

Off-equilibrium fluctuation-dissipation relations in the 3d Ising spin glass in a magnetic fieldA. Cruz,^{1,2,*} L. A. Fernández,^{3,2,†} S. Jiménez,^{1,2,‡} J. J. Ruiz-Lorenzo,^{4,2,§} and A. Tarancón^{1,2,**}¹Depto. de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain²Instituto de Biocomputación (BIFI), Universidad de Zaragoza, Zaragoza, Spain³Depto. de Física Teórica, Facultad de CC. Físicas, Universidad Complutense de Madrid, 28040 Madrid, Spain⁴Depto. de Física, Facultad de Ciencias, Universidad de Extremadura, 06071 Badajoz, Spain

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We study the fluctuation-dissipation relations for a three dimensional Ising spin glass in a magnetic field both in the high temperature phase as well as in the low temperature one. In the region of times simulated we have found that our results support a picture of the low temperature phase with broken replica symmetry, but a droplet behavior cannot be completely excluded.

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I. INTRODUCTION

The understanding of the behavior of a spin glass in a magnetic field is a challenging issue from both experimental and theoretical sides. On the theoretical side, there are two competing theories. In the droplet model the spin glass phase is unstable (for any amount of magnetic field) and so there is no phase transition: there is only a pure state describing the entire Ising spin glass in a magnetic field.¹ On the other side, the mean field (MF) approximation predicts a phase transition between two phases. The first one is characterized by one pure state, and the low temperature phase is described by a countable number of pure states. In the mean field approximation a third order phase transition² has been found between those two phases^{3,4} separated by the de Almeida-Thouless line.⁵ See Ref. 4 for a description and Ref. 6 for a critique of the replica symmetry breaking (RSB) picture.

Hence, those two competing theories have opposite predictions about the overall behavior of a spin glass in the presence of a magnetic field. However, to perform experimental or numerical tests of the previous analytical predictions has proved very difficult despite the clear theoretical predictions (phase transition or not).

A further step in mean field computations is to take into account the effect of fluctuations. This can be done, for instance, using field theoretic methods, and has been done in the past. Working with a projected theory (by taking only the replicon sector which contains the most divergent terms of the initial Hamiltonian) no fixed points have been found in the model.⁷ It is important to mention that the existence or not of a transition in magnetic field affects the existence or not of a phase with RSB at zero magnetic field. In particular the absence of a fixed point for the Ising spin glass in a magnetic field supports the droplet picture against the mean field one.

A recent and detailed analysis⁸ reached the same conclusions as Ref. 7, and so three possibilities are opened: (i) no phase transition at all, (ii) a first order phase transition driven by fluctuations, and finally (iii) a second order phase transition dominated by a fixed point outside the accessible perturbative region (i.e., the region of small parameters). However, a fourth possibility was recently opened by Temesvári and De Dominicis,⁹ who extended the field theoretic analysis fur-

ther. They analyzed a field theory in which the replicon and anomalous sectors are both *critical* going beyond the old analysis where only the replicon sector was taken to be critical. The main result of this analysis is the existence of a new critical point (which appears at eight dimensions) taking the control of the phase transition at six dimensions. The authors also pointed out that this new fixed point provides a phase transition which has different features from that of the mean field.

On the numerical side the situation is a bit clearer (but not enough). Looking at the off-equilibrium numerical simulations, the difference between the mean overlap and the minimum overlap has been computed.¹⁰⁻¹² In four dimensions and not for too low temperatures there is a clear difference between these two measurements, which is a clear signature of replica symmetry breaking. Another off-equilibrium approach is to compute the violation of the fluctuation-dissipation theorem out of equilibrium. This has been done using a slightly modified version of the four dimensional Gaussian spin glass,¹⁰ and it was found that the violation is well understood in terms of a nontrivial low temperature phase. In this paper we will follow this approach but working in three dimensions and simulating the Edwards-Anderson model. It is important to notice that the same kind of studies on the violation of fluctuation-dissipation out of equilibrium can be done in real experiments. In fact, in a recent paper,¹³ the violation of the fluctuation-dissipation relations in an Ising spin glass (in zero magnetic field) was reported, and the experiment can be explained in terms of replica symmetry breaking.

Another numerical method is to use exact ground state techniques in order to understand the qualitative features of the low temperature phase. This has been done in three dimensions, and a RSB behavior has been found between zero and a magnetic threshold (for the Gaussian Ising spin glass in 3d, this threshold is near 0.65); however, this work cannot completely exclude a droplet behavior.¹⁴ A recent study¹⁵ pointed out that there is no phase transition at all (at finite temperature), but one cannot exclude a critical field below 0.4.

We can cite different numerical studies working at equilibrium. Those studies have been mainly done in four dimensions in order to avoid the proximity to the lower critical

dimension (which is between two and three, at least in the Ising spin glass without magnetic field). Those studies are not fully conclusive, but the existence of a finite temperature phase transition emerges as the most likely explanation for the numerical data.^{16,17}

On the experimental side the situation is not clear. There is strong experimental evidence about an irreversibility line (where the zero field cooled and the field cooled magnetizations start to be different), but unfortunately, that line depends on the time, and so, we have only off-equilibrium information about what happens in the presence of a magnetic field. In the literature, one can find some attempts to analyze the scaling behavior of the freezing temperatures, and the conclusion is that no phase transition exists.¹⁸

However, recent experimental studies based in the fluctuation-dissipation relations point out the existence of a phase transition in the presence of a magnetic field.¹⁹ Moreover, a phase transition has been reported in a Heisenberg spin glass (AuFe) in three dimensions in the presence of a magnetic field against the droplet prediction (we recall that the droplet model predicts no phase transition independently of the number of components of the spin).²⁰

We will study a three dimensional Ising spin glass using an off-equilibrium approach based on the computation of the fluctuation-dissipation relations. This method has provided an important tool to investigate the low temperature properties of disordered systems (and it has been very useful in the study of nondisordered systems such as glasses).²¹⁻²⁴

II. THEORETICAL BASIS

We have focused this paper on a study of fluctuation-dissipation relations in the off-equilibrium regime. To do this we need to define the spin-spin autocorrelation function and the response of the magnetization to a small change of the magnetic field of the system.

In order to make the paper self-contained and to fix the notation, we shall recall some important results about the off-equilibrium fluctuation-dissipation relations. We have simulated a binary Ising spin glass in three dimensions on a cubic lattice of volume $V=L^3$ with helical boundary conditions. The Hamiltonian of the system is given by

$$\mathcal{H} = - \sum_{\langle ij \rangle} \sigma_i J_{ij} \sigma_j - h \sum_i \sigma_i. \quad (1)$$

By $\langle ij \rangle$ we denote the sum over nearest neighbor pairs. J_{ij} are chosen from $\{+1, -1\}$ randomly, and h is the external magnetic field. We have studied systems with magnetic field $h=0.2$ and lattice sizes $L=20, 30$ and 60 .

We have used the SUE parallel computer. SUE is a dedicated machine with an overall performance of 0.22 ns per spin flip. See Refs. 25 and 26 for a detailed description of this computer.

