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Violation of the fluctuation-dissipation theorem in finite-dimensional spin glasses

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Abstract. We study the violation of the fluctuation-dissipation theorem in the three- and four-dimensional Gaussian Ising spin glasses using on and off equilibrium simulations. We have characterized numerically the function $X(C)$ that determine the violation and we have studied its scaling properties. Moreover we have computed the function $x(C)$ which characterize the breaking of the replica symmetry directly from equilibrium simulations. The two functions are numerically equal and in this way we have established that the conjectured connection between the violation of fluctuation-dissipation theorem in the off-equilibrium dynamics and the replica symmetry breaking at equilibrium holds for finite-dimensional spin glasses. These results point to a spin-glass phase with spontaneously broken replica symmetry in finite-dimensional spin glasses.

1. Introduction

One of the characteristics of disordered systems at low temperatures (and also of real glasses) is that its approach to equilibrium is very slow, and it is difficult to study equilibrium properties. Obviously in the high-temperature regime there is a fast approach to the equilibrium.

Due to these large timescales, the out of equilibrium regime becomes very important since in nature the system remains in this regime for long times (minutes, days or even years). From a theoretical point of view it is interesting to develop a theory to describe this regime [1].

In this paper we will only discuss the low-temperature phase (i.e. below the phase transition point of the system) and centre the discussion on Ising spin glasses above their lower critical dimension (that clearly lies below three dimensions [2]).

In the disordered case and using the mean-field approximation (i.e. infinite-range interactions) Cugliandolo and Kurchan have derived a generalization of the fluctuation-dissipation theorem (FDT) that involves a new function (denoted by X) that determines multiplicatively (see below) the off-equilibrium regime. In the equilibrium regime $X = 1$ and we recover FDT. It is possible to link this X function with the static (equilibrium)

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function $x(q)$ (or its inverse $q(x)$) that appears in the replica symmetry breaking solution of infinite-dimensional spin glasses [3].

Unfortunately a direct check of this relation between static and dynamic in realistic models (such as finite-dimensional spin glasses) is still lacking. One of the aims of this paper is to check this static-dynamic link in finite-dimensional spin glasses.

The crucial point of the relation between the static and dynamic is that it is possible to compute the complete functional form of the order parameter (the order parameter is a number in ordered systems but is a function, $q(x)$, in infinite-dimensional spin glasses) using off-equilibrium simulations. Violations of the FDT relations have been reported for fragile glasses [4], but in this case the corresponding equilibrium computations are still missing.

On the other hand, equilibrium simulations of the three-dimensional spin glasses are very difficult [2]. It is interesting to examine different methods than can provide us with equilibrium information without performing (expensive) equilibrium simulations. These methods exist and are based on off-equilibrium simulations (see for instance [5–7]). They have been used, for example, in the four-dimensional Ising spin glass to extract the Edward–Anderson order parameter [6]. One clear advantage is that, after a fast initial transient, no thermalization is needed. Another advantage is that it is possible to simulate large lattices and so the final results have irrelevant finite-size effects.

Following this philosophy we have computed the order-parameter function† both from off-equilibrium numerical simulations and equilibrium ones, and we have obtained an impressive agreement between both approaches that confirm the link between static and dynamics in finite-dimensional spin glass and provide us with off-equilibrium numerical methods to compute static quantities such as the probability distribution of the overlap ($P(q) = \mathrm{d}x/\mathrm{d}q$) and the Edward–Anderson order parameter.

We have simulated the Gaussian Ising spin glass in three and four dimensions on a hypercubic lattice with periodic boundary conditions. The Hamiltonian of the system is given by

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

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

The plan of the paper is as follows. In section 2 we fix the notation and develop some analytical results. In sections 3 and 4 we show the numerical simulation for the three- and four-dimensional Ising spin glasses (respectively). Finally we present the conclusions.

2. Analytical results

Let us fix our notation. We will study the quantity $A(t)$ that depends on the local variables of our original Hamiltonian ($\mathcal{H}$). We can define the associate autocorrelation function

$$C(t, t') \equiv \langle A(t)A(t')\rangle \tag{2}$$

and the response function

$$R(t, t') \equiv \left.\frac{\delta\langle A(t)\rangle}{\delta\epsilon(t')}\right|_{\epsilon=0} \tag{3}$$

† We have computed directly an integrated version of the order parameter $P(q)$, from which $P(q)$ can be reobtained by double derivative.

