Measuring Equilibrium Properties in Aging Systems

Silvio Franz*
Abdus Salam International Center for Theoretical Physics, Strada Costiera 11, P.O. Box 563, I-34100 Trieste, Italy

Marc Mézard†
Laboratoire de Physique Théorique de l'Ecole Normale Supérieure,‡ 24 rue Lhomond, F-75231 Paris Cedex 05, France

Giorgio Parisi§
Dipartimento di Fisica and Sezione INFN, Università di Roma "La Sapienza," Piazzale Aldo Moro 2, I-00185 Rome, Italy

Luca Peliti‖
Dipartimento di Scienze Fisiche and Unità INFM, Università "Federico II," Mostra d'Oltremare, Padiglione 19, I-80125 Napoli, Italy
(Received 7 May 1998)

We corroborate the idea of a close connection between replica-symmetry breaking and aging in the linear response function for a large class of finite-dimensional systems with short-range interactions. In these systems, which are characterized by a continuity condition with respect to weak random perturbations of the Hamiltonian, the "fluctuation dissipation ratio" in off-equilibrium dynamics should be equal to the static cumulative distribution function of the overlaps. This allows for an experimental measurement of the equilibrium order parameter function. [S0031-9007(98)06959-2]

PACS numbers: 05.20.–y, 05.40.+j, 75.10.Nr

The glassy state of matter can appear in systems with quenched disorder (like spin-glasses), or in nondisordered systems. Ergodicity breaking takes a special form in these systems. A rather generic situation is the existence of many solid, "glass," phases, which are very different from one another, and unrelated among themselves by symmetry transformations. Hence the Gibbs equilibrium measure decomposes into a mixture of many pure states. This phenomenon was first studied in detail in the mean field theory of spin-glasses, where it received the name of replica-symmetry breaking [1]. But it can be defined in a straightforward way and easily extended to other systems, by considering an order parameter function, the overlap distribution function. This function measures the probability that two configurations of the system, picked up independently with the Gibbs measure, lie at a given distance from each other [2]. Replica-symmetry breaking is made manifest when this function is nontrivial.

The existence of nontrivial overlap distributions, first found in mean field systems, has been shown unambiguously, through numerical simulations, in finite-dimensional spin-glass systems with short-range interactions [3]. This order parameter function is a very important tool for the mathematical description of the Gibbs state. Unfortunately it seems impossible to access it experimentally for two reasons: (1) Large glassy systems never reach equilibrium at low temperatures; (2) The measurement of the distance between configurations requires a detailed observation at the microscopic—atomic—level, which is impossible. (In simulations, the second objection disappears, and one can get around the first one by working with smart algorithms and small enough systems.)

The first objection is a very basic one: experimentally, glassy systems exhibit a nonequilibrium behavior, which requires a dynamical description. Quite often, they exhibit a special type of dynamical behavior called aging, i.e., the property that extensive one-time quantities like the energy, magnetization, etc., are asymptotically close to time-independent values, whereas two-time quantities, like the autocorrelation functions and their associated linear response functions, continue to depend on the time elapsed after the quench even for long times. Aging, defined in this way, appears in mean field spin-glasses and has been exhibited in spin-glass experiments [4,5]. We will not discuss systems undergoing "stabilization" [6] (sometimes called "physical aging" [7]), where one-time quantities cannot be considered close to their asymptotic values during typical experiments. (This phenomenon has been recently observed in a lattice gas model with constrained dynamics [8].) In aging dynamics the usual equilibrium properties do not hold. The analysis of some spin-glass mean field models [9] has suggested, in particular, that the usual fluctuation-dissipation relation between the correlation and the response should be modified in a well-defined way. This modification, which holds when both the age of the system and the measurement time are large, involves the rescaling of the temperature

 0031-9007/98/81(9)/1758(4)$15.00

by a "fluctuation-dissipation ratio" (FDR), which depends on the relation between the two times involved [10,11]. This FDR can be found experimentally by simultaneous measurements of the noise and the response on various time scales and age scales.

The aim of this paper is twofold. We shall first show that, in *finite dimensional* systems with *short-range* interactions, there exists an identity relating the—experimentally accessible—FDR to an equilibrium order parameter function. This static order parameter function is an interesting new object. We shall then discuss its relationship to the usual distribution of overlaps. Our argument relies on a perturbation of the original Hamiltonian by the addition of some weak—but thermodynamic—random perturbations. This method has been recently used to derive interesting properties of the overlap distribution at equilibrium [12,13].

