

Generalized off-equilibrium fluctuation-dissipation relations in random Ising systems

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Abstract. We show that the numerical method based on the off-equilibrium fluctuation-dissipation relation does work and is very useful and powerful in the study of disordered systems which show a very slow dynamics. We have verified that it gives the right information in the known cases (diluted ferromagnets and random field Ising model far from the critical point) and we used it to obtain more convincing results on the frozen phase of four-dimensional spin glasses. Moreover we used it to study the Griffiths phase of the diluted and the random field Ising models.

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1 Introduction

In the last years more and more interest has been devoted to systems which show a very slow dynamics [1]. Major examples are spin glasses and structural glasses, which can be viewed as a supercooled liquid which slowly evolves never reaching equilibrium. In the study of such systems is clear the important role played by the off-equilibrium dynamics, which describes the behavior of the real system, in contrast with the equilibrium thermodynamic properties (which may differ from that of a not well thermalized system) [2].

Two well-known spin systems which show very slow approach to equilibrium are spin glasses [3,4] and diluted ferromagnets. In both cases it has been found that the effective dynamical exponent z in the frozen phase is quite large. Such effect makes the dynamics of those models very slow in the frozen phase.

In the last years we have used and compared two different kinds of simulations: a) Monte Carlo simulations by which we measure the *statics* of the model, *i.e.* we sample the configurational space according to the usual equilibrium Gibbs-Boltzmann distribution; b) a second kind of Monte Carlo during which we keep the system in the out of equilibrium regime, we let it relax during a very large waiting time and then we measure quantities slowly varying in time (the *dynamics* of the model). Hereafter with the word “dynamical” we will always refer to the out of equilibrium dynamics and never to the dynamics at the equilibrium. Thanks to some relations which link the thermodynamical observables to these off-equilibrium quantities we are able

to calculate, for the Edwards-Anderson (EA) model, the critical exponents measuring the relaxational dynamics at the critical point [5], and, as we will show in the present work, also the (functional) order parameter in the frozen phase.

The advantages of these dynamical studies are manifold. We do not need to thermalize the system (which is a very hard task in disordered systems) and so we are not restricted to study very small volumes. On the contrary we must use very large volumes to keep the sample in the off-equilibrium regime ($\xi(t) \ll L$, where $\xi(t)$ is the dynamical correlation length, which is the typical distance over which the system is equilibrated at time t) and therefore the finite size effects are irrelevant for not too large times. We can obtain information on the statics of the model *via* the dynamical scaling and we can predict the value of not self-averaging quantities (like the $P(q)$ in spin-glasses) only measuring self-averaging ones, and so we do not need to average over a large number of disorder realizations. This very important feature could also be exploited by the experimentalists to calculate the distribution function of the overlap in a spin glass sample, which until today was measurable only in numerical simulations¹.

In this work we present the results of a dynamical study on the diluted ferromagnetic and the random field models on one side and the spin glass model on the other. These models behave very differently in their statics, even if they age similarly in the out of equilibrium regime. Using the numerical method based on the off-equilibrium fluctuation-dissipation relation (OFDR), introduced

¹ An indirect experimental determination of $P(q)$ has been done in [6].

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for the study of the EA model by Franz and Rieger [7] and summarized in the next section, we can measure the correct equilibrium properties of the model. The presence of a large number of metastable states in all the models does not invalidate the method, which succeed in predicting the right thermodynamical state. Once checked the validity of the method, we can use it to determine whether the frozen phase of the spin glass model in finite dimensions is better described by the mean-field like solution [2, 4, 5, 8–10] or by the droplet model [11].

This last question is very interesting and still not completely answered, even if in the last years an impressive collection of numerical tests has been obtained [2, 8, 10, 12–14], suggesting a mean-field like picture. Recently, some criticisms have been raised against the mean-field picture, especially in the papers by Newman and Stein [15] and in that by Moore *et al.* [18].

We have given a numerical counter-example to the recipe that Newman and Stein provides in reference [15] in order to obtain the “right” $P(q)$. Our counter-example has been published in [16]. This numerical counter-example suggests that the results by Newman and Stein are based on heuristic assumptions which seems to be wrong. We leave a detailed analysis of this point to a paper, which is in the process of being written [14].

Moreover in a recent comment [17] to the work of Moore *et al.* [18] has been shown that the result stated in the cited paper was only a numerical coincidence. In particular, for the energy overlap has been found [17] that the Migdal-Kadanoff approximation used in [18] fails to describe even the numerical data for small lattice sizes.

From the experimental point of view, we can address the interested reader to some recent experimental papers that support an analysis of a mean-field type for the low temperature phase of the three dimensional spin glass [19, 20] and that ruled out clearly the droplet picture [20]. In [20] the behavior of the dynamical critical exponent was computed. The agreement with the previous numerical simulations is very good even to a quantitative level. The authors tried a fit to the droplet formula but the exponents of the fit were very different to that computed in numerical simulations (in this case, the quality of the fit was poor) and the value of the ψ exponent was dangerously at the lower bound imposed by the droplet theory. This implies that the droplet theory has been ruled out clearly in this experiment. In order to complete the discussion on the experimental results we should cite those by the Upsala group. However, this group avoid to analyze its experimental data using non real space models, in its words [21]: “... and we do not try to interpret our results on aging in spin glasses in term of non real space models”.

This paper gives one little step more in the direction of explaining the low-temperature phase of the four dimensional spin glass model in term of a mean-field like picture.

Few analytical results and the definitions of the models studied will be presented in the next section. In the third and fourth sections we show the numerical results and in the last one our conclusions. In the last year the

OFDR has been measured in many different systems. A clear classification of the models seems to come out from these studies. This classification will be presented in the Appendix.

