

Equilibrium and off-equilibrium simulations of the $4d$ Gaussian spin glass

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Abstract

In this paper we study the on and off-equilibrium properties of the four dimensional Gaussian spin glass.

In the static case we determine with more precision than in previous simulations both the critical temperature as well as the critical exponent.

In the off-equilibrium case we settle the general form of the autocorrelation function, and show that it is possible to obtain dynamically, for the first time, a value for the order parameter.

1 Introduction

Nowadays, the problem of the full characterization of the phase transition both from the static and dynamical approaches in finite dimensional spin glasses is still opened.

We center the present discussion in the four dimensional case (the same applies in the more physical case, the three dimensional system).

From the static simulations is very clear the cut of the Binder cumulant, clear signal of a phase transition at finite temperature with an order parameter (the Edward-Anderson order parameter, that we will denote hereafter as q_{EA}). We can identify this order parameter with the position of a Dirac delta in the probability distribution of the overlap, $P(q)$. Up to now, the SRSB theory (Spontaneous Replica Symmetry Breaking)[1, 2] and the droplet theory [3] are compatibles with this result. The differences begin with the rest of $P(q)$. In the droplet theory $P(q)$ is the sum of two Dirac deltas, one in q_{EA} and another in the opposite overlap: this distribution has a Binder cumulant equal to 1. The SRSB theory maintains this structure but adds a continuous part between $(-q_{EA}, q_{EA})$. This is a non trivial distribution and has a Binder cumulant different from 1, and goes to 1 as T goes to zero (the SRSB theory predicts two pure states like the droplet theory at $T = 0$).

The main problem is the impossibility of a direct measure of the order parameter, q_{EA} . From the scaling of the peak of $P(q)$ seems compatible a behaviour like Kosterlitz-Thouless (KT) transition, i.e. $q_{peak} \sim 1/L^\alpha$, but also is compatible a behaviour like $q_{peak} = q_{EA} + a/L^\rho$. Obviously the KT scenario goes against the cut of the Binder cumulant. The explanation of this phenomena could be that the term a/L^ρ is bigger than q_{EA} for the range of lattice sizes that has been simulated and then unobservable. The solution is to simulate bigger lattices in order to get $q_{EA} \gg a/L^\rho$.

The dynamical approach [4] have the same problematic that the just discussed static. The main object of this approach is the spin-spin autocorrelation, defined as:

$$C(t, t_w) = \frac{1}{N} \sum_{i=1}^N \overline{\langle \sigma_i(t_w) \sigma_i(t_w + t) \rangle} , \quad (1)$$

Usually in the literature [5] it finds the empirical formula

$$C(t, t_w) = t^{-x} f(t/t_w) , \quad (2)$$

for instance in the Mean Field case [6] and in the three dimensional case [7]¹.

The static limit (on equilibrium situation) is achieved send t_w to infinite, and then to simulate large t . With the formula (2) the spin-spin autocorrelation function goes to zero. But, in the case of a non zero order parameter, this autocorrelation function must go to q_{EA} . It is clear that a formula like

$$C(t, t_w) = (q_{EA}/f(0) + at^{-x})f(t/t_w) , \quad (3)$$

must be possible to find in the regime of $t_w \gg t \gg 1$, and again we need to do a very long numerical simulation to observe both the terms q_{EA} and at^{-x} . In the present work we show for the first time numerical evidence of this kind of behaviour.

¹Also in an on-equilibrium numerical simulation in the three dimensional case [8]: $C(t) \sim t^{-x}$.

Up to now, the only numerical studies of off-equilibrium dynamics in finite dimensional spin-glass are those of H. Rieger [7] in the three dimensional case.

The four dimensional case seems more easy to do: is far away from the lower critical dimension of the spin glasses ($d_l < 3$ [9, 10]) and so the static is very clear. In this paper we will study mainly the off-equilibrium dynamics of this model in order to compare with the three dimensional results by Rieger and to examine if it is possible to extract a finite value for the order parameter. In addition we have done static (on equilibrium) runs to characterize with higher precision the location of the critical temperature and the critical exponents.

In the off and on equilibrium cases we review the numerical results from the optics of the previous discussion and we will try to link both approaches in order to obtain a conclusion according with the existence of a finite temperature phase transition, with non zero order parameter.

2 Model, simulation and static observables

We have studied the 4- d Ising spin glass with nearest neighbor interactions and zero external magnetic field, whose Hamiltonian is

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j \quad , \quad (4)$$

where $\langle i, j \rangle$ denotes nearest neighbor pairs and the couplings are extracted from a Gaussian distribution with zero mean and unit variance.

The static and dynamical behaviour of the model have been investigated by several different simulations during which have been measured quite different observables. In this section will be analyzed the way we have measured the static exponents and the critical temperature with a precision higher than that present in the literature [11, 12].

The equilibrium simulations have been performed on small lattices ($L = 3, 4, 5, 6, 7, 8$) to ensure the system can reach equilibrium. The main work has been made in a range of temperature around the critical one, T_c . To take the mean over the disorder, we have simulated simultaneously 2048 samples for all the lattice sizes. For each realization of the quenched disorder we have simulated two replicas with spin σ_i and τ_i . This enable us to measure the k -th cumulant of the distribution of the overlaps, $q^{(k)} \equiv \int q^k P(q) dq$, simply by averaging the quantity $(N^{-1} \sum_i \sigma_i \tau_i)^k$ over a large number of independent configurations.

All the calculation have been carried on a *tower* of the parallel supercomputer APE100 [13], with a real performance of about 5 Gigafllops.