We use the language of magnetic systems, and denote by S_x the spin at a point x of a lattice of size L^d in d dimensions. We work with classical spins which are real variables in a double well potential, and the Ising limit will often be considered for simplicity. We call $H(S)$ the Hamiltonian. Our argument is rather general, and we do not have to specify much the Hamiltonian: it contains short-range interactions, in a d dimensional space; it may contain quenched disorder or not. The evolution of the spin dynamics is governed by the Langevin equation at temperature T

$$\dot{S}_x = -\frac{\partial H}{\partial S_x} + \eta_x , \tag{1}$$

where η_x is a white noise of variance $\langle \eta_x(t)\eta_y(t')\rangle = 2T\delta_{xy}\delta(t-t')$. (We denote by angular brackets thermal averages, i.e., either in the dynamic framework, the average with respect to the realization of the random noise, or in the static framework, the average with respect to the Gibbs measure.) The system starts at time $t=0$ from a random initial condition. Important quantities are the correlation function, $C(t,t') = (1/N)\sum_x \langle S_x(t)S_x(t')\rangle$, and the response function, which measures the response of the spins at time t to an instantaneous field at time t',

$$R(t,t') = \frac{1}{N}\sum_x \frac{\delta\langle S_x(t)\rangle}{\delta\eta_x(t')} . \tag{2}$$

The quantity which is measured experimentally (thermoremanent magnetization) is the integrated response function, defined by $\chi(t,t') = T\int_0^{t'} dt''\, R(t,t'')$.

The FDR $X(q)$ is obtained by considering the infinite-time limit of the response function, fixing the correlation function $C(t,t')$ to a given value q [9–11],

$$X(q) = \lim_{\substack{t,t'\to\infty \\ C(t,t')=q}} \frac{\partial\chi(t,t')}{\partial t'} \Big/ \frac{\partial C(t,t')}{\partial t'} . \tag{3}$$

The usual equilibrium dynamics is obtained by sending the two times t,t' to infinity while keeping their difference $\tau = t - t'$ fixed. Then the correlation and response functions, $C(t,t')$ and $R(t,t')$, reach their equilibrium values, $c(\tau)$ and $r(\tau)$. In short-range systems this regime relates to the property of "local equilibrium," i.e., to the fact that any finite region of space reaches equilibrium locally. The Edwards-Anderson order parameter is defined dynamically by $q_{\rm EA} = \lim_{\tau\to\infty} c(\tau)$, and the usual fluctuation-dissipation theorem asserts that, for $q > q_{\rm EA}$, $X(q) = 1$. The aging regime concerns systems with weak ergodicity breaking, such that the correlation $C(t,t')$ relaxes below $q_{\rm EA}$ when $t\to\infty$ (at fixed t') [14]. Then the FDR $X(q)$ can become different from unity in the regime $q < q_{\rm EA}$. Numerical measures of the FDR have been performed in short-range spin-glasses, ferromagnets, and structural glass models [15], through parametric plots of the integrated response function versus the correlation [5]. The ratio $T/X(q)$ can be interpreted as an effective temperature [16].

We wish to relate the FDR to an equilibrium order parameter. Let us add to the original Hamiltonian a perturbation of the form ϵH_2, with

$$H_2 = \sum_x h_x S_x S_{\mathcal{T}(x)} , \tag{4}$$

where the h_x's are independent Gaussian random variables of variance one, and $\mathcal{T}$ is a translation of length $L/2$ in a fixed direction e, say, the x axis [so that $\mathcal{T}(x) = x + (L/2)e$]. The thermal expectation value of the perturbation $\langle H_2\rangle$ is a contribution to the internal energy of the system which is extensive and self-averaging, i.e., independent (in the thermodynamical limit) of the particular realization of the disorder contained in either H or H_2. The interaction H_2, which looks long range, is, in fact, a local perturbation in a different space. Let us divide the space into two halves (S_l and S_r) and rename the spins in the right-hand part so that if $x \in S_l$ then $\mathcal{T}(x) \in S_r$ and $S_{\mathcal{T}(x)} = S'_x$. The total Hamiltonian can now be written as

$$H(S,S') = H_l(S) + H_r(S') + B(S,S') + \epsilon \sum_{x\in S_l} h_x S_x S'_x . \tag{5}$$

The Hamiltonian H_l and H_r refer, respectively, to the spins in S_l and S_r. The term $B(S,S')$ is a surface term whose presence does not affect the average of H_2. Dropping it, the Hamiltonian (5) characterizes a spin system of size $L^d/2$, with two spins S_x, S'_x on each site, and a purely local interaction. Notice that in the case of disordered systems the spin systems S and S' taken individually contain two independent realizations of the disorder.

