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Study of the phase transition in the 3D Ising spin glass from out-of-equilibrium numerical simulations

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Abstract

Using the decay of the out-of-equilibrium spin–spin correlation function we compute the equilibrium Edward–Anderson order parameter in the three-dimensional binary Ising spin glass in the spin glass phase. We have checked that the Edward–Anderson order parameter computed from out-of-equilibrium numerical simulations follows with good precision the critical law as determined in experiments and in numerical studies at equilibrium (which allow us to estimate the β critical exponent). Finally, we present a large time study of the off-equilibrium fluctuation–dissipation relations and find strong discrepancies (in the low-temperature region) between the numerical data and the droplet theory predictions and agreement with the predictions of the replica symmetry breaking theory.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The characterization, using numerical simulations, of the phase transition in the three-dimensional Ising spin glasses has been a challenging problem. Recently, a clear picture of the phase transition and good estimates of the critical exponents have been obtained for both Gaussian and bimodal disorder by working at equilibrium [1–3].

However, a characterization of the phase transition using out-of-equilibrium techniques is still lacking (see [4] for a detailed discussion). In the first part of this paper we will address this problem (simulating the bimodal disorder). In particular, we will compute the

order parameter using out-of-equilibrium techniques [5] and will characterize the transition using this observable. In addition, we will confront our data with previous estimates of the critical point and critical exponents for this model (obtained from numerical simulations and experiments). The behaviour of this observable will permit us to discard (again) a Kosterlitz–Thouless-like phase transition (as done in equilibrium [1], that we will refer in the following as *XY*-like scenario) for the transition [4]. Moreover, we have studied the dependence of the order parameter with the size of the system. Hence, we will present in this paper the first direct numerical computation of the Edwards–Anderson order parameter in the three-dimensional Ising spin glass (obtained out of equilibrium).

This kind of study was performed in the past in four dimensions [6] (see also [7, 8]) but is still lacking in three dimensions (the interesting physical dimensions).

The second part of the paper is devoted to the study of the fluctuation–dissipation theorem out of equilibrium. This kind of analysis has attracted a large amount of work (analytical, numerical and experimental) in the last few years [9–14].

Using the results of [14] and assuming that the three-dimensional Ising spin glass presents stochastic stability (until now it has not been rigorously proved but there are numerical evidences [17]) one can relate the fluctuation–dissipation curves with equilibrium properties and so, compute or measure the equilibrium probability distribution of the overlap. This computation or measurement is very important since it should discern between the different theoretical approaches in competition, which try to describe the behaviour of finite-dimensional spin glasses (e.g. the replica symmetry breaking (RSB) approach [16, 17] or the droplet model [18]).

The goal of this (last) part of the paper is twofold. First, to check if the order parameter computed in the first part of this paper matches well in the fluctuation–dissipation (FD) curves. This is important since this value marks the point in which the FD curve departs from its pseudo-equilibrium regime, and the behaviour of the curve from this departing point is a clear fingerprint whether or not the system behaves following the RSB theory or the droplet model.

And the second goal is to study the finite time behaviour (for really large times) of the curves in order to see how the asymptotic form of the FD curves is built up. This is important, since until now, the numerical simulations [12] and experiments [15] show up behaviour compatible with the replica symmetry breaking description and incompatible with droplet theory. One can argue that the curves reported in the literature [12, 15] are not asymptotic and that the asymptotic curve is compatible with droplet theory and not compatible with RSB.

Finally, we will draw the conclusions.

2. The model and numerical simulations

We have simulated a three-dimensional system in a cubic lattice with helicoidal boundary conditions of size L and volume $V = L^3$. The Hamiltonian is

$$\mathcal{H} = - \sum_{\langle i, j \rangle} J_{ij} \sigma_i \sigma_j, \quad (1)$$

where $\langle i, j \rangle$ denotes the sum over the first nearest neighbours, $\sigma_i = \pm 1$ are Ising variables and $J_{ij} = \pm 1$ are quenched random variables with a bimodal probability distribution with zero mean and unit variance. We have used the standard heat-bath algorithm (local dynamics) to simulate the three-dimensional lattice.