A detailed study has been performed to calculate the autocorrelation time at the equilibrium and consequently the sweeps needed to reach such equilibrium. At the conclusion of this study we have a termalization time of about 10^5 sweeps, been sure that using this value even the biggest system at the lowest temperature will be termalized. To verify the correctness of this value we have studied the biggest system ($L = 8$) at the lowest temperature ($T = 1.7$): we have choose three replicas of the system such that having, at the starting time, two overlaps set to zero and the third one equal to one; we have followed the evolution of these overlaps averaging over a large number of disorder configurations and

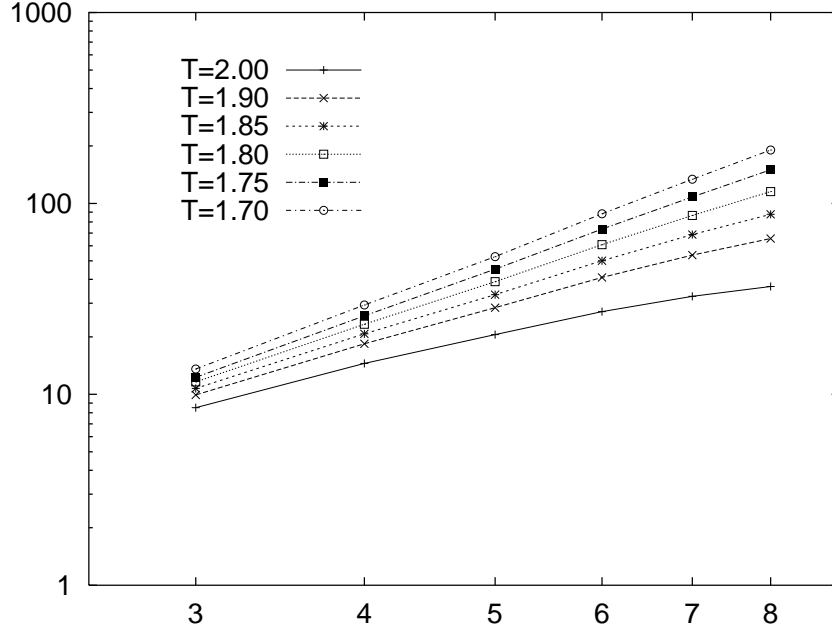


Figure 1: $\chi_{SG}(L, T)$ vs. L ; the errors are of the order of the symbol.

we have estimated the time needed in order that the three overlaps converge to a single value.

When the equilibrium has been reached, we have measured how much time is needed by the observables to decorrelate. In particular we have seen that the overlap between two replicas has a time correlation function that decreases exponentially, $C(t) \sim \exp(-t/\tau)$. This defines a characteristic time whose typical values at $T = 1.7$ are: for $L = 4$ $\tau \sim 200$, for $L = 6$ $\tau \sim 1000$ and for $L = 8$ $\tau \sim 3000$. Once we have thermalized the system, we measured every τ sweeps the overlap between the two replicas for a time longer than the equilibration one.

Defining the spin glass susceptibility as

$$\chi_{SG}(L, T) = \frac{1}{N} \sum_{i,j} \overline{\langle \sigma_i \sigma_j \rangle^2} = N q_L^{(2)} \quad , \quad (5)$$

where $N = L^4$, $\langle (\dots) \rangle$ is the thermodynamical average and $\overline{(\dots)}$ the mean over the disorder; and the Binder parameter as

$$g(L, T) = \frac{1}{2} \left(3 - \frac{q_L^{(4)}}{(q_L^{(2)})^2} \right) \quad , \quad (6)$$

the results of our simulations are plotted in fig.1 for the spin glass susceptibility and fig.2 for the Binder cumulant.

The errors on the plotted data are derived from a jackknife analysis, which also confirms that the overlaps measured every τ sweeps are decorrelated. Using finite size scaling we

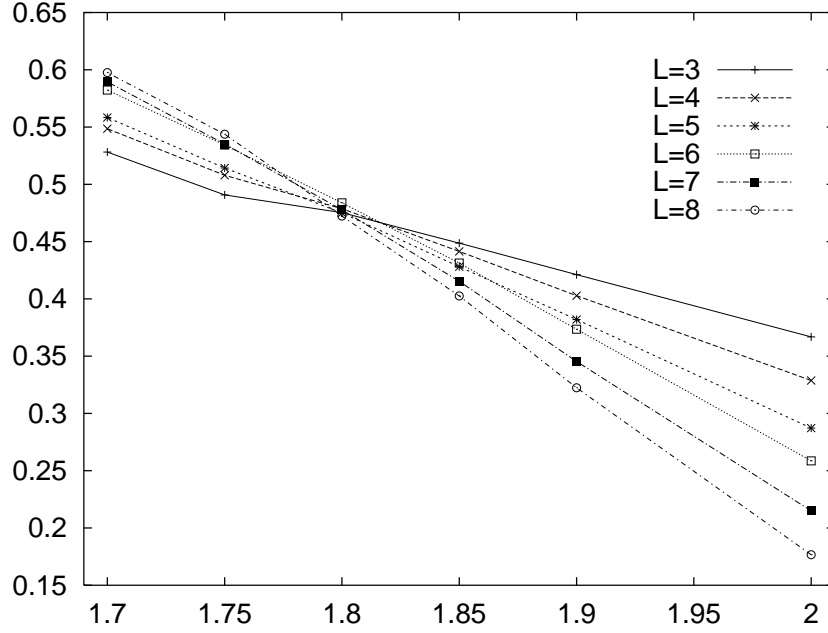


Figure 2: $g(L, T)$ against T ; the errors are of the order of the symbol.

see that $\chi_{SG}(L, T)$ and $g(L, T)$ scale as (in the scaling region)

$$\chi_{SG}(L, T) = L^{2-\eta} \tilde{\chi}_{SG}(L^{1/\nu}(T - T_c)) \quad , \quad (7)$$

$$g(L, T) = \tilde{g}(L^{1/\nu}(T - T_c)) \quad . \quad (8)$$

Note that at the critical temperature the Binder parameter does not depend on the size of the system, so T_c is the temperature where the curves of fig.2 cross themselves.

