J. Phys. A: Math. Gen. **33** (2000) 891–905. Printed in the UK PII: S0305-4470(00)09100-9

Quasi-equilibrium interpretation of ageing dynamics

S Franz and M A Virasoro

The Abdus Salam International Center for Theoretical Physics, Strada Costiera 11, PO Box 563, 34100 Trieste, Italy

Received 1 November 1999

Abstract. We develop an interpretation of the off-equilibrium dynamical solution of mean-field glassy models in terms of quasi-equilibrium concepts. We show that the relaxation of the 'thermo-remanent magnetization' follows a generalized version of the Onsager regression postulate of induced fluctuations. We then find the rationale for the equality between the *fluctuation–dissipation ratio* and the rate of growth of the configurational entropy close to the asymptotic state, found empirically in mean-field solutions.

1. Introduction

Ageing is a scaling dynamical regime characteristic of glassy systems [1]†. In this regime, typical features of equilibrium systems, such as the asymptotic absence of macroscopic heat currents, coexist with non-stationary aspects such as the dependence of the correlation and response functions on the system's 'age', i.e. the time spent in the low-temperature phase. The solution of mean-field spin-glass models [2–5]‡ has given a general framework to understand ageing phenomena, and has produced detailed predictions, which have been verified in numerical simulations of long- [6] and short-range [7] glassy systems. A characteristic prediction of this solution is the existence, at low temperature, of a dynamical regime where extensive quantities depending on the configuration of the system at a single time (one-time observables in the following) are well thermalized (or evolve very slowly), while two-time correlation functions and susceptibilities exhibit non-stationary scale-invariant behaviour.

Despite this coherent theoretical scheme, and recent progress in linking ageing dynamics to the nature of the equilibrium regime [8], a physical understanding of some fundamental aspects of ageing dynamics is still lacking. While the investigation of both equilibrium and asymptotic off-equilibrium regimes give solutions that show unexpected coincidences, all efforts to interpret ageing as a quasi-equilibrium condition have been thwarted by facts such as:

(a) No matter how large we take the ageing time, if we then wait long enough the system eventually wanders away from any finite region of phase space [2].
(b) Two identical systems starting from the same condition at any given ageing time will always come apart as far as possible [9].

† For a recent review on ageing in spin-glass materials see [1] (second reference).
‡ For a recent review on ageing mean-field theory see [5].

In this paper we try to make ends meet. In particular, we try to give a physical and intuitive explanation of the link between the so-called 'fluctuation–dissipation ratio' (FDR) (the factor $x(q)$) and the Parisi function (in Sherrington–Kirkpartick-like models) or the derivative of the configurational entropy close to the threshold state (in p-spin-like models). Our work should be understood as a physical interpretation of mean-field ageing dynamics in terms of a quasi-equilibrium scenario and not as an alternative derivation of the results of the theory.

We show that a modified version of the Onsager postulate on regression of fluctuations applies to the relaxation of the magnetization in thermo-remanent magnetization experiments. The observed anomalies in the response are then analysed. In this paper we discuss ageing mainly in the case of a 'one-time-sector' approximation, which is the dynamical counterpart of the 'one-step replica symmetry breaking' (1RSB) approximation in the equilibrium analysis. This is exact in models like the p-spin model, while it is only an approximation, and a rather crude one, when continuous replica symmetry breaking is present, like in the Sherrington–Kirkpatrick (SK) model or the random manifold model. We will refer to the first class of models as 'p-spin-like' and to the second as 'SK-like'. We discuss only this 'one-time-sector' approximation to unify the argument, and simplify the notation. However, we expect the reader to be able to generalize it without effort.

The picture that emerges from our analysis is simple and intuitive: the age of an ageing system determines the rate of entropy decrease, i.e. the flow rate of heat towards the thermal bath. A small force in the linear response regime cannot change this rate. Acquiring a non-zero magnetization means entropy reduction which has then to be compensated by an increase (or reduced decrease) of the free energy associated with the spin-couplings. As a consequence, the response becomes proportional to the growth of the logarithm of the number of *quasi-states* (to be defined later) with free energy. It is as if the slow degrees of freedom respond to external forces by sampling states that lie above in free energy, while they are blocked from exploring those that are at the same or at a lower level. This paper presents what we believe are convincing arguments in favour of this assertion. As a by-product the time-scale-dependent effective temperatures will appear [10] and their connection with the derivative of the logarithm of the number of quasi-states (or configurational entropy) with respect to free energy is explained [11]†.

We organize this paper as follows. In section 2 we review some properties of ageing in a mean-field model. In section 3 we discuss our definition of quasi-equilibrium and how it relates to the dynamics. In section 4 we recall the Onsager regression postulate and generalize it to ageing systems. In section 5 we discuss the origin of the FDR in SK-like models, while we treat the case of p-spin-like models in section 6. Finally, we present a summary and the conclusions.

2. A short review

We consider a mean-field spin-glass quenched at a given time $t = 0$ into the glassy phase. For simplicity we will imagine that the degrees of freedom consist of Ising spins $S_i = \pm 1$, $i = 1, \ldots, N$ ($N \to \infty$). We are interested on the long-time dynamics of such a system,

† The relation between the Parisi parameter βx and the derivative of the cluster entropies with respect to the cluster free-energies in equilibrium theory was well known (see the first reference of [11]). That the factor βx appearing in mean-field dynamics in the p-spin model is the derivative of the configurational entropy with respect to free energy was noticed soon after the Kurchan–Cugliandolo paper (see [12]). This observation is at the origin of an ambitious program to introduce a multi-temperature thermodynamics for the glassy state (see [13] and references therein).

i.e. on a regime where it has thermalized for a long time t_w before any measurements. The long-time limit $t_w \to \infty$ is always taken after the thermodynamic limit.

The free energy, and its derivatives with respect to the control parameters (e.g. temperature), tend to some asymptotic time-independent values. More interesting is the behaviour of observables depending on two time variables, such as correlation and response functions. Ageing behaviour manifests itself as an asymptotic non-stationary dependence on time of these quantities.