We will introduce the observables measured in our work. Firstly, the order parameter (the Edwards Anderson one) is defined as:

$$q_{\text{EA}} = \overline{\langle \sigma_i \rangle^2}, \quad (2)$$

where, as usual, we use $\langle \cdot \cdot \cdot \rangle$ and $\overline{\langle \cdot \cdot \cdot \rangle}$ to denote thermal and quenched disorder average respectively.

In addition, the spin–spin correlation function has been computed using

$$C(t, t_w) = \frac{1}{V} \sum_{i=1}^V \sigma_i(t) \sigma_i(t_w). \quad (3)$$

We can obtain formally the order parameter from this correlation as the double limit:

$$q_{\text{EA}} = \lim_{t \rightarrow \infty} \lim_{t_w \rightarrow \infty} C(t, t_w). \quad (4)$$

Note that the order of the limit is crucial in obtaining the order parameter. We will use this equation to extract q_{EA} from the out-of-equilibrium data.

We will study in the last part of the paper the finite time behaviour of the violation of the fluctuation–dissipation relation in the three-dimensional spin glass. We will review shortly the main equation of the off-equilibrium fluctuation–dissipation equations (see [19] for more details):

$$R(t_1, t_2) = \frac{1}{T} X(C(t_1, t_2)) \frac{\partial C(t_1, t_2)}{\partial t_2}, \quad (5)$$

where $t_1 > t_2$, $R(t_1, t_2)$ is the response of the system to the magnetic field perturbation (i.e. the magnetic susceptibility of the system: $R(t_1, t_2) = m(t_1, t_2)/h$) and $X(C)$ is the, in principle unknown, function which controls the violation of the fluctuation–dissipation theorem. Integrating this equation in t_2 and taking the perturbing field as $h(t) = h\theta(t - t_w)$ we finally obtain (working in the linear-response region):

$$m(t) \simeq \beta h \int_{C(t, t_w)}^1 du X(u). \quad (6)$$

In the regime $t_1 \gg t_2 \gg 1$ we reach the equilibrium, and it is possible to show that $C(t_1, t_2) \rightarrow q$. In addition $X(q) \rightarrow x(q) \equiv \int_{q_{\text{min}}}^q dq' P(q')$, where $x(q)$ is the integral of the probability distribution of the overlap at equilibrium [16]. Hence, in this regime [9–14],

$$m(t) \simeq \beta h \int_{C(t, t_w)}^1 du x(u). \quad (7)$$

Furthermore, we can define

$$S(C) \equiv \int_{C(t, t_w)}^1 dq x(q), \quad (8)$$

so,

$$\frac{m(t)T}{h} \simeq S(C(t, t_w)). \quad (9)$$

Both, in droplet theory and RSB (see [21], in particular its figure 10), $S(C)$ is the straight line $1 - C$ for $C \in [q_{\text{EA}}, 1]$. However, for $C < q_{\text{EA}}$ the behaviour is very different: in the droplet theory $S(C)$ is constant in this region and in RSB $S(C)$ is a growing function with curvature. We recall that knowing the initial point, $S(C = 0)$, we can compute q_{EA} in the droplet theory as

$$q_{\text{EA}}^{\text{droplet}} = 1 - S(C = 0). \quad (10)$$

This technique allows us to compute, taking the appropriate limit, the equilibrium function $x(q)$.

Finally, we report that all the numerical simulations have been obtained with the SUE machine [22]. This is a dedicated machine, designed for the simulation of the three-dimensional Edwards–Anderson model with first neighbour couplings [16], the system that is being studied in the present work. It consists of 12 identical boards. Each single board is able to simulate 8 different systems, updating all of them at each clock cycle. SUE reaches an update speed of 217 ps spin with a clock frequency of 48 MHz. The on-board reprogrammability permits us to change in an easy way the lattice size, or even the update algorithm or the Hamiltonian. The SUE machine is connected to a Host Computer running under Linux. SUE is in charge of the update of the configurations, and the host computer is in charge of measurements and analysis. The main electronic devices of each SUE board are the Altera family, that performs the update. Other devices store the spins and couplings variables. One of the Alteras is devoted to generating random numbers in a fast way (for more details, see [22]). Up to our knowledge, SUE has been the fastest dedicated machine in the simulation of the three-dimensional Edwards–Anderson model.