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

$$\mathcal{H}' = \mathcal{H} + \int \epsilon(t) A(t)\, \mathrm{d}t. \tag{4}$$

In the dynamical framework assuming time translational invariance it is possible to derive FDT, that reads as

$$R(t, t') = \beta\theta(t - t')\frac{\partial C(t, t')}{\partial t'}. \tag{5}$$

As we are interested in spin models we have chosen $A(t) = \sum_i \sigma_i(t)$. The brackets $\langle(\cdots)\rangle$ in equation (2) imply here a double average, one over the dynamical process and a second over the disorder.

The FDT holds in the equilibrium regime, but in the early regimes of the dynamic we expect a breakdown of its validity. Mean-field studies [8] suggest the following modification of the FDT:

$$R(t, t') = \beta X(t, t')\theta(t - t')\frac{\partial C(t, t')}{\partial t'}. \tag{6}$$

It has also been suggested in [8, 9] that the function $X(t, t')$ is a function of the autocorrelation function: $X(t, t') = X(C(t, t'))$. We can then write the following generalization of FDT, which should hold in early times of the dynamics, the off-equilibrium fluctuation-dissipation relation (OFDR), that reads

$$R(t, t') = \beta X(C(t, t'))\theta(t - t')\frac{\partial C(t, t')}{\partial t'}. \tag{7}$$

We can relate the previous formula, equation (7), with observable quantities such as the magnetization. The magnetization in the dynamics is a function of the time and a functional of the magnetic field (that is itself a function of the time: $h(t)$) and so we can denote it $m[h](t)$. Using the functional Taylor expansion we can write

$$m[h](t) = m[0](t) + \int_{-\infty}^{\infty} \mathrm{d}t' \left.\frac{\delta m[h](t)}{\delta h(t')}\right|_{h(t)=0} h(t') + \mathrm{O}(h^2). \tag{8}$$

We define the response function

$$R(t, t') \equiv \left.\frac{\delta m[h](t)}{\delta h(t')}\right|_{h(t)=0} \tag{9}$$

and using the fact that in an Ising spin glass $m[0](t) = 0$, we obtain

$$m[h](t) = \int_{-\infty}^{\infty} \mathrm{d}t'\, R(t, t')h(t') + \mathrm{O}(h^2). \tag{10}$$

Using causality we can reduce the range of the integration to $(-\infty, t)$:

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

This is nothing but the linear-response theorem if we neglect the terms proportional to h^2.

By applying the OFDR we obtain the dependence of the magnetization with time in a generic time-dependent magnetic field (with a small strength), $h(t)$†,

$$m[h](t) \simeq \beta \int_{-\infty}^{t} \mathrm{d}t'\, X[C(t, t')]\frac{\partial C(t, t')}{\partial t'} h(t'). \tag{12}$$

† The symbol $\simeq$ means that the equation is valid in the region where linear response holds.

Now, we can perform the following experiment. We let the system evolve in the absence of magnetic field from $t = 0$ to $t = t_w$, and then turn on a constant magnetic field, h_0: $h(t) = h_0\theta(t - t_w)$†. Finally, with our choice of the magnetic field, we can write‡

$$m[h](t) \simeq h_0\beta \int_{t_w}^{t} \mathrm{d}t'\, X[C(t,t')] \frac{\partial C(t,t')}{\partial t'} \tag{13}$$

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

$$m[h](t) \simeq h_0\beta \int_{C(t,t_w)}^{1} \mathrm{d}u\, X[u] \tag{14}$$

where we have used the fact that $C(t, t) \equiv 1$ (we work with Ising spins). In the equilibrium regime (FDT holds, $X = 1$) we must obtain

$$m[h](t) \simeq h_0\beta(1 - C(t, t_w)) \tag{15}$$

i.e. $m[h](t)T/h_0$ is a linear function of $C(t, t_w)$ with slope -1.