Let us consider the spin–spin time-dependent autocorrelation function

$$C(t,u) = \frac{1}{N}\sum_{i=1}^{N} S_i(t)\, S_i(u) \qquad t > u \gg t_w. \tag{1}$$

A first, short-time, dynamical regime is obtained by considering the difference $\tau = t - u$ finite to derive stationary correlations $C^*_{st}(\tau)$. Let us denote q_{EA} as the long-τ limit of C^*_{st}. In the ageing regime $C(t,u)$ relaxes below q_{EA}. In the 'one-time-sector' approximation scheme, the correlation function in this regime can be written as [2],

$$C(t,u) = C_{ag}(\mathtt{h}(u)/\mathtt{h}(t)) \tag{2}$$

where $\mathtt{h}(\cdot)$ is an increasing function not derivable from the present theory and t, u are large with $\lim_{t,u\to\infty} \mathtt{h}(u)/\mathtt{h}(t) =$ finite. The formulae in the two regimes are summarized in:

$$C(t,u) = C_{st}(t-u) + C_{ag}(\mathtt{h}(u)/\mathtt{h}(t)) \tag{3}$$

where $C_{st}(t-u) = C^*_{st}(t-u) - q_{EA}$ is a monotonically decreasing function equal to $1 - q_{EA}$ for $t - u = 0$ and tending to zero for $t - u \to \infty$, while $C_{ag}(\mathtt{h}(u)/\mathtt{h}(t))$ is equal to q_{EA} for $\mathtt{h}(u)/\mathtt{h}(t) = 1$ ($u = t$) and tends to q_0 for $\mathtt{h}(u)/\mathtt{h}(t) \to 0$. In order to simplify the notation we will suppose that the 'time reparametrization' $\mathtt{h}(t)$ is the identity $\mathtt{h}(t) = t$ and $C_{ag}(\mathtt{h}(u)/\mathtt{h}(t)) = C_{ag}(u/t)$. We will also suppose that $q_0 = 0$, but this will not affect any of our following arguments.

We stress that the form (3) of the correlation function implies that if we fix the value of u and let t run, the time spent at the value of the correlation equal to q_{EA} is much larger then the time needed to reach it. This is an aspect of the 'time-scale separation' observed in glassy systems that will play a crucial role in our discussion.

We are also interested in the behaviour of the linear response function,

$$R(t,u) = \frac{1}{N}\sum_{i=1}^{N} \frac{\delta}{\delta h_i(u)} \langle S_i(t)\rangle|_{h=0} \qquad t > u \gg t_w \tag{4}$$

and the corresponding integrated function

$$\chi(t,u) = \int_{t_w}^{u} \mathrm{d}s\, R(t,s) \qquad t > u \gg t_w \tag{5}$$

which represent the susceptibility at time t in a 'thermo-remanent magnetization' experiment in which a constant small field has acted from the time t_w up to time u. By the condition $u \gg t_w$ we mean $t_w/u \to 0$ for $t_w \to \infty$. The linear response theory requires that the limit $h \to 0$ be taken *before* sending the time u to infinity.

While in the stationary regime the fluctuation–dissipation relation $R(t,s) = R_{st}(t-s) = \beta\, \partial C(t,s)/\partial s$ is verified, in the ageing regime the relation is substituted by having a non-trivial fluctuation–dissipation ratio:

$$x(q) = \lim_{\substack{t,s\to\infty \\ C(t,s)=q}} \frac{T R(t,s)}{\partial C(t,s)/\partial s} \tag{6}$$

which turns out to coincide with the function $x(q)$ appearing in the replica approach that in principle applies to equilibrium of different kinds [14, 15]. In the one-sector scenario $x(q)$ is constant throughout the ageing regime.

The FDR $x(q)$ verifies the mathematical properties of a cumulative probability distribution, a feature that has been explained in recent work where it has been shown that there is a deep connection between the dynamic properties during ageing and the property of ergodicity-breaking in equilibrium [8]. Using only the hypothesis of equilibration of one-time observables (OTO) and the existence of a linear response regime for the correlation functions (stochastic stability), it was proved that the function $x(q)$ is related to the function $P(q)$ describing the statistics of equilibrium pure states [16] through the equation

$$P(q) = \frac{\mathrm{d}x(q)}{\mathrm{d}q}. \tag{7}$$

The theorem was originally formulated for finite-dimensional systems, where the OTOs are guaranteed to thermalize but can be generalized to mean-field long-range models of the SK-like class. A different situation is found in p-spin-like models [17]† where one of the hypotheses of the theorem is violated because the asymptotic value of the dynamic energy is higher than that of the states dominating the partition function.

3. The quasi-equilibrium hypothesis

From now on we will work on the 'one-time-sector' approximation described in the previous section.

Let us consider a large time u and the corresponding spin configuration $S_i(u)$. Our previous observations suggest that the value of q_{EA} can be used to decompose the spin configuration into a 'fast part' and a 'slow part' according to

$$S_i(u) = [S_i(u) - m_i(u)] + m_i(u) \tag{8}$$

where the slow variable $m_i(u)$ can be estimated immediately from the running average

$$m_i(u) \simeq \frac{1}{\Delta t}\int_u^{u+\Delta t} \mathrm{d}w\, S_i(w) \qquad \text{with} \quad C(u+\Delta t, u) = q_{EA}. \tag{9}$$

We will see later how to improve on this estimate. From (8) and (9) we obtain correctly the corresponding decomposition of the correlation function into two time domains

$$\langle [S_i(t) - m_i(t)][S_i(u) - m_i(u)]\rangle = C_{st}(t-u) \tag{10}$$

while

$$\langle m_i(t) m_i(u)\rangle = C_{ag}(u/t). \tag{11}$$

Any other decomposition, obtained by averaging the spins over times such that the value of $C(u, v)$ is different from q_{EA}, would mix C_{st} and C_{ag}.