3. Computation of the Edward–Anderson order parameter

In order to compute the Edward–Anderson order parameter (q_{EA}), we have carried out several runs for two lattice sizes and different temperatures: $\beta = 1/T = 2.00, 1.67, 1.25, 1.05, 1.00, 0.95$ and 0.91 for $L = 30$; and $\beta = 2.00, 1.67, 1.25$ and 1.00 for $L = 60$. For all of them we have averaged over 58 samples. In figure 1 we report the curves $C(t, t_w)$ as a function of time t .

We have checked that the behaviour of $C(t, t_w)$ for $t_w \gg 1$ follows with high precision the behaviour (as in higher dimensions, see [6, 7]; this is just an Ansatz):

$$C(t, t_w) = a(t) + b(t)t_w^{-c(t)}, \quad (11)$$

where $a(t)$ is related to the value of q_{EA} . In order to find it out we have first obtained, from figure 1 (top), the curves $C(t, t_w)$ versus t_w for several fixed values of t (typically, from 8192 to $\sim 3.7 \times 10^8$ Monte Carlo steps) (see figure 1, bottom). We have fitted these curves to the functional form defined in (11) obtaining in this way the behaviour of $a(t)$ as a function of t (we show these fits in figure 1). From $a(t)$ and for $t \gg 1$, we can obtain the value of q_{EA} (since asymptotically $a(t)$ must become q_{EA}). To achieve this aim, we have fitted the last points of $a(t)$ versus t to a constant function (since $a(t)$ shows a clear plateau, see figure 2). In this way, we have implemented the double limit in equation (4). The results obtained from these fits are shown in figure 3.

We have checked that for $\beta > 1.00$ the values for q_{EA} are the same for both $L = 30$ and $L = 60$. In $\beta = 1.00$ the difference is about 1.5 standard deviations. In addition, we have run a $L = 20$ lattice at $\beta = 0.91$ and $\beta = 1.00$: these data show finite-size effects as expected since they lie near the critical point (see figure 3).

4. Characterizing the phase transition

As we mentioned before, we have checked that the q_{EA} , which we have computed out of equilibrium, follows with good precision the critical law of the order parameter

$$q_{EA}(\beta) = A(\beta - \beta_c)^{\beta_q}, \quad (12)$$

where we have denoted by β_q the usual β exponent of the order parameter (in order to avoid confusion with the usual notation $\beta = 1/T$)