2 Analytical results

2.1 Off-equilibrium fluctuation-dissipation relation

Assuming time translation invariance (TTI), which is valid in the evolution of a system at the equilibrium, can be proved the fluctuation-dissipation theorem (FDT), that reads

$$R(t, t') = \beta \theta(t - t') \frac{\partial C(t, t')}{\partial t'}, \quad (1)$$

where β is the inverse temperature and $\theta(t - t')$ is the step function, given by causality. Here TTI implies that $C(t, t') = C(t - t')$ and $R(t, t') = \mathcal{R}(t - t')$. The autocorrelation (a two times function) and the response function are defined as follows

$$C(t, t') \equiv \overline{A(t)A(t')}, \quad R(t, t') \equiv \left. \frac{\overline{\delta A(t)}}{\delta \epsilon(t')} \right|_{\epsilon=0}, \quad (2)$$

where we assume that the original Hamiltonian has been perturbed by a term

$$\mathcal{H}' = \mathcal{H} + \int \epsilon(t) A(t). \quad (3)$$

A common choice in spin models is $A(t) = \sum_i \sigma_i(t)$ and $\epsilon(t)$ as an external magnetic field. The brackets $\langle \langle \dots \rangle \rangle$ imply here an average over the dynamical process and the overbar $\overline{(\dots)}$ a second one over the disorder.

In the out of equilibrium evolution (starting for example from a random configuration) the FDT does not hold any more. Nonetheless some years ago has been proposed by Cugliandolo and Kurchan [22] a generalization of this theorem which should be valid in the early times of the dynamics, when the system is too far from the equilibrium. Such generalization, that we call off-equilibrium fluctuation-dissipation relation (OFDR), has been obtained in the study of spin glass mean-field models. Only recently has been numerically verified that such generalization is also valid in a short-range spin glass model [10].

Let us recall how this relation can be obtain. In the off-equilibrium regime TTI is no longer valid and so all two-times functions depend explicitly on both times and not only on their difference. The fundamental assumption [22] is that, in this regime, FDT is modified simply by a multiplicative factor $X(t, t')$. This assumption have been verified in reference [10] for the EA model. In the large times region ($t \gg 1, t' \gg 1$) the violation factor depends on the times t and t' only *via* the autocorrelation function [23]: $X(t, t') = X[C(t, t')]$.

Assuming OFDR

$$R(t, t') = \beta X[C(t, t')] \theta(t - t') \frac{\partial C(t, t')}{\partial t'}, \quad (4)$$

we can now extract the violation factor $X(C)$ from the measures of autocorrelation and magnetization, which are self-averaging quantities.

In the linear-response regime ($h \ll 1$) we can write the magnetization as

$$m[h](t) = \int_{-\infty}^t dt' R(t, t') h(t'), \quad (5)$$

where the upper limit of the integral has been set to t due to causality.

Substituting equation (4) into equation (5) we have that

$$m[h](t) = \beta \int_{-\infty}^t dt' X[C(t, t')] \frac{\partial C(t, t')}{\partial t'} h(t'). \quad (6)$$

The way we perturb the system is important for the numerical purposes² and we choose to switch on a random field of intensity h_i , that depends on the site, at time t_w : $h_i(t) = h_i \theta(t - t_w)$, where h_i is a Gaussian variable with zero mean and variance h_0 . The corresponding magnetization and susceptibility are defined by

$$m[h](t) = \overline{\langle \sigma_i h_i \rangle} / h_0, \quad (7)$$

$$\chi(t, t_w) = \lim_{h_0 \rightarrow 0} \frac{m[h](t)}{h_0}. \quad (8)$$

Then we have that

$$\chi(t, t_w) = \beta \int_{t_w}^t dt' X[C(t, t')] \frac{\partial C(t, t')}{\partial t'}, \quad (9)$$

and by performing the change of variables $u = C(t, t')$ we finally obtain the key equation

$$\chi(t, t_w) = \beta \int_{C(t, t_w)}^1 du X(u), \quad (10)$$

where we have used the fact that $C(t, t) \equiv 1$ in Ising models.

From equation (10) the violation factor $X(C)$ can be easily extracted simply measuring the autocorrelation function $C(t, t_w)$ and the integrated response to a small external field $\chi(t, t_w)$.

Equation (10) can be rewritten as

$$T\chi(t, t_w) = S[C(t, t_w)], \quad (11)$$

where we have defined

$$S(C) = \int_C^1 du X(u). \quad (12)$$

We remark that all the information we need is encoded in the shape of the function $S(C)$.

If the system is at equilibrium the violation factor is equal to one and the relation becomes

$$T\chi(t, t_w) = 1 - C(t, t_w) \quad \text{or} \quad S(C) = 1 - C. \quad (13)$$

² In the first work on the subject Franz and Rieger [7] used $h_i(t) = h\theta(t_w - t)$, that gives less clear results.

2.2 Link between the statics and the dynamics

To get information on the thermodynamical properties of the model we should match the violation factor $X(C)$ to some static observable. This can be done using the following conjecture [22, 24] (proved under some assumptions in [25]) on the large times behavior of the $X(C)$, which has already been verified in [10]. Sending $t \rightarrow \infty$ and $t_w \rightarrow \infty$, keeping $C(t, t_w) = q$

$$X[C(t, t_w)] \longrightarrow x(q). \quad (14)$$

The function $x(q)$ is well-known in spin glass theory [4] and it is linked to the thermodynamical order parameter $P(q)$ via

$$x(q) = \int_0^q dq' P(q'), \quad (15)$$

where the overlap distribution function $P(q)$ is the thermodynamic probability of finding two copies of the system with overlap q . Moreover, we can define

$$s(C) = \int_C^1 du x(u). \quad (16)$$

Now we have all the ingredients for our numerical recipe: we measure the autocorrelation function and the integrated response to a small external field for large times, then we make a derivation and we obtain the function $P(q)$. The meaning of the outcoming function $P(q)$ is well described in [4].