Through this decomposition one can define a dynamical notion of 'quasi-state' in which the system (almost) equilibrates before relaxing further. The quasi-equilibrium hypothesis can be formulated by considering the probability distribution of finding the system in a given

† A review on the spherical p-spin model can be found in [17] (first reference). The model was first introduced in [17] (second reference).

configuration of the slow and the fast variables at time t induced by the thermal noise and the flat distribution of initial conditions

$$P_t(\{S_i\}, \{m_i\}) = \left\langle \prod_i \delta(S_i(t) - S_i)\delta(m_i(t) - m_i) \right\rangle_{\substack{\text{thermal noise} \\ \text{initial conditions}}} \tag{12}$$

which can be written as

$$P_t(\{S_i\}, \{m_i\}) = P_t(\{S_i\}|\{m_i\}))P_t(\{m_i\})). \tag{13}$$

All the known properties of the dynamical solution, and in particular the short-time response to external perturbations, are consistent with the proposition that the conditional probability $P_t(\{S_i\}|\{m_i\})$ becomes independent of time, and takes asymptotically the form of a restricted Boltzmann measure†:

$$P(\{S_i\}|\{m_i\}) = \frac{\mathrm{e}^{-\beta H(\{S_i\})}\delta\left(\sum_i S_i m_i - N q_{EA}\right)}{\sum_{\{S_i\}} \mathrm{e}^{-\beta H(\{S_i\})}\delta\left(\sum_i S_i m_i - N q_{EA}\right)}. \tag{14}$$

We stress that the same property manifestly would not hold had we chosen time scales such that $C(t, u) < q_{EA}$ in the average (9). This proposition is implicit in the definition of the ageing regime, where there is no ambiguity in the definition of q_{EA}. The measure should be restricted to the transverse configuration space projecting out those directions along which the system evolves (*transverse* quasi-states) where the energy landscape is flat or has negative eigenvalues. In these conditions, the free energy of the quasi-state (see below), as well as the value of q_{EA} entering in (14) are close to their asymptotic values, but still depend on time. We can safely assume that in the asymptotic regime the number of negative directions become vanishingly small. Note that, if we take two macroscopically different sets of slow variables $\{m_i\}$ and $\{m_i'\}$ then, by construction, the corresponding conditional probabilities $P(\{S_i\}|\{m_i\})$ and $P(\{S_i\}|\{m_i'\})$ are mutually orthogonal. This can be easily understood from the fact that the mutual overlap among a configuration with non-zero weight in the first distribution and a configuration with non-zero weight in the second one is almost surely smaller then q_{EA}. It is therefore convenient to think of a discretized m_i-sphere such that the centres of the neighbouring cells correspond to disjoint quasi-states. In general, we expect different quasi-states to define disjoint regions in configuration space and that the union of all such regions define a partition of all relevant configurations. We will use α as the index of the quasi-state which of course will change with the slow time. In (9) therefore $m_i(u)$ should rather read m_i^α with α a function of u. The finiteness of Δt limits the accuracy of the running average estimate. To derive a better estimate of m_i^α we could clone the trajectory from time u on and take a weighted average along all trajectories.

It is useful to define thermodynamic quantities such as the dynamical free energy,

$$\mathcal{F}_t = \sum_\alpha P_t(\{m_i^\alpha\})\left[F(\{m_i^\alpha\}) + T\log\left(P_t(\{m_i^\alpha\})\right)\right] \tag{15}$$

where T is the temperature of the thermal bath and

$$F(\{m_i^\alpha\}) = \int \prod_i \mathrm{d}S_i\; P(\{S_i\}|\{m_i^\alpha\})\left[H(\{S_i\}) + T\log\left(P(\{S_i\}|\{m_i^\alpha\})\right)\right] \tag{16}$$

is the free energy of the (transverse) α quasi-state.

† To be more precise we should define the measure in such a way that each S_i has average m_i. One can check with a detailed calculation that this condition is automatically fulfilled by the measure (14).

Observe that $\mathcal{F}_t$ includes the average free energy of the quasi-states

$$F_t = \sum_\alpha P_t(\{m_i^\alpha\})\, F(\{m_i^\alpha\}) \tag{17}$$

and a slow entropy term

$$\mathcal{S}_t = -\sum_\alpha P_t(\{m_i^\alpha\}) \log\big(P_t(\{m_i^\alpha\})\big). \tag{18}$$

An explicit computation shows that, due to the disjointness property of the quasi-states, the sum $S_t + \mathcal{S}_t$ coincides with the entropy of the distribution $P_t(\{S_i\})$. We can identify $\mathcal{F}_t$ with the dynamical free energy $\int \prod_i \mathrm{d}S_i\, P_t(\{S_i\})[H(\{S_i\}) + T \log P_t(\{S_i\})]$.

This last quantity is known to decrease in any process verifying detailed balance. In our case, due to the white average over the initial conditions we expect, in addition, both F_t and $\mathcal{S}_t$ to decrease with time.

For typical trajectories extensive quantities are self-averaging and therefore the free energy F_t is a well defined function. The asymptotic value, F_∞, is the free energy of the equilibrium state for SK-like systems, and the free energy of the threshold Thouless–Anderson–Palmer (TAP) solutions for the p-spin class.

The role of $\mathcal{S}_t$ in the dynamical relaxation is not immediately obvious. By construction, it does not say anything about the number of quasi-states accessible starting from a generic point of a trajectory at time t. In fact, we expect that the support of $P_t(\{m_i\})$ decomposes in non-overlapping, mutually inaccessible, regions of phase space that become more and more isolated as time advances.