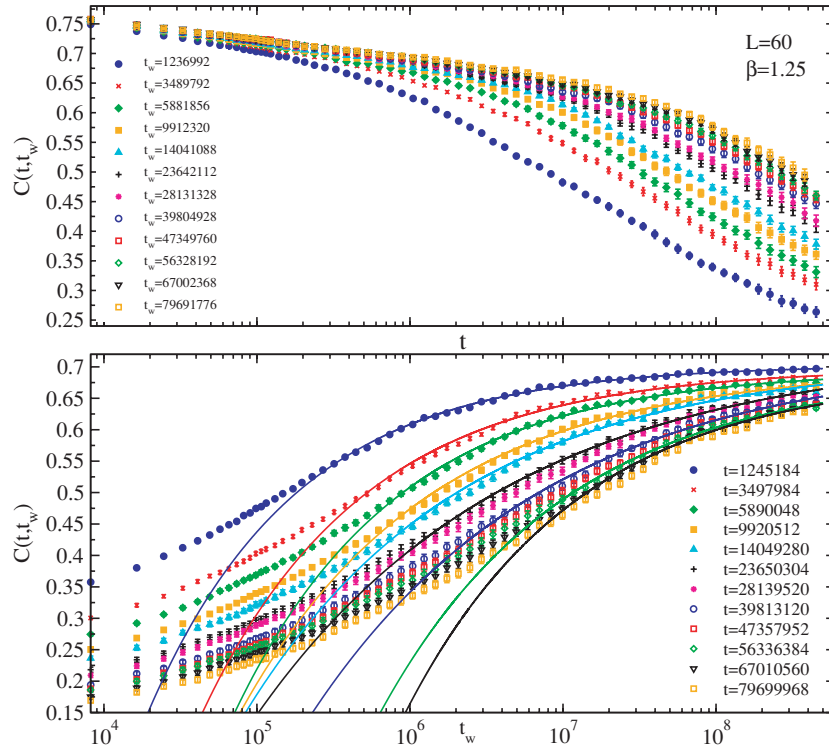


Figure 1. Out-of-equilibrium spin–spin correlation function $C(t, t_w)$ computed for $L = 60$ and $\beta = 1.25$. *Top:* $C(t, t_w)$ versus time, t . *Bottom:* $C(t, t_w)$ versus waiting time, t_w , obtained by studying the figure in the top for several fixed times t in order to find the limit $t_w \rightarrow \infty$ behaviour of $C(t, t_w)$. The continuous lines in the plot are the fits to equation (11). Note that for the curves with larger waiting time we have chosen to show not all the fits to (11) in order to present a clean figure (the quality of the fits is the same for all the waiting times).

By fitting only the points closer to the critical one (satisfying $\beta < 1.25$) we obtain

$$\beta_c = 0.866(2), \quad \beta_q = 0.52(9), \quad (13)$$

with a $\chi^2/\text{d.o.f} = 1.13$. These figures compare really well with the numerical values obtained at equilibrium [1], namely: $\beta_c = 0.88(1)$ and $\beta_q = 0.71(5)$. In particular the difference between the two estimates of β_q is $0.19(11)$, less than two standard deviations^{4,5}.

In addition, we can compare with experiments. In [23] was found $\beta_q = 0.54(10)$ ⁶ which is in a very good agreement with our out-of-equilibrium value.

We have also checked that q_{EA} follows with good precision the critical law

$$(q_{EA}(\beta))^{1/\beta_q} = A(\beta - \beta_c). \quad (14)$$

Again, we have only used in the fit the points with $\beta < 1.25$ (critical region). Moreover we can fix β_q to the experimental value, obtaining again a compatible value with the equilibrium one: $\beta_c = 0.8603(6)(236)$, where the first error is statistical and the second error comes from

⁴ Note that in [1] corrections to scaling were taken into account. In our estimate there is no scaling correction, hence our error is smaller than the error quoted in [1]: i.e. our error bars are underestimated.

⁵ See also [24] for a non-universality scenario: they reported $\beta_c = 0.84(1)$.

⁶ Note that both results in [1, 23] come from different methods.

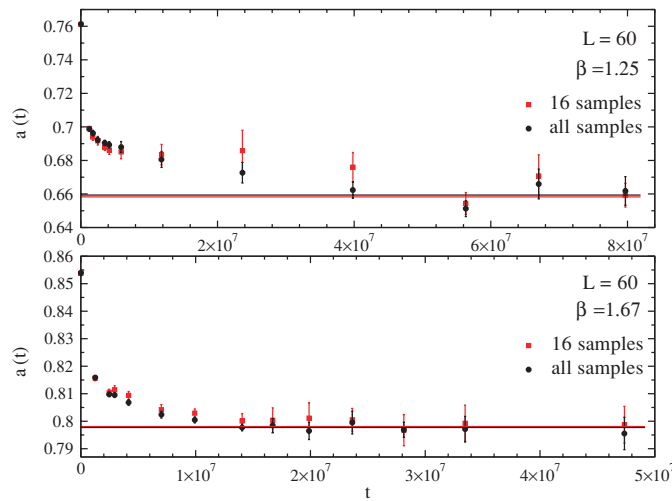


Figure 2. Function $a(t)$ defined in equation (11) computed for $L = 60$ lattice size and $\beta = 1.25$ (top) and $\beta = 1.67$ (bottom). Note that the last points of the curve can be fitted to a constant in the two plots. In addition, we have drawn the function $a(t)$ with only 16 samples in order to show the dependence of the extrapolated value (i.e. the plateau) on the number of samples.