A classification of the models can be given in terms of the violation factor X . We will report this classification in the Appendix.

3 The models

We simulate Ising spin models on cubic ($d = 3$) or hypercubic ($d = 4$) lattices with the following Hamiltonian

$$\mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} \sigma_i \sigma_j - \sum_i h_i \sigma_i, \quad (17)$$

where the first sum runs over the first-neighbors pairs. Depending on the model the couplings J_{ij} and the fields h_i are fixed to some value or are taken randomly with some distribution function.

The three random models we are interested in are:

SDIM (Site-Diluted Ising Model) where $J_{ij} = J\epsilon_i\epsilon_j$ and $h_i = 0$. Every ϵ_i follows the probability distribution $P(\epsilon_i) = c\delta(\epsilon_i - 1) + (1 - c)\delta(\epsilon_i)$, where c is the spin concentration. The dimensionality will be $d = 3$.

RFIM (Random Field Ising Model) where $J_{ij} = 1$ and every h_i follows the probability distribution $P(h_i) = \frac{1}{2}[\delta(h_i + h_r) + \delta(h_i - h_r)]$. The dimensionality will be $d = 3$.

EA (Edwards-Anderson Model) where J_{ij} is a Gaussian distributed variable of zero mean and unit variance. Moreover, in this case, we have set the magnetic field to zero ($h_i = 0$). We will study this model in four dimensions.

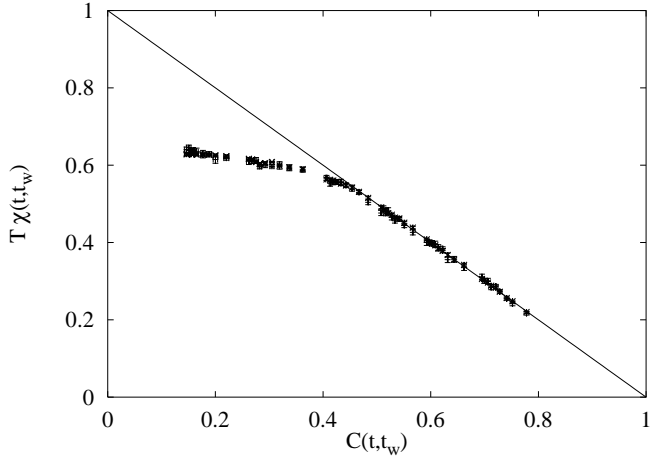


Fig. 1. This plot shows that we are working in the linear response regime. The data obtained from the simulation of a spin glass model ($T = 1.35 = \frac{3}{4}T_c$ and $t_w = 10^4$) using two different magnetic fields ($h_0 = 0.1$ and $h_0 = 0.05$) used to compute the response function, are perfectly superimposed. In the following we will use a perturbing field of intensity $h_0 = 0.1$.

4 Numerical results

All the simulations have been performed on a *tower* of the parallel computer APE100 [26], with a peak performance of 25 Gigafllops.

We have numerically computed the function $S(C)$ for the models presented in Section 3. All the plots present the integrated response multiplied by the temperature versus the autocorrelation. These plots should be read from right to left and from bottom to top, since during the simulation $C(t, t_w)$ starts from 1 and falls off, while $\chi(t, t_w)$ starts from zero and increases. The equation of the line is always $1 - C$ and we define $q_{EA}(t_w)$ as the value of the autocorrelation when the data with waiting time t_w left the straight line $1 - C$. In the model which present a ferromagnetic transition we often use m_0^2 instead of q_{EA} , being m_0 the spontaneous magnetization.

We have checked that we work in the linear response regime by simulating all three models with perturbations of intensity $h_0 = 0.1$ and $h_0 = 0.05$. We have checked that both magnetic field gives the same response function. For example, in Figure 1, the data for $h_0 = 0.1$ and $h_0 = 0.05$ coincide in the four dimensional spin glass. Moreover, we always simulated very large volumes with a small number of disorder realization (typically from 2 to 6), since we are measuring correlation and response functions, which are self-averaging.

4.1 Site-diluted Ising model

In Figure 2 and 3 we show the data for the site-diluted ferromagnetic model in $d = 3$, with concentration respectively $c = 0.65$ and $c = 0.8$.

A great care has to be taken in order to keep the system in the out of equilibrium situation in the whole run. We require the off-equilibrium correlation length $\xi(t)$

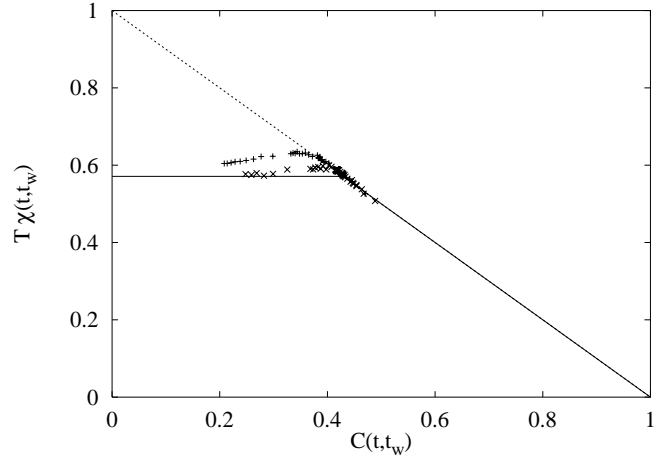


Fig. 2. The function $S(C)$ for the 3d diluted Ising model with a spin concentration $c = 0.65$. We used a volume of 400^3 and a temperature $T = 2.4314 = 0.9 T_c$. The two sets of data have been measured after a waiting time $t_w = 10^3$ (uppermost) and $t_w = 10^4$ (lowermost). The line $1 - C$ is the FDT regime, while the horizontal line is the infinite time limit of the data. See the text for more details.