Given a quantity $A(t)$ that depends on the local variables of our original Hamiltonian (\mathcal{H}), we can define the autocorrelation function

$$C(t_1, t_2) \equiv \langle A(t_1) A(t_2) \rangle, \quad (2)$$

and the response function

$$R(t_1, t_2) \equiv \left. \frac{\delta \langle A(t_1) \rangle}{\delta \Delta h(t_2)} \right|_{\Delta h=0}, \quad (3)$$

where we have assumed that the original Hamiltonian has been perturbed to

$$\mathcal{H}' = \mathcal{H} + \int \Delta h(t) A(t) dt. \quad (4)$$

The brackets $\langle \dots \rangle$ in Eqs. (2) and (3) here imply a double average, one over the dynamical process and one over the disorder. As usual one could choose $A(t) = \sigma_i(t)$ and the response function should be

$$R(t_1, t_2) \equiv \left. \frac{\delta m(t_1)}{\delta \Delta h(t_2)} \right|_{\Delta h=0} = \left. \frac{\delta \langle \sigma_i(t_1) \rangle}{\delta \Delta h(t_2)} \right|_{\Delta h=0}, \quad (5)$$

where $m(t) = \langle \sigma_i(t) \rangle$

However, to improve the signal of the autocorrelation in the present paper we have used:

$$C(t_1, t_2) \equiv \frac{1}{V} \sum_{i=1}^V \langle \sigma_i(t_1) \sigma_i(t_2) \rangle, \quad (6)$$

and $m(t) = (1/V) \sum_i \langle \sigma_i(t) \rangle$. We remark that we are interested in global fluctuation dissipation relations. Recently work has been done in local microscopic fluctuation dissipation relations,²⁷ but we will not study them in this paper.

In the dynamical framework, assuming time translational invariance, it is possible to derive the fluctuation-dissipation theorem (FDT), that reads

$$R(t_1, t_2) = \beta \theta(t_1 - t_2) \frac{\partial C(t_1, t_2)}{\partial t_2}, \quad (7)$$

where the inverse temperature is $\beta = 1/T$.

The fluctuation-dissipation theorem holds in the equilibrium regime, but in the early times of the dynamics we expect a breakdown of its validity. Mean field studies²⁸ suggest the following modification of the FDT:

$$R(t_1, t_2) = \beta X(t_1, t_2) \theta(t_1 - t_2) \frac{\partial C(t_1, t_2)}{\partial t_2}. \quad (8)$$

It was also suggested in Refs. 28–30 that the function $X(t, t')$ is only a function of the autocorrelation: $X(t, t') = X(C(t, t'))$. We can then write the following generalization of the FDT, which should hold in early times of the dynamics, the off-equilibrium fluctuation-dissipation relation (OFDR), that reads

$$R(t_1, t_2) = \beta X(C(t_1, t_2)) \theta(t_1 - t_2) \frac{\partial C(t_1, t_2)}{\partial t_2}. \quad (9)$$

We can use the previous formula, [Eq. (9)], to relate the observable quantities defined in Eqs. (2) and (3). Using the functional Taylor expansion we can write

$$m[h + \Delta h](t) = m[h](t) + \int_{-\infty}^t dt' \left. \frac{\delta m[h'](t')}{\delta h'(t')} \right|_{h'(t')=h(t)} \times \Delta h(t') + O(\Delta h^2), \quad (10)$$

and so

$$\Delta m[h, \Delta h](t) = \int_{-\infty}^t dt' R(t, t') \Delta h(t') + O(\Delta h^2). \quad (11)$$

where we have defined $\Delta m[h, \Delta h](t) \equiv m[h + \Delta h](t) - m[h](t)$. Equation (11) is just the linear-response theorem neglecting higher orders in Δh . By applying the OFDR we obtain the dependence of the magnetization with time in a generic time-dependent magnetic field (with a small strength), $\Delta h(t)$,

$$\Delta m[h, \Delta h](t) \approx \beta \int_{-\infty}^t dt' X[C(t, t')] \frac{\partial C(t, t')}{\partial t'} \Delta h(t'). \quad (12)$$

Next we let the system evolve with the unperturbed Hamiltonian of Eq. (1) from $t=0$ to $t=t_w$, the so called waiting time, and then we turn on the perturbing magnetic field Δh (hence, the system “feels” a magnetic field $h + \Delta h$). Finally, with this choice of the magnetic field, we can write (ignoring in our notation the fact that Δm also depends on t_w)

$$\Delta m[h, \Delta h](t) \approx \Delta h \beta \int_{t_w}^t dt' X[C(t, t')] \frac{\partial C(t, t')}{\partial t'}, \quad (13)$$

and by performing the change of variables $u = C(t, t')$, Eq. (13) reads

$$\Delta m[h, \Delta h](t) \approx \Delta h \beta \int_{C(t, t_w)}^1 du X[u], \quad (14)$$

where we have used the fact that $C(t, t) \equiv 1$ (always true for Ising spins). In the equilibrium regime ($X=1$ as the fluctuation-dissipation theorem holds) we must obtain

$$\Delta m[h, \Delta h](t) \approx \Delta h \beta [1 - C(t, t_w)], \quad (15)$$

i.e., $\Delta m[h, \Delta h](t)T/\Delta h$ is a linear function of $C(t, t_w)$ with a slope -1 . We remark that we can use this formula to obtain q_{\max} as the point where the curve $\Delta m[h, \Delta h](t)$ against $C(t, t_w)$ leaves the line with slope $-\beta\Delta h$.

In the limit $t, t_w \rightarrow \infty$ with $C(t, t_w) = q$, one has that $X(C) \rightarrow x(q)$, where $x(q)$ is given by

$$x(q) = \int_{q_{\min}}^q dq' P(q'), \quad (16)$$

where $P(q)$ is the equilibrium probability distribution of the overlap. Obviously $x(q)$ is equal to 1 for all $q > q_{\max}$, and we recover the FDT for $C(t, t_w) > q_{\max}$. This link between the dynamical function $X(C)$ and the static one $x(q)$ has

been already verified for finite dimensional spin glasses.²² The link has been analytically proved for systems with the property of stochastic stability.³¹

For future convenience, we define

$$S(C) \equiv \int_C^1 dq x(q), \quad (17)$$

or, equivalently,

$$P(q) = - \left. \frac{d^2 S(C)}{d^2 C} \right|_{C=q}. \quad (18)$$

In the limit where $X \rightarrow x$ we can write Eq. (14) as

$$\frac{\Delta m[\Delta h](t)T}{\Delta h} \approx S(C(t, t_w)). \quad (19)$$

Looking at the relation between the correlation function and the integrated response function for large t_w we can thus obtain q_{\max} , the maximum overlap with nonzero $P(q)$, as the point where the function $S(C)$ becomes different from the function $1 - C$.

From the function $S(C)$ we can get information on the overlap distribution function $P(q)$, through Eq. (18). Let us recall which is the prediction for the $S(C)$ assuming the validity of each one of the competing theories described in the introduction. The droplet model predicts $P(q) = \delta(q - \hat{q})$ and, consequently,

$$S(C) = \begin{cases} 1 - \hat{q} & \text{for } C \leq \hat{q} \\ 1 - C & \text{for } C > \hat{q}. \end{cases} \quad (20)$$

In models with only one state, as the droplet model predicts for this model, the equilibrium time is finite irrespective of the value of the volume of the system; hence we can always thermalize any volume, and so the asymptotic behavior, for waiting times larger than the equilibration time, is composed only for the straight line $1 - C$. There is no horizontal part.