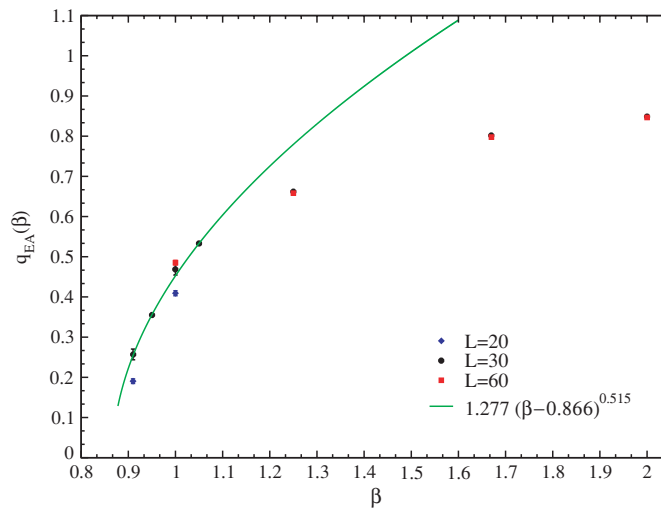


Figure 3. q_{EA}^{dyn} versus β for three lattices sizes $L = 20, 30$ and 60 . The continuous line is the fit reported in the text.

the error of the experimental β_q . In addition, by fixing β_q to the numerical simulations value we obtain $\beta_c = 0.820(3)(13)$, less than three standard deviations from the numerical value.

All figures reported in this analysis are compatible with latest estimates of the critical exponents. In [2] $\beta_c = 0.893(3)$ and $\beta_q = 0.723(25)$ were reported. In addition, a diluted version of this model was studied in [3] and $\beta_q = 0.723(50)$ was reported.

Finally, we remark that our numerical results from both β_c and β_q must suffer from the systematic error coming from the dependence of q_{EA} with L near the critical point (as shown

the $L = 20$ runs). At $\beta = 1.00$ we have three different values of the order parameter that fit to the law

$$q_{\text{EA}}(L) = q_{\text{EA}}(\infty) + \frac{b}{L^c},$$

where b and c are constants. This is the finite volume correction equation which holds in the low-temperature phase⁷. We have obtained $c = 3.54$ and $q_{\text{EA}}(\infty) = 0.49$ (note that we are fitting three points to a three-parameter function) to be compared with $q_{\text{EA}}(L = 60) = 0.485(6)$ and $q_{\text{EA}}(L = 30) = 0.47(1)$. At $\beta = 0.91$ (the nearest value we have to the critical point) we have only two points, that anyhow, we can try to fit to equation (4) fixing $c = 3.54$, obtaining $q_{\text{EA}}(\infty) = 0.278$ (no error bars can be reported since, again, the number of degrees of freedom in this fit is zero) to be compared with the value of our largest lattice $q_{\text{EA}}(L = 60) = 0.26(1)$, so this limited analysis suggests that the $L = 30$ lattice is asymptotic in its error bars in the region $\beta \geq 0.91$. Hence, we are confident that our final estimates of β_c and β_q should have small systematic error coming from finite-size effects.

We remark that testing the dependence of q_{EA} with the lattice size, for large lattices (e.g. $L = 60$) near the transition is not accessible even using the SUE machine.

5. Finite time effects in the fluctuation–dissipation relations

We have performed several runs again with the SUE machine, in a lattice of size $L = 60$ for different temperatures: $\beta = 1.25, 1.10, 1.05, 1.00$ and 0.95 . We have used the following standard procedure. We let the system evolve during a time t_w , just after this time, a field $h = 0.03$ is plugged, seeing the response of the system and recording the magnetization and the correlation function. Then it is possible to extract the value of q_{EA} , for the particular β being analysed at that moment, from the point where the curve leaves the linear regime, that is, where mT/h does not follow the pseudo-equilibrium line $(1 - C)/T$.