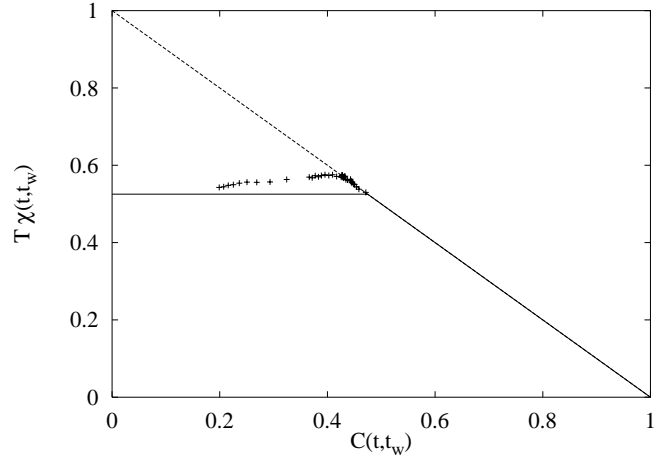


Fig. 3. The function $S(C)$ for the 3d diluted Ising model with a spin concentration $c = 0.8$. The volume is 520^3 , the temperature $T = 3.1497 = 0.9 T_c$ and $t_w = 10^3$. The line $1 - C$ is the FDT regime, while the horizontal line is the infinite time limit of the data. See the text for more details.

[5, 8, 9] to be always much less than the sample size L . This requirement is quite easy to satisfy in a spin glass due to the high value of the dynamical exponent z : working in the frozen phase ($T \simeq \frac{3}{4} T_c$) is practically impossible to thermalize a sample with $L = 32$, which is the size that we use in the simulations described in Section 4.3. In a diluted ferromagnet the situation is much more subtle because two main reasons. Firstly the dynamics is slow but not so much like in spin glasses, especially for small dilution (on the time scales we use the “effective” dynamical exponent z seems to increase with the dilution [27, 28]). On the other hand, we must simulate in the frozen phase, where the spontaneous magnetization m_0 is different

from zero, but near to the critical temperature in order to have a small order parameter.

To solve this problem we have used always large volumes (up to 140 millions of spins) and we have checked how far from equilibrium the system was during all the simulation. The simplest way to do that is to measure the absolute value of the instantaneous magnetization, which is very small in the off-equilibrium dynamics and which grows, around the thermalization time, converging to m_0 . All the data presented here come out from runs where the magnetization is statistically compatible with zero in the whole simulation.

Two different regimes can be clearly distinguished. In the regime $(t - t_w) < t_w$, or equivalently $C(t, t_w) > m_0^2(t_w)$ the data stay on the line $T\chi(t, t_w) = 1 - C(t, t_w)$, which means that the system is in a quasi-equilibrium regime where the relation between the correlation and the response is like that at the equilibrium. In the regime $(t - t_w) > t_w$ (*i.e.* $C(t, t_w) < m_0^2(t_w)$) the data leave the straight line and the violation of the FDT can be summarized in the X factor, which is nothing but the derivative of the curve followed by the data (with the opposite sign).

It is clear from the plots that the diluted ferromagnetic model belongs to the category A defined in the Appendix, with $X = 0$ and the data which stay on a horizontal line.

In Figures 2 and 3 we draw also the lines corresponding to the infinite time limit. As explained in the Appendix, in the ferromagnetic phase the model should have an

$$s(C) = \begin{cases} 1 - C & \text{for } C > m_0^2, \\ 1 - m_0^2 & \text{for } C \leq m_0^2, \end{cases} \quad (18)$$

being m_0 the equilibrium spontaneous magnetization.

The spontaneous magnetization have been calculated from equilibrium simulations, in order to check the convergence of the data measured in the out of equilibrium regime. As it can be seen the data presented are already very near to the asymptotic regime. The horizontal line in Figures 2 and 3 is given by $1 - m_0^2$. For our purposes the main information is that the shape of $S(C)$ does not depend strongly on the value of t_w in a large time range.

A further remark on these data is needed in order to justify why $\chi(t, t_w)$ slightly decreases with time in the region $(t - t_w) > t_w$. Being $\chi(t, t_w)$ the integral of the response, which we would expect that is a non-negative function, it is surprising that it is a decreasing function of the time. The little decrease is mainly due to the high susceptibility of the spins placed on the interfaces (domain walls), which give to the response an extra contribution which will disappear for longer times, when the fraction of spins on the domain boundaries gets smaller. This effect has been already found by Barrat [29] in the study of the OFDR in a coarsening pure ferromagnet.