Since the perturbation H_2 is a sum of local terms, the thermal expectation value (for almost all realizations of the disorder) $\langle H_2(t)\rangle$ measured in the dynamics has a long-time limit which is equal to its equilibrium expectation value. The proof of this fact is standard for systems with short-range interactions. We first notice that the free energy density $f(t)$ must reach, at long times, its equilibrium value $f_{\rm eq}$: if it were to converge to a value $f(\infty)$ larger than the equilibrium one, one could always nucleate a bubble of radius r with the equilibrium free energy, with a cost of free energy less than or equal to $cr^{d-1} + [f_{\rm eq} - f(\infty)]r^d$, which becomes negative for large enough r. Therefore the free energy reaches equilibrium, as well as its derivative with respect to ϵ, proving the convergence of $\langle H_2(t)\rangle$. (Notice that we do not discuss here the time scale for reaching this equilibrium, which may become very long in some systems: what matters here is that it is finite when $L \to \infty$.)

We now compute the expectation value of the perturbation H_2 in the dynamics and in the statics. Since $\langle H_2(t)\rangle$ is self-averaging, it is equal to its average over the random field h and all other possible quenched disorder in the system, which we denote by $E_h\langle H_2(t)\rangle$. In the dynamical framework, starting from the Langevin equation in the presence of the perturbation ϵH_2, we express the average of H_2 in the Martin-Siggia-Rose formalism [17] as a path integral,

$$\begin{aligned}\langle H_2(t)\rangle &= E_h\langle H_2(t)\rangle \\ &= E_h \int \mathcal{D}(S)\,\mathcal{D}(\hat S)\, e^{I[S,i\hat S]} \sum_x h_x S_x(t) S_{\mathcal{T}(x)}(t)\,,\end{aligned} \tag{6}$$

with the dynamical action

$$\begin{aligned} I[S,i\hat S] = \int dt' \sum_x i\hat S_x(t') \\ \times \left[\dot S_x + \frac{\partial H}{\partial S_x} + \epsilon \frac{\partial H_2}{\partial S_x} + iT\hat S_x\right]. \end{aligned} \tag{7}$$

Integrating by parts over the h_x's, and observing that the insertion of $i\hat S_x(t')$ acts as the derivative with respect to an impulsive magnetic field at site x and at time t', $\delta/\delta h_x(t')$, we obtain [18]

$$E_h\langle H_2(t)\rangle = 2\epsilon \sum_x E_h \frac{\delta}{\delta h_{\mathcal{T}(x)}(t)} \langle S_x(t) S_x(t') S_{\mathcal{T}(x)}(t')\rangle\,. \tag{8}$$

In the linear response regime $\beta\epsilon \ll 1$, the average of the product on far away sites factorizes up to terms of order ϵ, and one has

$$\begin{aligned} E_h \frac{\delta}{\delta h_{\mathcal{T}(x)}(t)} \langle S_x(t) S_x(t') S_{\mathcal{T}(x)}(t')\rangle = C(t,t')R(t,t') \\ + O(\epsilon)\,. \end{aligned} \tag{9}$$

Assuming that the bound holds uniformly in time (remember that the large volume limit is taken before the large time limit) and substituting the definition (3) of the FDR we obtain for large values of t

$$2\epsilon\beta N \int_0^1 dq\, X_\epsilon(q) q = \epsilon\beta N\left(1 - \int_0^1 dq\, \frac{dX_\epsilon}{dq}\, q^2\right), \tag{10}$$

where we have assumed $\lim_{t\to\infty} C(t,0) = 0$ for simplicity. We have denoted by X_ϵ the FDR of the system with the perturbed Hamiltonian. Notice that this is a very general result that holds for every sample in the case where there is quenched disorder.