The choice of the field strength applied to the system has not been arbitrary. We need to stay in the linear-response region. We have checked this by simulating different magnetic fields: $h = 0.01, 0.03, 0.05$ and 0.10 . Finally we have selected a safe value for h : $h = 0.03$, which is a compromise between large and small fields (note that small fields induce strong noise in the measures). In figure 4 we have shown the FDT curve for a waiting time and two perturbing magnetic fields ($h = 0.01$ and 0.003) in order to test that we are in the region in which linear response holds. It is clear from this figure that the curve, inside the error bars, is independent of the perturbing magnetic field.

In the droplet model, the curve $X(C)$ departs horizontally from the straight line $1 - C$, the final value of the horizontal line being $m_{\text{asyn}}T/h$ (i.e. $S(C = 0)$), where m_{asyn} is the equilibrium value of the magnetization in a field h at the temperature T . Hence, measuring m_{asyn} we can obtain the droplet theory estimate for the order parameter as:

$$q_{\text{EA}}^{\text{droplet}} = 1 - \frac{m_{\text{asyn}}T}{h}. \quad (15)$$

We will show in this section plots corresponding to $\beta = 1.25$ and $L = 60$. In order to obtain numerically m_{asyn} we have performed a very large in-field numerical simulation recording the value of the magnetization at the time t : $m(t)$. The asymptotic value is

⁷ In [20] it was checked that in the three-dimensional Gaussian Ising spin glass the position of the maximum of the equilibrium probability distribution of the overlap follows this law with $c = 1.5(4)$ by fitting $L \leq 16$. Note that in our case we are using $20 \leq L \leq 60$ data and simulate the $\pm J$ model and that the c exponent could depend on the temperature. Note that usually in equilibrium small lattices develop larger order parameter; however, in our dynamical approach we have found the opposite behaviour.

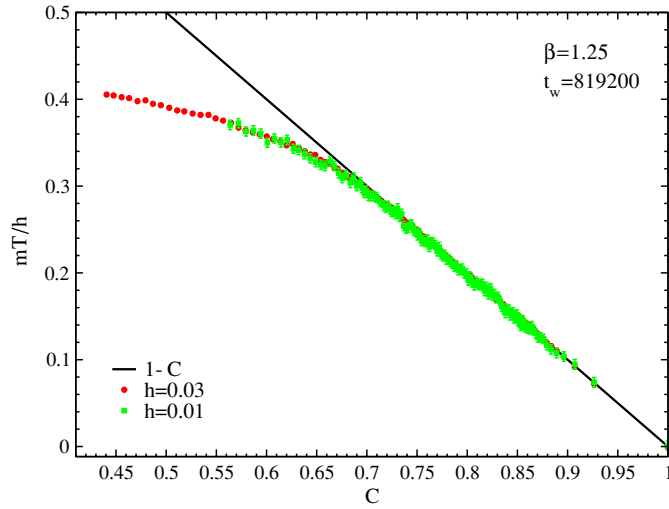


Figure 4. Fluctuation–dissipation curve out of equilibrium for one of the lowest temperatures simulated $\beta = 1.25$, $L = 60$ and one waiting time for two different perturbing magnetic fields, $h = 0.01$ and 0.03 , in order to check linear response.

Table 1. $q_{EA}(\beta)$ for $L = 60$ from $C(t, t_w)$ (obtained in the first part of the paper) and assuming droplet theory from mT/h . All the data showed in this table were obtained in a $L = 60$ lattice except for dynamical q_{EA} at $\beta = 0.95$ that was obtained simulating a $L = 30$ lattice.

β	$q_{EA}^{\text{dyn}}(\beta)$	q_{EA}^{droplet}
1.25	0.6583(34)	0.5573(13)
1.00	0.5071(31)	0.3957(17)
0.95	0.3554(7)	0.3404(21)

simply $m_{\text{asyn}} = m(\infty)$ (this observable shows really small dependence on L for the lattice sizes simulated in this paper). To avoid extrapolations we have continued the run until the magnetization shows a plateau (this means that the magnetization has reached its equilibrium value), and so we extract the value of m_{asyn} by computing the position of this plateau. For instance, we show in figure 5 the magnetization as a function of time for $\beta = 1.25$ and $L = 60$.