The results from the diluted ferromagnetic model are very important because they rule out the possibility that what we measured in spin glasses [10] was simply a dynamical artifact, which shadows the true static behavior. Now we are sure that the method based on the OFDR is able to give us information on the right thermodynamic

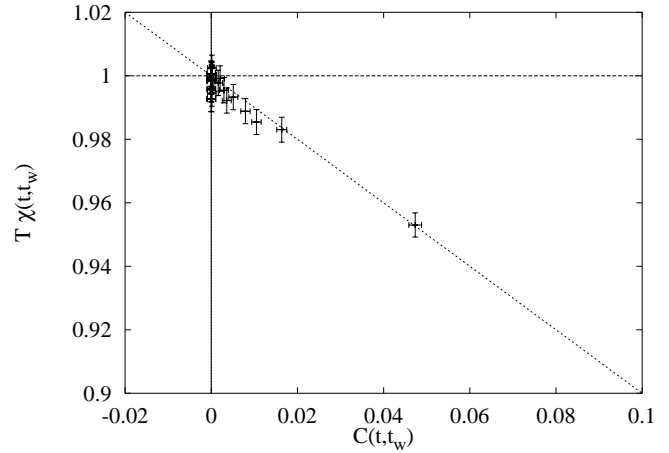


Fig. 4. The 3d diluted Ising model with $c = 0.8$ and $T = 4.0$, that is in the region, $T_c \simeq 3.5 < T < T_c^{(0)} \simeq 4.5$, where the Griffiths singularities [30] may break the replica symmetry, clearly behaves like in the paramagnetic and replica symmetric phase (*i.e.* the data always stay on the FDT line) with the autocorrelation decreasing to zero in a fast way. The results do not depend on t_w . Note that the plot range is zoomed in the upper left corner of the usual range.

state, no matter of how complex is the dynamics followed by the system in reaching that state.

One more result from these simulations is the strong hint that the diluted ferromagnetic model has no replica symmetry breaking in the Griffiths phase [30]. To this purpose a run was also performed in the temperature region between the critical temperature of the pure model ($T_c^{(0)} \simeq 4.5$ [31]) and that of the diluted one ($T_c \simeq 3.5$ [31]). In this region the model could show a replica symmetry breaking [32]. Our results (Fig. 4) show very clearly that there is no replica symmetry breaking and the data behaves in the same way they do in the paramagnetic region, *i.e.* they stay on the FDT line, while the autocorrelation decays rapidly to the limiting value, which is zero for the diluted ferromagnetic model in the high temperature phase.

A heuristic analytical argument can be provided in order to justify why in a diluted ferromagnetic model (with Z_2 as global symmetry) can not exist a phase transition from a paramagnetic to a spin glass phase. In the paramagnetic phase of a ferromagnetic model (diluted or not) the two-point correlation function is positive and obviously less than 1

$$0 < \langle \sigma_i \sigma_j \rangle \leq 1 \quad \forall i, j. \quad (19)$$

Using the definitions of the magnetic and spin glass susceptibility for $T > T_c$

$$\chi_m = \sum_{i,j} \overline{\langle \sigma_i \sigma_j \rangle} \quad \chi_q = \sum_{i,j} \overline{\langle \sigma_i \sigma_j \rangle^2}, \quad (20)$$

where the angular brackets $\langle \langle \dots \rangle \rangle$ stands for the thermal equilibrium average in a given sample and $\overline{\langle \dots \rangle}$ stands for average over the disorder. The inequality $\langle \sigma_i \sigma_j \rangle^2 \leq \langle \sigma_i \sigma_j \rangle$

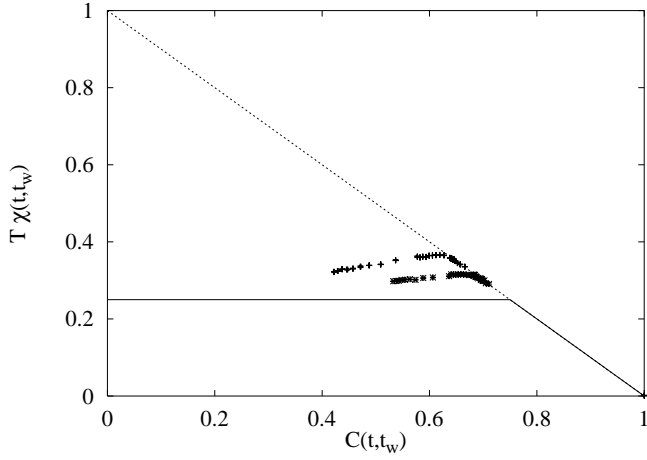


Fig. 5. The function $S(C)$ for the 3d RFIM with bimodal field distribution. The volume is 440^3 , the field $h_r = 1.2425$, the temperature $T = 3.2 = 0.9 T_c$ and the waiting time $t_w = 10^3$. The data behave like in a ferromagnet and they should converge to the horizontal line.

can be easily demonstrated, and so, above the critical temperature we have that

$$\chi_q \leq \chi_m \quad \forall T > T_c. \quad (21)$$

The transition to a spin glass phase is usually defined as the divergence of the spin glass susceptibility (χ_q), while the magnetic one (χ_m) remains finite. This can not happen if equation (21) holds.

4.2 Random field Ising model

In Figures 5 and 6 we show the results for the 3d random field Ising model (RFIM) with bimodal field distribution $h_i = \pm h_r = \pm 1.2425$, whose critical temperature is $T_c = 3.55$ [33]. We have simulated very large volumes, 440^3 , in a wide range of temperatures.

The main result in the low temperature phase, $T < T_c$, is that the function $S(C)$ converges quite rapidly to the right ferromagnetic equilibrium function (category A of the Appendix):

$$s(x) = \begin{cases} 1 - x & \text{for } x > m_0^2, \\ 1 - m_0^2 & \text{for } x \leq m_0^2, \end{cases} \quad (22)$$

where m_0 is the equilibrium spontaneous magnetization. This limiting function is plotted with a continuous line in Figure 5. The data plotted in that figure are relative to $t_w = 10^2$ (uppermost) and $t_w = 10^3$ (lowermost). The decrease of the data for $C(t, t_w) < m_0^2(t_w)$ is due to the same reason we explained before in the case of the diluted Ising model and, as it can be seen in Figure 5, the effect tends to disappear for larger t_w .