We now turn to the statics. The thermal equilibrium average of H_2 is self-averaging with respect to disorder. We can thus evaluate it as follows:

$$\langle H_2\rangle = E_h \frac{1}{Z} \sum_S e^{-\beta[H(S)+\epsilon H_2(S)]} \sum_x h_x S_x S_{\mathcal{T}(x)}\,. \tag{11}$$

Integrating by parts over the h_x's, we obtain

$$\langle H_2\rangle = \beta\epsilon N E_h\left(1 - \frac{1}{N}\sum_x \langle S_x S_{\mathcal{T}(x)}\rangle^2\right). \tag{12}$$

Invoking again linear response for small ϵ, together with the fact that x and $\mathcal{T}(x)$ are infinitely far apart in the thermodynamic limit, we can write

$$E_h\langle S_x S_{\mathcal{T}(x)}\rangle^2 = E_h\langle S_x S_y\rangle^2 + O(\epsilon)\,, \tag{13}$$

where x and y are two far away spins not directly coupled in H_2. We obtain then (up to higher orders in ϵ)

$$\langle H_2\rangle = \beta\epsilon N E_h\left(1 - \int dq\, P_\epsilon(q) q^2\right). \tag{14}$$

The last equality, involving the overlap distribution $P_\epsilon(q)$ for the perturbed system, results from the decomposition of the Gibbs measure into a sum of pure states characterized by a clustering property [2].

Comparing the two results, (10) and (14), for the dynamics and the statics, we see that the second moments of the dynamical order parameter function $dX_\epsilon(q)/dq$ and of the static one $P_\epsilon(q)$ coincide for the system in the presence of the perturbation ϵH_2. It is straightforward to generalize this derivation to perturbations of the type $H_p = \sum_x h_x S_x S_{\mathcal{T}_1(x)} \cdots S_{\mathcal{T}_{p-1}(x)}$, where $\mathcal{T}_k(x) = x + (k/pL)e$. (For $p = 1$ the perturbation is nothing but a small random field term.) This shows that the pth moments of the two functions $dX_\epsilon(q)/dq$ and $P_\epsilon(q)$ coincide.

Let us now consider the functions $\tilde X(q) = \lim_{\epsilon\to 0} X_\epsilon(q)$ and $\tilde P(q) = \lim_{\epsilon\to 0} P_\epsilon(q)$. (To be precise, we need to introduce simultaneously all the perturbations with arbitrary p and strength ϵ_p, and send all the ϵ_p's to 0.) These are two characteristic functions of our problem. One describes the violation of the FDR in the out of equilibrium dynamics, and the other describes some equilibrium correlations. These two functions are equal, and thus an unexpected link between statics and dynamics is established.

We now discuss the relationship between the new functions $d\tilde X/dq, \tilde P(q)$, and the more conventional definitions of the FDR and the overlap distribution. Let us first consider the equilibrium distribution $\tilde P(q)$. Clearly, in a situation with ergodicity breaking and several nearly degenerate pure states, the effect of the ϵ perturbation which scales as $\epsilon\sqrt{L^d}$ induces a reshuffling of the weights of the states. A simple example appears when there is an exact degeneracy due to a symmetry. For instance, in the case of an Ising Hamiltonian quadratic in the spin variables, the symmetry by reversal of all the spins implies that the overlap distribution $P(q)$ of the unperturbed system is symmetric: $P(q) = P(-q)$, each pure state appearing with the same weight as its symmetric one in the Gibbs measure. This symmetry will be violated by the perturbation terms H_p with odd p, leading (in the absence of further reshuffling) to the relation $\lim_{\epsilon\to 0^+} P_\epsilon(q) \equiv P_{0^+}(q) = 2\theta(q)P(q)$. Suppose now that care has been taken of all the symmetries of the system, by defining a modified $\hat{P}(q)$ measuring the distance between orbits of the symmetry group. It is reasonable to believe that, for a large class of systems, the reshuffling of the weights will lift only the degeneracy, so that $\tilde{P}(q) = \hat{P}(q)$. We shall refer to such systems as being *stochastically stable*. Mean field spin-glasses fall into this category, as well as Ising ferromagnets in dimensions $d \geq 2$ [19], but we do not know how to characterize this class in general. Turning to the case of dynamics, it is trivial to show that the limit of $\epsilon \to 0$ is smooth when it is taken before the limit of large times (the infinite volume limit is always taken first). If the limits commute, then the static $\tilde{X}(q) = \int_0^q dq' \tilde{P}(q')$ is identical to the dynamical (FDR) $X(q)$ of the unperturbed system, measured with *random* initial spin configurations. This result holds for Sherrington-Kirkpatrick spin-glasses, but is violated, e.g., in p-spin spherical spin-glass models, where the dynamics is dominated by infinitely long-lived metastable states.

