour; to study the system at long times, we therefore make the ansatz: $C(t, t') = C(t - t') = C(\tau)$, $R(t, t') = R(t - t') = R(\tau) = -\frac{1}{T}\frac{dC}{d\tau}$, with $\lim_{\tau \to \infty} C(\tau) = q$. This ansatz allows, with usual methods, to obtain coupled equations for the limiting values of the various one-time quantities, and moreover we have for the evolution of the asymptotic correlation function:

$$\frac{dC}{d\tau} = -\frac{T}{1 - q}(C(\tau) - q) - \beta \int_0^\tau du (f'(C(\tau - u)) - f'(q))C'(u). \qquad (5)$$

The equations for the values of q, q_0, $\tilde{p}$, c_1, c_0 are equivalent to the equations for the parameters q_{33}, q_{13}, q_{23}, w_{23}, z_{23} of the three-replicas potential§. This correspondence pushes forward the one noted in [1, 9] between the potential with two replicas and the dynamics with thermalized initial conditions. Here, the interpretation is that the first replica ρ lies in an equilibrium state at temperature T, the replica number 2 of the potential gives the initial conditions of the dynamics, while the dynamical system goes towards a minimum of the potential (given in the potential approach by the third replica) where it relaxes according to (5), which is exactly the equation of the relaxation in a TAP state of self-overlap q, as given in [9].

An important difference between the two approaches is that, while the potential can be explored for all values of q_{12}, q_{13}, q_{23} (i.e. all positions of both replicas 2 and 3), the only parameter of the studied dynamics is q_{12}: the initial conditions of the dynamics can be compared with the second replica of the potential, and all possible values of q_{12} can be studied, but the values of q_0, $\tilde{p}$ are *outcomes* of the dynamics and are not chosen. From the equivalence between potential and dynamics, it follows for the dynamics that, while for $q_{12} > \bar{q}$ only the solution M_1 exists, for $q_{12} < \bar{q}$ there are the two solutions M_1 and M_2. However, as the dynamical equations admit (within the one-step RSB ansatz we use) a unique solution for any finite time, only one of the two can be reached dynamically. The size of the basin of attraction of the equilibrium states is related to the smallest value of q_{12} for which the solution M_1 is reached.

In order to settle this question we integrate numerically the dynamical equations (A1). For simplicity we limit our analysis to the case $p = 3$ for which most of the analysis of [2] was perfomed. Then $T_s \approx 0.586$, $T_d \approx 0.612\,37$ and we will show results for $T = 0.6$: then $q_{EA} = 0.6$, $\bar{q} \approx 0.342$. The numerical integration is carried out using a simple iteration algorithm, discretizing the dynamical equations with a finite time step h. We proceed with

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† This means that $C_\alpha(t)$ is equal to $C(t, 0)$ for $\alpha = 1$, to $C_1(t)$ for $\alpha = 2, \ldots, x$, and to $C_0(t)$ for $\alpha = x+1, \ldots, n$.
‡ To recover the replica symmetric case, we take $r_1 = r_0$: then, at all times, $C_1(t) = C_0(t)$.
§ In the replica symmetric case, the equivalence is $q_{33} = q$, $q_0 = q_{13}$, $c_1 = c_0 = \tilde{p} = q_{23}$.
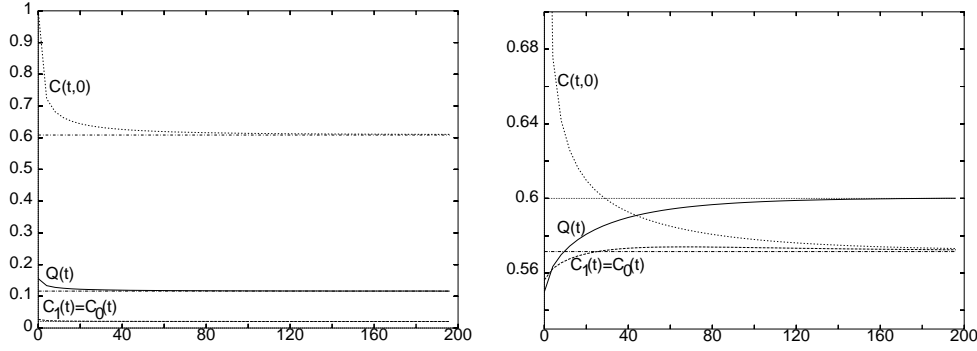
Figure 2. Evolution of $C(t, 0)$, $Q(t)$ and $C_1(t) = C_0(t)$ with time for $q_{12} = 0.155\,702$ (left) and $q_{12} = 0.55$ (right). These curves correspond to the extrapolation at $h \to 0$ of the results of the numerical integration with $h = 0.05, 0.1, 0.2$; we see that they go quite quickly to their limiting values $\tilde{p}$, q_0 and $c_1 = c_0$ (given by the horizontal lines) with $\tilde{p} = c_1 = c_0$ for $q_{12} = 0.55$.

three values h, $2h$, $4h$ and then do the interpolation at $h \to 0$ to compare the numerical values with the values obtained from the study of the potential V_3†.

