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On the 3D Ising spin glass

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Abstract. We study the 3D Ising spin glass with ± 1 couplings. We use a Hamiltonian with second and third nearest-neighbour interaction. We use finite-size scaling techniques and very large lattice simulations. We find that our data can be described equally well by a finite-T transition or by a $T = 0$ singularity of an unusual type.

1. Introduction

Three-dimensional spin glasses [1, 2] are a fascinating subject. Numerical simulations here are particularly interesting [3–9], since for such models (the real thing) it is very difficult to obtain reliable analytical results (see, however, [10]). Up to now numerical simulations for the Ising case have been shown to have a phenomenology very similar to the experiments on real spin glasses (for recent simulations and analytical results about, for example, *aging* phenomena, see [11]). The study of small-size systems (up to a linear size $L = 14$) has shown a reasonable agreement with the predictions of broken replica theory, but it is not clear how much information about the thermodynamic limit can be inferred from the behaviour of small systems. In particular one has to be careful about extrapolating the pattern of replica symmetry breaking from small to large lattices. Here our aim has been to reconsider the whole subject and try to clarify the emerging physical picture at low temperature T.

We will deal with the problem of the nature and the existence of a phase transition. A cursory look at the history of the subject is useful. If we look at the period that begins when people first investigated the subject of disordered spin systems we can easily establish that there have been periodic oscillations, with periods of the order of seven years. Researchers in the field have been oscillating between the credence that there is a sharp transition and the belief that there are no transitions at all (as is maybe true in real glasses) and that when lowering T there is only a gradual freezing of the dynamical degrees of freedom. At the beginning, theoreticians had (at the same time) a different credence from the experimental researchers. The two groups had a different frequency of oscillation, and now there is consensus that the system undergoes some kind of phase transition.

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We have run long numerical simulations at various temperatures, doing our best to distinguish between these two possibilities. In our analysis we have been very much inspired by the approach and the doubts of Bhatt, Morgenstern, Ogielsky and Young [3–6, 8, 9], and we have tried to build on and improve their results. We have found that the whole set of our data is closely compatible with the possibility that there is a transition at a given non-zero T. Such a transition would be characterized by a large value of the exponent γ, close to 2.5 (γ is the usual susceptibility exponent, which will be defined later in a more precise way). The whole set of data is also compatible with a large set of possible reasonable functional dependencies, which imply a transition temperature of zero. Recent studies using improved Monte Carlo techniques [12–14] also find that doubts about the existence of a finite-T critical behaviour are justified—see [15] and references therein. The difficulty of resolving between the two behaviours is because a large value of γ implies that the system is not far from being at its lower critical dimension (at which, according to the conventional wisdom, $\gamma \to \infty$). The distinction between a system at the critical dimension and a system very close to it is particularly difficult to make. We believe, however, that we are not too far from being able to distinguish between the two models, and that an increase in the simulation time of one or two orders of magnitude could clarify the situation. Of course, precise theoretical predictions on the behaviour of spin glasses at the lower critical dimension would be invaluable.

We have studied the 3D Ising spin glass, with ± 1 couplings, but have not used the standard first-neighbour model. Hoping for some gain, we have simulated a slightly modified model with second- and third-nearest coupling. The reason for introducing this model is that in the conventional model (on the usual cubic lattice) the interesting pseudo-critical region is at very low temperatures. In this region sensible numerical simulations are extremely demanding on computer time, due to the extreme difficulty in crossing even small barriers. We also believe that a systematic comparison of results obtained with different Hamiltonians may be useful in finding out those universal features that are independent of the detailed form of the Hamiltonian.

In section 2 we define the model we use and the quantities we measure. In section 3 we present the results obtained by using finite-size scaling on small lattices (from 4^3 to 14^3), while in section 4 we present the results obtained on a large lattice $64^2 \times 128$. Finally, in section 5 we present our conclusions.

2. The model and the observable physical quantities

We consider a three-dimensional Ising spin glass model on a body-centred cubic lattice. In this model, the lattice sites are labelled by an integer valued three-dimensional vector i. The spins are defined on each lattice point and take the values -1 or 1.

The Hamiltonian of the model (with couplings $J_{i,k}$ that can take the three values 0 and ± 1) is

$$H[\sigma] \equiv -\tfrac{1}{2} \sum_{i,k} J_{i,k} \sigma_i \sigma_k. \tag{1}$$

The couplings J may be zero or take randomly a value ± 1. In the simplest version of the model $J_{i,k}$ is different from zero if and only if

$$|i-k| \equiv \left((i_x-k_x)^2+(i_y-k_y)^2+(i_z-k_z)^2\right)^{1/2} \leqslant r. \tag{2}$$

Different models may be obtained by changing the value of r. In the limit $r \to \infty$ we recover the infinite-range SK model, while for $r = 1$ we have the usual short-range nearest-neighbour model. In this paper we will discuss the model with $r = 3^{1/2}$, which corresponds to having $J \neq 0$ when all the following three conditions are satisfied

$$|i_x - k_x| \leqslant 1 \qquad |i_y - k_y| \leqslant 1 \qquad |i_z - k_z| \leqslant 1 \tag{3}$$

and $|i - k| \neq 0$. A crucial parameter in the model is the effective coordination number z, which is the number of spins that interact with a given spin (for $r = 1$, $z = 6$ and for $r = 3^{1/2}$, $z = 26$). For large values of z the energy is proportional to $z^{1/2}$. On a Bethe lattice (which is a refined mean-field approximation) the critical temperature may be computed exactly [16], and one finds that

$$(z - 1)\tanh(\beta_{\mathrm{Bethe}})^2 = 1. \tag{4}$$

In this approximation one finds $T_{\mathrm{Bethe}}^{(z=6)} = 2.08$ and $T_{\mathrm{Bethe}}^{(z=26)} = 4.93$. One difficulty with the original $r = 1$ model is that the hypothetical critical temperature is small (about 1.1). Since under a single spin-flip the minimum change of the energy is 4, such a low value of the critical temperature implies a very small acceptance rate (about 2%) for Monte Carlo steps in which we try to change the energy. This effect should disappear for the $r = 3^{1/2}$ theory. Moreover, a different form of the lattice action may be useful to disentangle the lattice artifacts from the universal behaviour.

In the particular case of the 3D Ising spin glass a large value of z should increase the system similarity to the infinite-range model. In a system at the lower critical dimension for high values of z we should see a sharp change of behaviour from the predictions of the mean-field theory to the asymptotic low-energy behaviour.

In order to define interesting observable quantities it is convenient to consider two replicas of the same system (σ and τ). The total Hamiltonian reads

$$H = H[\sigma] + H[\tau]. \tag{5}$$

For the two replica systems we can define the *overlap*

$$q_i \equiv \sigma_i \tau_i \tag{6}$$

which will play a crucial role in our analysis. We introduce the correlation function of two q's as

$$G(i) \equiv \sum_k \langle q_{i+k} q_k \rangle = \sum_k \langle \sigma_{i+k}\sigma_k \rangle \langle \tau_{i+k}\tau_k \rangle = \sum_k \langle \sigma_{i+k}\sigma_k \rangle^2. \tag{7}$$

We can use this correlation function to define a correlation length. From high-temperature diagram analysis (or from the field theoretical approach) we expect that for large separation

$$G(i) \sim \frac{\mathrm{e}^{-|i|/\xi}}{|i|}. \tag{8}$$

We can define an *effective mass* as

$$m(i) \equiv \log\left(\frac{iG(i)}{(i+1)G(i+1)}\right). \tag{9}$$

We expect that at large i

$$\xi^{-1} = \lim_{i\to\infty} m(i). \tag{10}$$

In our numerical simulations we have not measured the full $G(i)$. We have measured the zero two-momentum Green functions

$$G^{(0)}(d) = \frac{1}{L_x \times L_y} \sum_{x-y \text{ plane}} G(i) \tag{11}$$

where d now runs only in one lattice direction. We will label with a superscript $^{(0)}$ this kind of quantity. We have also measured the site–site correlation function, but only summing over contributions where one single coordinate changes (by swapping the lattice in a single chosen direction). Here the coordinate increment has the form $(x, 0, 0)$. We will denote quantities defined in this way with a superscript $^{(1)}$.