On the other hand the MF like prediction for the overlap distribution³ $P(q) = (1 - x_M) \delta(q - q_{\max}) + x_M \delta(q - q_{\min}) + \tilde{p}(q)$ (where the support of $\tilde{p}(q)$ belongs to the interval $[q_{\min}, q_{\max}]$, $q_{\min} \propto h^{4/3}$ and q_{\max} mainly depends on the temperature-), implies that

$$S(C) = \begin{cases} S(0) & \text{for } C \leq q_{\min} \\ \tilde{s}(C) & \text{for } q_{\min} < C \leq q_{\max} \\ 1 - C & \text{for } C > q_{\max}, \end{cases} \quad (21)$$

where $\tilde{s}(C)$ is a quite smooth and monotonically decreasing function such that

$$\tilde{p}(q) = - \left. \frac{d^2 \tilde{s}(C)}{d^2 C} \right|_{C=q}. \quad (22)$$

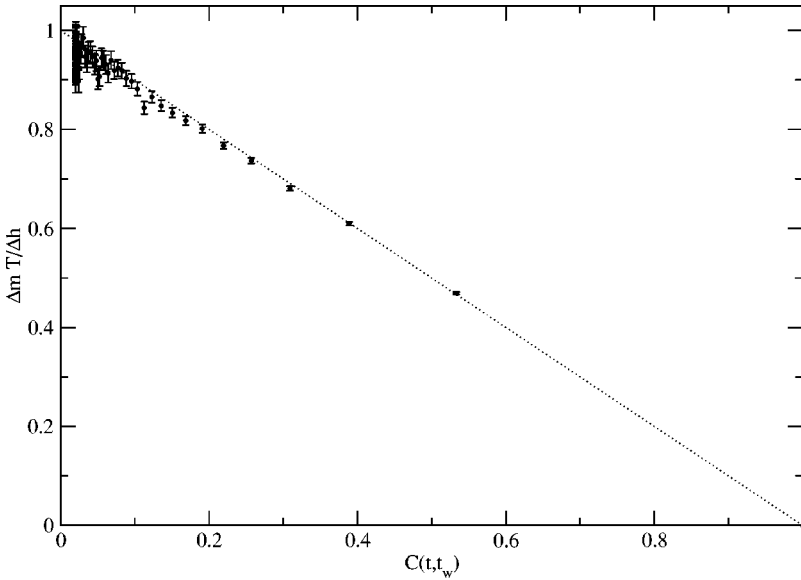


FIG. 1. Off-equilibrium fluctuation-dissipation relations for $T=2.5$, $h=0.2$, and $L=30$. We have drawn the equilibrium straight line $1 - C$. We plot $\Delta m T/h$ against $C(t, t_w)$ for the waiting time $t_w=819200$.

To finish this section we will recall an approximate scaling property of the probability distribution of the overlap that was introduced by Parisi and Thouless (hereafter PaT).³² In particular in Mean field the PaT hypothesis implies

$$S(C) = \begin{cases} 1 - C & \text{for } C \geq q_{\max} \\ T\sqrt{1 - C} & \text{for } q_{\min} \leq C \leq q_{\max}. \end{cases} \quad (23)$$

The result for $C \geq q_{\max}$ is general (and true for finite dimension) and for $q_{\min} \leq C \leq q_{\max}$ we make the following Ansatz: $S(C) = AT(1 - C)^B$ (in the mean field, $A=1$ and $B=1/2$). If we substitute this ansatz in Eq. (19) we obtain the scaling equation

$$\frac{mT}{h} T^{-\phi} = f[(1 - C)T^{-\phi}], \quad (24)$$

where f is a scaling function and $\phi = 1/(1 - B)$ (in the mean field, $\phi=2$). In order to be consistent the scaling function should be composed by a linear part (x) and by a power law part (Ax^B). We have only measured the autocorrelation function [see Eq. (6)] and the response function [see Eq. (5)].

III. NUMERICAL RESULTS

A. On the critical temperature

Assuming the existence of a phase transition in a magnetic field, we can estimate the shift of the critical temperature when a small magnetic field is turned on using the mean field approximation. The main formula is²

$$\frac{T_c(h) - T_c(0)}{T_c(0)} = \left(\frac{3}{4}\right)^{1/3} \left(\frac{h}{J}\right)^{2/3}, \quad (25)$$

where J is defined (in the mean field) as $\overline{J_{ij}^2} = J^2/N$, N being the volume of the system (or the coordination number in the

mean field approximation), J_{ij} being the random couplings between the spins, $T_c(0)$ being the critical temperature in absence of a magnetic field and finally $T_c(h)$ being the critical temperature in the presence of a magnetic field h . That is the formula that fixes the Almeida-Thouless (AT) instability in infinite dimensional spin glasses.

We can modify that formula [Eq. (25)] for a finite coordination number. Let z be the coordination number of our lattice. We recall that our J_{ij} have unit variance and so $J = \sqrt{z}$. Hence we can write

$$\frac{T_c(h) - T_c(0)}{T_c(0)} = \left(\frac{3}{4}\right)^{1/3} \left(\frac{h}{\sqrt{z}}\right)^{2/3}. \quad (26)$$

In our case $z=6$, $T_c(0) \approx 1.14$, and so $T(h=0.2) \approx 0.945$ ($h=0.2$ is the magnetic field simulated in the present work). Notice that near zero magnetic field the phase transition line has vertical slope ($dT(h)/dh \approx 1/h^{1/3}$).

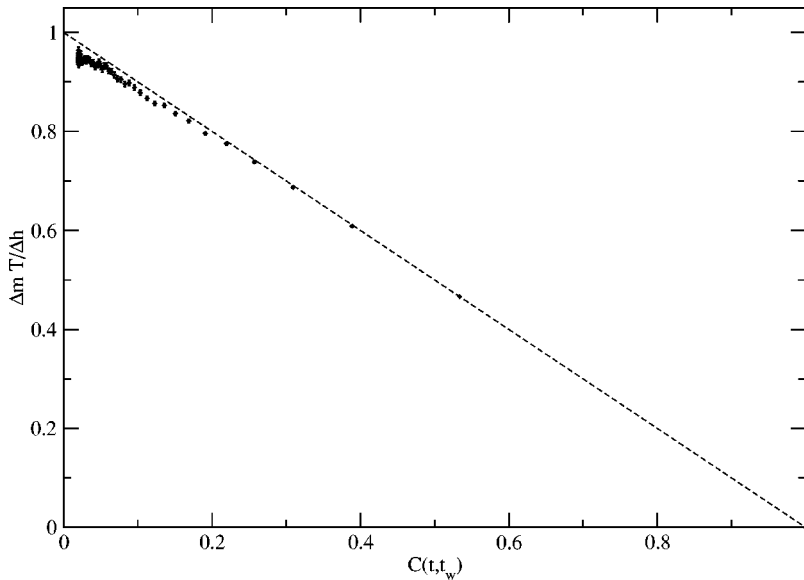
In order to check the existence or not of a phase transition (using the OFDR as a tool) we have simulated at very high temperature ($T=2.5$) and a lower temperature (which is below our previous estimate of the critical one, $T=0.714$).

