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Off-equilibrium dynamics at very low temperatures in three-dimensional spin glasses

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Abstract. We present a high-statistic systematic study of the overlap correlation function well below the critical temperature in the three-dimensional Gaussian spin glass. The off-equilibrium correlation function has been studied confirming the power law behaviour for the dynamical correlation length. In particular, we have computed the dynamical critical exponent z in a wide range of temperatures, $0.35 \leqslant T \leqslant 0.9$, obtaining a dependence $z(T) = 6.2/T$ in very good agreement with recent experiments. Moreover, we report a study of the violation of the fluctuation–dissipation theorem for very low temperatures $T = 0.5$ and 0.35. All our numerical results avoid a droplet model interpretation even when T is as low as $T = 0.35$.

1. Introduction

The nature of the low-temperature phase of finite-dimensional spin glasses is still a subject of controversy [1–5].

Recently Bray, Moore, Bokil and Drossel [5, 6] questioned many of the numerical results obtained with Monte Carlo methods in the three-dimensional Edwards–Anderson (EA) model [4, 7–10].

Inspired by the study of the Migdal–Kadanoff approximation (MKA) of the EA model, they argued that the numerical results, that were obtained at temperatures $T \geqslant \frac{3}{4}T_c$, could be strongly affected by finite-size effects and that one should go to sizes larger than the crossover length L^* in order to see the right (droplet) behaviour. They found (in the framework of the MKA) that the crossover length is $L^* \simeq 100$ for $T \simeq 0.7T_c$ and that it decreases for lower temperatures: $L^* \leqslant 10$ when $T \leqslant 0.5T_c$ [5, 6] (see also the comment [11]).

This is perhaps the main motivation that pushed us to study the EA model in the very low temperature region: verify whether the behaviour already found at $T \simeq 0.75T_c$ persists at $T \leqslant 0.5T_c$. In fact, at these temperatures we can simulate (using off-equilibrium techniques) a system of size larger than L^* (in this paper, we will present data for sizes $L = 24$ and 64).

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The numerical data presented in this paper have been measured in the off-equilibrium dynamical regime. This way of probing the system properties, apart from being much more similar to the experimental procedure, does not present the thermalization problems of a simulation performed at equilibrium, that would lead to insurmountable obstacles at such low temperatures. The efficiency of this way of measuring has been largely tested in the recent past [12–16]. Moreover, over the passing years the off-equilibrium dynamics of spin glasses has received a great deal of attention both from the experimental [17,18] and the analytical [19] points of view.

Taking the measurements in the off-equilibrium regime we are able to confront the droplet model (DM) [1] and the mean-field-like theory [4] on two grounds: the off-equilibrium regime itself and the equilibrium one, that can be obtained in the limit of very large times. We can take this limit quite safely thanks to the very large time reached in our simulations.

A preliminary analysis based on the data at temperatures $T = 0.7$ and 0.35 was reported in [12]. In this paper we present an extended analysis based on nine different temperatures obtaining a precise temperature dependence of the dynamical critical exponent in order to have an accurate comparison with recent experiments.

2. The model and the numerical method

We have simulated the Gaussian Ising spin glass on a three-dimensional cubic lattice of volume L^3 with periodic boundary conditions. The Hamiltonian of the system is

$$\mathcal{H} = -\sum_{\langle ij \rangle} \sigma_i J_{ij} \sigma_j. \tag{1}$$

We denote by $\langle ij \rangle$ the sum over nearest-neighbour pairs. J_{ij} are Gaussian variables with zero mean and unit variance.

We focus our attention on the study of the point–point overlap correlation function computed at distance x and time t

$$G(x,t) = \frac{1}{L^3} \sum_i \overline{\langle \sigma_{i+x} \tau_{i+x} \sigma_i \tau_i \rangle_t} \tag{2}$$

where σ and τ are two real replicas (systems which evolve with the same disorder) and the index i runs over all the points of the lattice. As usual we denote by $\overline{(\cdots)}$ the average over the disorder and, in this context, $\langle(\cdots)\rangle_t$ is the average over the dynamical process until time t (for a given realization of the disorder). The two replicas (σ and τ) evolve with different random numbers.