In a similar way, in a finite volume we can introduce the quantity

$$q \equiv \frac{1}{V} \sum_i q_i. \tag{12}$$

In the infinite-volume limit the *spin glass susceptibility* is defined as

$$\chi_0 \equiv \lim_{V\to\infty} V\overline{\langle q^2\rangle} \tag{13}$$

where the upper bar denotes the average over the different choices for the disorder.

We expect the spin glass susceptibility and the correlation length to diverge at the critical temperatures with critical exponents γ and ν, respectively. Below the critical temperature in the mean-field approach χ_0 is proportional to the volume. More generally in the broken replica approach one finds that

$$\lim_{V\to\infty} V\langle q^m\rangle = \int_0^1 \mathrm{d}x\, q(x)^m \tag{14}$$

where $q(x)$ is the order parameter function defined in [1].

In the high-temperature phase no interesting physical predictions can be obtained for the usual magnetic susceptibility (divided by β) defined as

$$\chi \equiv \lim_{V\to\infty} V\overline{\langle m^2\rangle} \tag{15}$$

m being the total instantaneous magnetization ($m \equiv (1/V)\sum_i \sigma_i$). Gauge invariance implies that at thermal equilibrium

$$\chi = 1. \tag{16}$$

At $T < T_c$ this equality is valid after summing over all configurations with the correct Boltzmann weight. If we restrict the sum only to configurations in a given equilibrium state this identity does not apply.

3. Finite size scaling

We will discuss here results obtained on small lattice sizes, in situations where typically $L \gg \xi$. Since our goal is to establish or disprove the existence of a critical behaviour for $T > 0$ let us start by sketching the predictions of a finite-size scaling analysis. If scaling is satisfied in the vicinity of a critical point (at $T > 0$), we expect

$$\chi_0 \sim L^{2-\eta} f(L/\xi) \tag{17}$$

where η is the anomalous dimensions of the operator q defined in (12) and ξ is the correlation length that is expected to diverge at the critical temperature. Moreover, to establish the existence of a finite critical temperature it is useful to use the Binder parameter to locate the transition point, it is defined by

$$g(T) = \tfrac{1}{2}\big(3 - \overline{\langle q^4\rangle}/(\overline{\langle q^2\rangle})^2\big). \tag{18}$$

If a finite-T phase transition exists we expect the curves $g(T)$ obtained for different lattice sizes to cross (asymptotically for large enough lattices) at T_c. This is quite a precise method of finding the location of a critical point. For a $T = 0$ singularity the same curves will merge into a single curve as $T \to 0^+$. We will see that the possibility that the exponent ν characterizing the divergence of the correlation length is greater than one makes it arduous to distinguish between these two cases.

As we have already discussed, we want to distinguish between two different scenarios. In one case there is a finite temperature transition and the correlation length diverges like $\xi \sim (T - T_c)^{-\nu}$. In our finite-size scaling analysis we will use the large lattice best fit to T_c, γ and ν from section 4. If a transition exists we have a precise determination of the critical exponents and parameters.

We should note here that if three is the lower critical dimension and we have a $T = 0$ singularity, it is not clear that the scaling relation (17) is satisfied. As we will discuss, our results suggest that if the scenario of a $T = 0$ phase transition holds such scaling behaviour could not hold. This violation of scaling appears in the Heisenberg model in two dimensions and is a consequence of the existence of the Goldstone modes. In the $O(N)$ symmetric Heisenberg model for $N > 2$ the correct scaling laws contain an effective exponent

$$\chi_0 \sim L^{2-\eta(L/\xi)} f(L/\xi) \tag{19}$$

where $\eta(0) = 0$. The dependence of the exponent on L/ξ is due to the instability of the $T = 0$ fixed point. In the $N = 2$ case, there is no renormalization of the coupling constant (i.e. of the temperature). In the low-temperature phase one finds the simpler equation

$$\chi_0 \sim L^{2-\eta(T)} f(L/\xi) \tag{20}$$

where the function $\eta(T)$ is not a universal function. Its value at the transition point, i.e. $\eta(T_c)$, is universal and it is equal to $\frac{1}{4}$.

We have simulated lattices with linear size $L = 4, 6, 8, 10, 12$ from $T = 5.4$ down to the lowest temperature at which we were sure to have thermalized ($T = 2.6$ for $L = 4$ and $T = 3.6$ for $L = 12$). We have computed the overlap between two identical copies of the system, defined in (12).

We have been careful to check that we have really reached thermal equilibrium. We have used as a basic criterion the condition that $\langle q\rangle$ was compatible with zero for each sample.

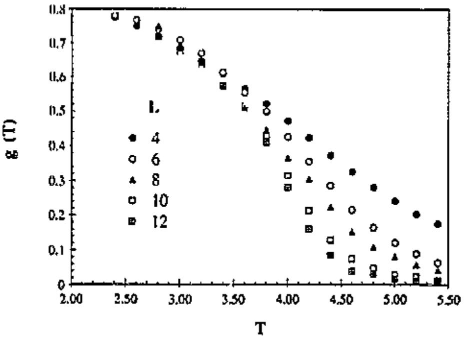

Figure 1. The Binder parameter $g(T)$ as a function of the temperature T for different lattice sizes.

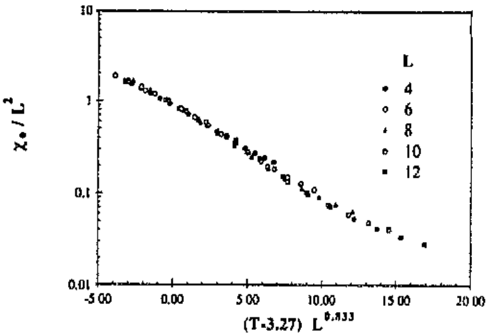

Figure 2. The scaled overlap susceptibility χ_0/L^2 plotted against the scaled reduced critical temperature $(T - T_c)\, L^{1/\nu}$.

We show in figure 1 the Binder parameter defined in (18), for different values of T. We cannot distinguish any crossing, but we can clearly see some merging of the different curves.

From the large lattice results (see section 4) we can use the values $T_c = 3.27$, $\gamma = 2.4$ and $\eta \sim 0$ (see (36)) to check the consistency of the finite-size behaviour with a finite-T transition. In figure 2 we plot χ_0/L^2 against $(T - T_c)\, L^{1/\nu}$. The data collapse into a single curve, showing a good scaling behaviour, on both sides of T_c. It is already clear from these first data (illustrated in figures 1 and 2) that it will be exceedingly difficult to distinguish between the two candidate critical behaviours (with $T_c = 0$ or $T_c \neq 0$).

To understand better what is happening in the pseudo-critical region, for T close to 3.3, it is interesting to apply a magnetic field h to the model. We expect q to scale as $h^{2/\delta}$. δ is related to η by the hyper-scaling relation

$$\delta = \frac{d+2-\eta}{d-2+\eta}. \tag{21}$$

In the presence of h the correct definition of the overlap susceptibility requires subtraction of the connected part, i.e.

$$\chi_0 \equiv \lim_{V\to\infty} V\left(\overline{\langle q^2\rangle} - \overline{\langle q\rangle}^2\right). \tag{22}$$

For a finite-T phase transition the scaling relation (17) is still satisfied, but now (we are sitting at T_c) ξ diverges as

$$\xi(h) \sim h^{-2(\delta+1)/d\delta}. \tag{23}$$

Equation (23) only depends on the critical exponent η. Once we have measured T_c, and established that a finite-T phase transition exists, we can use (23) to find η.

It turns out that the correct overlap susceptibility we have just defined in (22) is not a good observable for checking scaling. It depends on the first moment of $\langle q\rangle$ that is affected by strong finite-size corrections. This is because the region of negative overlaps with $q < 0$ is only suppressed in the infinite-size limit. We have found it preferable to study the behaviour of the non-subtracted $\overline{\langle q^2\rangle}$, i.e. the overlap susceptibility defined in the absence of h divided times the volume. Here we expect the scaling (17) divided times L^3, i.e. a scaling with L with the power $-(1+\eta)$.