In the neighborhood of T_c we can approximate the function \tilde{g} with a linear one and so we obtain the following critical temperature and ν exponent

$$T_c = 1.80 \pm 0.01 \quad , \quad (9)$$

$$\nu = 0.9 \pm 0.1 \quad . \quad (10)$$

The value of ν is confirmed also by the results of the analysis done, following [14], on the quantity

$$\left. \frac{dg}{dT} \right|_{T_0: g(T_0)=g_0} = \alpha L^{1/\nu} \quad , \quad (11)$$

obtaining

$$\nu = 1.06 \pm 0.06 \quad . \quad (12)$$

The prediction about the infinite volume limit of the Binder cumulant is different in the droplet theory ($g(L, T < T_c) \xrightarrow{L \rightarrow \infty} 1$) and in the SRSB picture ($g(L, T < T_c) \xrightarrow{L \rightarrow \infty} \bar{g}(T) < 1$). Unfortunately with our data ($L = 3$ to $L = 8$) is impossible to extrapolate the infinite value with a precision such that to discriminate between the two predictions.

The estimation of the anomalous dimension η can be done fitting the χ_{SG} data at $T = T_c$ with a power law

$$\chi_{SG}(L, T = T_c) \propto L^{2-\eta} \quad , \quad (13)$$

finding $\eta = -0.35 \pm 0.05$ (the error is almost all due to the indetermination on the critical temperature and to the rapid variation in the region around T_c of the exponent in eq.(13)). These results are in agreement with those found by Bhatt and Young in [11] using a maximum size of 6^4 and 200-800 samples: $T_c = 1.75 \pm 0.05$, $\nu = 0.8 \pm 0.15$ and $\eta = -0.3 \pm 0.15$

Using the scaling law $\gamma = \nu(2 - \eta)$ and the exponents values just calculated, we have $\gamma = 2.1 \pm 0.2$, which is in good agreement with the value obtained by the high temperature expansions $\gamma = 2.0 \pm 0.4$, [15].

By another series of computer runs and using the annealing procedure [16] we have measured the non connected susceptibility for a wide range of temperature in the spin glass phase ($T < T_c$). We clearly see that the data diverge with the increasing of the system size, but, cause the small lattices, we find that they can be fitted via different scaling functions: either by

$$\chi_{SG}(L, T) = A(T)L^4 \left[1 + B(T)L^{-\Lambda(T)} \right] \quad , \quad (14)$$

or by

$$\chi_{SG}(L, T) \propto L^{2-\eta(T)} \quad . \quad (15)$$

In this way we also obtain a further confirmation of the value of T_c , as the higher temperature where the power law fit is yet acceptable (by a χ^2 test).

3 Off-equilibrium dynamics

In the second part of our study we have simulated systems of greater dimensions (from 8^4 to 32×16^3). At the beginning of every simulation the system is frozen from an infinite temperature to one in the critical region, and then we immediately start to measure the autocorrelation functions, when the system is yet out of equilibrium. Due to the hughes thermalization times of the simulated systems, the off-equilibrium dynamics is the most realistic situation and also the most interesting. In fact, thanks to the enormous number of metastable states, the dynamics is very slow and besides it is reminiscent of the time passed in the spin glass phase, that we will call t_w . These effects can be clearly seen by the study of the autocorrelation functions defined as

$$C(t, t_w) = \frac{1}{N} \sum_{i=1}^N \overline{\langle \sigma_i(t_w) \sigma_i(t_w + t) \rangle} \quad , \quad (16)$$

where $\overline{(\cdot)}$ is the mean over the disorder and $\langle (\cdot) \rangle$ stands not for an average over the equilibrium thermodynamic state, cause we are not at the equilibrium, but for an average over the thermal histories. Nevertheless we have found that, for the system sizes we have considered, disorder fluctuations are always stronger, so generally we omit the angular brackets.

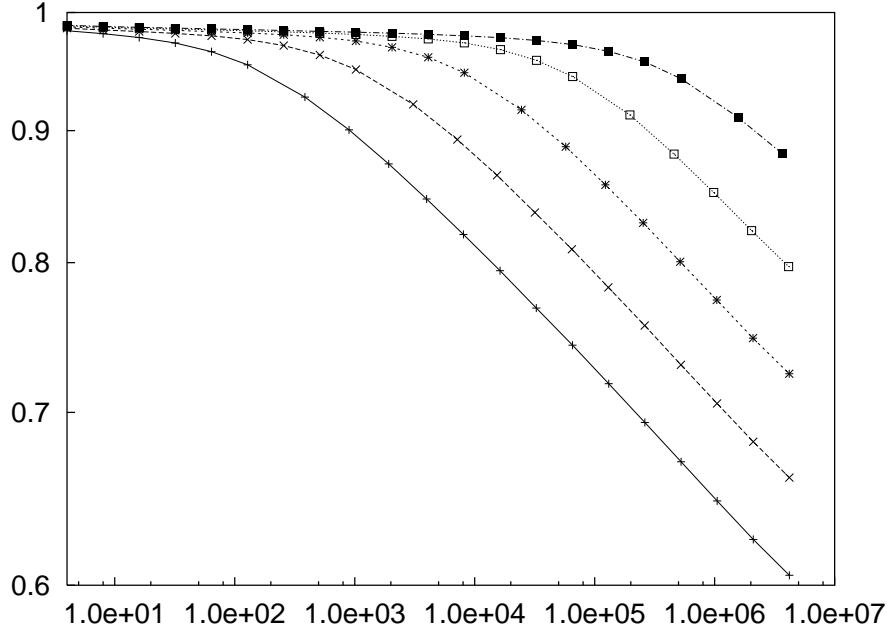


Figure 3: $C(t, t_w)$ vs. t at $T = 0.2$ with $t_w = 2^7, 2^{10}, 2^{13}, 2^{16}, 2^{19}$ (bottom to top).