The link with the static is the following. In the limit $t, t_w \to \infty$ with $C(t, t_w) = q$, $X(C) \to x(q)$, where $x(q)$ is given by

$$x(q) = \int_0^q \mathrm{d}q'\; P(q') \tag{16}$$

where $P(q)$ is the equilibrium probability distribution of the absolute value of the overlap. Obviously $x(q)$ is equal to 1 for all $q > q_{\mathrm{EA}}$, and we recover FDT.

For future convenience, we define

$$S(C) \equiv \int_C^1 \mathrm{d}q\, x(q) = \int_C^1 \mathrm{d}q \int_0^q \mathrm{d}q'\; P(q') \tag{17}$$

or equivalently

$$P(C) = -\frac{\mathrm{d}^2 S(C)}{\mathrm{d}^2 C}. \tag{18}$$

In the limit where $X \to x$ we can write equation (14) as

$$\frac{m[h](t)T}{h_0} \simeq S(C(t, t_w)) \tag{19}$$

for large t_w. The main aim of this paper is to test this last relation (equation (19)).

3. Three-dimensional results

The scheme of our off-equilibrium simulations has been the following. In a run without magnetic field we compute the autocorrelation function. We perform a second run where from $t = 0$ until $t = t_w$ the magnetic field is zero and then for $t \geqslant t_w$ we turn on a uniform magnetic field of strength h_0. The starting configurations were always chosen at random (i.e. we quench the system suddenly from $T = \infty$ to the simulation temperature T).

We have performed a first simulation with $h_0 = 0.1$ and $t_w = 10^5$, with a maximum time of 5×10^6. A second simulation was done with a smaller magnetic field, in order to check that linear response works: $h_0 = 0.05$ and $t_w = 10^4$ with the same maximum time. The lattice size in both cases was 64, the number of samples 4 and $T = 0.7$ (inside the spin-glass phase, the critical temperature is close to 1.0 [11]).

† Franz and Rieger [10] used a different magnetic-field function in their study of the FDT: $h_{\mathrm{FR}}(t) = h_0\theta(t_w - t)$.
‡ We ignore in our notation the fact that $m[h](t)$ depends on t_w.

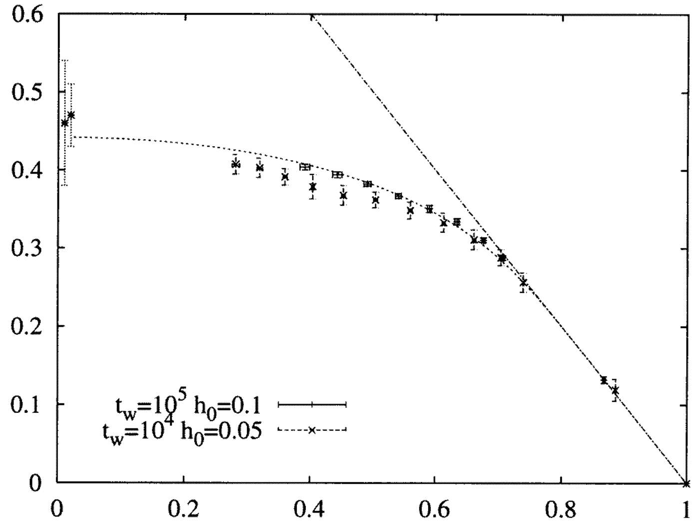

Figure 1. mT/h_0 versus C with $L = 64$ and $T = 0.7$ for the three-dimensional Ising spin glass. The curve is the function $S(C)$ obtained from the equilibrium data. The straight line is the FDT prediction. We have plotted the data of the two runs: $t_w = 10^5$, $h_0 = 0.1$ and $t_w = 10^4$, $h_0 = 0.05$.

We show in figure 1 the numerical results, mT/h_0 against $C(t, t_w)$. We have also plotted a straight line with slope -1 in order to control where the FDT is satisfied.