By inverting the relation F_t among free energy and time, we can define $\mathcal{S}(F) = \mathcal{S}_{t(F)}$ and derive that $\mathcal{S}(F_\infty)$ is the extensive part of the configurational entropy of ground states in SK-like models (zero in this case) and the configurational entropy of the threshold states in the p-spin. The *dynamical* entropy that we have defined weights different regions of phase space according to their basins of attraction. Here we are using the observation that since the threshold states are identical in all their properties, they must also have the same basin of attraction. Furthermore, with respect to those states which appear in exponentially smaller numbers there is the additional observation that their basin of attraction cannot be so much larger as to compensate for their smaller multiplicity.

For large time, the support of $P_t(\{m_i\})$ will be in regions of small TAP gradient. We can calculate $\mathcal{S}(F)$:

$$\mathcal{S}_t = \mathcal{S}(F_t) = \left.\frac{\partial \mathcal{S}(F)}{\partial F}\right|_{F_\infty} (F_t - F_\infty) + \mathcal{S}_\infty. \tag{19}$$

In our scenario $\mathcal{S}(F_t)$ measures the multiplicity of quasi-states at t which as before will have equal basins of attraction. A detailed calculation in the p-spin model is developed in the appendix. It shows that if we compute the multiplicity of minima of the modulus of the gradient of the TAP free energy then their number and derivative are continuous across the threshold value. Therefore, we propose to identify *the quasi-states with the minima of the gradient of the TAP free energy*. For SK-like models we conjecture instead $\mathcal{S}(F)$ to be equal to the number of stable TAP excites states at level F.

With this identification we now write $(\partial \mathcal{S}(F)/\partial F)|_{F_\infty}$ equal to βx. It is one of those remarkable coincidences, referred to in the introduction, that the same value of x appears in the anomalous FDR. We will interpret this coincidence in the following sections.

This identification of the quasi-states is crucial. An explicit calculation of the dynamical entropy could check its validity but unfortunately with our present techniques such a calculation is not feasible.

A strong hint in favour of it comes, however, from the study of the equilibrium dynamics of p-spin-like models at temperatures slightly larger then the dynamical transition temperature T_d. For $T - T_d \ll T_d$ there is a similar separation of two time scales controlled by the ratio $(T - T_d)/T_d$. This allows the definition of dynamical quasi-states along lines similar to the ones followed in the non-equilibrium case. The free energy obtained by considering the collection of the quasi-states of appropriate energy, should be coherent with the direct computation from the partition function. By an explicit computation that we sketch in the appendix, we verified that in the spherical p-spin model, up to second-order corrections in $T - T_d$, the thermodynamic entropy coincides with the TAP internal entropy plus the configurational entropy of the saddles.

4. Regression of fluctuations and the Onsager postulate

In order to discuss the behaviour of the response function we consider the set-up of 'thermo-remanent magnetization' (TRM) experiment [1]. The system is allowed to age in a small field h acting from time t_w to time u such that $C(u, t_w) \to 0$. At later times $t > u$ one detects the magnetization $M(t) = (1/N)\sum_{i=1}^{N} S_i(t) = h\chi(t, u)$†. Our set-up differs slightly from the one usually considered in the literature, in which the field acts directly from the quenching time. We switch the field on at time t_w because we find it conceptually clearer to discuss the behaviour of the magnetization starting from a situation where the system is already in the asymptotic regime. We notice that the response to any arbitrarily varying field $h(t)$ can be expressed as a linear superposition of TRM magnetizations.

In order to discuss the decay of $M(t)$ we will show that a generalization of the Onsager postulate of normal regression of fluctuations applies to the dynamical off-equilibrium process [18]. The principle, originally stated for equilibrium systems, concerns the behaviour of *macroscopic quantities* and states that in the linear response regime one cannot distinguish the regression of a spontaneous fluctuation of a certain quantity from the regression from the same value when imposed through a constraint on the equilibrium measure. Onsager's postulate means that for a large system, a spontaneous fluctuation must have the characteristic of the *most probable* fluctuations and therefore corresponds to constrained minimization of the free energy. This is equivalent to free-energy minimization in a conjugated field, thus leading to an immediate derivation of the fluctuation–dissipation theorem.

The argument can be phrased in greater detail as follows [18]. Consider a thermodynamic system in equilibrium and a given macroscopic (extensive) quantity α which takes the value zero at equilibrium. Let γ be the corresponding conjugate intensive variable. Suppose that at time zero the quantity α has a small but extensive spontaneous fluctuation α_0. This will occur with exponentially small probability, but when it occurs the subsequent evolution of $\alpha(t)$ will be independent of the thermal noise, i.e. $\alpha(t) = E(\alpha(t)|\alpha_0)$, where we have denoted by $E(\cdot|\alpha_0)$ the conditional expectation over the trajectories for fixed α_0 at time zero. As α_0 is small, we can write

$$\alpha(t) = E(\alpha(t)|\alpha_0) = A(t)\alpha_0. \tag{20}$$

Denoting by $E_{\alpha_0}(\cdot)$ the average over the distribution of α_0, and $C_\alpha(t) = E(\alpha(t)\alpha(0))$ the correlation function, it follows that $A(t) = C_\alpha(t)/E_{\alpha_0}(\alpha_0^2)$. Note that the typical values of α_0 entering in the correlation function are of the order of $\sqrt{N}$, while in relation (20) we consider values of order N. The validity of the above analysis relies on the smoothness of the probability

† It should be kept in mind that $M(t)$ denotes the magnetization at time t but can depend on both t and u.

distribution of α_0 in the crossover region, an assumption which is at the heart of linear response theory.