We have run numerical simulations in the presence of a magnetic field. In figure 3 we show $\overline{\langle q^2 \rangle}$ for several lattice sizes $L = 5, 7, 9, 11, 13$ and different values of the magnetic field (ranging from $h = 0$ up to $h = 1.5$). Again we find consistency with $T_c = 3.27$. The preferred value for η is negative and close to -0.1. Let us stress that none of the finite size scaling fits give very precise predictions. There are many free parameters, and that makes the fitting procedure questionable. Still we should note that all the exponents we find, when assuming a finite-T transition, are fully compatible with the ones found for the $r = 1$ model in the previous works [3–6].

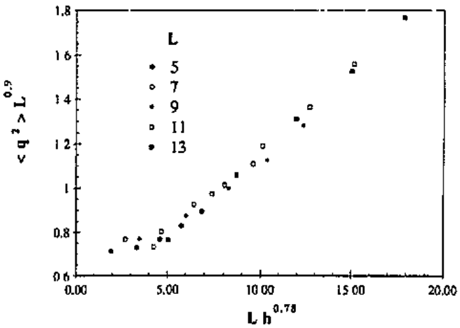

Figure 3. The rescaled $\langle q^2 \rangle$ as a function of the rescaled applied magnetic field, for different lattice sizes.

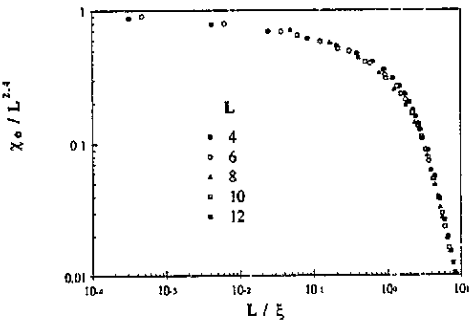

Figure 4. The rescaled χ_0 as a function of L/ξ. This scaling is compatible with a singularity at $T = 0$.

As we already hinted, the finite-size scaling results are also compatible with a $T = 0$ singularity. We will use the best value (45) of the parameters defined in (44). In figure 4 we show the rescaled susceptibility χ_0 (again without magnetic field, now) for the different lattice sizes. The curves for different lattice sizes scale tremendously well, and a comparison with figure 2 is instructive. This is, as we will discuss in the following, fully compatible with the results obtained for the large lattice size, in a regime where $\xi \gg L$.

If the transition is at $T = 0$ the usual scaling laws imply that the correlation function at large distance behaves as $x^{-\zeta}$, with $\zeta = d - 2 + \eta$. When the ground state is not degenerate the $T = 0$ correlation function tends to a constant value at large distance, implying $\zeta = 0$ and in 3D $\eta = -1$. The value we estimate for η turns out to be not so close to -1, and using $\eta = -1$ does not make our curves scale.

Here we see two options. One possibility is that $\zeta \neq 0$ in 3D Ising spin glasses (our best fit is close to $\zeta \sim 0.6$). This possibility cannot be excluded. For example in 2D [6] ζ is estimated to be in the range 0.2–0.3. In our case, where the coupling constants J take the values ± 1, the ground state is highly degenerate, and there are no general *a priori* reasons for $\zeta = 0$ to hold (however, it has been suggested in [17] that at the lower critical dimension we indeed expect $\zeta = 0$). The other possibility is that to get good scaling for η we have to go to lower values of T. Here we have been obliged to stop at not too low values of T, and it is quite possible that the value of η in this temperature range is quite different from its zero-temperature limit.

In figure 5 we have tried to show the scaling behaviour in a suggestive form. We plot $\chi_0(L)/\chi_0(\infty)$ as a function of L/ξ for the different lattice sizes. The values of $\chi_0(\infty)$ and ξ are those discussed in the next sections and computed on very large lattices (which we judge to be free from systematic errors in our statistical precision). The data smoothly collapse into a single curve.

From these data it is not clear if the 3D Ising spin glass undergoes a finite-T phase transition (and the puzzling behaviour of Binder cumulant generally seems to point toward something different). If we assume a finite T_c our predictions for the critical exponents agree with those reported in the literature (for the first-neighbour cubic lattice model).

Though high-temperature expansions predict a finite-temperature transition (which agrees with that found in numerical simulations) we consider the compatibility of our data with a $T = 0$ phase transition serious (and we will discuss this kind of evidence in more detail in the next section, when discussing our large lattice results).

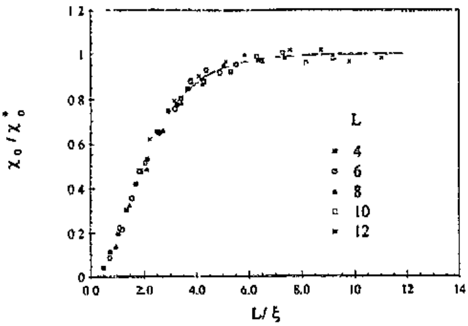

Figure 5. The overlap susceptibility divided by the asymptotic large lattice value (which we denote here by χ_0^*) plotted against L/ξ. The line is the best fit to the form (31).

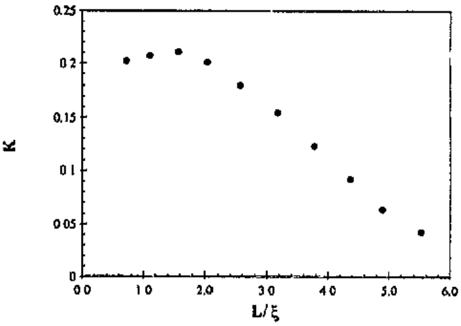

Figure 6. K as a function of L/ξ.

As we have already remarked, the behaviour of the Binder cumulant below T_c is different from what happens in normal spin systems. It is also very different from what one measures in spin glasses in high dimensions, and a few more comments may be in order. Let us consider what happens in the usual ferromagnetic Ising case, by defining the function

$$g(T) \equiv \lim_{L\to\infty} g(T, L) \tag{24}$$

where here $g(T, L)$ is defined in terms of the moments of the order parameter m, the total magnetization of the system. In this non-disordered case we have that

$$g(T) = \begin{cases} 1 & \text{for } T < T_c \\ 0 & \text{for } T > T_c. \end{cases} \tag{25}$$

Moreover, the quantity $g_c \equiv g(T_c)$ is a function of the dimensionality of the system. It increases when the dimension decreases, and tends to one at the lower critical dimension.

The situation is different in spin glass models. In this case in the mean-field approximation $g(T)$ is non-trivial at low temperature. One finds that below T_c

$$g(T) = \frac{3}{2} - \frac{1}{2}\frac{\int \mathrm{d}x\, q(x)^4}{\left(\int \mathrm{d}x\, q(x)^2\right)^2} = \frac{3}{2} - \frac{1}{2}\frac{\int \mathrm{d}P(q)\, q^4}{\left(\int \mathrm{d}P(q)\, q^2\right)^2}. \tag{26}$$

Using the mean-field expression for the dependence of $q(x)$ on T one finds that

$$g_{-} \equiv \lim_{T \to T_c^-} g(T) = 1 \tag{27}$$

but the function $g(T)$ is non-trivial. The statement $g \neq 1$ coincides with the fact that the $P(q)$ is not equal to a δ-function, and implies replica symmetry breaking. In the mean-field approximation no closed formula exists for g, however one finds that qualitatively g behaves as

$$1 - A\frac{T}{T_c}\left(1 - \frac{T}{T_c}\right). \tag{28}$$

In other words $1 - g(T)$ vanishes linearly both at zero temperature and at the critical temperature. For $T > T_c$ one still finds that $g(T) = 0$. Below the upper critical dimension ($d_c^{(u)} = 6$), according to the prediction of [17], g_{-} becomes different from one. Slightly below $d = 6$ the function $g(T)$ is not monotonic, but it is possible that it becomes monotonic at sufficient low dimensions, i.e. near three dimensions. It is tempting to conjecture that near the critical dimension one finds that g_c becomes close to g_{-}. It is difficult to assess quantitatively the values of these two quantities. If we use our best estimate for T_c we find $g_{-} \simeq (0.65 \pm 0.05)$ (using our small lattice data for $T < T_c$), and a very similar value for g_c (from the data at the estimated critical temperature). We can only tentatively conclude that:

- The L independence of $g(L, T)$ in the (pseudo-)low-temperature phase and the fact that $g(L, T)$ is different from 1 is a clear signal that replica symmetry is effectively broken in this region. This is because $g \neq 1$ in the thermodynamic limit implies a non-trivial function $P(q)$. Obviously if there is no finite-T phase transition this symmetry breaking will eventually disappear for very large lattices, but it will correctly describe the physics of the system for large lattices with L smaller than the exponentially large correlation length ξ.
- The shape of the function $g(T)$ is in qualitative agreement with the predictions of the renormalization group and it suggests that the lower critical dimension is close to three (and very probably exactly three [18]).