We have also plotted the function $S(C)$, see equation (17), obtained at equilibrium (i.e. using the equilibrium probability distribution of the overlaps, $P(q)$) by means of a simulation of a 16^3 lattice using parallel tempering [12, 13, 2]. We have simulated, with the help of the APE100 supercomputer [14], 900 samples of a $L = 16$ lattice using the parallel tempering method simulating 23 temperatures, from $T = 1.8$ down to $T = 0.7$ with a step of 0.05. In order to control the thermalization we have checked that the $P(q)$ is completely symmetric in q. We have used 10^6 sweeps to thermalize and 10^6 more sweeps to measure, each sweep consisting of one metropolis step and one attempt at exchanging the temperatures (a detailed analysis of the static of the three-dimensional Ising spin glass will be presented elsewhere [11]).

Finally we have plotted two points, in the left of the figure, that are obtained with the infinite-time extrapolation of the magnetization assuming a law

$$m(t) = m_\infty + \frac{A}{t^B} \tag{20}$$

with $B = 0.18(6)$ and $m_\infty T/h_0 = 0.46(8)$ in the $h_0 = 0.05$ run, and $B = 0.21(7)$ and $m_\infty T/h_0 = 0.47(4)$ in the $h_0 = 0.1$ run. The agreement between the two Tm_∞/h_0 results is very good. Within statistical error there are (almost) no differences between the numerical curves corresponding to the two runs.

From this figure we can estimate the order parameter at this temperature, that is precisely where the numerical curve and the straight line with -1 slope begin to be different, i.e. where the violation of FDT starts. So we can estimate $q_{\rm EA} \simeq 0.68$. We can relate this number with the estimate of $q_{\rm EA} = 0.70(2)$ obtained in [15] using equilibrium simulations. It is clear that the agreement is very good.

Surprisingly the $S(C)$ curve fits the numerical data very well even in the region where

FDT does not hold, i.e. the equilibrium distribution determines where the violation of the FDT begins and moreover the function $x(C)$ is very similar to $X(C)$ even in the very off-equilibrium regime, in the whole range of C. For instance $S(0) = 0.45$ to compare with the off-equilibrium data $Tm_\infty/h_0 = 0.47(4)$.

In this case we have been able to control down to $C \simeq 0.28$, but with an optimal combination of h_0 and t_w it should be possible to reach the region of smaller C. In any case the infinite-time extrapolation of mT/h_0 gives us the final point of the $S(C)$ and so it should not be difficult to reconstruct (by means of educated fits) the curve $S(C)$ in the region of small C.

This analysis implies that the ansatz $X(t,t') = X(C(t,t'))$ is correct in finite-dimensional spin glasses and that equation (19) holds in the three-dimensional Ising spin glass even for intermediate waiting times.

4. Four-dimensional results

In this section we study in detail the scaling properties of the function $X(T,C)$ and its dependence on the waiting time. We have used the same procedure as in the three-dimensional runs.

For the static measurements we have simulated an $L = 8$ lattice using the parallel-tempering method. We have simulated 1536 samples in a range of temperatures $T = 1.35$–1.95 with a step of 0.05 (we remark that the transition temperature is 1.80 [6]). We have performed 10^5 sweeps (metropolis + exchange) to thermalize and we have made measurements, using metropolis + exchange, during 10^5 sweeps. This takes about one month on the parallel computer APE100 [14]. We checked that thermalization was achieved by analysing the symmetry of the overlap probability distribution. From these simulations we have extracted the function $S(C)$ shown in figure 2.

For the dynamical measurements we have performed off-equilibrium simulation using the same procedure described in the previous section.