The data for $T > T_c$ are plotted in Figure 6 and the four data spots correspond to temperatures, from bottom to top, $T = 3.9, 4.5, 5.0, 8.0$. Note that the abscissa range

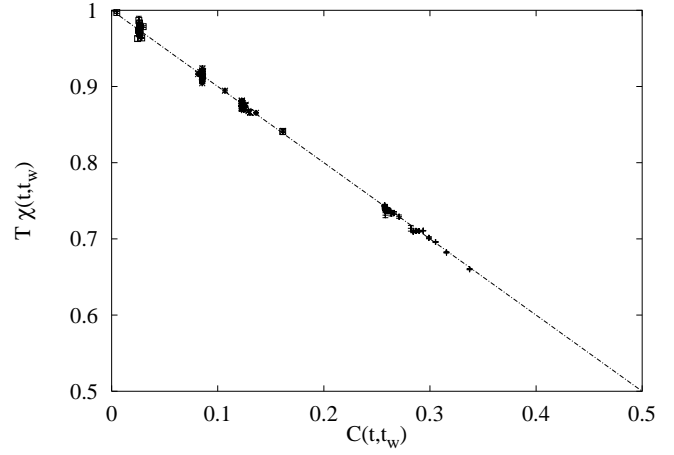


Fig. 6. High temperature behavior of the RFIM with bimodal field distribution. We have used a volume of 440^3 and a field $h_r = \pm 1.2425$. The four data spots correspond to temperatures (from below to top) $T = 3.9, 4.5, 5.0, 8.0$. The results are t_w -independent.

used is smaller than the typical one, because the data converges rapidly to the equilibrium value. The aging effects quickly disappear and the results become independent of the value of t_w and so we are able to use always a quite small value for the waiting time $t_w = 10^2$. Note that in the RFIM the autocorrelation function does not tend to zero even in the high temperature range. This can be simply understood writing a mean-field equation, that it should work in the high temperature region even at a quantitative level, for the equilibrium magnetization of a given sample

$$m_i = \tanh \left(\beta \sum_j m_j + \beta h_i \right), \quad (23)$$

where $m_i = \langle \sigma_i \rangle$ and the angular brackets $\langle (\cdot) \rangle$ stands for the thermal equilibrium average in a given sample. For high temperatures the first term in the hyperbolic tangent argument in equation (23) will be smaller than the second one. In fact assuming that $m_i \simeq \tanh(\beta h_i) \propto \beta$ for small β values, we have that $\beta \sum_j m_j \propto \beta^2$, which is much smaller than βh_i .

For large times the equilibrium autocorrelation function tends to $\lim_{\tau \rightarrow \infty} C(\tau) = N^{-1} \sum_i m_i^2$ (we call this limit C_∞) and then we have that in the RFIM this limit is non-zero even in the high temperature region and equals

$$C_\infty(\beta, h_r) = \int dh P(h) \tanh^2(\beta h) = \tanh^2(\beta h_r), \quad (24)$$

where the last equality holds only for the bimodal random field distribution we have used. We have verified that the autocorrelation function at temperatures $T = 5.0$ and $T = 8.0$ converges to the C_∞ value given by equation (24), as it should.

Our conclusion are that all the data behave in the same way of the diluted Ising model, showing no replica symmetry breaking, even in the temperature region between

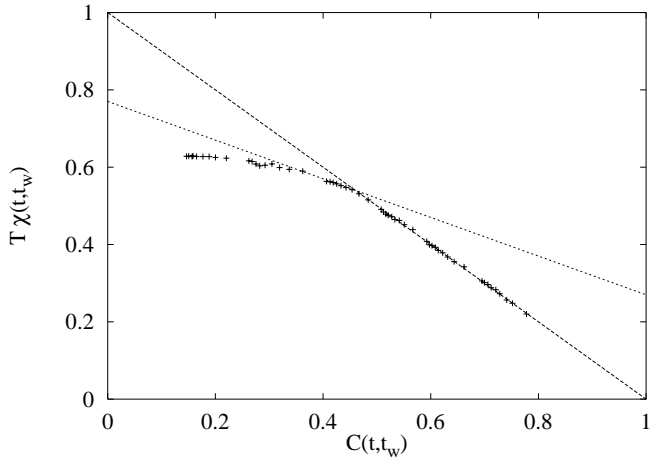


Fig. 7. The function $S(C)$ for the $4d$ Ising spin glass. The volume is 32^4 , the temperature $T = 1.35 = 0.75 T_c$ and $t_w = 10^4$. The line $1 - C$ is the FDT regime, while the other one is only a guide for the eyes (see text).

the critical temperatures of the random model and that of the pure one (this region defines the Griffiths phase of the model). A spin glass phase could be expected just above the critical temperature [34] (which is $T_c \simeq 3.55$ in our case), but from our data measured at $T = 3.9 \simeq 1.1 T_c$ we can conclude that, if this phase exists, it should be in a very narrow temperature range. In fact in the work of Sacconi [35] in $d = 4$ the spin glass critical temperature was found to be only few percent greater than the ferromagnetic one. The region very close to the critical one (*i.e.* $3.55 < T < 3.9$) is not yet explored and we are actually investigating it.

4.3 Edwards-Anderson model

The data plotted in Figure 7 are obtained from a simulation of an Edwards-Anderson (EA) model in $d = 4$ spatial dimensions. They are of the same type of the ones already presented in [10]. In addition to previous data [10] we have simulated very large waiting times. Moreover, we report them to make a comparison between the models belonging to categories A and C. Anyhow note that the data reported here come out from longer runs and now we can assert with higher confidence that the EA model belongs to category C, contradicting the droplet theory [11] which assign it to category A.