With our simulations we have analyzed the cold phase (from $T = T_c = 1.8$ down to $T = 0.2$) using the set of waiting times $t_w = 2^k$ with $k = 7, 8, \dots, 21$ and averaging over 3072 disorder realizations systems of volumes from 8^4 to 12^4 .

In the four-dimensional Ising spin glass the presence of a critical temperature and the subsequent spin glass phase has been widely accepted, so the principal question that remain to answer is which kind of phase space arises for $T < T_c$. In the literature there are principally two theories that try to describe the spin glass systems in their low temperature phase: one is based on a mean field like approximation which predicts a spontaneous replica symmetry breaking (SRSB picture) and the other that starting from a Migdal-Kadanoff renormalization group technique concludes that the system remain trivial, with only one pure state (droplet model). The predictions of the two theories about the autocorrelation function are different: the SRSB picture says that in the limit of $t_w \rightarrow \infty$ it must be a power law that converge to the Edward-Anderson parameter (q_{EA})

$$C(t, t_w) = (q_{EA} + at^{-x}) \frac{f(t/t_w)}{f(0)} , \quad (17)$$

while in the droplet model the relaxation is slower

$$C(t, t_w) = (\log t)^{-\theta/\psi} C' \left(\frac{\log(t/\tau)}{\log(t_w/\tau)} \right) . \quad (18)$$

The data we are collect (see fig.3 and fig.4) seem to follow well the scaling law used in [7] and in [6]

$$C(t, t_w) = t^{-x'(T)} \tilde{C}(t/t_w) , \quad (19)$$

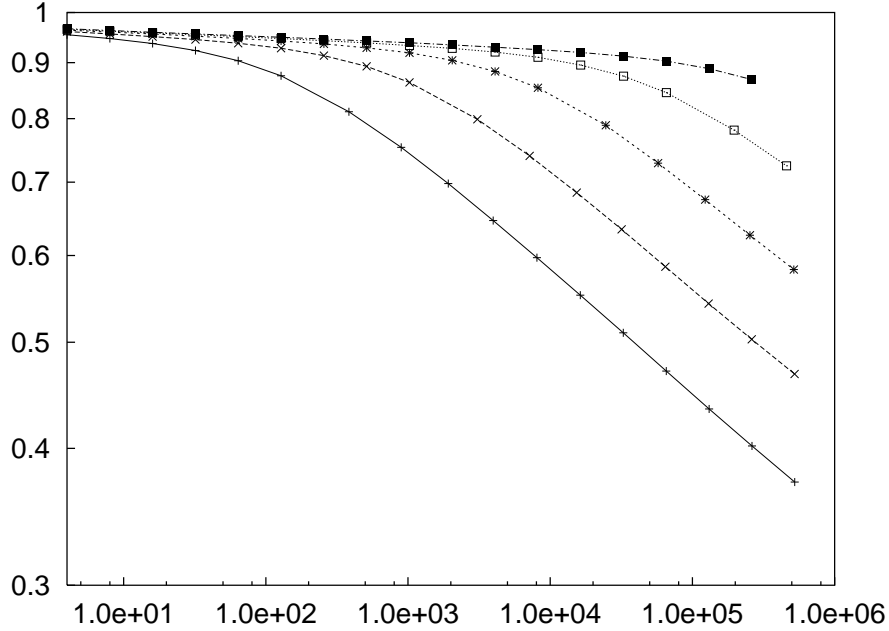


Figure 4: $C(t, t_w)$ vs. t at $T = 0.45$ with $t_w = 2^7, 2^{10}, 2^{13}, 2^{16}, 2^{19}$ (bottom to top).

with a scaling function

$$\tilde{C}(z) = \begin{cases} \text{constant} & \text{for } z \rightarrow 0 \\ z^{x'(T)-\lambda(T)} & \text{for } z \rightarrow \infty \end{cases} \quad (20)$$

The values of the exponent $x'(T)$ will be plotted together with the values of $x(T)$ in fig.9, while $\lambda(T)$ is plotted in fig.7 .

To evaluate the goodness of the two proposed scaling formulas eq.(19) and eq.(18) we have plotted in fig.5 the $T = 0.45$ data rescaled following the former law, noting that they collapse very well on a single curve. On the contrary, following the droplet model scaling law, it was impossible for us to find a value for the parameters θ/ψ and τ such to force the data over a single curve; in fig.6 we show the best scalings we could obtain in order to make the data collapsing in the $t < t_w$ or in the $t > t_w$ region.

Nevertheless the very good rescaling of the data in fig.5 we have performed a deeper analysis to find the value of the Edward-Anderson parameter, q_{EA} , which is assumed to be zero in eq.(19). The value of q_{EA} can be found performing the $t \rightarrow \infty$ limit *after* the $t_w \rightarrow \infty$ limit; for this purpose we have done very long simulations (more than 4 millions Monte Carlo sweeps). We note that the scaling laws followed by the data in the two regions $t \gg t_w$ and $t \ll t_w$ are essentially different. In the former the data can be well fitted by a power law of the ratio t/t_w , while in the latter we obtain a law equal to that of eq.(17) times a function of t/t_w which is almost a constant.