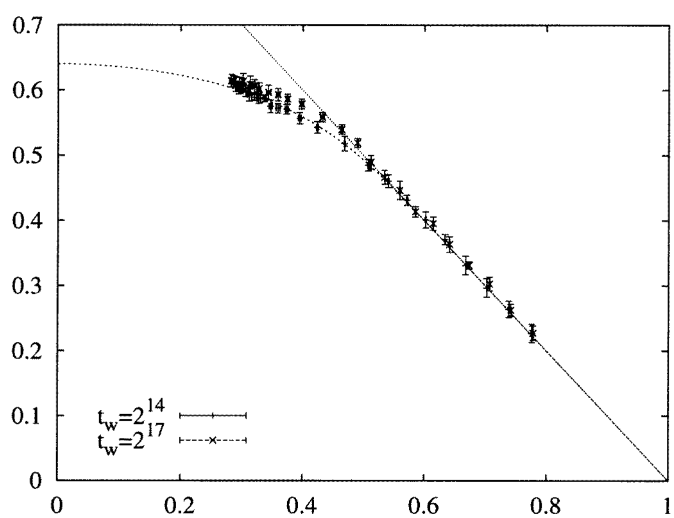

Figure 2. mT/h_0 versus C with $L = 32$ and $T = 1.35$ for the four-dimensional Ising spin glass. The curve is the function $S(C)$ obtained from the equilibrium data. The straight line is the FDT prediction. Here $h_0 = 0.1$.

We take a few samples (six in this case) of a very large system ($L = 24$ and $L = 32$) such that it cannot thermalize in any computer accessible time. We have measured the correlation (runs without magnetic field) and the response functions of the system for various waiting times ($t_w = 2^8, 2^{11}, 2^{14}, 2^{17}$) verifying that for increasing t_w the data of mT/h_0 versus $C(t, t_w)$, plotted in figure 2, collapse on a single curve losing the dependence on the waiting time. We have simulated almost all the runs with $h_0 = 0.1$: except in one run of a $L = 32$ lattice at $T = 1.0$ we have put $h_0 = 0.05$.

The clear agreement between the static and dynamical data supports (again) the correctness of the theoretical hypothesis. Nevertheless the data for the largest waiting times lie a little above the static curve. We justify this discrepancy noting that in a numerical simulation of a relatively small volume ($L = 8$ in our case) the delta function for $q = q_{\rm EA}$ in the $P(q)$ is replaced by quite a broad peak. This effect smooths the cusp we expect in $S(C)$ at the value $C = q_{\rm EA}$ lowering the numerical curve with respect to the right one. In the three-dimensional case the data obtained from the simulation of the 16^3 lattice are very close to asymptotic values (by comparing, for instance, with $S(C)$ obtained in 8^3 and 12^3 lattices [11]).

Once we have verified that we can obtain information on the overlap distribution function $P(q)$ (measuring the linear response of a large system kept in the out-of-equilibrium regime) we have performed a systematic study in the whole frozen phase.

We wish to stress that the data from the $L = 24$ and the $L = 32$ systems coincide within error, suggesting that our results are not affected by a finite-size bias. Anyhow, we present data for both the lattice sizes.

In figure 3 we plot the integrated response against the correlation function for different temperatures. The straight lines ($m/h_0 = (1-C)/T$) represent the quasi-equilibrium regime in which the system stays while $C > q_{\rm EA}$. Note how the data measured in the regime where $C < q_{\rm EA}$ collapse on a single curve independently of the temperature.

We can understand this fact by recalling a hypothesis that was developed in the study of the $P(q)$ in the mean-field approximation by one of the authors (GP) and Toulouse [16, 17].

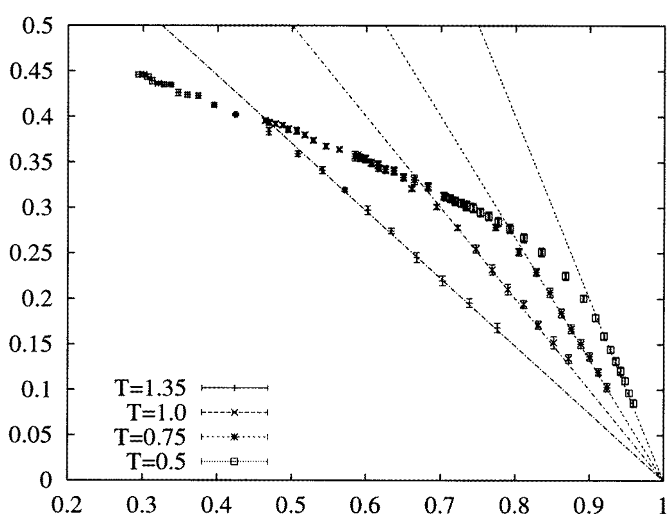

Figure 3. m/h_0 versus C with $L = 32$ and different temperatures for the four-dimensional Ising spin glass. The lines are the FDT regime: $(1 - C)/T$. Note how the data stay on a single curve when they leave the straight line (the FDT regime). Here $h_0 = 0.1$.