Summarizing, we have introduced a new order parameter function for systems at equilibrium, which can be related in general, in finite-dimensional systems, to the FDR of a weakly perturbed system. This new order parameter is interesting since its moments are obtained as expectation values of extensive quantities. It is thus much more robust than the usual overlap distribution, and will not have the same chaotic behavior under weak perturbations. It is interesting to notice that in mean field spin-glasses, the order parameter appearing from the replica computation is naturally related to this new order parameter. For stochastically stable systems, this new order parameter is equal to the overlap distribution of symmetry classes of the states, and can be measured experimentally. The relation implies that in any finite-dimensional system replica-symmetry breaking and aging in the response functions either appear together or do not appear at all. Although we have used the language of the magnetic systems, the arguments put forward here can be generalized to systems of a different nature, using different random perturbations of the Hamiltonian.

S. F. thanks Professor D. Sherrington for kind hospitality at the Department of Theoretical Physics of the University of Oxford, where part of this work was elaborated. We thank A. Barrat, A. Cavagna, I. Giardina, D. Sherrington, and M. Virasoro for valuable discussions.

*Email address: franz@ictp.trieste.it
†Email address: mezard@lpt.ens.fr
‡Unité propre du CNRS, associée à l'Ecole Normale Supérieure et à l'Université de Paris Sud.
§Email address: giorgio.parisi@roma1.infn.it
‖Email address: Luca.Peliti@na.infn.it

[1] Reviews can be found in K. Binder and A. P. Young, Rev. Mod. Phys. **58**, 801 (1986); M. Mézard, G. Parisi, and M. A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987); K. H. Fischer and J. A. Hertz, *Spin Glasses* (Cambridge University Press, Cambridge, 1991); *Spin Glasses and Random Fields,* edited by A. P. Young (World Scientific, Singapore, 1997).
[2] G. Parisi, Phys. Rev. Lett. **50**, 1946 (1983).
[3] For a recent review see E. Marinari, G. Parisi, and J. J. Ruiz-Lorenzo, in the last of Ref. [1].
[4] L. Lundgren, P. Svedlindh, P. Nordblad, and O. Beckman, Phys. Rev. Lett. **51**, 911 (1983); P. Nordblad, P. Svedlindh, L. Lundgren, and L. Sandlund, Phys. Rev. B **33**, 645 (1986); M. Alba, J. Hamman, M. Ocio, and Ph. Refrigier, J. Appl. Phys. **61**, 3683 (1987); F. Lefloch, J. Hamman, M. Ocio, and E. Vincent, Europhys. Lett. **18**, 647 (1992). For a recent review see P. Norblad and P. Svendlindh, in the last of Ref. [1].
[5] For a recent review see J.-P. Bouchaud, L. Cugliandolo, M. Mézard, and J. Kurchan, in the last of Ref. [1].
[6] J. Zarzycki, *Glasses and The Vitreous State* (Cambridge University Press, Cambridge, 1991).
[7] L. C. E. Struik, *Physical Aging in Amorphous Polymers and Other Materials* (Elsevier, Houston, 1978).
[8] J. Kurchan, L. Peliti, and M. Sellitto, Europhys. Lett. **39**, 365 (1997).
[9] L. F. Cugliandolo and J. Kurchan, Phys. Rev. Lett. **71**, 173 (1993).
[10] S. Franz and M. Mézard, Europhys. Lett. **26**, 209 (1994); Physica (Amsterdam) **210A**, 48 (1994).
[11] L. F. Cugliandolo and J. Kurchan, J. Phys. A **27**, 5749 (1994).
[12] F. Guerra, Int. J. Mod. Phys. B **10**, 1675 (1997).
[13] M. Aizenmann and P. Contucci, e-print cond-mat/9712129 [J. Stat. Phys. (to be published)].
[14] J.-P. Bouchaud, J. Phys. (Paris) **2**, 1705 (1992).
[15] S. Franz and H. Rieger, J. Stat. Phys. **79**, 749 (1995); G. Parisi, Phys. Rev. Lett. **79**, 3660 (1997); J. Phys. A **30**, 8523 (1997); E. Marinari, G. Parisi, F. Ricci-Tersenghi, and J. J. Ruiz-Lorenzo, J. Phys. A **31**, 2611 (1998); G. Parisi, F. Ricci-Tersenghi, and J. J. Ruiz-Lorenzo, Phys. Rev. B **57**, 13 617 (1998); A. Barrat, Phys. Rev. E **57**, 3629 (1998).
[16] L. Cugliandolo, J. Kurchan, and L. Peliti, Phys. Rev. E **55**, 3898 (1997).
[17] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Clarendon Press, Oxford, 1989).
[18] A similar technique was first used in [9] in order to relate the FDR to the expectation value of a long-range perturbation in the p-spin systems.
[19] S. Franz, M. Mézard, G. Parisi, and L. Peliti (to be published).