As one is conditioning (20) by the value of α_0 only, then the overwhelming majority of the configurations $\mathcal{C}$ giving rise to the fluctuation are the ones 'typical' of the restricted canonical distribution

$$\frac{\mathrm{e}^{-\beta H(\mathcal{C})}\delta(\alpha(\mathcal{C})-\alpha_0)}{\int \mathrm{d}\mathcal{C}\,\mathrm{e}^{-\beta H(\mathcal{C})}\delta(\alpha(\mathcal{C})-\alpha_0)} \tag{21}$$

which is equivalent to

$$\frac{\mathrm{e}^{-\beta(H(\mathcal{C})-\gamma\alpha(\mathcal{C}))}}{\int \mathrm{d}\mathcal{C}\,\mathrm{e}^{-\beta(H(\mathcal{C})-\gamma\alpha(\mathcal{C}))}} \tag{22}$$

in which γ is fixed by $\langle\alpha\rangle_\gamma = \alpha_0$. Since to linear order in γ we have $\langle\alpha\rangle_\gamma = \beta\gamma\langle\alpha^2\rangle_{\gamma=0}$, it follows that the relaxation of $\alpha(t)$ induced by the field is given by

$$\alpha(t) = \beta\gamma C_\alpha(t). \tag{23}$$

which is the fluctuation–dissipation theorem in its integral form.

Here we would like to show how a generalized form of the regression principle holds in ageing dynamics where the time-scale separation suggests that, besides the fluctuations of the instantaneous magnetization $M(u)$, one should also consider possible fluctuations of the running global magnetization $m(u)$, defined as

$$m(t) = \frac{1}{N}\sum_{i=1}^{N} m_i(t). \tag{24}$$

We consider the conditional expectation value of the magnetization at time t given small values of the instantaneous and running magnetizations $M(u)$ and $m(u)$: $E(M(t)|M(u), m(u))$. This can again be expanded to first order:

$$E(M(t)|M(u), m(u)) = A(t,u)[M(u) - m(u)] + B(t,u)m(u) \tag{25}$$

and the functions A and B can be fixed by a continuity hypothesis, leading to

$$E(M(t)|M(u), m(u)) = \left[\frac{C_{st}(t-u)}{1-q_{EA}}[M(u)-m(u)] + \frac{C_{ag}(u/t)}{q_{EA}}m(u)\right] \tag{26}$$

where we have used $\langle(M(u)-m(u))^2\rangle = (1-q_{EA})/N$ and $\langle m(u)^2\rangle = q_{EA}/N$.

Onsager's argument demonstrates two things:

(a) that the decay of a spontaneous fluctuation with time is governed by the correlation function; and

(b) that a fluctuation induced by a conjugate field will decay as a spontaneous fluctuation if the probability distribution defining the state of the system immediately after the induced field is turned off is equal to the unperturbed probability distribution projected on the hypersurface defined by the equations

$$\frac{1}{N}\sum_{I=1}^{N} m_i(u) = m(u) \qquad \frac{1}{N}\sum_{I=1}^{N} S_i(u) = M(u) \tag{27}$$

where now, $m(u)$ represents the value of an average as (9) for times immediately *after* the field is turned off.

This second condition is consistent with our scenario of quasi-equilibrium in the dynamical relaxation process. In the following sections we will deal with the problem of computing the slow part of the magnetization induced by a field. We will first discuss the case of SK-like models whose OTOs during the dynamical relaxation tend to the ground state values. Then we will discuss those systems where the asymptotic state is different from the ground state. In this case, the argument is further complicated by the extensive multiplicity of the threshold states.

5. The case of SK-like models

We first recall that the equilibrium analysis of these models [19] in the 'one-step replica symmetry breaking' approximation determines the multiplicity of states at low free energy F [20] as

$$\mathcal{N}(F)\,\mathrm{d}F = \mathrm{e}^{\beta x(F-F_{GS})}\,\mathrm{d}F \tag{28}$$

where F_{GS} is the ground state free energy and x is the Parisi parameter in this approximation.

We then quote from the dynamical solution the expression of the magnetization in the TRM experiment described in the previous section:

$$M(t) = C_{st}(t-u)\beta h + C_{ag}(u/t)\beta hx. \tag{29}$$

The comparison of this with equation (26) tells us the following remarkable fact: the action of an external field h from time t_w to u produces at u a state of the system (in the sense of a measure in the microscopic variables) which is identical to the one we can obtain through infinite realizations of the thermal noise and selection of those trajectories with

$$\begin{aligned} M(u) - m(u) &= \beta h(1-q_{EA}) \\ m(u) &= \beta hxq_{EA}. \end{aligned} \tag{30}$$

Therefore, thanks to the use of Onsager's postulate it is enough to calculate the response at time u immediately after the magnetic field has been turned off. We have assumed t_w and u sufficiently large so that the system is in a quasi-state with free energy F slightly larger than that of the ground state. Equations (30) separate the response to the magnetic field into two components: (a) inside the same quasi-state the more probable configurations will change and (b) the quasi-state will change. The response (a) is the equilibrium intrastate response and is trivial. To isolate (b) we imagine turning off the magnetic field at time u and then waiting a finite time Δt such that $C_{st}^{(\Delta t)}$ is q_{EA}, while $\Delta t/u$ is still zero. Then we know that the system has gone from one quasi-state at time t_w to another at time $u + \Delta t$, both defined with zero magnetic field. The distribution of (zero-magnetic-field) quasi-states with this free energy is given by (28). Each of them may have a magnetization, uncorrelated from the free energy and with variance $\langle m^2\rangle = q_{EA}/N$. The typical number of quasi-states with free-energy density F and magnetization m is therefore given by

$$\mathcal{N}(F,m) = \mathrm{e}^{\beta x(F-F_{GS})}\mathrm{e}^{-Nm^2/2q_{EA}} \tag{31}$$

implying that

$$\mathcal{S}(F,m) = \beta x(F-F_{GS}) - \frac{m^2N}{2q_{EA}} \geqslant 0. \tag{32}$$

We first note that if we send u to infinity before sending h to zero, i.e. we consider fields such that the induced magnetization m verifies $\beta x(F_u - F_{GS}) \ll m^2N/2q_{EA}$ we can derive the result (30) in a quite straightforward way. In fact, we obtain that a non-zero magnetization has to be compensated by an increase of free energy so as to keep the configurational entropy $\mathcal{S}(F, m)$ non-negative

$$F - F_{GS} = \frac{m^2 N}{2q_{EA}\beta x}. \tag{33}$$

Along this line in the (F, m)-plane the state with lowest total free energy $F - hmN$ has

$$F = F_{GS} + \tfrac{1}{2}\beta N h^2 q_{EA} x \tag{34}$$

implying $m = \beta x h q_{EA}$.