B. OFDR in the high temperature region

We have simulated the system at temperature $T=2.5$ in a magnetic field $h=0.2$ and with perturbing fields $\Delta h=0.01$ and 0.03 (in order to check linear response) and different waiting times: 409600 and 819200. The number of samples simulated was about 6400 samples for each waiting time. In Fig. 1 we show the plot for $t_w=819200$ and $L=30$.

For the largest value of the waiting time simulated all the data stay on the equilibrium line $1 - C$ (i.e., this waiting time is greater than the equilibration time for this lattice size).

In the paramagnetic phase, droplet and RSB agree: for a “finite” volume and very large times (greater than the equilibration time) all the points should lie on the straight line $\Delta m(t)T/\Delta h = 1 - C$ with $C \in [0, q_{EA}]$ (equilibrium situa-

FIG. 2. As Fig. 1, but with $t_w=409600$.

tion). For intermediate situations (i.e., not so large waiting times) the curves lie below the straight line (see Fig. 2), and the final straight line is built from below (i.e., curves with lower waiting times lie below those with higher ones). This behavior is similar to that found in the two dimensional Ising spin glass in a magnetic field for a finite temperature (the system is paramagnetic).³³ Also see Fig. 5 of Ref. 10 for an example of a FDT plot in a paramagnetic phase in the four dimensional Ising spin glass.

C. OFDR in the low temperature region

The situation at a lower temperature is dramatically different. We start by showing the numerical results for one of the lowest temperature simulated, $T=0.714$. All the simulations reported in this subsection have been done at $h=0.2$ as the external magnetic field. In Fig. 3 we show $\Delta m T/\Delta h$ against $C(t, t_w)$ for different waiting times t_w and perturbing magnetic field $\Delta h=0.03$ for the $L=30$ lattice.

The first check we have performed is to control that we are in the linear response regime. To do this we have computed the OFDR for different perturbing magnetic fields $\Delta h=0.01$ and 0.03 . We have found that the results are independent of these two values of Δh . In the following we show the results obtained with $\Delta h=0.03$.

The second check has been to verify that our results are lattice size independent. In Fig. 4 we can see the results for $L=30$ and $L=60$, with perturbing field $\Delta h=0.03$. For $L=20$, the perturbing field $\Delta h=0.03$ has proved too noisy, and we have used $\Delta h=0.06$. It can be seen that the behavior of $L=30$ is asymptotic in this kind of simulations (i.e., for the time scales that we have simulated): the $L=20$ points are still a bit noisy but $L=30$ and $L=60$ coincide. Using this information we will focus on the $L=30$ lattice in the rest of the paper. We can state that we have simulated 512 samples for $t_w=81920$, 416 samples for $t_w=163840$ and 3232 for $t_w=327680$ and 1638400 in the $L=30$ lattice. In addition

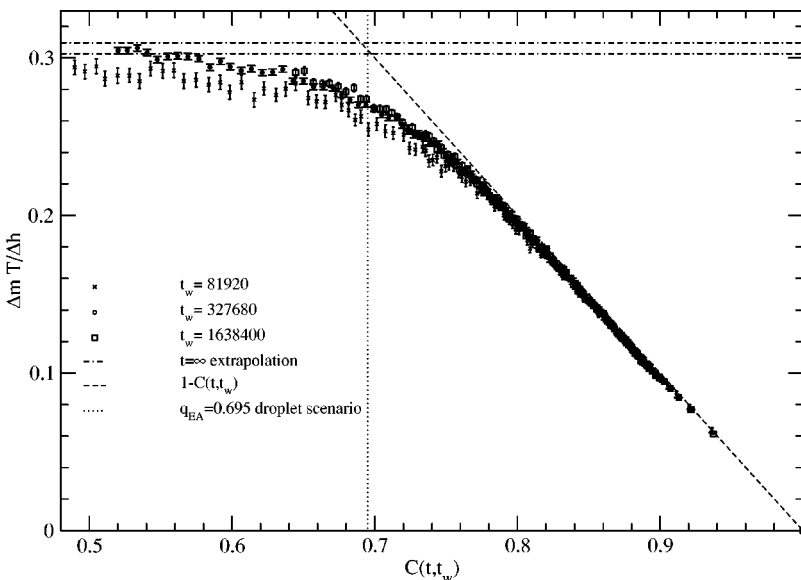


FIG. 3. Off-equilibrium fluctuation-dissipation relations for $T=0.714$, $L=30$ and $h=0.2$. We have marked the equilibrium straight line $1-C$. We plot $\Delta m T/h$ against $C(t, t_w)$ for three different waiting times. We have also plotted the error band for the asymptotic value of $\Delta m T/h$.

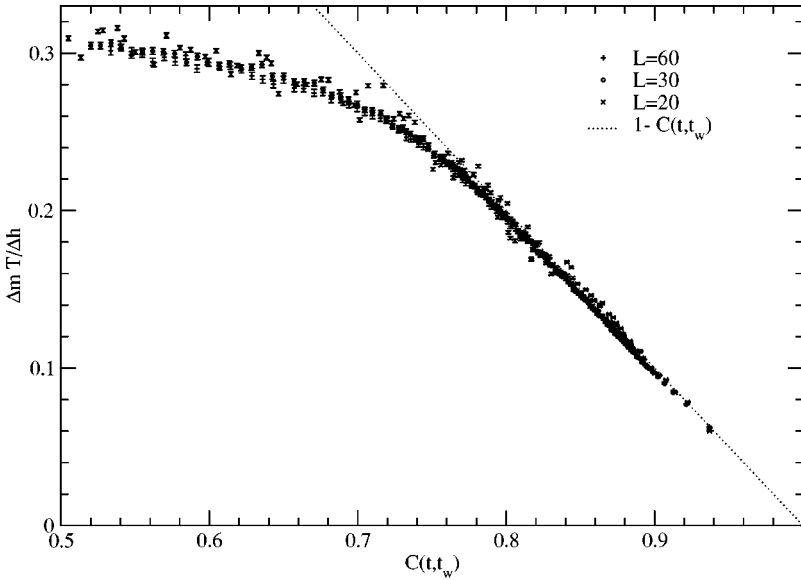


FIG. 4. Off-equilibrium fluctuation-dissipation relations for $T=0.714$ and three different lattice sizes $L=60, 30$ and 20 . The perturbing field is 0.03 for $L=30$ and 60 lattices and 0.06 for the $L=20$ lattice. We show the data for one of the larger waiting time simulated $t_w = 327680$.

6200 samples in the $L=20$ lattice and 412 in the largest lattice that we have simulated ($L=60$).

The third goal is to study the dependence on the waiting times of the OFDR curves. We have simulated $t_w = 81920, 163840, 327680$, and 1638400 , and from Fig. 3 it is possible to see that the curves rise as the waiting time is larger. Moreover, the curves for the larger waiting times are just compatible within our error bars. In this sense we are confident that the curve corresponding to $t_w = 1638400$ represent very well the overall behavior of the system (very large volumes and times or equivalently infinite volume and waiting times). This behavior is very important because our final curve (i.e., $t_w = 1638400$) has a clear curvature which should be absent if the droplet model holds [see Eq. (20) for the droplet prediction and Eq. (21) for the RSB predictions].