The simulation has been performed in a similar way to the experimental procedure: the system is prepared in a high-temperature configuration (actually the initial configurations were chosen at random, i.e. $T = \infty$) and it is suddenly quenched below the (estimated) critical temperature, $T_c = 0.95(3)$ [8]. Immediately we start taking the measurements, which obviously depend on time. The equilibrium behaviour is recovered in the large-time limit. As a dynamical process we have used the standard Metropolis method.

We have simulated four samples (eight systems) of an $L = 64$ lattice, measuring the correlation function at times $t = 100 \cdot 2^k$ (with $k = 0, \ldots, 13$) and temperatures $T = 0.9$, 0.8, 0.7, 0.6, 0.5, 0.4, and 0.35. In addition, we have simulated 4096 samples of an $L = 24$ lattice measuring at times $t = 2^k$ (with $k = 7, \ldots, 19$) and at three temperatures: $T = 0.7$, 0.5 and 0.35.

For the study of the fluctuation–dissipation relation we have used $L = 64$ systems and have simulated them for more than 10^7 Monte Carlo steps. All the simulations have been performed with the help of the parallel computer APE100 [20].

Table 1. Parameters of the point–point correlation function.

T	$z(T)$	δ	$B^{-\delta}$	α
0.9	6.85(1.0)	1.37(11)	1.02(4)	0.60(7)
0.8	7.5(1.3)	1.37(9)	1.06(4)	0.49(9)
0.7	9.3(0.7)	1.50(5)	1.02(4)	0.53(5)
0.6	10.3(1.2)	1.38(3)	1.09(4)	0.49(16)
0.5	11.7(1.8)	1.43(2)	1.04(4)	0.59(20)
0.4	14.1(2.4)	1.45(4)	0.99(3)	0.60(26)
0.35	19.9(3.8)	1.41(6)	1.03(7)	0.29(32)

3. Results on the correlation function

First, we analyse the correlation functions computed with $L = 64$ runs. The study of the numerical data suggests to us the following Ansatz for the time and spatial dependences of the correlation function [12]:

$$G(x,t) = \frac{\text{const}}{x^{\alpha}} \exp\left[-\left(\frac{x}{\xi(t)}\right)^{\delta}\right] \tag{3}$$

where $\xi(t)$ is the dynamical correlation length. The numerical data clearly show that the dynamical correlation length depends on the time following a power law $\xi(t) = Bt^{1/z}$ where z is the dynamical critical exponent. The exponents α, δ and z and the amplitude B could, in principle, depend on the temperature. However, we obtain (see below) that α, δ and B are almost temperature independent, while $z(T)$ is inversely proportional to T.

In table 1 we report the results of our fits (always performed using the CERN routine MINUIT [21]). We remark that, for a given temperature, we have fitted our numerical data to the Ansatz of equation (3) in two steps. In the first step we fix the distance in the correlation function and perform the following three-parameters fit in the variable t:

$$\log G(x,t) = A(x) - B(x)t^{-\delta/z}. \tag{4}$$

We have found that δ/z is independent of x. In the second step we extract from $A(x)$ and $B(x)$ the exponents α and δ and the amplitude B using the formulae: $A(x) = \text{const} - \alpha \log x$ and $B(x) = B^{-\delta}x^{\delta}$. We report our final values of z, δ, B and α in table 1.

The resulting values for $z(T)$ (see table 1) can be fitted to a power law (using all the temperatures of table 1) obtaining

$$z(T) = 6.4(6)T^{-0.96(20)}. \tag{5}$$

From the previous fit we can guess a simpler law for the dynamical critical exponent $z(T) = a/T$, obtaining†

$$z(T) = \frac{6.2(3)}{T}. \tag{6}$$

This kind of behaviour suggests that the low-temperature dynamics in spin glasses is dominated mainly by activated processes with free-energy barriers diverging logarithmically with the size of the system.