Let us now discuss in some detail the form of finite-size effects. This is very interesting, mainly since we have to plan larger scale numerical simulations, and we want to be sure to optimize the use of our computer time. We will describe here the strategy that should eventually lead us to a numerical simulation in which we can establish in a clear way which kind of singularity the 3D Ising spin glass undergoes. For lattice sizes much larger than the correlation length one finds that (in the presence of periodic boundary conditions) the finite-volume corrections are exponentially small. The leading correction can be computed in perturbation theory, giving

$$\chi_0(L) = \chi_0(\infty)\left(1 - C\xi^3\lambda^2 e^{-L/\xi}\right) \tag{29}$$

where C is some computable constant, and λ is the coupling constant of a ϕ^3-like interaction in a field-theoretical framework. Close to the critical point the usual scaling laws imply that the quantity $\xi^3\lambda^2$ tends to a constant. So we obtain

$$\chi_0(L) = \chi_0(\infty)\left(1 - Ce^{-L/\xi} + O(e^{-2L/\xi})\right). \tag{30}$$

We have fitted our data for the correlation length on small lattices, divided by the large-lattice result, as

$$\frac{\chi_0(L)}{\chi_0(\infty)} \simeq (1 - C\mathrm{e}^{-L/\xi}). \tag{31}$$

The best fit works very well. We show it in figure 5. For a finite temperature transition C is important. It is universal, and in principle it can be computed in a field-theoretical renormalization approach.

These data are relevant since they are crucial for planning simulations free of finite-size effects on large lattices. We see that if we require finite-size effects to be smaller than 1% we need to have $L/\xi > 6$, while to reach a 10% accuracy we can accept $L/\xi > 3.5$.

In a similar way it is interesting to compute

$$K = \frac{\overline{\chi_0^2} - \overline{\chi_0}^2}{\overline{\chi_0}^2}. \tag{32}$$

The quantity K measures the susceptibility to system-to-system fluctuations. We expect it to have similar properties to the Binder cumulant g. In particular at low temperatures mean-field predicts that

$$K = \frac{1}{3}\left(\frac{\int \mathrm{d}x\, q(x)^4}{\left(\int \mathrm{d}x\, q(x)^2\right)^2} - 1\right). \tag{33}$$

In other words mean-field theory predicts that

$$\overline{\langle q^4 \rangle - \langle q^2 \rangle^2} = 2\left(\overline{\langle q^2 \rangle^2} - \overline{\langle q^2 \rangle}^2\right). \tag{34}$$

The size dependence of K can be used to estimate the number of different realizations of the quenched disorder we need to extract an accurate value of χ_0.

The measurement of K is rather delicate because for each system we must know the value of $\langle q^2 \rangle$ with high accuracy. In figure 6 we plot K as a function of L/ξ for $L = 6$. The knowledge of K is useful in estimating the size of sample-to-sample fluctuations when planning a numerical simulation. Our result indicates that, for example, one must go to L/ξ greater than four in order to have fluctuations of less than 30% in the spin glass susceptibility.

4. Large-lattice results and discussion

Our *large* lattice runs have been done on a $64 \times 64 \times 128$ lattice, on the 8192 processor DECmpp at Syracuse NPAC. We have always studied the evolution of two replicas of the system in the same realization of the quenched disorder. In this way we have been able to compute the overlap between two replicas.

We have studied the behaviour of the system for two different realizations of the quenched random couplings. We give in table 1 the details about the two series of runs (the

Table 1. The number of millions of MC sweeps we used for the two different realizations of the couplings. We give the number of thermalization sweeps, plus (+) the number of sweeps used for measuring.

T	Sample 1	Sample 2
$6.0 \to 4.4$	$0.005 + 0.5$	
$4.3 \to 3.8$	$0.5 + 2.0$	$0.5 + 2.0$
3.7	$0.5 + 4.5$	$0.5 + 14.5$
3.6	$2.5 + 9.0$	$2.5 + 30.0$

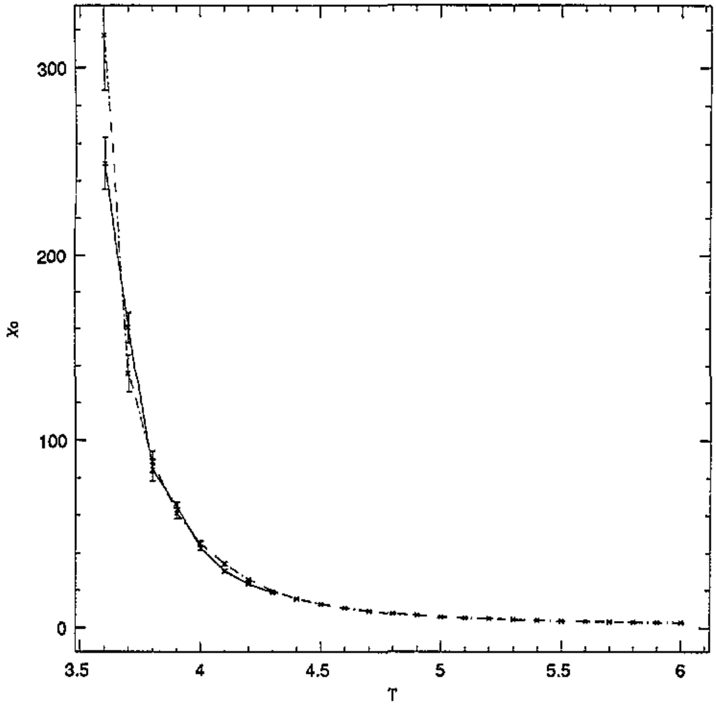

Figure 7. χ_0, the overlap susceptibility, for the two realizations of the random couplings.

number of millions of sweeps is for each of the two replicas we studied in a given coupling realization).

We studied two different realizations of the random noise, mainly to check the size of the fluctuations of χ_0. We wanted to be sure that even for our T point closer to criticality ($T = 3.6$) sample-to-sample fluctuations are not too dramatic. In figure 7 we show that in the worst case the two results for χ_0 deviate by less than two standard deviations (in this and in the following figures the smooth curves just join the Monte Carlo data points with straight segments). But we know from our binning analysis that the error we quote is probably slightly underestimated at the lower T values. So we find this result reassuring and consistent with the serious critical slowing down that we observe and with critical fluctuations.