In Fig. 3 we plot two additional straight lines. The first line, horizontal, corresponds to the asymptotic value of $\Delta m(t)T/\Delta h$. To obtain this value, we have performed a simulation reaching times much longer than the ones used in

the OFDR curves, but using a smaller number of samples. In Fig. 5 we can see the evolution of $m(t)$. The horizontal lines are the error band related to the asymptotic value of $\Delta m(t) = 0.1286(15)$. For this value we do not need to do any kind of extrapolation since we have reached the thermodynamic value of $\Delta m(t)T/\Delta h$ in this long simulation [$O(10^8)$ Monte Carlo steps].

If the droplet model holds, the final (asymptotic) curve should be composed by the $1 - C$ straight line ($C \in [q_{EA}, 1]$) as explained above. This implies that we can estimate the “droplet” prediction for the order parameter as $q_{EA} \approx 0.694(4)$. We have marked this value with a vertical line in Fig. 3.

We make the following points at the end of this section.

(i) We have obtained a t_w -independent (and L -independent) final curve, at least within our statistical precision. We believe that this curve represents with high accuracy the behavior for large volumes and times of an Ising spin-glass at $T=0.714$ and $h=0.2$. In this scenario we can

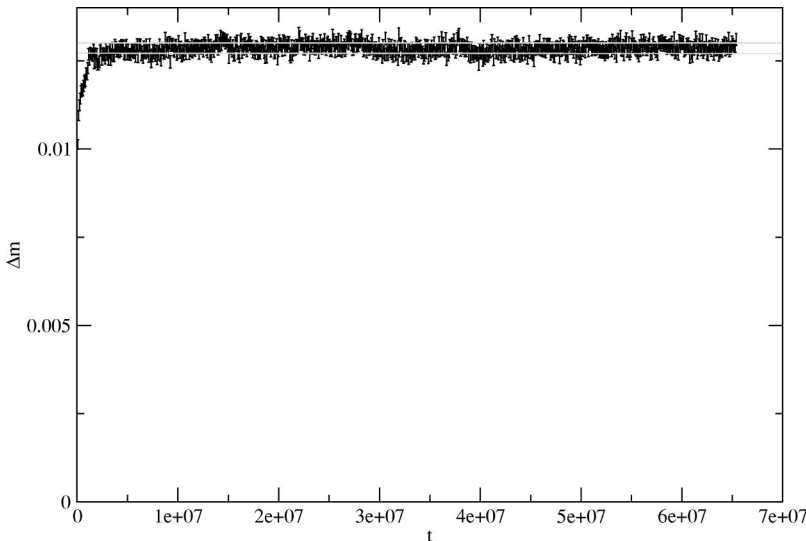


FIG. 5. $\Delta m(t)$ against t for $t_w = 327680$ and $L=30$ in a simulation longer in time than the ones used in the figures of the FDT, but with much less samples 1152. The fit to equilibrium plateau is also shown (we again show the error band for the mean value).

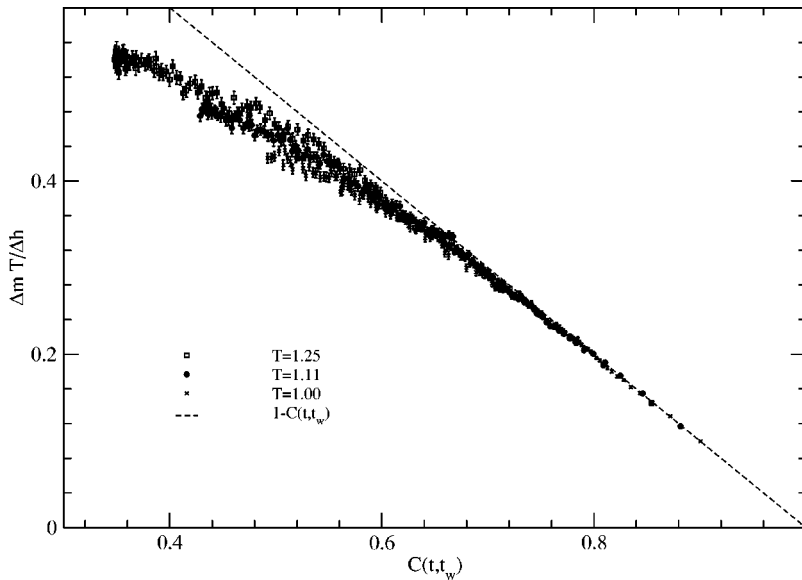


FIG. 6. We show the OFDR for three temperatures, for $t_w = 327680$ and $L = 30$.

estimate that $q_{EA} \approx 0.76(2)$ (the points in which the points leave the straight line) which differs from the droplet value $0.694(4)$.

(ii) We cannot avoid a dependence on the waiting times beyond our numerical precision, and so we can not exclude completely a droplet phase with $q_{EA} = 1 - \Delta m(\infty)T/\Delta h \approx 0.694(4)$.

(iii) As we cited above, the final curve is built from below. At low temperature, in the droplet scenario, we should expect the same behavior as at high temperature and so the final curve should build from below. The point is whether the curves for large waiting times stop or not before they reach the droplet prediction. Our numerical data suggest that the curves stop before the droplet final curve, and that the asymptotic curve shows the characteristic curvature of a phase with RSB.

We end this section by showing a figure corresponding to the crossover region. In the following discussion we will restrict ourselves to a qualitative level. In Fig. 6 we have shown the OFDR for the three values of temperature ($T = 1.25, 1.11, \text{ and } 1.0$) and $t_w = 327680$. It is clear that the largest temperature shows a clear signature of a paramagnetic phase (i.e., a small curvature and almost a straight line). One can compare these curves with a clear paramagnetic one, (see Fig. 2, which also shows a small curvature at the end of the curve). We remark that the critical temperature of the model with no magnetic field is about 1.14, and so we are (qualitatively) exploring the region near the vertical of this point. On the basis of the mean field approximation we should expect that the line of transitions emerges from the point at zero magnetic field with vertical slope. Hence, this plot and a transition temperature near 1.1 is compatible with this scenario. The prediction using Eq. (26) was 0.95. Obviously, in order to see a clear paramagnetic curve with no violations, we refer to Fig. 1. We remark that this method based on a violation of the fluctuation-dissipation relation is not so powerful as to be determinable with precision transition points; is a good method to decide if one point (T, h) (well inside the phase in order to avoid the crossover region) behaves in a way or not.

D. OFDR in the high magnetic field region

In this section we study the properties of the OFDR at a fixed low temperature when the magnetic field grows. The goal of this section is to find when the behavior of the OFDR relations change from a nontrivial one (as found for $T = 0.714$ and $h = 0.2$) to a trivial one (droplet) as the magnetic field becomes larger. Notice that this temperature ($T = 0.714$) is far away from the critical temperature of the model with no magnetic field ($T = 1.138$), and so avoiding crossover effects between the phase transition at zero field. In Figs. 7 and 8 we show the results obtained at $T = 0.714$ and $h = 0.4$ and 0.6 , respectively.