For 'small' values of q_{12}, the dynamics converge rapidly towards an equilibrium behaviour with time tranlsation invariance and fluctuation-dissipation relation. The numerical integration yields limits in excellent accordance with the resolution of the aforementioned equations for q, q_0, $\tilde{p}$, c_1, c_0, and coincide with the values of the various parameters in the minimum M_2 of the three-replicas potential. (e.g. see figure 2, $q_{12} = 0.155\,702$, then $r_1 = r_0 = 0.027\,15$, $q_0 = 0.116\,338$, $c_1 = c_0 = 0.020\,5437$, $q = 0.608\,423$, $\tilde{p} = 0.609\,467$. These values coincide with the values respectively of q_{13}, $w_{23} = z_{23}$, q_{33}, q_{23} in the minimum M_2.) This means that the system $\sigma(t)$ stays in the state found by the replica $\sigma(0)$, with finite overlap with ρ. We are therefore in the minimum M_2, and out of the attraction basin of the equilibrium state where ρ lies.

For q_{12} 'large', conversely, we expect that the system, which starts close to ρ, remains in the same state. This is indeed what we find (e.g. for $q_{12} = 0.817\,272$, then $r_1 = r_0 = 0.7859$; we obtain $q_0 = q = q_{\text{EA}}$, $c_1 = c_0 = \tilde{p} = 0.633\,625$; the integration of two-times equations coincide well with the integrations of the equation on $C(\tau)$ and with these values). For a somewhat smaller value of q_{12} (e.g. see figure 2, $q_{12} = 0.55$, $r_1 = r_0 = 0.556\,345$) the same behaviour is obtained: the two-times equations yield the same results as the equations using the equilibrium ansatz, with $q_0 = q = q_{\text{EA}}$, $c_1 = c_0 = \tilde{p} = 0.571\,534$).

For these values of q_{12}, the system thermalizes therefore in the TAP state found by ρ. The long-time dynamics is the relaxation dynamics in a TAP state of equlibrium at T, and therefore does not depend on the initial conditions.

The outcome of the dynamics for small and large values of q_{12} show that both minima M_1 and M_2 can be dynamically reached. We can then naturally ask if a minimum is always reached, and what the limiting value is of q_{12} for which the system goes towards ρ. We therefore study the behaviour of the system for values of q_{12} decreasing towards $\bar{q}$, and also for values lower than, but close to $\bar{q}$. We observe that, while for large values of q_{12} (or also for values of q_{12} lower than $\bar{q}$) the one-time quantities go directly to their limiting values, upon decreasing q_{12} a plateau appears at an intermediate value between the initial and the

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† After checking that the interpolation at $h \to 0$ coincides well with the values obtained via the potential, we used a unique value of the time step for some runs that involved larger timescales, at values of q_{12} close to the limit of the attraction basin.
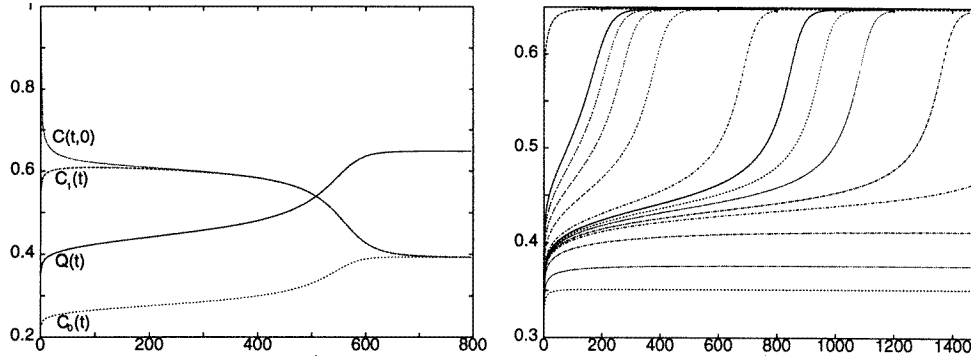
Figure 3. Left: evolution with time of the one-time quantities $C(t, 0)$, $C_1(t)$, $C_0(t)$, $Q(t)$, for $q_{12} = 0.353$. We observe the presence of a plateau until $t^* \approx 500$ before the quantities reach their final values corresponding to M_1. Right: evolution with time of $Q(t)$ for various values of q_{12}. From bottom to top, $q_{12} = 0.32, 0.33, 0.34$ ($< \bar{q}$), and $q_{12} = 0.344, 0.345, 0.346, 0.347, 0.348, 0.35, 0.36, 0.37, 0.38, 0.39, 0.55$ ($> \bar{q}$): we see the growth of the timescale given by the length of the plateau as q_{12} decreases towards $\bar{q}$. For $q_{12} > \bar{q}$, we see that all the curves go to the same limit corresponding to M_1, while the limiting value depends on q_{12} for $q_{12} < \bar{q}$. In both figures, the time step used is $h = 0.2$.
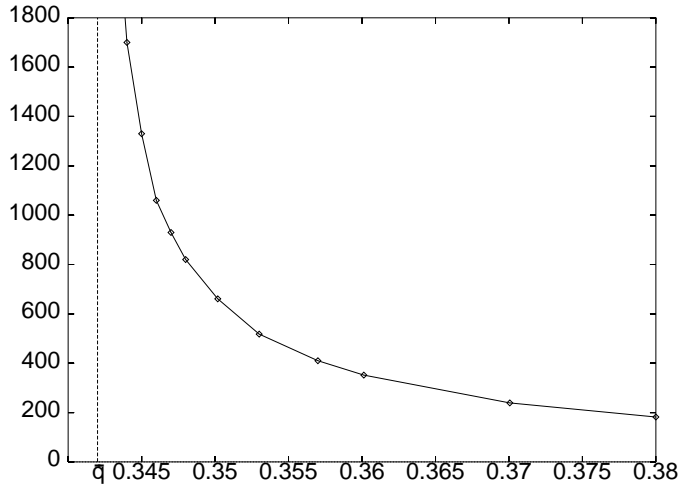