Such a behaviour for $C(t, t_w)$ can be justified supposing that the system evolves as long as $t \ll t_w$ with a quasi equilibrium dynamics which converges to q_{EA} while for $t \gg t_w$ it decorrelates faster and toward zero ($C \sim t^{-\lambda}$ with $\lambda(T) \gg x(T) \forall T$), but always with a critical slowing-down.

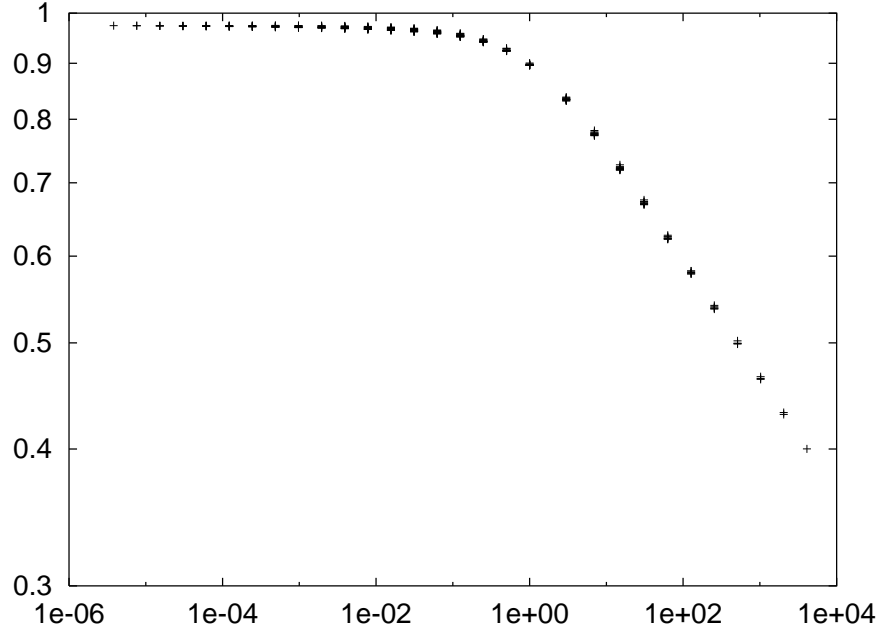


Figure 5: $T = 0.45$ aging autocorrelation function rescaled following eq.(19), with $x = 0.0054$. We plot $t^x C(t, t_w)$ against t/t_w .

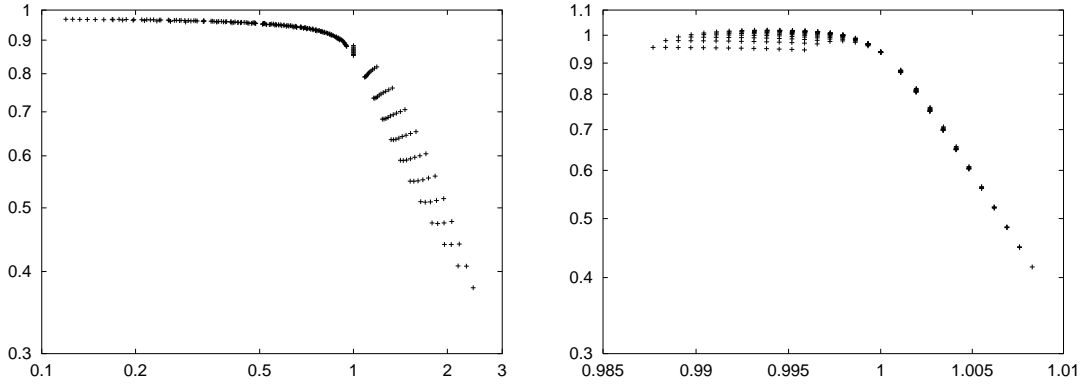


Figure 6: Tentatives of rescaling following the droplet model law eq.(18): in the left plot $\theta/\psi = 0.0054$ and $\log(\tau) = -1$; in the right plot $\theta/\psi = 0.043$ and $\log(\tau) = -1000$.