We start by discussing the $h = 0.4$ plot (Fig. 7). If we compute, as above, q_{EA} as the minimum value of the correlation (starting from $C = 1$), for which the points do not lie (using one standard deviation as criteria) on a straight line, we obtain that this value of the field is still not statistically compatible with the droplet value. If we relax the one standard deviation criteria to two or three standard deviations, the behavior can be described as droplet behavior. Obviously for larger magnetic field we can show analytically that the behavior is a droplet behavior (the magnetic contribution in the Hamiltonian becomes dominant and we can drop the spin glass term).

For a larger magnetic field, $h = 0.6$, the situation is clearer (Fig. 8). Practically all the points are on a straight line (slightly below but always at a distance less than a one-two standard deviations). We have a horizontal part (the system has reached its asymptotic magnetization), since our largest waiting time is still smaller than the equilibration time for this magnetic field (in the droplet, this time is finite).

The conclusion of this section is that for $h = 0.4$ the situation is still not clear but that $h = 0.6$ is a droplet situation. We have observed a clear change in the behavior of the OFDR in the region $h \approx 0.4 - 0.6$. Assuming a phase transition (between RSB and droplet behavior) this implies that $h_c(T = 0.714) \sim 0.6$.

This figure compares very well with that obtained at zero temperature in a related model (which uses Gaussian cou-

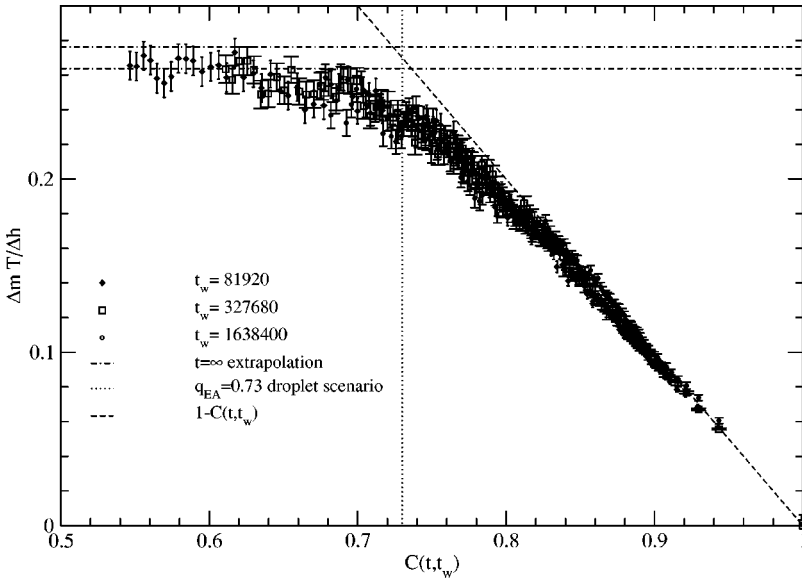


FIG. 7. Off-equilibrium fluctuation-dissipation relations for $T=0.714$, $L=30$, and $h=0.4$. We have marked the equilibrium straight line $1-C$. We plot $\Delta m T/h$ against $C(t, t_w)$ for three different waiting times. We have also plotted the error band for the asymptotic value of $\Delta m T/h$.

pling). A critical magnetic field at zero temperature of 0.6,¹⁴ or 0.4 if we use Ref. 15, has been obtained.

E. Scaling properties of OFDR in the low temperature region

In this section we will study the scaling properties of the t_w - and L -independent fluctuation dissipation curves obtained for different temperatures. The main goal of this section is to study the degree of accuracy of the approximate PaT ansatz in a three dimensional Ising spin glass in a magnetic field. That ansatz has been found to be very adequate to describe the low temperature fluctuation-dissipation curves both in three and four dimensions in the presence of a magnetic field. Moreover this scaling ansatz has been checked in experiments, and found to describe very well the experimental data. The ansatz has also been studied in a two dimensional spin glass (no phase transition), and it has been found that the curves computed for different temperatures at the same

t_w ($t_w=10^4$) for a large lattice ($V=400^2$) also follow this ansatz (see Fig. 1-a of Ref. 33). Notice that this waiting time is not an asymptotic one (see Fig. 1-b of Ref. 33).

In Fig. 9 we show the t_w and L -independent fluctuation dissipation curves obtained at five different temperatures. In particular, in Fig. 10 we show the fluctuation-dissipation plot for the lowest temperature we have simulated, $T=0.625$, and for two different and large waiting times ($t_w=162840$ and 327680). It is clear that these two waiting times are asymptotic (within error bars) and so we are again confident in that our curves plotted in Fig. 9 are asymptotic.

We have deleted the temperature factor in the ordinate axis, and so each FDT straight line has a slope $1/T$. We can see that when the data leave the pseudoequilibrium region (i.e., the straight line), they go to the same curve (independently of their temperatures). This is a strong signature that the PaT ansatz works. In Fig. 11 we have tried this kind of

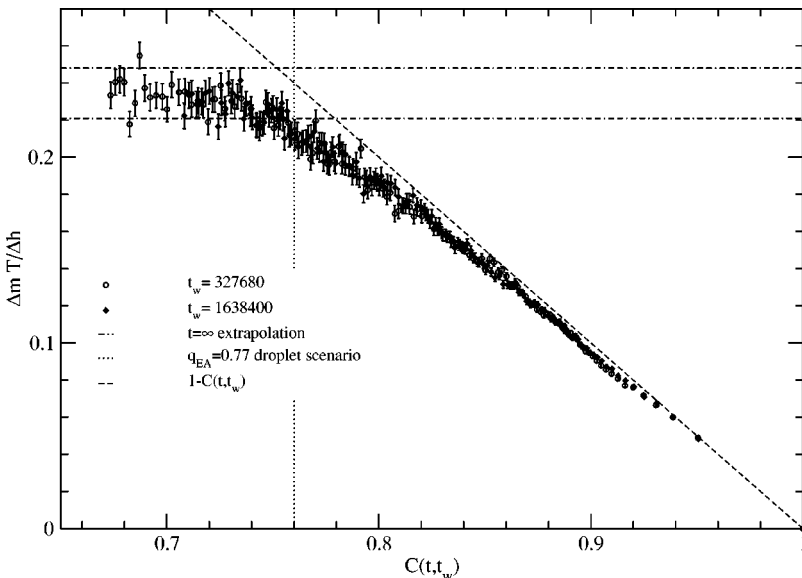


FIG. 8. Off-equilibrium fluctuation-dissipation relations for $T=0.714$, $L=30$, and $h=0.6$. We have marked the equilibrium straight line $1-C$. We plot $\Delta m T/h$ against $C(t, t_w)$ for two different waiting times. We have also plotted the error band for the asymptotic value of $\Delta m T/h$.