Figure 4. Timescale t^* as a function of q_{12} ($\bar{q} \approx 0.342$).

limiting values. This plateau gives a timescale t^* that grows and diverges when $q_{12} \rightarrow \bar{q}$. We show the various one-time quantities for a particular value of q_{12}, and the evolution of the plateau and of the timescale with q_{12}, in figures 3 and 4. For q_{12} lower than $\bar{q}$, we observe that the dynamics converges towards the values of the parameters in the minimum M_2 of the potential, and no more reach M_1.

The situation is therefore that, for any $q_{12} > \bar{q}$, the system reaches the state where the first replica, ρ, lies, but after a transient which length diverges as q_{12} goes to $\bar{q}$. For initial conditions farther from ρ than $\bar{q}$, i.e. as soon as the minimum M_2 of the potential exists, the system relaxes in the state corresponding to M_2, which is a metastable state at finite overlap with ρ, and is no more able to 'reach' ρ. We can therefore understand $\bar{q}$ as the

limit of the attraction basin of the state where ρ lies. It is worth noting that $\bar{q}$ is quite small ($\bar{q} \approx 0.342$ for $T = 0.6$) which means that it is possible to find configurations that will dynamically evolve towards a TAP state, and thermalize in it within a finite time, even at quite large distances from typical configurations of this state.

This is the situation that we find if we weight the initial condition with the Boltzmann probability. Let us turn now briefly to the case of initial conditions with overlap q_{12} with ρ, but otherwise uniformly distributed. In this case the basins of attraction are vanishing. Indeed for any value of q_{12} we find that the asymptotic value of the energy is larger than the equilibrium value $E_{\rm eq}$ (the energy of ρ). As far as the correlations with the initial state are concerned we have found two different regimes, separated by a (rather large) threshold value q^* of q_{12} (e.g. $q^* \approx 0.99$ for $p = 3$, $T = 0.6$). For $q > q^*$ the system reaches a time translation invariant situation, with final energy that depends continuously on q_{12} (see figure 5). The overlap with the initial condition tends to a nonzero value in this case, and the relation between the asymptotic energy and the Edwards–Anderson parameter is the one verified in the TAP states, indicating equilibration within a metastable state. For $q < q^*$ instead, the system loses the correlation with the initial state (and with ρ) and irrespectively of q_{12}, falls into an ageing state with asymptotic energy equal to $E_{\rm dyn}(T)$ analogous to the one discussed in [8], where the dynamics starts from a completely random initial condition. The situation can be understood analysing the energy of the initial state. For each value of q_{12} this energy takes with probability one a fixed value $E(q_{12})$, which is a decreasing function of q_{12} and equals $E_{\rm eq}(T)$ for $q_{12} = 1$. It is tempting at this point to interpret the initial states as *typical* states with that energy, i.e. as equilibrium states at a corresponding temperature $T(q_{12})$. If this is true then for $T(q_{12}) < T_d$ the typical initial configuration is in the basins of metastable states that survive at temperature T [1, 9, 10], although they are slightly deformed. The dynamics at temperature T leads then to equilibrium in these states. For $T(q_{12}) > T_d$, the typical initial configuration belongs to the paramagnetic state, and ageing has to be expected; this means that $T(q^*) = T_d$. We have checked that this is
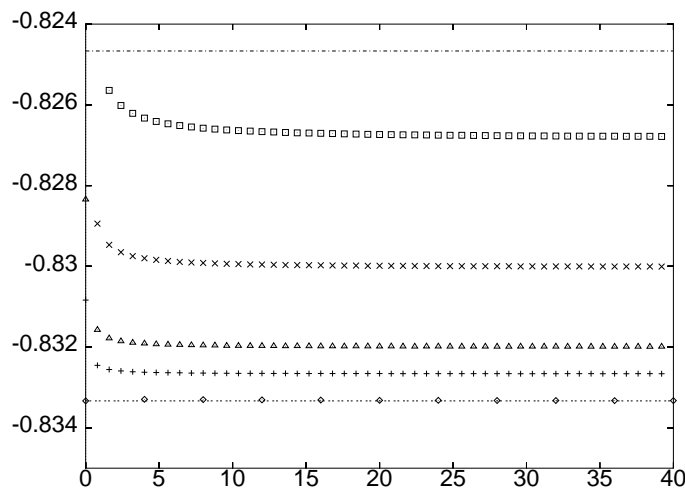