We can finally write down the dependence of the dynamical correlation length on the time as well as on the temperature:

$$\xi(t,T) \propto t^{T/6.2(3)} = t^{0.161(8)\ T} = t^{0.153(12)\ T/T_c} \tag{7}$$

† This law was found by Kisker *et al* for the ± 1 three-dimensional spin glass (see [22, 23]). Moreover, this law was guessed for the Gaussian model using numerical data taken at temperatures $T = 0.7$ and 0.35 in [12].

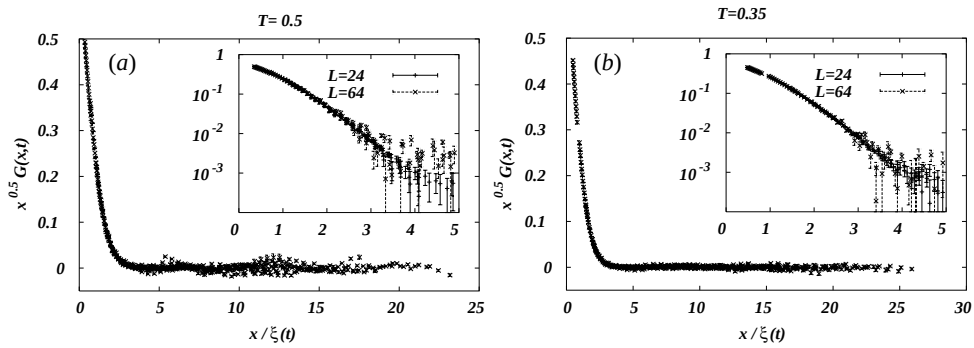

Figure 1. Scaling plot for the correlation function $G(x, t)$ measured at two very low temperatures, $T = 0.5$ and 0.35, and two lattice sizes, $L = 24$ and 64. It shows that the finite-size effects are negligible and it also gives reliability to our estimate for $\xi(t)$.

where we have assumed that the temperature of the phase transition is $T_c = 0.95(3)$ [8]. The agreement of the previous formula with the experiments is very good. We recall that in experiments [17] it was found the following dependence for the dynamical correlation length

$$\xi(t, T) \propto t^{0.170\ T/T_g} \tag{8}$$

where T_g is the experimental critical temperature (the authors of this result do not quote the error in the exponent).

A further check of equation (3) would be the collapse of the data (measured at different times and different temperatures) when plotting $G(x, t)x^{\alpha}$ versus $x/t^{1/z(T)}$. To this purpose we use the data from four samples of the 64^3 runs, together with those measured on 4096 samples of 24^3 runs. We remark that, in the 24^3 runs, the volume is nearly 19 times less than the $L = 64$ runs but we have computed 1000 times more samples and therefore expect the errors to be smaller.

In figure 1 we plot the correlation function for two low temperatures ($T = 0.5$ and 0.35) using as variables $x/\xi(t)$ and $x^{\alpha}G(x, t)$ (we have taken $\alpha = 0.5$, see table 1). In the plots we use the data from both runs ($L = 24$ and 64) and they superimpose perfectly. In the insets we present the same data in a log–linear scale in order to let the reader better evaluate the collapse. It is clear that the scaling is impressive even at the lowest temperature $T = 0.35$. We can also state that the finite-size effects are negligible for the lattice sizes used.

Scaling arguments tell us that the more general scaling function for the correlation function is (for large x and t)

$$G(x, t) \propto x^{-\alpha}\mathcal{G}\left(\frac{x}{\xi(t)}\right) \tag{9}$$

where the scaling function $\mathcal{G}(y)$ is smooth. Moreover, in the scaling regime, $\mathcal{G}(y)$ should not depend on either the temperature nor on the lattice size. Note that in our Ansatz (3) we have chosen an exponential function for the scaling function: $\mathcal{G}(y) \propto \exp(-y^{\delta})$, and we show that it fits very well with the data. However, to check that our estimates of α and $\xi(t)$ are correct we do not need to know $\mathcal{G}(y)$. We can simply plot $x^{\alpha}G(x, t)$ versus $x/\xi(t)$ (as in figure 1) and check how well the data collapse.