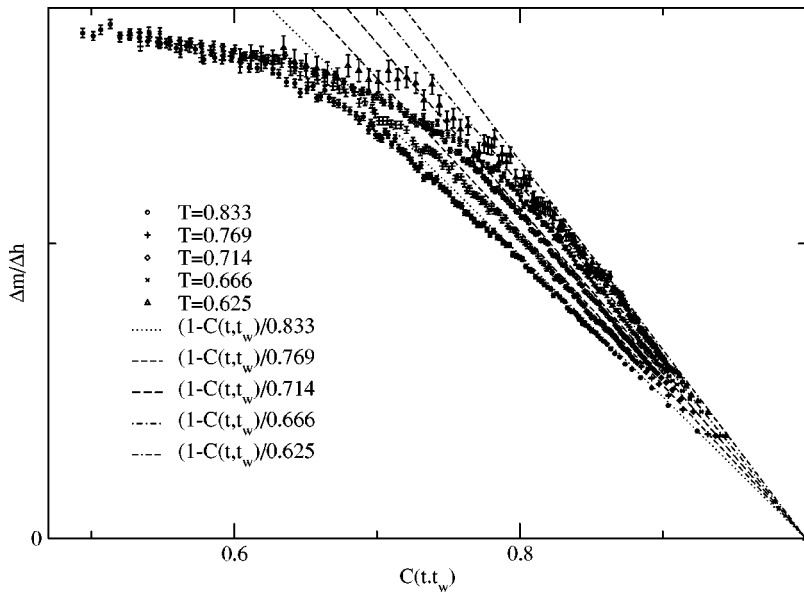


FIG. 9. Off-equilibrium fluctuation-dissipation relations for five different temperatures. We have marked the equilibrium straight lines. Notice that we plot $\Delta m/h$ instead $\Delta mT/h$ as in previous plots, hence the slopes of the equilibrium lines are $1/T$. We show only the data computed with the largest waiting time $t_w = 327680$.

ansatz, and the scaling is very good; thus we are confident that the PaT scaling describes with great accuracy the behavior of the fluctuation dissipation curves in a large temperature window.

Notice that the PaT scaling works for our L - and t_w -independent curves. We have found a good scaling for values of $\phi \in (1.2, 1.4)$. In Fig. 11 we use central value for $\phi = 1.3$. Two clear and distinctive regimes can be seen in that figure. The first one corresponds to the quasiequilibrium regime: in that part of the figure the behavior is linear and so it matches the quasiequilibrium regime $\Delta mT/h = 1 - C$. The second one corresponds to the aging regime: that part of the plot can be parametrized with a power law with the B exponent introduced above in the paper. We have obtained $B = 0.27(3)$ which provides $\phi = 1.37(6)$, which is a compatible value with the ϕ value used in the scaling plot (this is a check of consistency of the scaling law). For completeness we report the value of A [we remark that the aging region follows a law Ax^B , where x is the scaling variable $T^{-\phi}(1 - C)$]: $A = 0.52(1)$.

We can compare the values obtained for A and B with previous results published in the literature. In the $3d$ Ising spin glass with no magnetic field $A = 0.7$ and $B = 0.41$.³⁴ For the $4d$ Ising spin glass again with no magnetic field, $A = 0.52$ and $B = 0.41$.²² We can see that in absence of magnetic field the B value is close to the mean field value (0.5) whereas the magnetic field value in three dimensions is clearly far from the MF value.

Following Ref. 33 this kind of scaling is not enough to detect a RSB phase (they found in the two dimensional Ising model—with no phase transition at finite temperature—a PaT scaling for their OFDR). Nevertheless, in Ref. 33 the PaT scaling only works for points with the same waiting time, instead, in our plot we have points computed with different waiting times. In effect, we remark again, our scaling is t_w independent (at least in our numerical precision) which is a behavior completely different from the two dimensional spin glass (paramagnetic phase). For a paramagnetic phase and very long waiting time (i.e. all the points lie in the 1

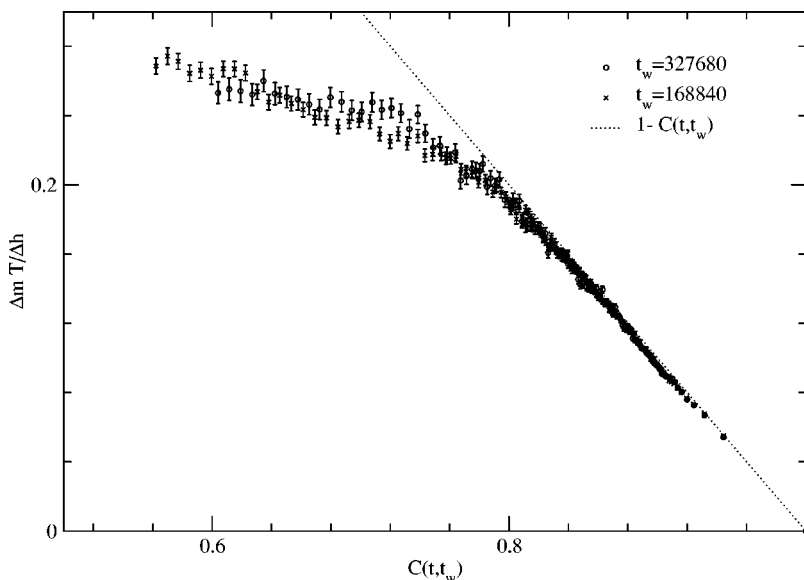


FIG. 10. Off-equilibrium fluctuation-dissipation relations for $T=0.625$ (the coldest temperature we have simulated) for $L=30$, $h=0.2$, and $\Delta h=0.03$. We show the data for the largest waiting time simulated $t_w=327680$ and for $t_w=162840$. The data seem to be asymptotic in the statistical error.

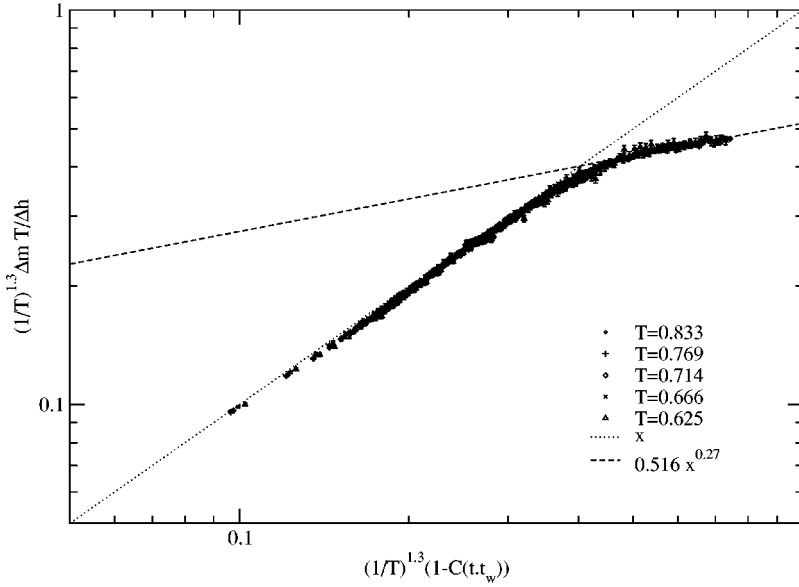


FIG. 11. Scaling plot of the off-equilibrium fluctuation-dissipation relations for four different temperatures in the low temperature region.

– C straight line; see, for example, our Fig. 1, where we have equilibrated the system) the PaT scaling plot should consist in points over the linear part (quasiequilibrium regime), and no one in the power law part (aging regime). We finally remark that this scaling in addition with the analysis of the OFDR (see above) provides us with a picture that could be explained assuming a low temperature phase with RSB.