Figure 5. Evolution of the energy of the system starting at overlap $q_{12} = 1, 0.999, 0.998, 0.995, 0.99$ (symbols, from bottom to top) from an equilibrium configuration ρ at $T = 0.6$ ($p = 3$), but otherwise randomly; the curves give the equilibrium energy $E_{\rm eq} \approx -0.833\,33$ and $E_{\rm dyn} \approx -0.824\,67$.

indeed the right scenario, using the techniques of [1, 9, 10], finding the interesting result that, arbitrarily close to an equlibrium state at temperature T, there are states which are of equilibrium at some other temperature.

In this letter, we have studied, by a dynamical approach, the attraction basin of an equilibrium state at temperature $T_s < T < T_d$ (and established the correpondence with the static three-replicas potential). If we weight with the Boltzmann distribution we find wide basins of attraction. Almost all initial conditions with overlap larger than a threshold value $\bar{q}$, are in the basin of attraction of the reference state. Conversely if we perform a white average we find zero size basins of attraction. Starting close enough to the reference configuration, the system equilibrates in a TAP state close to the starting point, while if the initial overlap is larger than this threshold the system ends up ageing. This combination of facts indicates a highly non trivial structure of the various states and basins of attraction in configuration space.

Appendix A. Dynamical equations

Denoting $f(q) = 1/2q^p$, and using the methods of [1, 9, 11, 12] one can show that the following dynamical equations are obeyed:

$$\mu(t) = \int_0^t ds \, (f'(C(t,s)) + f''(C(t,s))C(t,s))R(t,s) + \beta f'(Q(t))Q(t)$$

$$+ \beta \sum_{\alpha=1}^m f'(C_\alpha(t))C_\alpha(t)$$

$$\frac{\partial R(t,t')}{\partial t} = -\mu(t)R(t,t') + \int_{t'}^t ds \, f''(C(t,s))R(t,s)R(s,t')$$

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

$$+ \beta f'(Q(t))Q(t') + \beta \sum_{\alpha=1}^m f'(C_\alpha(t))C_\alpha(t') \qquad \text{(A1)}$$

$$\frac{dC_\alpha}{dt} = -\mu(t)C_\alpha(t) + \int_0^t ds \, f''(C(t,s))R(t,s)C_\alpha(s) + \beta f'(Q(t))q_{12}$$

$$+ \beta \sum_{\beta=1}^m f'(C_\beta(t))Q_{\alpha\beta}^{22}$$

$$\frac{dQ_a}{dt} = -\mu(t)Q_a(t) + \int_0^t ds \, f''(C(t,s))R(t,s)Q_a(s) + \beta f'(Q_a(t))$$

$$+ \beta \sum_{\alpha=1}^m f'(C_\alpha(t))Q_{a,\alpha}^{12}$$

where Q^{12} and Q^{22} are the matrices used in the two-replicas potential [1]. Using the one-step RSB ansatz, i.e. $C_\alpha(t) = (C(t,0), C_1(t), C_0(t))$ with breaking point x, with initial

conditions $C_1(0) = r_1$; $C_0(0) = r_0$, $Q(0) = q_{12}$, we can obtain the equations for $C(t, t')$, $R(t, t')$, $C_1(t)$, $C_0(t)$, $Q(t)$ by expanding the sums in the previous equations; for example:

$$\sum_{\alpha=1}^{m} f'(C_\alpha(t))C_\alpha(t') = f'(C(t, 0))C(t', 0) + (x - 1)f'(C_1(t))C_1(t') - xf'(C_0(t))C_0(t').$$

(A2)

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