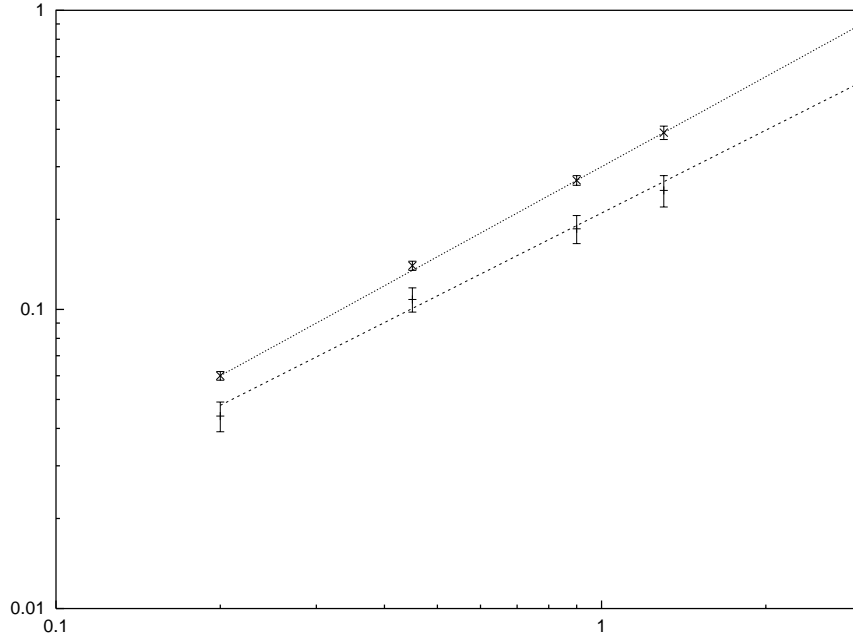


Figure 7: $\lambda_{t_w=0}(T)$ (top) and $\lambda_{t_w \neq 0}(T)$ (bottom) against T ; the lower line represents the power fit $\lambda(T) = 0.21(1) T^{0.92(7)}$; the upper line both the linear and the power fit: respectively $\lambda(T) = 0.000(3) + 0.30(1) T$ and $\lambda(T) = 0.303(8) T^{1.00(3)}$.

The values for $\lambda(T)$ have been obtained fitting the $C(t, t_w = 0)$ data with a power law and for $t_w \neq 0$ with

$$C(t, t_w) \propto \left(\frac{t}{t_w} \right)^{-\lambda(T)}, \quad (21)$$

in the range $t/t_w \geq 15$. In fig.7 we plot the results either for $t_w = 0$ and for $t_w \neq 0$. We note that both the fits are compatible with the linear dependence in the temperature predicted from the experimental measurements [17].

In the region $t_w/t \geq 32$ we have performed the analysis assuming that the correlation function could be factorized as

$$C(t, t_w) = (q_{EA} + at^{-x}) \overline{C}(t/t_w), \quad (22)$$

where we have approximated $\overline{C}(z) = 1 - c_1 z^{c_2}$ for $z \rightarrow 0$. In a first step has been calculated the rescaling function $\overline{C}(t/t_w)$ fitting the correlation function at a fixed value of t . Secondly, divided the data by this rescaling function, we have verified that the curves for different ratios t/t_w collapse over a single curve and we interpolate the data via a power law plus constant, following eq.(17). In fig.8 we plot in a log-log scale typical $C(t, t_w)/\overline{C}(t/t_w)$ data with the best fit; we note that until today this data have been fitted via a simple power law, while it is evident that the points in fig.8 are not on a straight line.

From the just described fit we obtain the values of q_{EA} and x as a function of the temperature (see fig.9 and fig.10). As a guide to the eye we plot in fig.10 the simpler

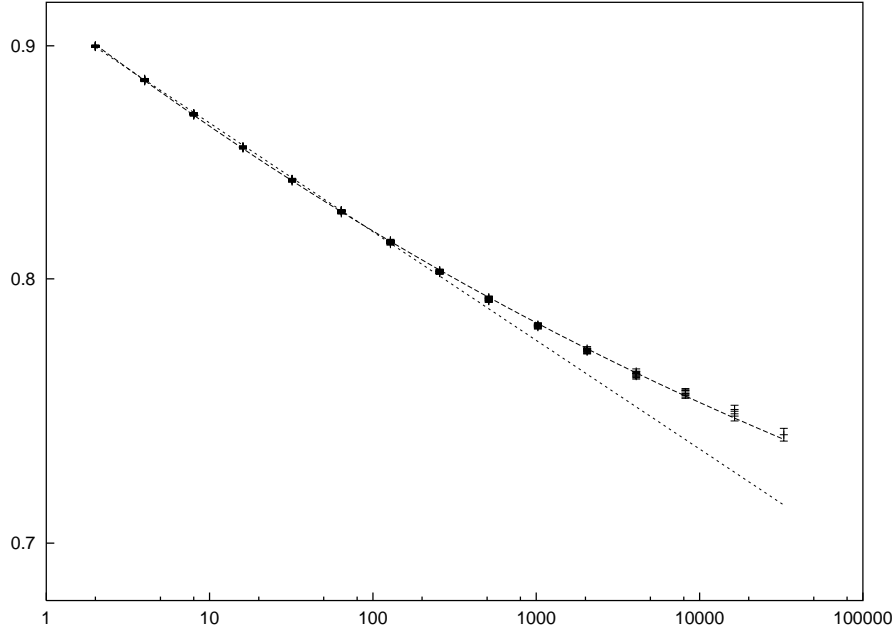


Figure 8: $\frac{C(t, t_w)}{\bar{C}(t/t_w)}$ data at $T = 0.9$ versus t ; the upper line is the best power plus constant fit: $0.60(4) + 0.32(4)t^{-0.08(1)}$, while the lower line is the best power fit.

function that behaves like $|T - T_c|^\beta$ near the critical temperature and tends to 1 for $T = 0$

$$q_{EA}(T) = \left(\frac{T_c - T}{T_c}\right)^\beta, \quad (23)$$

where $T_c = 1.8$ and $\beta = \frac{\nu}{2}(d - 2 + \eta) = 0.74$ (using the values found in the previous section). From fig.9 we note that only the quantity $x(T)$, not $x'(T)$, is such that $x(T)/T$ is roughly independent from the temperature, so that only in this parametrization the $t_w = \infty$ autocorrelation function ($R(t; T) = C(t, t_w = \infty)$ at temperature T) can be written as

$$R(t; T) - R(\infty; T) = b(T) \exp(-BT \log(t)) . \quad (24)$$

The relevance of the variable $T \log(t)$ has been observed in experiments on magnetic remanence in a wide region [17].