The internal energies of the two systems are completely compatible (figure 8), as is the specific heat (which we measure both from equilibrium fluctuations and from the T derivative of the internal energy; figure 9). We feel confident that on the $64 \times 64 \times 128$

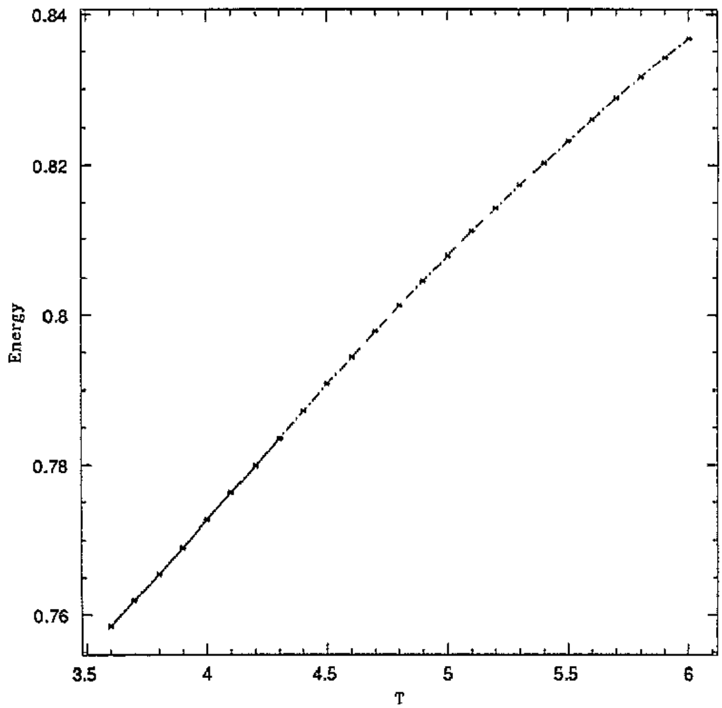

Figure 8. As in figure 7, but for the two internal energies.

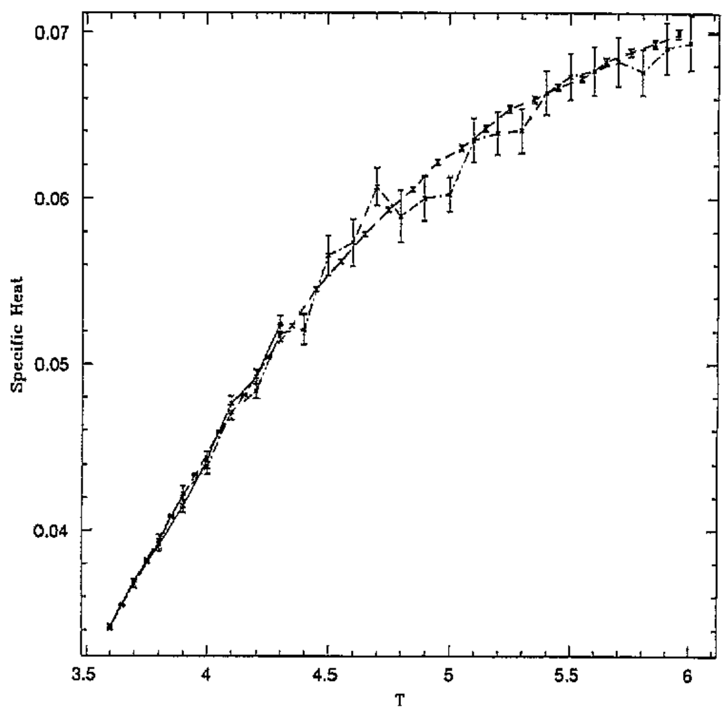

Figure 9. As in figure 7, but for the specific heats. The points with large statistical noise are from the energy fluctuations, while the ones with smaller noise are from T derivatives of the internal energy.

lattice results do not vary much with the sample, and in the following we will discuss results averaged over the two realizations of the quenched disorder.

We have estimated statistical errors by a binning analysis. We have systematically blocked the data in increasingly coarse sub-samples, to check statistical independence of the configuration groups eventually used for the final error analysis. Apart from for the two lower T values (3.6 and 3.7) we have always reached a very reliable estimate of the true statistical error. In the two last cases the error seems to be stabilizing under binning, but the evidence is less compelling, and we would allow for a possible small underestimation of the statistical error (of less, say, than 50%).

For T going from 6.0 down to 4.4 we present errors based on nine blocks of the order of 50 000 configurations (the actual measurements were taken just once in 200 sweeps). From 4.3 down to 3.8 we have nine blocks of the order of 400 000 configurations each. At $T = 3.7$ we have used five blocks of 3×10^6 configurations, and at $T = 3.6$ six groups of 6.5×10^6 configurations.

In figure 10 we plot the final overlap susceptibility, averaged over the two coupling realizations, as a function of the temperature T.

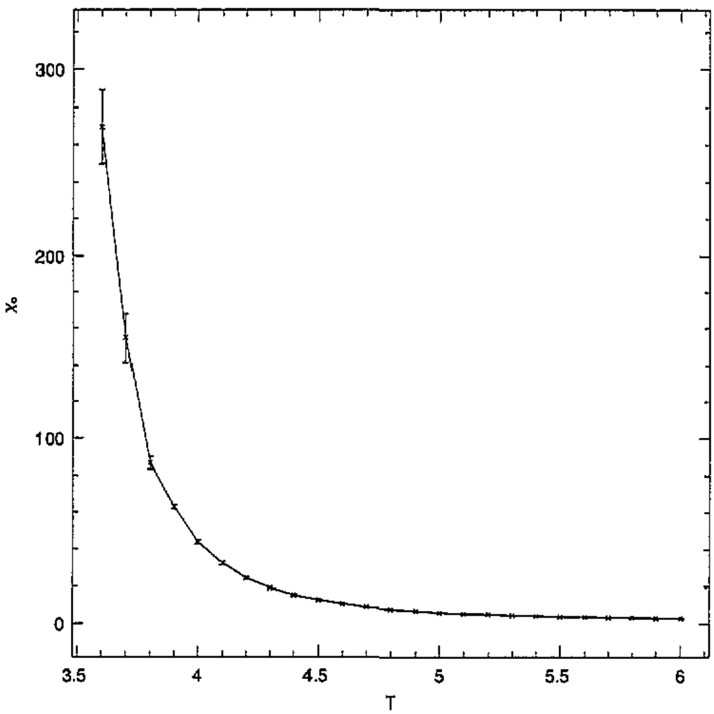

Figure 10. The overlap susceptibility, averaged over the two different samples.

Our main goal has been to try and establish (or disprove) the existence of a finite-T phase transition for the 3D spin glass model under study. Since correlation times diverge very fast when approaching the low-temperature region (or T_c^+, if it exists), we are not in an easy situation. On a large lattice we have to look at data far away in the warm phase (the one we can check and trust to be thermalized), and try to decide which kind of critical behaviour they have.

At first we have tried fitting χ_0 with a power divergence at the critical temperature T_c, i.e.

$$\chi_0 \simeq 1 + \frac{A_p^\chi}{(T - T_c)^\gamma} \tag{35}$$

where the subscript p stands for *power* fit. We show in figure 11(*a*) our best fit, obtained by using all the data points shown in the figure. The results are

$$A_p^\chi = 19.3 \pm 1.1 \qquad T_c = 3.27 \pm 0.02 \qquad \gamma = 2.43 \pm 0.05. \tag{36}$$

We do not attach much significance to the statistical errors quoted here. They are reasonable estimates of a standard fitting routine, but not the result of a detailed study of a very complex three-parameter fit. We will see in a moment that the main issue here is not the statistical error, but the systematic error, which is, as far as we can judge from the present data, infinite (see later).