The interpretation of this result is particularly illuminating. Turning on the magnetic field is a way of making energy available to the system. The thermal bath would normally absorb part of this energy. However, this is possible only if the entropy of the system decreases in the process. This cannot happen here as by hypothesis the available entropy is much smaller than that required to increase m. We conclude that the equilibration must occur only between the magnetic free energy hmN and the unperturbed, zero magnetic field F.

With this argument in mind we can now understand the limit which is more relevant to the dynamical approach. In this case $F(u) - F_{GS}$ is extensive and large with respect to the potential energy introduced by the external magnetic field. In this situation there is, formally, enough entropy to allow the magnetization to reach the value of equilibrium with the thermal bath $m = \beta h q_{EA}$. However, with the same token one would argue that the thermal bath could have absorbed that entropy to decrease the spin–spin interaction energy. We know that this is not the case, or rather that entropy/heat is absorbed at a certain rate basically determined by the barriers. The external force is uncorrelated to the direction of relaxation of the system, and therefore it is reasonable to assume that the turning on of the magnetic field *will not modify the rate of entropy decrease (heat transfer to the thermal bath)*. We conclude as before that the equilibration must occur between the magnetic free energy hmN and F. In formulae if we call $F^h(u)$, $F(u)$ the free energy (associated with the inter-spins coupling) that the system would reach in the presence of the magnetic field or in its absence at time u, then

$$\mathcal{S}(F^h(u), m(u)) = \mathcal{S}(F(u)) \tag{35}$$

so that

$$\beta x(F^h(u) - F_{GS}) - \frac{m(u)^2 N}{2q_{EA}} = \beta x(F(u) - F_{GS}). \tag{36}$$

The previous argument now follows minimizing $F^h(u) - Nhm(u)$.

We remark that both entropy reductions refer to the same degrees of freedom and therefore respond on the same time scale. The result is that the thermal bath acts as if it was uncoupled, while the two forms of (free) energy mutually equilibrate†. In other words, the transition time to higher free-energy states is much smaller than the one required to go to equal or lower free-energy states.

This argument is so crucial to our picture that we feel it necessary to try to confirm it with a detailed model of the dynamical process.

† This represents an instance of the recent proposal that a system and a thermometer responding on the same time scale will equalize their effective temperatures [10]. In fact, the inverse temperature of the magnetic field interaction energy is $\mathrm{d}S/\mathrm{d}E_h = \mathrm{d}(-m^2/2q_{EA})/\mathrm{d}(-mh) = m/(q_{AE}h) = \beta x$. However, our entropic interpretation suggests that time scales will depend strongly on βx—the lower the effective temperature, the slower the evolution of the system. If two different ageing systems starting with different effective temperatures and equal time scales are put into contact, they will quickly develop different time scales before equilibrating.

Let us imagine the dynamical trajectory from a (large) time u to a time t such that $C(t, u) \approx 0$. We discretize the dynamics in k steps such that $u = t_0 < t_1 < \cdots < t_k = t$ such that $C(t_{i+1}, t_i) = q_{EA} - \epsilon$ with ϵ small. At time t_i the system will have free energy F_i and $F_{i+1} - F_i$ will be small but extensive. The model we make of the dynamical process consists of assuming that when going from time t_i to time t_{i+1} the system can access different quasi-states with the lower one at free energy F_{i+1} and the higher ones distributed exponentially

$$\mathcal{N}(F) = \mathrm{e}^{\lambda(F-F_{i+1})} \tag{37}$$

while the probability of transition to a state with free energy F is proportional to

$$\mathrm{e}^{-\beta F}. \tag{38}$$

The model is consistent for $\lambda < \beta$ (otherwise the free energy would grow with time) and incorporates the following two features.

(a) The decrease in extensive free energy is deterministic.
(b) If we fix the initial condition, the increase in entropy in a single step is finite†. In fact, this can be calculated following the lines of [21] for the random energy model, with the result

$$\Delta S = \Gamma'(1) - \frac{\Gamma'(1-\lambda/\beta)}{\Gamma(1-\lambda/\beta)}. \tag{39}$$

In k steps the entropy generated will be $k\Delta S$ and therefore negligible with respect to $Nm^2/(2q_{EA})$. Although non-extensive, $k\Delta S$ can be arbitrarily large, thus explaining the divergence of two cloned trajectories. In this model we have heavily used the self-averaging character of the macroscopic quantities along the trajectories. It is again clear that the only way to develop a magnetization is by compensating it with an increase in the (zero-magnetic-field) free energy.

6. *p*-spin-like models

For p-spin-like models even the limit $t_w \to \infty$ before $h \to 0$ is non-trivial. In fact, it is well known that for this kind of system the properties of the quasi-states encountered in the dynamics are closer and closer to these of the threshold TAP states, which have extensive configurational entropy S_{th}. If this entropy were accessible in the dynamical process the equality (19) would be valid with $\mathcal{S}_\infty = S_{th}$. The condition that the total configurational entropy at time u should be positive would then read

$$S_{th} + \beta x(F_u - F_{th}) - \frac{m^2 N}{2q_{EA}} \geqslant 0 \tag{40}$$

which could be satisfied even if $F_u - F_{th}$ is small and negligible in front of $-m^2N/2q_{EA}$. In more physical terms we can say that among the $\mathrm{e}^{S_{th}}$ states there are $\mathrm{e}^{S_{th}-m^2/2q_{EA}}$ states with magnetization m. If all of these states were available to a single trajectory the response would be normal, $m = \beta h q_{EA}$. If we want the response to be anomalous we must show that the system, while wandering in phase space has no access to the configurational entropy‡.