We call off-equilibrium correlation length, $\xi(t)$, the typical distance over which the system is thermalized after a time t . For this domain growth the SRSB picture predicts a power law [9]

$$\xi(t) \propto t^{1/z(T)}, \quad (25)$$

while in the droplet model, where the energy barriers scales proportional to L^ψ , the law is

$$\xi(t) \propto (T \log t)^{1/\psi} . \quad (26)$$

At least at the critical temperature there is a scaling relationship between the dynamical exponent $z(T_c)$ and the one which describe the dynamics in the quasi equilibrium regime,

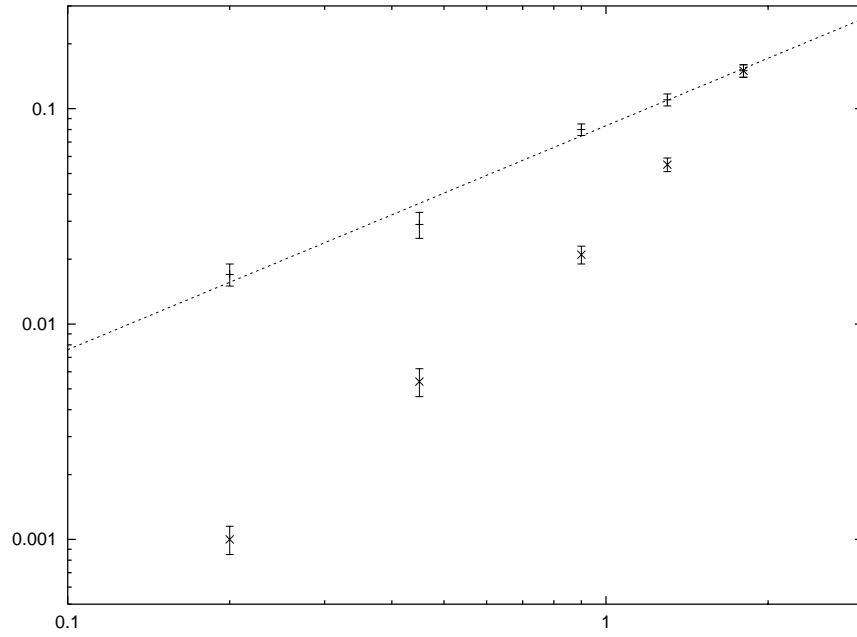


Figure 9: $x(T)$ (top) and $x'(T)$ (bottom) against T (the value at the greater temperature is equal: $x(T_c) = x'(T_c)$); the line is best power fit $x(T) = 0.083(3) T^{1.04(7)}$.

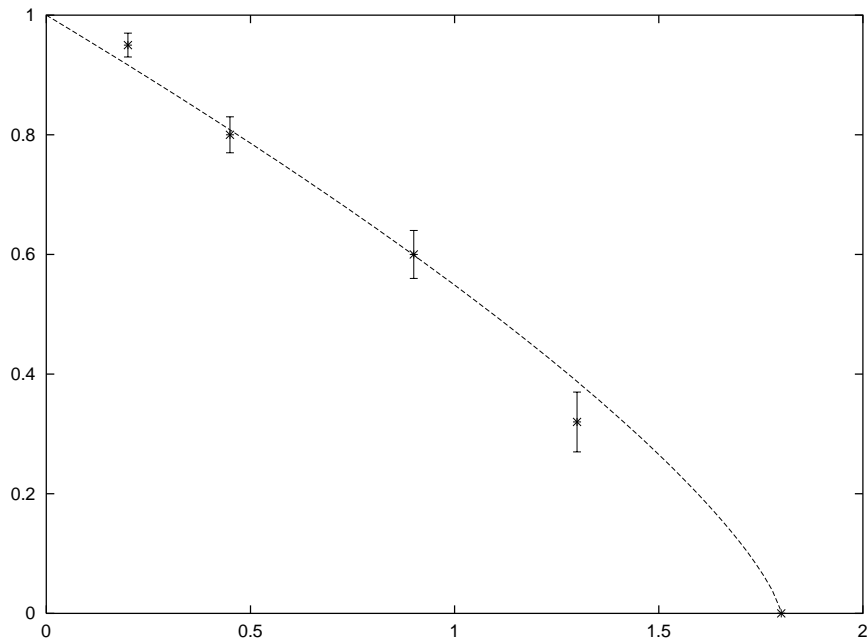


Figure 10: Edward-Anderson order parameter against T ; the line is only a guide to the eye as explained in the text.

$x(T_c) = x'(T_c)$ (because $q_{EA}(T = T_c) = 0$)

$$x = \frac{d - 2 + \eta}{2z} . \quad (27)$$

This equation is satisfied by all the exponents we have estimated at the critical temperature: $x = 0.15$, $\eta = -0.35$ and $z = 5.3$.

To find the behaviour of the off-equilibrium correlation length we have measured, like in [9], the equal time spatial correlation functions

$$G(r, t) = \frac{1}{N} \sum_{i=1}^N \overline{\langle \sigma_i(t) \sigma_{i+r}(t) \rangle^2} , \quad (28)$$

where the averages are the same as in eq.(16) and t is the time since the cooling. This study has been performed on systems of volume 32×16^3 .

From scaling concepts we know that, at large values of r , $G(r, t)$ must behave like

$$G(r, t) \propto r^{-(d-2+\eta)} f\left(\frac{r}{\xi(t)}\right) , \quad (29)$$

and, supposing $f(y) = A \exp(-By^D)$, we have fitted our data with the function

$$G(r, t) = Ar^{-(2+\eta)} \exp\left[-B(rt^{1/z})^D\right] . \quad (30)$$

In the $t \rightarrow \infty$ limit the exponential term tends to 1 and we obtain a spatial correlation function that decrease with a power law: in fig.11 we plot such function at the critical temperature ($T_c = 1.8$). Note that from the slope of the curve we obtain an estimation of the η exponent compatible with that of section 2.