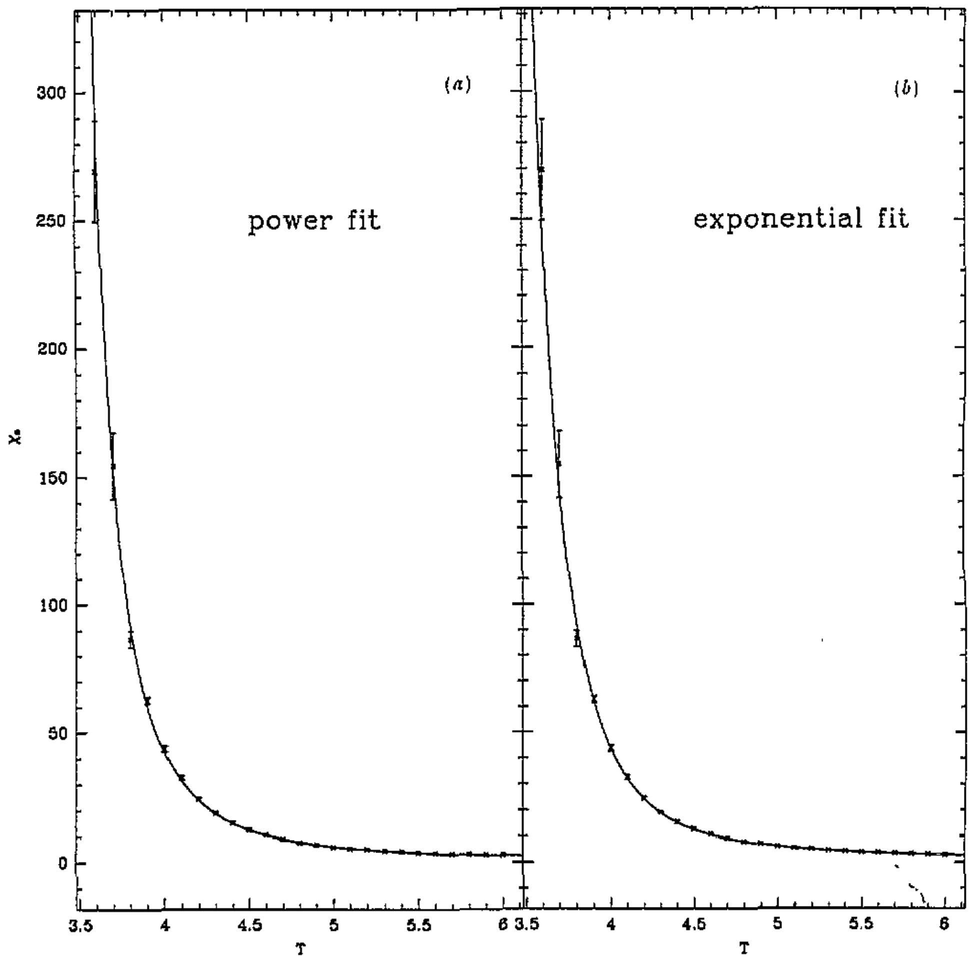

Figure 11. The overlap susceptibility, as in figure 10. Here the curves are the results of the best fits. In (*a*) the result of the power fit to the form (35) are shown, and in (*b*) the result of the power fit to the form (38).

Obviously one would like to select a T region that would allow a good scaling behaviour to be exposed (and to be obliged from the fit to discard a high-T region where scaling corrections are important and a region close to T_c where finite-size effects become sizeable). This would amount, in some sense, to finding at least the size of the first corrections to scaling. In the present case we have to compromise on the quality of the results in (36), which is, still, reasonably good. We have checked that by fitting only points close to T_c we get results that are not so different from the ones given in (36). For example if we fit from $T = 5.0$ down to $T = 3.6$ we obtain $\gamma = 2.67 \pm 0.06$ and $T_c = 3.20$.

Let us repeat that here the problem will turn out to be mainly the systematic error.

The second functional behaviour we have tried assumes no critical point, but an essential singularity at $T = 0$. We have first tried the form

$$\chi_0 \simeq A_e^\chi \left(\exp\{(B_e^\chi / T)^P\} - 1 \right) + C_e^\chi \tag{37}$$

where the subscript e stands for *exponential* fit. The power P turned out to be very close to 4 (as it did also for the exponential fit to the correlation length ξ, see later). We have tried fits with different fixed power P, and for the fit to χ_0 (the fit to $\xi^{(1)}$ has a larger indetermination, see later) we find that a power of 3 or 5 gives cleary worse results than a power 4. So we have eventually used the three-parameter fit to the form

$$\chi_0 \simeq A_e^\chi \left(\exp\{(B_e^\chi / T)^4\} - 1 \right) + C_e^\chi \tag{38}$$

which gives results

$$A_e^\chi = 1.67 \pm 0.05 \qquad B_e^\chi = 5.38 \pm 0.01 \qquad C_e^\chi = 1.28 \pm 0.05. \tag{39}$$

The best fit is very good, and we show it in figure 11(*b*). The value of χ^2 is much better than for the power fit (12 compared with 29 with some slightly arbitrary normalization).

The divergence of the correlation length as a function of $(T - T_c)$ gives, if a phase transition exists, the exponent ν. We have repeated here the analysis we have discussed for χ_0. In figure 12 we give $\xi^{(1)}$ (which we have defined earlier) as a function of T. $\xi^{(0)}$ is always compatible with $\xi^{(1)}$, but has a larger statistical error.

Our estimator for $\xi^{(1)}$ is defined by taking the weighted average of the effective mass estimator at distance d

$$\tilde{m}(d) \equiv \log \left(\frac{G^{(1)}(d)}{G^{(1)}(d+1)} \right) \tag{40}$$

(where $G^{(1)}$ was defined after (11)) for d going roughly from ξ to 2ξ. In this way we are making systematic effects (coming from small distance contributions) and statistical errors small. A typical fitting window is d from 2 to 3 at large T down, for example, to 8 to 15 at $T = 3.7$. We have estimated errors by using a standard binning plus jack-knife procedure. Our conclusions about the statistical significance of the sample coincide with the ones we have drawn for χ_0.

Also in this case we have tried a power fit and an exponential fit. For the power fit we used the form

$$\xi^{(1)} \simeq \frac{A_e^\xi}{(T - T_c)^\nu} \tag{41}$$

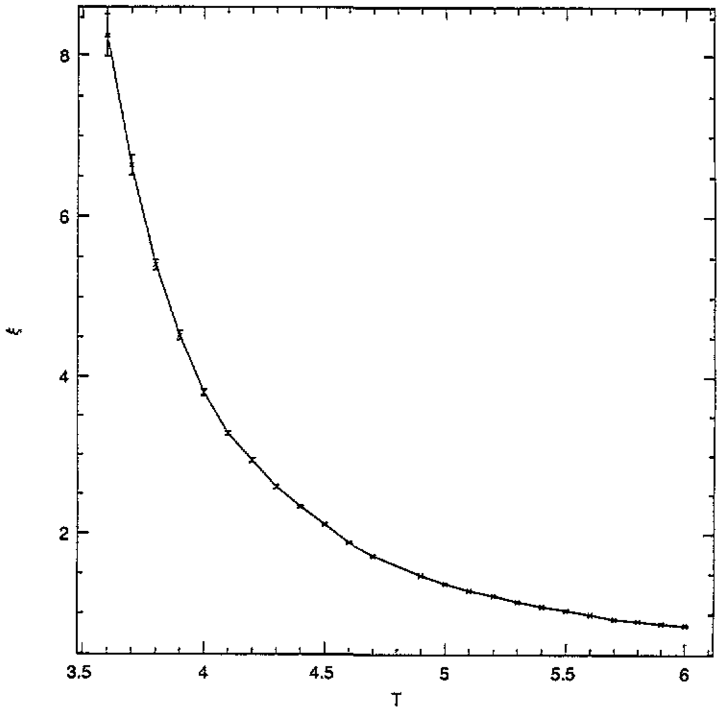

Figure 12. The correlation length $\xi^{(1)}$, averaged over the two different samples. The curve is here only to join neighbouring points.

with the result

$$A_e^\xi = 2.73 \pm 0.11 \qquad T_c = 3.24 \pm 0.03 \qquad \nu = 1.20 \pm 0.04. \tag{42}$$

Even if the results are very reasonable, the fit is not good (as shown in figure 13(*a*)). The value of χ^2 is very high ($\simeq$ 120), and the points close to T_c are the ones that do not fit (very dangerous *caveat*!). Still, if we take these data seriously, we have to notice that T_c is the same we estimated by using χ_0, and that by means of the scaling relation

$$\gamma = \nu(2 - \eta) \tag{43}$$

we get $\eta \simeq 0$.

The exponential fit has the form

$$\xi \simeq A_e^\xi\big(\exp\{(B_e^\xi/T)^4\} - 1\big) + C_e^\xi \tag{44}$$

and gives

$$A_e^\xi = 1.41 \pm 0.05 \qquad B_e^\xi = 4.21 \pm 0.02 \qquad C_e^\xi = 0.46 \pm 0.01. \tag{45}$$

This best fit is very good, and we show it in figure 13(*b*). The χ^2 is four times smaller than for the power fit. This fit is by far a better fit than the fit to a power-law behaviour.