IV. DISCUSSION AND CONCLUSIONS

We have studied how the fluctuation-dissipation relations work off-equilibrium in the three dimensional Ising spin glass with a magnetic field. We have shown numerical data that has been obtained by simulating very large lattices ($L = 20, 30,$ and 60) and for extremely large times for the three dimensional Ising spin glass. In order to achieve these lattice sizes and time we have used a dedicated machine (SUE).

With this tool we have identified a paramagnetic phase in the high temperature region (as expected), and a phase where we have found strong violations of fluctuation-dissipation. We can describe very well (within our statistical precision) these violations assuming a RSB scenario, yet we can not exclude completely a droplet scenario.

Moreover we have shown the crossover, both moving in

temperature as well as moving in magnetic field, between a spin glass behavior and a paramagnetic one. We have a picture of the phase diagram composed by three points [using the notation (T, h)]: $(1.138, 0)$, $(\sim 1.1, 0.2)$, and $(0.714, \sim 0.6)$ (by the symbol \sim we denote that the figure that follows is only indicative). In addition we know that for the Gaussian model there is a critical point at $(0, 0.6)$, but this critical magnetic field should be modified to take into account that we are using binary couplings. Finally we have checked that the overlap probability distribution of our model, $P(q)$, [obtained via the static-dynamics link: $X(C) \rightarrow x(q)$], which is not trivial (at least within our numerical precision, see Sec. II), satisfies the PaT Ansatz.

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¹W. L. McMillan, J. Phys. C **17**, 3179 (1984); A. J. Bray and M. A. Moore, *ibid.* **18**, L699 (1985); G. J. Koper and H. J. Hilhorst, J. Phys. (Paris) **49**, 429 (1988); D. S. Fisher and D. A. Huse, Phys. Rev. B **38**, 386 (1988); *ibid.* **38**, 373 (1988).

²K. Binder and P. Young, Rev. Mod. Phys. **58**, 801 (1986).

³M. Mézard, G. Parisi, and M. A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987).

⁴E. Marinari, G. Parisi, F. Ricci-Tersenghi, J. Ruiz-Lorenzo, and F.

Zuliani, J. Stat. Phys. **98**, 973 (2000).

⁵J. R. L. de Almeida and D. J. Thouless, J. Phys. A **11**, 983 (1978).

⁶C. N. Newman and D. S. Stein. cond-mat/0105282 (unpublished).

⁷A. J. Bray and S. A. Roberts, J. Phys. C **13**, 5405 (1980).

⁸I. R. Pimentel, T. Temesvári, and C. De Dominicis, Phys. Rev. B **65**, 224420 (2002).

⁹T. Temesvári and C. De Dominicis, cond-mat/0207512 (unpublished).

¹⁰G. Parisi, F. Ricci-Tersenghi, and J. J. Ruiz-Lorenzo, Phys. Rev. B **57**, 13617 (1998).

¹¹E. Marinari, G. Parisi, and F. Zuliani J. Phys. A **31**, 1181 (1998).

¹²E. Marinari, G. Parisi, and F. Zuliani, Phys. Rev. Lett. **84**, 1056 (2000).

- ¹³D. Herisson and M. Ocio, Phys. Rev. Lett. **88**, 257202 (2002).
- ¹⁴F. Krazakala, J. Houdayer, E. Marinari, O.C. Martin, and G. Parisi, Phys. Rev. Lett. **87**, 197204 (2001).
- ¹⁵J. Lamarq, J.-P. Bouchaud, and O.C. Martin. cond-mat/0208100 (unpublished).
- ¹⁶S. Caracciolo, G. Parisi, S. Patarnello, and N. Sourlas, Europhys. Lett. **11**, 783 (1990); J. Phys. (Paris) **51**, 1877 (1990). E. R. Grannan and R. E. Hetzel, Phys. Rev. Lett. **67**, 907 (1991); J. C. Ciria, G. Parisi, F. Ritort, and J. J. Ruiz-Lorenzo, J. Phys. I **3**, 2207 (1993); M. Picco and F. Ritort, *ibid.* **4**, 1619 (1994); cond-mat/9702041; E. Marinari, C. Naitza, and F. Zuliani, J. Phys. A **31**, 6355 (1998).
- ¹⁷E. Marinari, G. Parisi, and J. J. Ruiz-Lorenzo, in *Spin Glasses and Random Fields*, edited by P. Young (World Scientific, Singapore, 1997); cond-mat/9701016 (unpublished).
- ¹⁸P. Norblad and P. Svendlish, in *Spin Glasses and Random Fields* (Ref. 17).
- ¹⁹V. S. Zotev and R. Orbach, cond-mat/0112489 (unpublished); cond-mat/0201226 (unpublished).
- ²⁰D. Petit, L. Fruchter, and I. A. Campbell, Phys. Rev. Lett. **83**, 5130 (1999).
- ²¹S. Franz and H. Rieger, J. Stat. Phys. **79**, 749 (1995).
- ²²E. Marinari, G. Parisi, F. Ricci-Tersenghi, and J. J. Ruiz-Lorenzo, J. Phys. A **31**, 2611 (1998).
- ²³G. Parisi, F. Ricci-Tersenghi, and J. J. Ruiz-Lorenzo, Eur. Phys. J. B **10**, 317 (1999).
- ²⁴G. Parisi, Phys. Rev. Lett. **79**, 3660 (1997).
- ²⁵A. Cruz, J. Pech, A. Tarancón, P. Téllez, C. L. Ullod, and C. Ungil, Comput. Phys. Commun. **133**, 165 (2001).
- ²⁶H.G. Ballesteros, A. Cruz, L.A. Fernández, V. Martín-Mayor, J. Pech, J.J. Ruiz-Lorenzo, A. Tarancón, P. Tellez, C.L. Ullod, and C. Ungil, Phys. Rev. B **62**, 14237 (2000).
- ²⁷H. Castillo *et al.*, Phys. Rev. Lett. **88**, 237201 (2002); A. Montanari and F. Ricci-Tersenghi, cond-mat/0207416 (unpublished); G. Parisi, cond-mat/0208070 (unpublished).
- ²⁸L. F. Cugliandolo and J. Kurchan, Phys. Rev. Lett. **71**, 173 (1993); Philos. Mag. **71**, 501 (1995); J. Phys. A **27**, 5749 (1994).
- ²⁹S. Franz and M. Mézard, Europhys. Lett. **26**, 209 (1994).
- ³⁰A. Baldassarri, L. F. Cugliandolo, J. Kurchan, and G. Parisi, J. Phys. A **28**, 1831 (1995).
- ³¹S. Franz, M. Mezard, G. Parisi, and L. Peliti, Phys. Rev. Lett. **81**, 1758 (1998); J. Stat. Phys. **97**, 459 (1999).
- ³²G. Parisi and D. J. Thouless, J. Phys. (France) Lett. **41**, L361 (1980).
- ³³A. Barrat and L. Berthier, Phys. Rev. Lett. **87**, 087204 (2001).
- ³⁴E. Marinari, G. Parisi, and F. Ricci-Tersenghi, J. Phys. A **33**, 2373 (2000).