In order to check the temperature independence of $\mathcal{G}(y)$ we show in figure 2 the scaling function for three different temperatures ($T = 0.35$, 0.5 and 0.7), together with the exponential function $\exp[-y^{1.42(2)}]$ (see table 1) obtained through the fitting procedure. It is clear that the

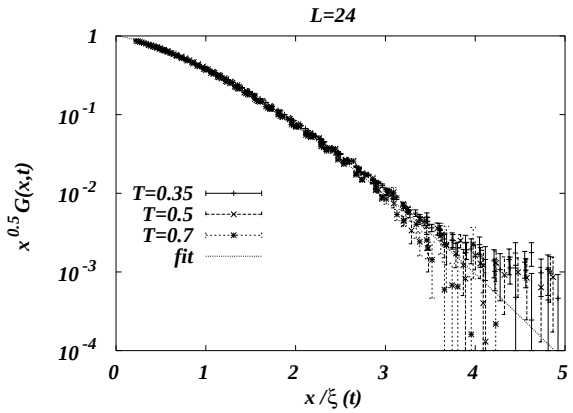

Figure 2. The scaled data for $G(x, t)$ are well described by a temperature-independent scaling function, that can be very well approximated by our fit.

scaling function is really temperature independent and it can be very well approximated by the exponential function as we have chosen in our Ansatz.

Another interesting issue is the extrapolation of the correlation function to infinite time. In this limit we can compare again our numerical results with the predictions of the droplet model and with that of the RSB theory. In the former the extrapolated correlation function tends to the value q_{EA}^2 for large distances, whereas the RSB prediction is a pure power law going asymptotically to zero [24]. Our Ansatz, which describes perfectly the numerical data, supports the RSB prediction even for the lowest temperatures.

Nevertheless, we have tried to fit our data with a functional dependence compatible with the droplet model, that is, $G(x, t) = G_\infty(x)\mathcal{G}(x/\xi(t))$, where $G_\infty(x) = Ax^{-\alpha} + C$. If $C = 0$, then the previous formula is exactly our Ansatz (and it implies a breaking of the replica symmetry), while if $C = q_{\mathrm{EA}}^2$ then it would support a droplet picture. Fitting the data to the previous formula, $G_\infty(x)$, we have found that at every temperature and even at $T = 0.35$ (our lowest temperature), the best value for C is always compatible with zero. At very low temperatures, i.e. $T = 0.35$, the Edwards–Anderson order parameter is so close to one ($q_{\mathrm{EA}} \simeq 1$) that we can safely distinguish between the two competing theories. In fact, in the droplet-like formula we have that $G_\infty(x)$ is almost constant† and so we should simply fit the data into the scaling formula of equation (9) without the factor $x^{-\alpha}$ in order to check the correctness of the droplet model.

In figure 3 we present the data rescaled with the formula suggested by the droplet model (left plot) and with that implied by RSB (right plot). It is clear that the RSB prediction fits much better with the numerical data. Note that the data error is sufficiently small to affirm safely that the data in the left plot have no collapse at all. It should be noted that the maximum correlation length we have been able to reach is quite small (of the order of three lattice spacing). Since we cannot thermalize the system at such low T values we cannot estimate an equilibrium correlation length (that is infinite in all the phase where q_{EA} is nonzero), but it is certainly larger than $\xi(t)$ (q_{EA} is substantially different from zero in thermalized samples up to $L = 16$). Still we believe it is relevant that our scaling works so well in all the region we have been able to analyse (in complete agreement with static simulations, that thermalize deep in the cold phase lengths up to 16, and are well fitted with a RSB-like scaling behaviour [9]).

† Actually it slowly decreases from 1 to $q_{\mathrm{EA}}^2 \simeq 1$, but for all our purposes it can be considered as a constant.