We tried to fit the data to a two-lines behavior (categories A and B), but the result was discarded because of the high χ^2 value. The only prediction which seems to be compatible with our data is the one coming from the mean-field-like scenario of finite-dimensional spin glasses [8, 12, 14], which predicts a full replica symmetry breaking solution for the Edwards-Anderson model and assign it to category C. In Figure 7 we also plot a second straight line to emphasize the curvature of the data in the aging regime.

The data plotted in Figure 7 have $t_w = 10^4$ and we believe that they have an $S(C)$ function very similar to the asymptotic one.

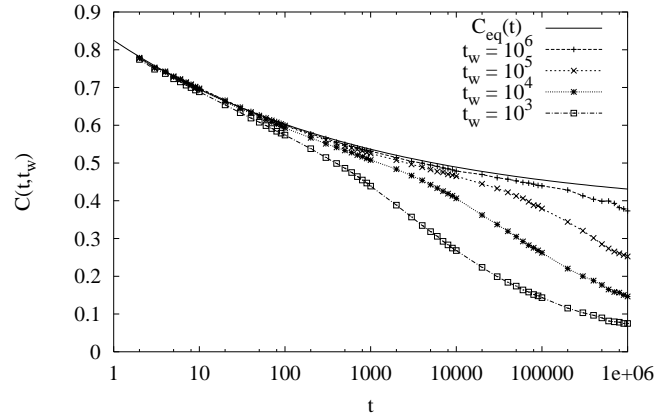


Fig. 8. The autocorrelation functions of a system of volume 32^4 and temperature $T = 1.35$ with many different waiting times. The higher curve is the infinite time extrapolation: $C_{\text{eq}}(t) = 0.37(1) + 0.455(5)t^{-0.145(3)}$.

The time dependence of the fluctuation-dissipation ratio in spin glasses is a subject to be dealt with very much care, because of the very slow dynamics. We dedicated to the study of this subject a great numerical effort (several weeks of the parallel computer APE100) to be able to extrapolate our results to the infinite times limit where we can link it with the statics. We simulated 12 systems of size 32^4 with waiting times as large as $t_w = 10^6$ and magnetic fields of intensity $h_0 = 0.1$ and $h_0 = 0.05$. With such very high values of t_w we can safely extrapolate to infinite waiting times our data.

To confute the prediction of the droplet theory that assign the EA model to category A, we focus our attention on two points of the function $S(C)$:

- the point where the system leaves the quasi-equilibrium regime to enter the aging one, whose coordinates in the plane $(C, T\chi)$ are $(q_{\text{EA}}, 1 - q_{\text{EA}})$;
- the point where the system, with a finite t_w , converges for very large times ($t \rightarrow \infty$), whose coordinates are $(0, T\chi_0)$.

Note that the first point also represent the equilibrium state into a single pure state, that can be obtained sending first $t_w \rightarrow \infty$ and then $(t - t_w) \rightarrow \infty$. In a model belonging to category A the two points must have the same height, while we show that $T\chi_0 > 1 - q_{\text{EA}}$.

We obtain $q_{\text{EA}} = 0.37(1)$ from the data of the autocorrelation function (see Fig. 8) and

$$T\chi_0(t_w) = T \lim_{t \rightarrow t_w + \infty} \chi(t, t_w) = 0.75(1), \quad (25)$$

from the data of the response with $t_w = 10^6$. This value should be considered as a lower bound for χ_0 , defined as

$$\chi_0 = \lim_{t_w \rightarrow \infty} \chi_0(t_w), \quad (26)$$

because the data slightly increase with increasing t_w ³.

³ If we take the limits in the reversed order we obtain a relation valid in a single pure state $T\chi_{\text{eq}} = 1 - q_{\text{EA}}$.

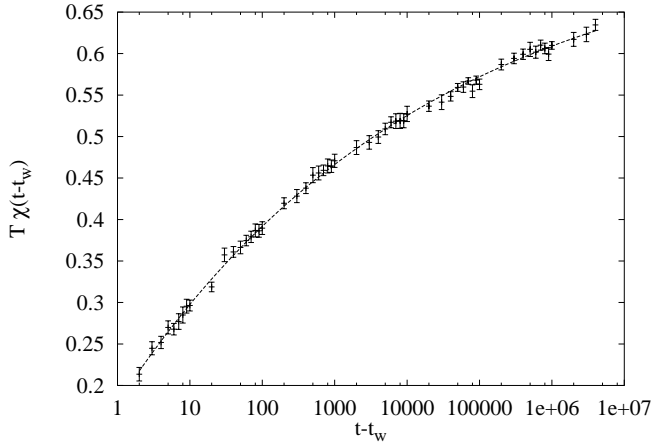


Fig. 9. Numerical data for the linear response in a system of volume 32^4 , temperature $T = 1.35$ and perturbation $h_0 = 0.05$ applied after a waiting time $t_w = 10^6$. The curve is the best fitting power law (see text).

The extrapolation of the $\chi(t, t_w)$ data is shown in Figure 9 together with the best fitting power law function:

$$T\chi(t) = 0.75(1) - 0.571(7)t^{-0.102(4)}, \quad (27)$$

Even if the exponent is very small, we think our extrapolation to be very trustworthy because we used more than six time decades and the fit is very good: $\chi^2/\text{d.o.f} = \frac{24.2}{54}$, where d.o.f stands for degrees of freedom.

An exponent so small like the one we found, though in agreement with previous numerical works [13], could be interpreted as an hint for a logarithmic law. We tried to fit the data with some logarithmic law and we found an asymptotic value greater than the one obtained with the power law. So we can assert, with high confidence, that the value found is a good lower bound for χ_0 and the inequality holds.