† The entropy which we are talking about here corresponds to the dynamical probability in which the initial condition is fixed, and is therefore increasing with time.
‡ A moment of reflection reveals that otherwise the system, wandering in such a large space, would pass to lower-lying states and relax below F_{th}.

The logarithm of the number of states in the vicinity of any given TAP state has been computed by Cavagna *et al* in [22] in the case of the spherical p-spin model. Below threshold all states are isolated; there are no states closer than a given distance $q_{EA} - q_{\max}$, where $q_{\max}$ is a level-dependent overlap which tends to q_{EA} at threshold. Right at the threshold, the logarithm of the number of states as a function of the distance $(q_{EA} - q)$ is

$$N\Sigma(q) \propto N(q_{EA} - q)^5. \tag{41}$$

Let us again imagine a discretization of the dynamics in which at each step the system can jump a distance $\delta = (q - q_{EA})$. Then after n steps the log of the number of accessible states would be at most of the order of $n\delta^5$†. On the other hand, the distance travelled will be $\Delta = n\,\delta$ if all the steps are in the same direction and $\Delta = \sqrt{n}\,\delta$ if the steps are uncorrelated. In both cases it is easy to see that if we take the limit $\delta \to 0$ and $n \to \infty$ fixing Δ we find that $\log(\mathcal{N})/N$ goes to zero ($n\delta^5 \to 0$).

Note that the argument is based on the scarcity of states in the vicinity of a given state. This should be a generic feature for p-spin-like systems other then the p-spin model.

Having eliminated the configurational entropy from the balance, the argument proceeds as in the case of SK-like models.

Let us conclude by pointing out that threshold states with a large magnetization (of order $\beta h q_{EA}$) do exist, but are non-critical in the presence of the field. Therefore, with probability one such states would be isolated and unreachable.

7. Summary and conclusions

The main point of our analysis has been to give an explanation of the anomalous response function. We have found the physical origin of the equality between the FDR and the growth rate of the configurational entropy close to the asymptotic state. The value of the anomalous response can be traced to the lack of available entropy when the system is close to the low-lying states. Our interpretation clarifies the relation among equilibrium properties and off-equilibrium dynamics. For p-spin-like systems we have argued that the extensive configurational entropy of the threshold states does not play any thermodynamical role. We have seen that the classical Onsager argument on the equivalence between the regression of a spontaneous, noise-caused, fluctuation of the magnetization and the one induced by an external field can be generalized to ageing systems.

Our analysis can be summarized by saying that in ageing systems the rate of entropy decrease is a function of age and does not change due to small forces. Thus the balance is always between the value of the unperturbed free energy and that of the perturbation, without taking into account the thermal bath. We expect this conclusion to also hold in short-range systems with ageing.

In spin-glass materials, one-time observables equilibrate, and the picture we have developed relates to the structure of configuration space close to the ground state. In ageing experiment of structural glasses on the other hand, OTOs are far from their asymptotic values. Still, one can observe quasi-scaling ageing dynamics on two-time observables. The structure of the phase space visited on this time scale cannot be related to 'true' asymptotic properties of the system. We would like to speculate that even here the fluctuation–dissipation ratio, which could be a slowly varying function of time, is related to the derivative of the available

† This estimate could correspond to a severe double counting, as one can realize by applying the estimate to finite-dimensional Brownian motion. In infinite-dimensional problems we expect it to give essentially the correct result. However, in any case, we only need it as an upper bound in our argument.

phase space with the free energy also varying along the dynamical path. This could be true even if the system were to eventually reach equilibrium on a different time scale where FDT is asymptotically obeyed.

Finally, the case of multiple time sectors or multiple replica symmetry breakings will need trivial modifications.

Acknowledgments

We thank M Mezard, R Monasson, G Parisi and L Peliti for important discussions at the early stages of this work.

Appendix

The aim of this appendix is twofold. We first show that in the spherical p-spin model the derivative of the configurational entropy of the saddles is continuous at the threshold. Then, we prove that above T_d the paramagnetic state can be seen, to first order in $T - T_d$ as a collection of quasi-states identifiable with the points of least gradient of the TAP free energy.

Let us start from the expression of the TAP free energy for the spherical p-spin model [23]

$$F_{TAP}[m_i = \sqrt{q} S_i] = E_0 q^{p/2} - \tfrac{1}{4}\beta(1 - p(1-q), q^{-1+p} - q^p) - \frac{\log(1-q)}{2\beta} \tag{A1}$$

where E_0 is the angular part of the energy as a function of the angular variables S_i. It is well known that while one can find stationary points of the angular part for all the values of E_0 in the range $|E_0| > -E_{GS}$. Conversely, at finite temperature one finds solutions for the radial parts only in the range $-E_{th} > |E_0| > -E_{GS}$. The overwhelming majority of these solution are free-energy minima.

The stationary points of the angular part for $-E_{th} < |E_0|$ turn out to be saddles, with a number of unstable directions which depends on E_0. The number of stationary points as a function of E_0 is given by [24]

$$\Sigma(E_0) = \frac{1}{2}\left[\frac{2-p}{p} - \frac{2}{p^2 z^2} + \frac{(-1+p)z^2}{2} - \log(\tfrac{1}{2} p z^2)\right] \tag{A2}$$

where z is an auxiliary variable given by

$$-\frac{E_0}{-1+p} - \frac{\sqrt{E_0^2 - E_{th}^2}}{-1+p}. \tag{A3}$$

For the saddles $E_0 > E_{th} = -(\sqrt{2}\sqrt{(-1+p)/p})$ the formula becomes complex. This is due to the fact that the Hessian which appears in the computation [24] has negative eigenvalues and one has to compute the absolute value of its determinant. As suggested in [22] this can be done by just taking the real part of expression (A2), which gives the parabolic shape

$$\Sigma(|E_0| < -E_{th}) = -E_0^2 \frac{(p-2)}{2(p-1)} + \frac{1}{2}\log(p-1). \tag{A4}$$

An explicit computation using this formula shows that the E_0-derivative of (A2) and (A4) is continuous at the threshold energy.