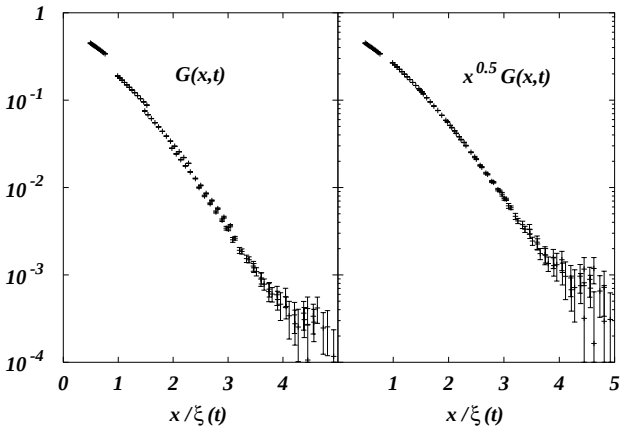

Figure 3. The comparison of these two scaling plots clearly shows that the $\sqrt{x}$ factor is essential in order to collapse the correlation function data. The temperature is $T = 0.35$ and the lattice size $L = 24$.

It is also appropriate to note that the droplet theory is a large-scale theory, but just how large this scale is remains completely unknown (we do not consider that as a strong point of the droplet approach): in this sense our numerical evidence, as all the numerical evidence one can hope to obtain, does not represent a complete refutation of the droplet theory. A scaling plot like the left one presented in figure 3 has been recently presented by Komori *et al* in [25] (see also [26]). We believe that the rather poor collapse of their data (see figure 5 in [25]) is due to the fact that they neglect the factor $x^{-\alpha}$ in the scaling formula. A much better collapse would be obtained by plotting $\sqrt{x}\ G(x,t)$ versus $x/\xi(t)$ (see [26]).

4. Fluctuation dissipation relation at very low temperatures

Now, we present the results of the analysis based on the generalization of the fluctuation–dissipation theorem (FDT) in the out-of-equilibrium regime [27]. In this section we will focus on the scaling properties of the ageing region and the violation of fluctuation–dissipation at very low temperatures.

A preliminary analysis was performed in [28] studying the violation of FDT at temperature, $T = 0.7$. Here we have simulated different lower temperatures and so, as byproduct, we can study the scaling properties of the violation of FDT. An analogous analysis, with many temperatures, was performed in [28] but on the four-dimensional EA model.

For the sake of conciseness, we do not repeat all the formalism and we address the interested reader to one of the previous publications on the subject [15, 27–30]. Here we simply recall the main formulæ that we use. As usual we define the integrated response to a very small external field as

$$\chi(t, t_w) = \lim_{h_0 \to 0} \frac{1}{h_0} \int_{t_w}^{t} R(t, t') h(t')\, \mathrm{d}t' \tag{10}$$

where $h(t) = h_0 \theta(t - t_w)$ and $R(t, t') = \frac{1}{N} \sum_i \frac{\partial \langle s_i(t) \rangle}{\partial h(t')}$. The autocorrelation function is defined as

$$C(t, t_w) = \frac{1}{N} \sum_i \langle s_i(t) s_i(t_w) \rangle. \tag{11}$$

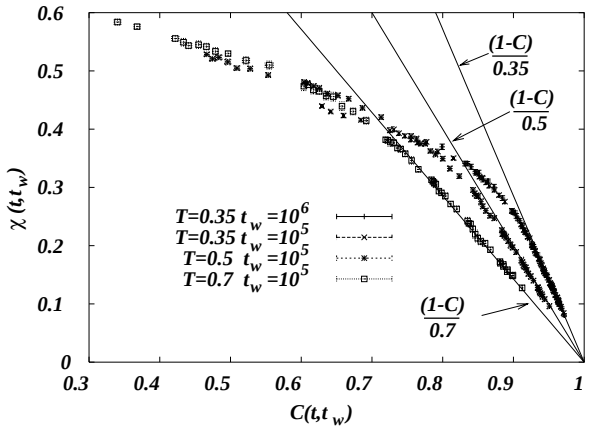

Figure 4. Response against the autocorrelation function for three different temperatures and lattice size $L = 64$. Note that in this figure we plot $\chi(t, t_w)$ versus $C(t, t_w)$. The data stay on a single universal curve when they leave the FDT lines. This curve is clearly non-horizontal and this hints for a breaking of the replica symmetry in the very low temperature phase of the EA model.