For ξ the evidence for the power in the exponential being 4 is less compelling than for χ_0. Here fits with power 2, 3 or 5 are acceptable; also if the χ^2 is a minimum at power

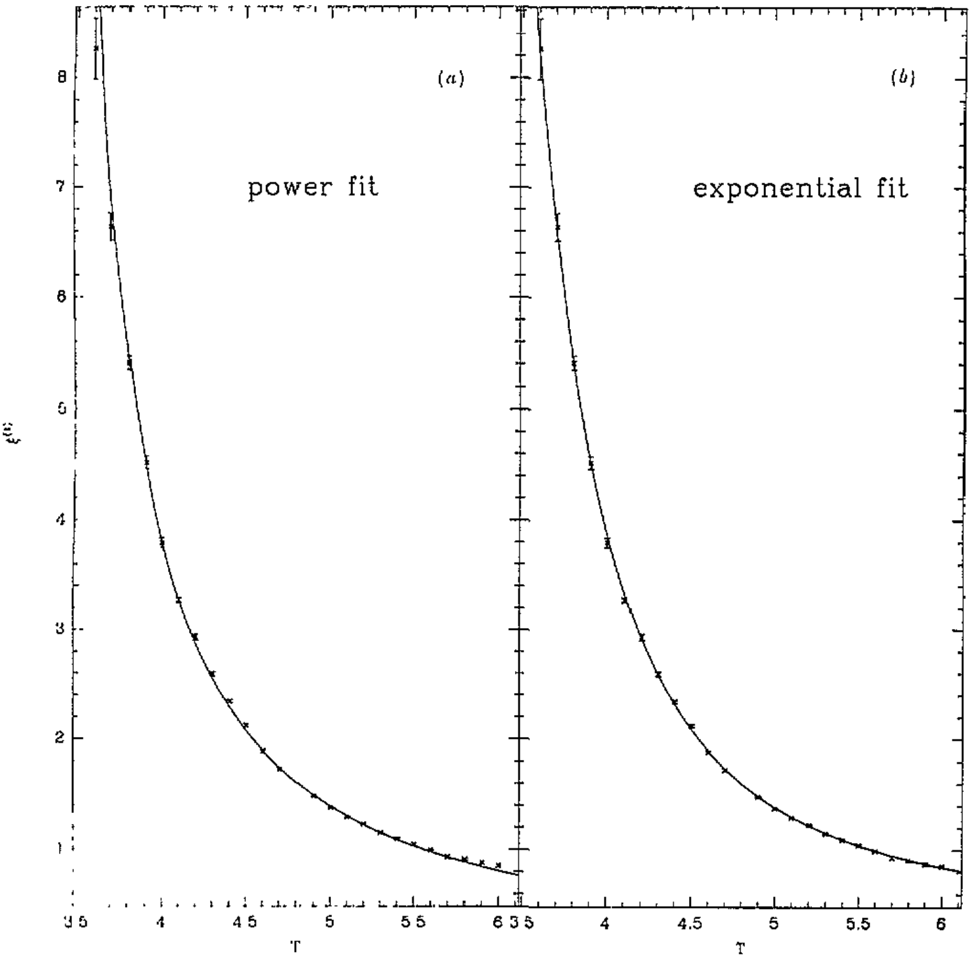

Figure 13. The correlation length, as in figure 12. Here the curves are the results of the best fits. In (*a*) we show the result of the power fit to the form (41), and in (*b*) the result of the power fit to the form (44).

4 (or 5, which gives a very similar fit; for power 3 a small decrease in quality is already apparent).

In figure 14 we show the data for

$$Z_0 \equiv \chi_0 m^2 \qquad Z_1 \equiv \left(\sum_i i G^{(1)}(i) \right) m \tag{46}$$

from the data we have already shown for m, the inverse correlation length. We expect both quantities to diverge as m^{η} in the small-m limit. Both quantities are well fitted by a power law with $\eta \sim -0.25$.

An independent way to measure η is to study directly the data for the correlation function $G^{(1)}$. At large distances the data can be fitted by

$$\frac{\mathcal{Z}(\beta)}{r} \mathrm{e}^{-mr}. \tag{47}$$

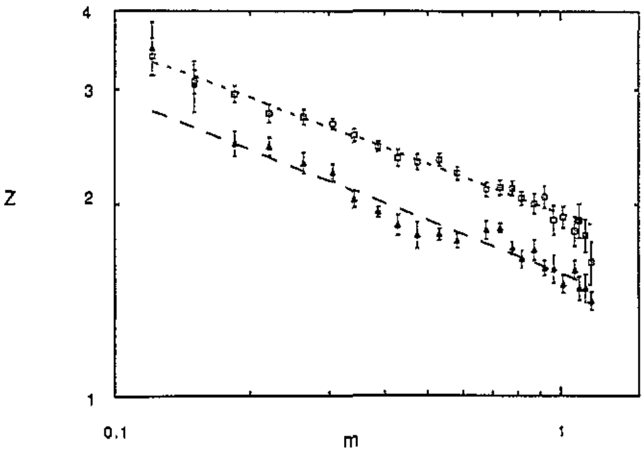

Figure 14. The quantities Z_0 (lower curve) and Z_1 (upper curve) as functions of m on a logarithmic scale.

$\mathcal{Z}(\beta)$ seems to diverge close to the critical temperature, with a very small power $\sim m^{-0.1}$, making this estimate of η quite different from the previous one. The discrepancy between the two estimates of η is likely to be related to the small asymptotic value of η.

As a check we have analysed the data for the correlation function

$$C(s) \sim rG^{(1)}(r)/\mathcal{Z}(\beta) \tag{48}$$

in the scaling region as a function of $s \equiv r/\xi$. The fact that the exponentially decaying fits to the correlation function are good implies that for $s > 1$ the function $C(s)$ is well approximated by e^{-s}. At small values of s the function should go to zero as s^{η}. Alas, since we cannot reach very small values of s it is difficult to use this method to get a precise determination of η.

Let us insist on the difficulty in reaching a definite conclusion about the critical regime by presenting some more fits (figures 15 and 16). Here we are analysing the overlap susceptibility χ_0 as a function of β. In figure 15 we show the best fit to the form (35) with the parameters given in (36) (with a transition at a critical temperature), and we superimpose a second fit of the form

$$\log(\chi_0) = Ae^{(B\beta)} \tag{49}$$

with $A = 0.085$ and $B = 15.16$. Again, although the two functional forms imply a very different critical behaviour, in the region we have studied they are indistinguishable.

We can try more. A similar phenomenon is displayed in figure 16. Here we show dependencies that imply a transition at zero temperature

$$\begin{aligned} \log(\chi_0) &= A\beta^{\omega} \\ \log(\chi_0) &= A + B\beta + C\beta^2. \end{aligned} \tag{50}$$

In the first-best fit we find $A = 383$ and $\omega = 3.33$, while in the second-best fit we get $A = 5.9$, $B = -69.8$ and $C = 246$. ω turns out to be not so far from 4, as we have already remarked.

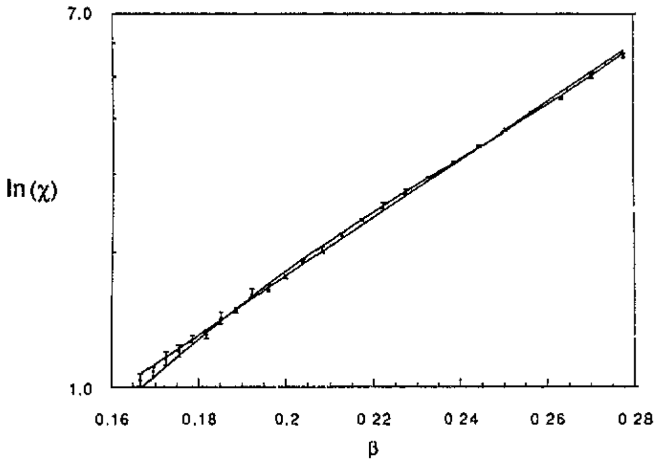

Figure 15. Two fits to the data for the susceptibility χ_0, as a function of β, according to equations (35) and (49).