Let us now pass to our second task. We would like to identify the quasi-states close to threshold as points of minima of the TAP gradient. Unfortunately, we were not able to prove this directly in the ageing regime at low temperature, for we do not know how to compute the dynamical entropy. We start then from the observation that for temperatures higher, but close to T_d one observes a slowing down of the dynamics with time-scale separation which becomes sharper and sharper as $T \to T_d$. So we can define dynamic quasi-states even above T_c, where the role of a small but finite $T - T_d$ is similar to the role of a finite t_w in the low-temperature dynamics. We put these quasi-states in relation with the TAP free energy, supposing that they coincide with the points of least TAP gradient for fixed internal energy equal to the paramagnetic value $-\beta/2$. These are saddle points of the angular part, while the radial part is an inflection point, i.e. we fix q in the value of the minimum of $\mathrm{d}F_{TAP}/\mathrm{d}q$. By explicit computation from (A1) and (A4) we find that the total free energy $F_{TAP} - T\Sigma(E_0)$ is equal to the paramagnetic free energy $-\beta/4$ up to terms which are of the second order in $T - T_d$. For instance, for $p = 3$ one finds that $F_{TAP} - T\Sigma(E_0) = -\beta/4 - 8\sqrt{2/3}(T - T_d)^2$.

References

[1] Struik L C E 1978 *Physical Aging in Amorphous Polymers and Other Materials* (Houston, TX: Elsevier)
Norblad P and Svendlindh P 1997 *Spin Glasses and Random Fields* ed A P Young (Singapore: World Scientific)
[2] Cugliandolo L F and Kurchan J 1993 *Phys. Rev. Lett.* **71** 173
[3] Franz S and Mézard M 1994 *Europhys. Lett.* **26** 209
Franz S and Mézard M 1994 *Physica* A **210** 48
[4] Cugliandolo L F and Kurchan J 1994 *J. Phys. A: Math. Gen.* **27** 5749
[5] Bouchaud J-P, Cugliandolo L, Mézard M and Kurchan J in 1997 *Spin Glasses and Random Fields* ed A P Young (Singapore: World Scientific)
[6] Cugliandolo L F, Kurchan J and Ritort F 1994 *Phys. Rev.* B **49** 6331
Baldassarri A 1998 *Phys. Rev.* E **58** 7047
[7] Franz S and Rieger H 1995 *J. Stat. Phys.* **79** 749
Parisi G 1997 *Phys. Rev. Lett.* **79** 3660
Parisi G 1997 *J. Phys. A: Math. Gen.* **30** 8523
Marinari E, Parisi G, Ricci-Tersenghi F and Ruiz-Lorenzo J J 1998 *J. Phys. A: Math. Gen.* **31** 2611
Parisi G, Ricci-Tersenghi F and Ruiz-Lorenzo J J 1998 *Phys. Rev.* B **57** 13 617
Barrat A 1998 *Phys. Rev.* E **57** 3629
Sellitto M 1998 *Euro. J. Phys.* B **4** 135
Franz S and Ricci-Tersenghi F 1998 *Preprint* cond-mat/9812059
Barrat J L and Kob W 1998 *Preprint* cond-mat/9806027
Barrat J L and Kob W 1999 *Physica* A **263** 234
Barrat J L and Kob W 1999 *Preprint* cond-mat/9905248
[8] Franz S, Mezard M, Parisi G and Peliti L 1998 *Phys. Rev. Lett.* **81** 1758
Franz S, Mezard M, Parisi G and Peliti L 1999 *J. Stat. Phys.* to appear
(Franz S, Mezard M, Parisi G and Peliti L 1999 *Preprint* cond-mat/9903370)
[9] Barrat A, Burioni R and Mezard M 1996 *J. Phys. A: Math. Gen.* **29** L81
[10] Cugliandolo L, Kurchan J and Peliti L 1997 *Phys. Rev.* E **55** 3898
[11] Mézard M, Parisi G and Virasoro M A 1985 *J. Phys. Lett.* **46** L217
Mézard M, Parisi G and Virasoro M A 1986 *Europhys. Lett.* **1** 77
[12] Monasson R (private communication)
Virasoro M A (unpublished)
[13] Nieuwenhuizen Th M 1999 *Phys. Rev.* E at press
(Nieuwenhuizen Th M 1998 Thermodynamic picture of the glassy state gained from exactly solvable models *Preprint* cond-mat/9807161)
[14] Baviera R and Virasoro M A 1997 *Physica* D **107** 151
[15] Monasson R 1995 *Phys. Rev. Lett.* **75** 2847
[16] Parisi G 1983 *Phys. Rev. Lett.* **50** 606

[17] Barrat A 1997 *Preprint* cond-mat/9701031 (unpublished)
Crisanti A and Sommers J 1992 *Z. Phys.* B **87** 341
Crisanti A, Horner H and Sommers J 1993 *Z. Phys.* B **92** 257
[18] Onsager L 1931 *Phys. Rev.* **37** 405
Onsager L 1931 **38** 2265
Onsager L 1996 *The Collected Works of Lars Onsager* (Singapore: World Scientific) (reprint)
[19] Mézard M, Parisi G and Virasoro M A 1987 *Spin Glass Theory and Beyond* (Singapore: World Scientific)
[20] Mézard M, Parisi G and Virasoro M A 1985 *J. Phys. Lett.* **46** L217
Mézard M, Parisi G and Virasoro M A 1986 *Europhys. Lett.* **1** 77
[21] Gross D and Mezard M 1984 *Nucl. Phys.* B **240** 431
[22] Cavagna A, Giardina I and Parisi G 1997 *J. Phys. A: Math. Gen.* **30** 7021
[23] Kurchan J, Parisi G and Virasoro M A 1993 *J. Physique I* **3** 1819
[24] Crisanti A and Sommers H J 1995 *J. Physique I* **5** 805