Relating these two functions, in the large-times limit, via

$$T\chi(t, t_w) = S(C(t, t_w)) \tag{12}$$

we have that, at the equilibrium, the FDT holds and $S(C) = 1 - C$, while in the ageing regime the function $S(C)$ can be linked to the equilibrium overlap distribution through $P(q) = -\frac{\partial^2 S(C)}{\partial C^2}|_{C=q}$ [28, 31].

Models that, in the frozen phase, do not show any breaking of the replica symmetry, have, at the equilibrium level, a static $P(q) = \delta(q - q_{\rm EA})$, which dynamically corresponds to the absence of response in the ageing regime. This means that, plotting $\chi(t, t_w)$ versus $C(t, t_w)$, we obtain a horizontal line in the range $C \leqslant q_{\rm EA}$ [30] (in the quasi-equilibrium regime, $C \geqslant q_{\rm EA}$, and it always holds $T\chi = 1 - C$ independently of the model).

In figure 4 we show the results for different temperatures in the usual plot $\chi(t, t_w)$ versus $C(t, t_w)$. Note that in this plot the FDT line is $\chi = (1-C)/T$ and so it is different for different temperatures. It is quite clear that, even for very large times, the curves are far from being horizontal when they leave the FDT line. This result gives more evidence in favour of a replica symmetry breaking in the very low temperature phase of the 3D EA model [28].

We present the data for different temperatures on a single plot in order to make more evident the fact that the numerical data seem to stay on the same curve once the system enters into the ageing regime, i.e. when the points leave the FDT line. This kind of behaviour has been observed in the four-dimensional EA model [28] and it is reminiscent of the mean-field solution.

Indeed in the SK model, using the Parisi–Toulouse (PAT) hypothesis [32], it can be shown [28] that

$$S(C) = \begin{cases} 1 - C & \text{for} \quad C \geqslant q_{\rm EA}(T) \\ T\sqrt{1 - C} & \text{for} \quad C \leqslant q_{\rm EA}(T). \end{cases} \tag{13}$$

The formula can be easily generalized assuming a generic power law behaviour in the aging regime: $S(C) = TA(1 - C)^B$ (the mean-field value for the exponent is $B = \frac{1}{2}$).

We use this generalization to fit the data and we obtain very good results. The best-fit parameters have been estimated from the collapse of the data reported in figure 4 and they are

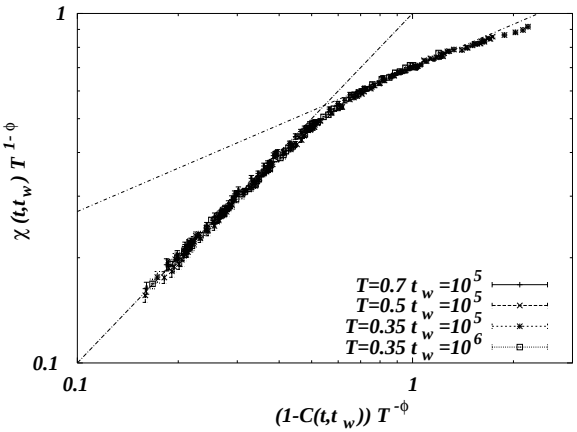

Figure 5. Scaling plot of the curves shown in the previous figure: $\chi T^{1-\phi}$ versus $(1-C)T^{-\phi}$ with $\phi = 1.7$. In the FDT regime (left part of the figure) the scaled data stay on the line $y = x$, while in the off-equilibrium regime (right part of the figure) they follow the plotted power law $y = Ax^B$ with $B = 0.41$.