By computing the asymptotic value of the magnetization for different temperatures, we obtain a reliable estimate for the order parameter in the droplet theory. In table 1 we report these values for the droplet theory estimates and, in addition, we write the values for the order parameter obtained in the first part of this paper, which we will denote in the rest of the paper as $q_{EA}^{\text{dyn}}(\beta)$.

We recall that the values of $q_{EA}^{\text{dyn}}(\beta)$ reported in table 1 have small finite-size effects (taking into account their error bars) as checked in figure 3. Moreover, we have found strong discrepancies between $q_{EA}^{\text{dyn}}(\beta)$ and q_{EA}^{droplet} for small temperatures.

We will describe in the rest of the paper our results for the violation of FDT out of equilibrium.

In figure 6 we report the FD data out of equilibrium for one of the lowest temperatures simulated. We have shown a vertical band which marks our estimate of q_{EA}^{dyn} , a straight line

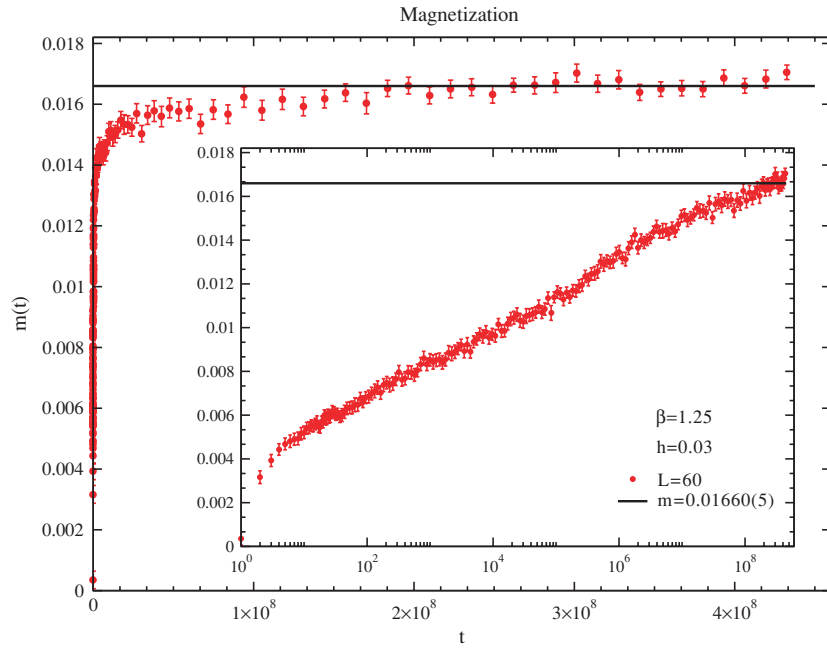


Figure 5. Magnetization as a function of time for $\beta = 1.25$, $L = 60$ and $h = 0.03$. We have plotted in the inset the main plot with logarithmic scale in the abscissas, in order to make sure we had found a plateau. We have marked in the main figure the plateau of the magnetization with a horizontal line.

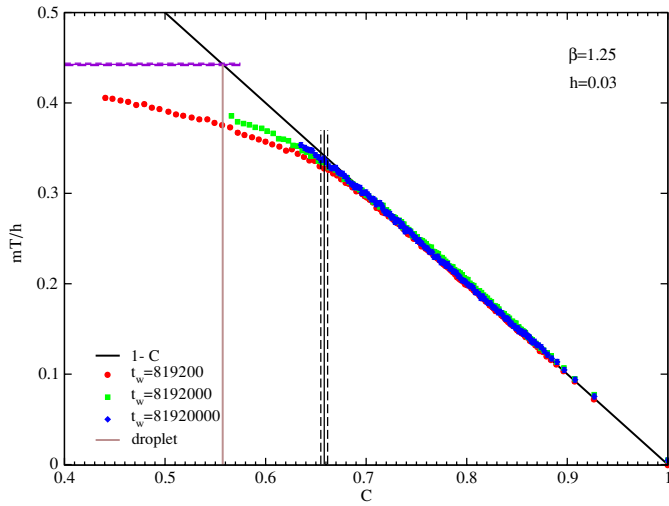


Figure 6. Fluctuation–dissipation curve out of equilibrium for one of the lowest temperatures simulated $\beta = 1.25$, $L = 60$ and three waiting times. We have marked using three vertical lines the interval in which lies q_{EA}^{dyn} for this β computed in the first part of the paper. In addition, we have marked with three horizontal lines the value and the statistical error for $m_{asyn}T/h$. Finally, we have marked a vertical line with the droplet theory prediction for q_{EA} (the left part of the plot).