It assumes that the order parameter $q(x, T)$ [3], in the mean-field theory, is a function of the ratio x/T for $q < q_{\mathrm{EA}}$. This implies that we can write, in this approximation,

$$x(q, T) = \begin{cases} T\tilde{x}(q) & \text{for } q \leqslant q_{\mathrm{EA}}(T) \\ 1 & \text{for } q > q_{\mathrm{EA}}(T) \end{cases} \tag{21}$$

and, integrating $x(q, T)/T$, we obtain the relation between m/h_0 and C

$$\frac{m}{h_0} = \frac{S(C)}{T} = \begin{cases} \displaystyle\int_C^{q_{\mathrm{EA}}} \tilde{x}(q)\,\mathrm{d}q + (1 - q_{\mathrm{EA}})/T & \text{for } C \leqslant q_{\mathrm{EA}}(T) \\ (1 - C)/T & \text{for } C > q_{\mathrm{EA}}(T). \end{cases} \tag{22}$$

The terms in the r.h.s. of equation (22) describe the two regimes present in figure 3: the first gives an expression for the curve followed by the data in the off-equilibrium regime, while the second is the straight line (FDT regime).

In the following we will show that this hypothesis [16, 17] also implies that the off-equilibrium part is independent of the temperature (i.e. in the region where $C < q_{\mathrm{EA}}$, $[m/h_0](C)$ is independent of the temperature). Using the fact that the magnetic susceptibility is 1 in the spin-glass phase and with the help of equation (21) it is possible, with a little algebra, to show that

$$\frac{1 - q_{\mathrm{EA}}(T)}{T} + [1 - T\tilde{x}(q_{\mathrm{EA}}(T))]\frac{\mathrm{d}q_{\mathrm{EA}}(T)}{\mathrm{d}T} = 0. \tag{23}$$

Now is very easy to demonstrate that the curves describing the off-equilibrium regime ($C \leqslant q_{\mathrm{EA}}(T)$ in equation (22)) do not depend on the temperature. By deriving the curve expression with respect to T we obtain

$$\frac{\mathrm{d}}{\mathrm{d}T}\left[\frac{m}{h_0}\right] = \frac{\mathrm{d}}{\mathrm{d}T}\left[\frac{S(C)}{T}\right] = \tilde{x}(q_{\mathrm{EA}}(T))\frac{\mathrm{d}q_{\mathrm{EA}}(T)}{\mathrm{d}T} - \frac{1}{T}\frac{\mathrm{d}q_{\mathrm{EA}}(T)}{\mathrm{d}T} - \frac{1 - q_{\mathrm{EA}}(T)}{T^2} = 0 \tag{24}$$

where in the last equality we have made use of equation (23). So we have verified that the first expression in equation (22) does not depend on T. We finally write that for $C \to q_{\mathrm{EA}}^-$ the hypothesis [16, 17] implies

$$S(C) \simeq \sqrt{1 - C}. \tag{25}$$

At this point we have seen that mean field predicts qualitatively the behaviour plotted in figure 3 for a finite-dimensional spin glass. Now we will examine quantitatively the data of figure 3.

For $C < q_{\mathrm{EA}}$ we have seen (figure 3) that the numerical data can be approximated by a power law of the variable $1 - C$

$$\frac{mT}{h_0} = \begin{cases} TA(1 - C)^B & \text{for } C \leqslant q_{\mathrm{EA}}(T) \\ 1 - C & \text{for } C > q_{\mathrm{EA}}(T) \end{cases} \tag{26}$$

with $A \simeq 0.52$ and $B \simeq 0.41$ (not very far from the mean-field behaviour, $(1 - C)^{1/2}$). Multiplying both sides of the previous expression by $T^{-1/(1-B)}$ we have

$$\frac{mT}{h_0}T^{-\frac{1}{1-B}} = \begin{cases} T^{-\frac{B}{1-B}}A(1 - C)^B = A[(1 - C)T^{-\phi}]^B & \text{for } C \leqslant q_{\mathrm{EA}}(T) \\ T^{-\frac{1}{1-B}}(1 - C) = (1 - C)T^{-\phi} & \text{for } C > q_{\mathrm{EA}}(T) \end{cases} \tag{27}$$

where we have introduced $\phi = 1/(1 - B) \simeq 1.7$ for convenience. Doing so we can rescale the data for all the temperatures on a single curve like the one shown in figure 4.