$A \simeq 0.7$ and $B \simeq 0.41$ (to be compared with the mean-field values $A = 1$ and $B = \frac{1}{2}$, and those obtained for the four-dimensional EA model $A \simeq 0.52$ and $B \simeq 0.41$ [28]).

In order to show the validity of the fitting formula, we present in figure 5 the collapse of the scaled data using the variables $x = (1-C)T^{-\phi}$ and $y = \chi T^{1-\phi}$, where $\phi = \frac{1}{1-B} = 1.7$. It is easy to see that, if the previous scaling holds, the data should stay on two power laws: $y = x$ and $y = Ax^B$ in the quasi-equilibrium and ageing regime, respectively. The two power laws are reported in figure 5.

Even if we expect a breakdown of the assumed scaling for large values of the scaling variable x (i.e. the scaled data are no longer described by a power law), we note however that for a quite large range the collapse is very good and very well approximated by a power law. Moreover, we remark that the collapse has been obtained adjusting only one parameter.

5. Discussion

We have studied the off-equilibrium dynamics of the three-dimensional Gaussian spin glass in the very low temperature phase. In particular, we have studied the scaling properties of the dynamical overlap correlation functions and the scaling properties of the violation of the fluctuation–dissipation.

We have tried to fit our correlation functions to the functional form predicted by the droplet model but the fits were poor. Moreover, a correlation length diverging following a power law with the time implies, as was noted by Rieger [23], barriers diverging not as L^{ψ} (as predicted by the droplet model with the lower bound $\psi \geqslant \theta \simeq 0.2$) but as $\log L$. This latter results implies $\psi = 0$, hence violating the droplet lower bound.

It is interesting to note that the experimental data could be fitted to the droplet formula assuming that $\psi = \theta$ [17]. However, while both the results of numerical simulations and the experiments are in very good agreement with a power law fit for $\xi(t, T)$, the numerical fit assuming a droplet formula for $\xi(t, T)$ [22] disagrees with the experimental fit assuming the same hypothesis [17].

As it has been noted above, our final result for the dynamical correlation length is in a very good agreement with the experimental result.

We remark that the same scenario (power law dependence of $\xi(t, T)$ and linear dependence of $1/z$ with temperature) also emerges in four and six dimensions. In the latter case it was found that $z(T) = 4T_c/T$ [14] ($z = 4$ at the transition is the value predicted by mean field) while in the former one $z(T) = 5.5T_c/T$ [13]. Moreover, in these two dimensions the overlap correlation function constrained to zero overlap follows a pure power law as in three dimensions.

If we send to infinity the time in our Ansatz for the overlap–overlap correlation function we obtain a pure power decay $G(x) \propto x^{-\alpha}$ with $\alpha \simeq 0.5$, with a small dependence of α on the temperature for the whole spin glass phase. We recall again that the droplet prediction is $G(x) \to q_{\mathrm{EA}}^2$ in contradiction with our numerical correlation functions (this fact was already noted in [12]). Instead, the pure power behaviour is supported by the Gaussian approximation using the mean-field solution [4, 24].

One could argue that the simulated temperatures are not low enough and the times and sizes not large enough in order to see the 'true' (droplet) behaviour of the EA model. However, as we stressed in the introduction, $L = 64$ is large enough for temperatures as low as $T = 0.35$ and 0.5. Moreover, our large times extrapolations are very safe thanks to the measurements having been taken over six time decades.

We have shown numerical results that contradict the droplet predictions over a wide range of temperatures ($0.35 \leqslant T \leqslant 0.9$). In particular, we point out that our results (both for correlation functions and for violation of FDT) at a very low temperature, $T = 0.35$, support a mean-field picture.

Finally, we remark that using the PAT mean-field scaling relations for the $P(q)$ [32] we have obtained a very good scaling plot of the violation of fluctuation–dissipation (like in four dimensions [28]). This provides us another strong evidence calling for a low-temperature phase being well described by mean field [4].

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