The validity of the inequality $T\chi_0 > 1 - q_{\text{EA}}$ confirms that in the EA model there is a breaking of the replica symmetry.

5 Conclusions

In this work we have shown how the complexity of the frozen phase of a disordered system can be obtained *via* the measurements of autocorrelation and response functions in the out of equilibrium regime.

We have checked that the generalization of the fluctuation-dissipation theorem, proposed by Cugliandolo and Kurchan, is valid for all the models where we have tested it.

In the case of the diluted ferromagnetic model and of the random field Ising model the off-equilibrium fluctuation-dissipation relation succeed in predicting the existence of a single pure state at the equilibrium, even if the out of equilibrium dynamics is very slowed by the large number of metastable states (like in spin glasses).

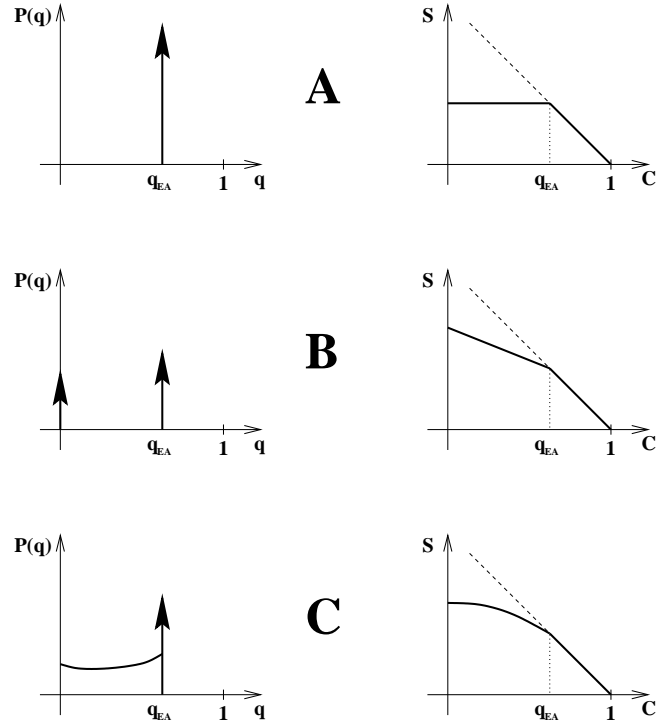


Fig. 10. A possible model classification based on the function $S(C)$. The big arrows represent delta functions.

We believe that this is a further step in the proof that the method is robust and we think that this method will give the opportunity of studying disordered systems with less expensive simulations.

The results obtained with this method and reported here show that in the temperature region under study (still far away from the critical point) no evidences of replica symmetry breaking have been found in the diluted ferromagnetic and the random field models. While the frozen phase of the four dimensional Edwards-Anderson model is well described by a mean-field-like solution.

Appendix

In Section 2 we obtained the link between the statics and the dynamics, *i.e.* between the OFDR and the $P(q)$. With this link we can now translate to the dynamical framework the usual classification of complex systems based on the form of replica symmetry breaking [4]: one step or full replica symmetry breaking.

We will consider always only the positive part of the distribution function of the overlaps ($P(q)$ for $q > 0$), assuming that the Hamiltonian is invariant under a global flip of the spins.

In a model whose frozen phase is well described by a single pure state (no replica symmetry breaking) the distribution function of the overlap is a single delta function: *e.g.* for the pure ferromagnetic model with $T < T_c$ we have $P(q) = \delta(q - m_0^2)$, where $m_0(T)$ is the spontaneous magnetization at a given temperature T . These models

are the simplest in the sense that their frozen phase can be described simply giving one parameter. To such a simple thermodynamic description correspond an OFDR like the one depicted in Figure 10a, with an horizontal line in the region $C < q_{EA} = m_0^2$. We group these models in category A.

The second category (B) groups such models which show a transition with only one step of replica symmetry breaking (p -spin models with $p > 2$ in the mean-field approximation, binary mixtures of soft spheres [36] and Lennard-Jones mixtures [37]) and which seem to well describe the real glass transition. The mean-field version of the p -spin model in the cold phase has a solution with two delta functions, $P(q) = m \delta(q) + (1 - m) \delta(q - q_{EA})$ where m is a function of the temperature (*e.g.* $m = T/T_c$ in the Random Energy Model), and so their OFDR is given by two straight lines like the one shown in Figure 10b.

In the category C we include all the models which show an infinite number of steps of replica symmetry breaking (like the Sherrington-Kirkpatrick model and the Edwards-Anderson one). They have a $P(q)$ different from zero in a whole range $q \in [0, q_{EA}]$ with a delta function on the greater allowed value q_{EA} . These models have an OFDR like the one shown in Figure 10c.

In any case there is a time region ($(t - t_w) < t_w$ and $C > q_{EA}$), which we call of *quasi-equilibrium*, where the FDT holds and $S(C) = 1 - C$. The differences arise in the *aging* regime ($(t - t_w) > t_w$ and $C < q_{EA}$), where only the models belonging to category A do not show any aging effect in the response, that is their integrated response is flat and $S(C)$ is constant. On the other hand, models of categories B and C do also respond in the aging regime, in a way that depends on the value of the waiting time. This memory effect is an important feature of a kind of disordered systems and the method based on the OFDR is able to measure it.

In the aging regime can be naturally defined an effective temperature *via* [38]

$$\hat{T} = \frac{T}{X(C)} \quad \text{or} \quad \hat{\beta} = X(C)\beta. \quad (\text{A.1})$$

This effective temperature is infinite for the models that do not have memory in the response (cat. A), is finite for the category B models and takes values in a broad distribution for systems with full replica symmetry breaking (cat. C).

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