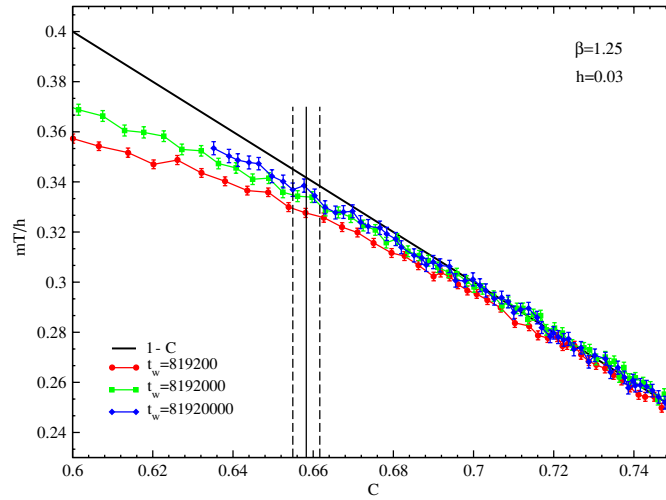


Figure 7. Magnification of figure 6 showing up the region in which the FD curves depart from the straight line $1 - C$. We have marked using three vertical lines the interval in which lies q_{EA}^{dyn} computed in the first part of the paper.

$1 - C$ to monitor the departure of this linear behaviour and a horizontal band which marks $m_{asyn}T/h$ (see figure 5). In addition, we have plotted data from three different waiting times.

Figure 6 shows that our estimate for q_{EA}^{dyn} matches very well in the plot and marks the region in which the FD data start to depart from the linear behaviour (for all the temperatures simulated). In figure 7 we have drawn a magnification of this region. In addition, in this figure one can see that the finite time effects in the building of the asymptotic curve are small. Practically, the two biggest waiting times are compatible in the error (there is a factor 10 in waiting time). With the current dedicated computers it is impossible to simulate larger waiting times. We can conclude from this figure that we are unable to see dependence in waiting time for the two largest waiting times in the region in which they depart from the linear behaviour. The dependence on the waiting time for larger times is smaller than our statistical errors. From our numerical data a droplet theory fluctuation–dissipation asymptotic curve seems unlikely.

6. Conclusions

We have studied numerically and out of equilibrium the three- dimensional Ising spin glass with bimodal disorder.

By computing the off equilibrium spin–spin correlation function we have been able to extract the order parameter of the phase transition. The study of the behaviour of this order parameter with temperature permits us to compute the critical temperature and the associated critical exponent: both figures compare very well with the previous numerical simulations and experiments. We have also discarded a XY -like scenario (we have found a non-vanishing order parameter in the low-temperature region). We have also monitored the dependence of $q_{EA}(\beta)$ with the lattice size in the low-temperature region for one β .

In the second part of the paper we have extracted the droplet prediction for the order parameter by computing the asymptotic value of the susceptibility (mT/h). The droplet

prediction compares (for all the β 's simulated) well with the order parameter computed in the first part of the paper for high temperature (of course, slightly below the critical temperature), but for lower temperatures the comparison is bad.

Moreover, the analysis (for larger waiting times) of the FD curves shows behaviour that can be described in the RSB theory and points out that the droplet scenario seems unlikely (only a really small dependence on waiting time, outside the precision of this work, could build a final FD curve compatible with the droplet theory). Moreover the point at which the numerical data depart from the linear behaviour compares well with the estimate obtaining in the first part of this paper, supporting the RSB scenario.

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