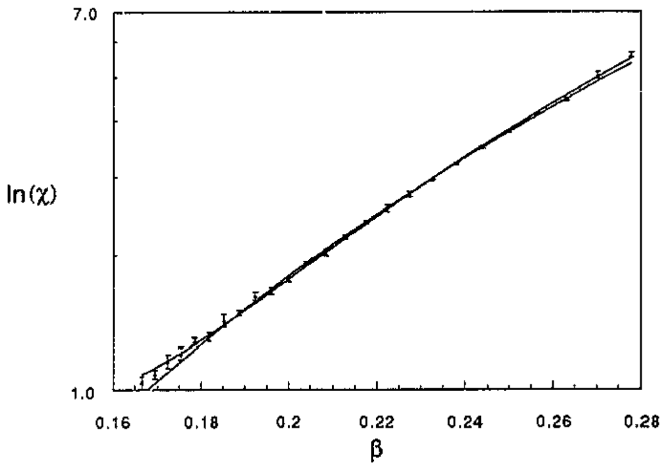

Figure 16. Two fits to the data for the susceptibility χ_0, as a function of β, according to equation (50).

The four fits all give reasonable results. It is impossible to use the data to reject one of them. Of course we could choose the one with smallest χ^2, but this procedure may give an incorrect answer since we have neglected sub-asymptotic terms, inducing a systematic error which is out of control.

From these data, we tend to conclude that we have a hint about the absence of a phase transition in the 3D spin glass. If, on the contrary, such a phase transition is present, than we have given a reasonably precise estimate of the critical exponents.

5. Conclusions

We believe we have pointed out an open problem that in recent papers was quoted as solved. Nowadays it is usually said that the existence of a phase transition is established.

For example in [9], which is about aging phenomena (see [11] for more aging papers), it is claimed that it is common lore that 3D spin glasses undergo a finite T_c phase transition. It does not seem to us that the existence of a phase transition is well established at all.

The possibility of three being the lower critical dimension is appealing. We have in mind a scenario where the predictions of the mean-field theory describe fairly well the behaviour of the system down to $d = 3$, where the transition disappears. In no cases, as it is sensible to expect, does the system behave as a normal ferromagnet. At low T in 3D the system is reminiscent of the mean-field picture up to a critical length which is function of T, and diverges at $T = 0$.

As was noted many years ago in [19], at the lower critical dimension we expect $1/f$ noise for the power spectrum of the magnetization; this agrees with what has been observed experimentally [20].

It is clear that there is an apparent critical temperature. Close to this pseudo-T_c the correlation length becomes so large that it cannot be measured on the lattice sizes that are normally studied. Below this temperature the system behaves as if it is in the low-temperature phase, irrespective of the existence of the transition (think about the 1D normal Ising model for low values of T).

The only way to disprove the existence of a transition at finite temperature would be to show that the data for the susceptibility and the correlation length cannot be fitted with power-law singularities at finite temperature. On the other hand, to present evidence for a transition at finite temperature one should show that the data can be fitted as power-law singularities and cannot be fitted with functions having only singularities at zero temperature. Our data, as well those from the very long simulations of Ogielski and Morgenstern [3, 5], can be fitted in both ways. As we already said, we do not think that we can discriminate between the two admissible behaviours from the value of χ^2, i.e. of the quality of the fit, especially in an approach where corrections to scaling have been neglected. Unfortunately, in the absence of clear predictions about the low-temperature behaviour, it is difficult to exclude the possibility of a transition at $T = 0$.

To visually discriminate among the two possibilities we plot in figure 17 the quantity

$$\Gamma \equiv \frac{d\beta}{d\log(\chi_0)} \tag{51}$$

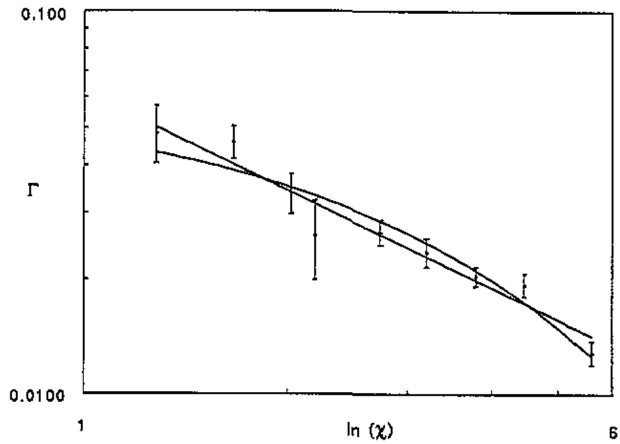

Figure 17. Γ plotted against τ (see the definitions in the text).

against $\tau \equiv \log(\chi_0)$. A finite-T transition implies that

$$\Gamma \simeq e^{-A\tau} \tag{52}$$

with $A = 1/\gamma$, while a transition at $T = 0$ with a divergence of the form $\exp(\beta^{\omega})$ implies

$$\Gamma \simeq \frac{1}{\tau^B} \tag{53}$$

with $B = 1 - 1/\omega$. $B = 1$ corresponds to an $\exp(e^{\beta})$ behaviour. Our best fits give $A = 0.29$ and $B = 0.86$. The data are noisy at high temperature (low τ). Clearly it is difficult to select one fit, especially since we have neglected corrections to scaling. The data seem to prefer a straight line with a coefficient not far from one, but we are unwilling to rely on this kind of evidence.

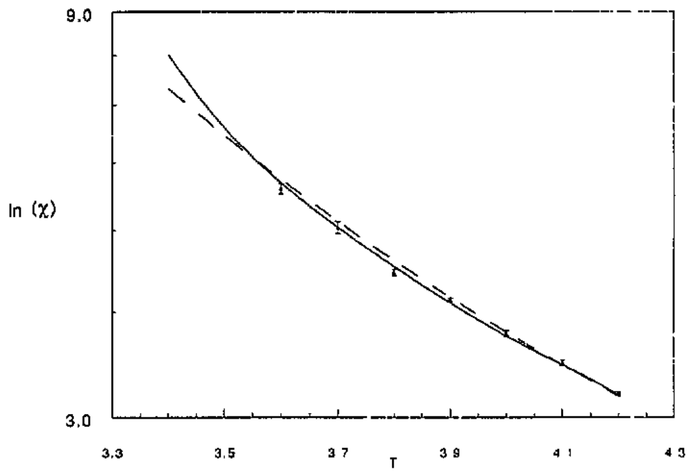

Figure 18. $\log \chi_0$ plotted against T. Fit 1 (full curve) is to a power-law singularity, as in (35); fit 2 (broken curve) has a $T = 0$ singularity, as in (49).

What can be done with a better numerical simulation? To get a hint we have extrapolated two typical fits at a reasonable low T. We show them in figure 18. We have considered a simple power singularity at $T \neq 0$, and a divergence at $T = 0$ of the form $\exp\{Ae^{B}\}$. From our present best fits we can deduce that at, say, $T = 3.4$, we would be able to discriminate between the two. If the data really followed the finite-T singularity scenario (the first case), the strong increase of the susceptibility could not be fitted by the double exponential scenario, and the zero-temperature transition would be refuted.

In the opposite case, where the hypothetical data follows a form of the second kind (a double exponential singularity at $T = 0$) we find that a power fit would still be a good fit, but with a larger value of γ and smaller value of T_c. This variation of the value of the best-fit parameters with the temperature interval used for the fitting would then be taken as good evidence for the existence of a zero-temperature transition.

If the double exponential singularity behaviour is correct, the correlation length should increase by a factor of about 2.5 when going from $T = 3.6$ to $T = 3.4$. This means that a reliable estimate would be possible on 128^3 lattice, only slightly larger than that we used here, and not out of the reach of the present technology. An increase in the computer time of more than one order of magnitude seems unfortunately necessary, but this is also a reasonable goal. Such a computation seems possible in the not too distant future.

It is also possible that a careful analysis of the model at low T could allow one to show the absence of a phase transition [21–23]. In this case it would be essential to identify the renormalization group flow away from the zero-temperature fixed point.

Acknowledgments

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