At the lower temperatures the value of η depends strongly on the r range we interpolate over, cause the fitting function diverges at $r = 0$. On the contrary, trying to fit the data in different ranges of r , we find that the dynamical exponent $z(T)$ is a robust parameter which remains unchanged for every r range (plotted in fig.12)

Fitting the plotted data with a power law we obtain, up to the critical temperature

$$z(T) = A T^{-\alpha} , \quad (31)$$

with $A = 9.7 \pm 0.5$ and $\alpha = 1.0 \pm 0.1$.

A preliminar analysis of a new set of data at $T = 0.9 = T_c/2$ suggests a value of $\eta \simeq -1$ with a large error. The fact that the value of z at this temperature is higher than the correspondent value at T_c makes the evaluation of the exponent η proner to systematic error. Nevertheless this rough estimation of η is compatible with the prediction of the reference [18].

4 Conclusions

In this paper we have studied the on and off-equilibrium properties of the four dimensional Gaussian spin glass.

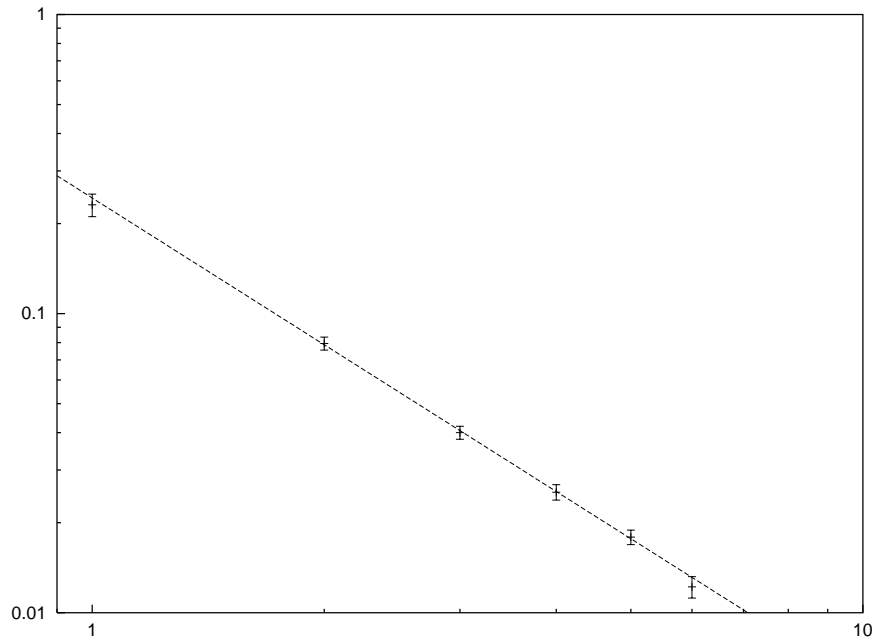


Figure 11: $G(r, t = \infty)$ vs. r at $T = T_c = 1.8$; the line is the power fit $0.24(1) r^{-1.63(5)}$.

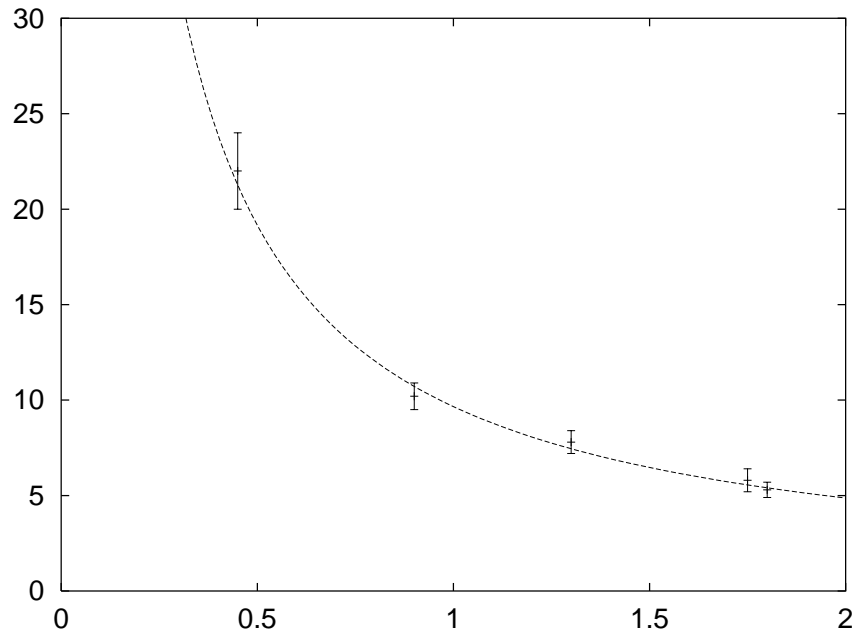


Figure 12: $z(T)$ vs. T ; the line is the power fit, eq.(31).

In the static case we have determined with more precision than in previous simulations both the critical temperature as well as the critical exponent.

In the off-equilibrium case we have settled the general form of the autocorrelation function, and shown that it is possible to obtain dynamically, for the first time, a value for the order parameter. We have plotted this value as a function of the temperature. Also we have established the temperature dependence of the exponents that appear in this off-equilibrium dynamics, linear in all the cases.

An open problem leaves the estimation, using the static spin glass susceptibility, of the order parameter simulating much more large lattices. We plan to study in the future this problem.

5 Acknowledgments

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