The good scaling of data (figure 4) obtained with different magnetic fields is a confirmation that we are working in the linear response regime. We should also note the absence of different finite-size effects for the lattices we have considered (24^4 and 32^4).

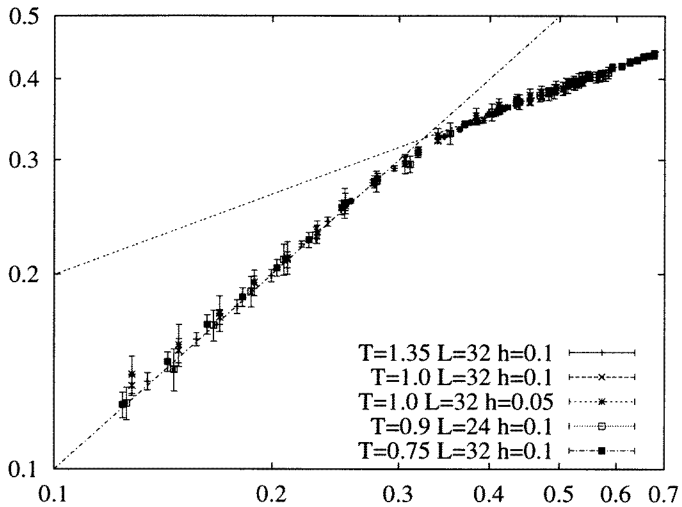

Figure 4. $(mT/h_0)T^{-\phi}$ versus $(1-C)\ T^{-\phi}$ with $\phi = 1.7$. Note that in the plot we have included data measured on different lattices and in the presence of different magnetic fields. In the FDT regime (left part of the figure) the factor $T^{-\phi}$ has no effect because in this region $mT/h_0 = 1-C$. The off-equilibrium regime (right part of the figure) follows a power law with power $B = 0.41$.

5. Conclusions

In this paper we have found that the violation of the FDT in finite-dimensional spin glasses follows the lines of the violation of the theorem in mean-field models.

We have also found that the function that determines the violation is given, even for not very long waiting times, by the double integral of the probability distribution of the overlap calculated at equilibrium.

This fact gives us a further confirmation that the ansatze used in [8] are correct even in finite-dimensional models (i.e. X depends only on C, as was established in [10]). We have also obtained that the violation of the theorem is determined by the static behaviour (i.e. we can express $X(C)$ as a function of static quantities).

Moreover we have seen that by controlling the scaling of the waiting times it is possible to construct the $X(C)$ curve without doing equilibrium simulations. Also these curves provide us an useful and precise method to compute the Edward–Anderson order parameter.

The form of the $X(C)$ function is very different from that in the droplet approximation, in the ferromagnetic case and in one step replica symmetry breaking systems [4], and so we have obtained additional evidence that the finite-dimensional Ising spin glasses cannot be described by the droplet model.

Finally, we have studied the scaling properties of $X(C)$ finding that it is possible parametrize it using static mean-field analytical results. It gives us further evidence of spontaneously broken replica symmetry (infinite steps of replica symmetry breaking).

In this paper we have found that the finite-dimensional Ising spin glass behaves in the way predicted by the mean-field approximation and in contrast to the heuristic predictions by Newman and Stein [18]. We remark that in the numerical calculation we have computed well-defined observables (i.e. self-averaging quantities) such as the autocorrelation function and the magnetization and there is no reference to the replica–replica overlap. Moreover, it has been shown that there is no conflict between the rigorous part of the Newman–Stein work [18] and the predictions of the mean-field approximation with replica broken symmetry, if this last theory is correctly interpreted [19].

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