Search for a Transition in the Three-Dimensional $\pm J$ Ising Spin-Glass

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The three-dimensional Ising spin-glass in zero field with nearest-neighbor interactions having a $\pm J$ distribution is studied by Monte Carlo simulations for samples of linear dimension L with $3 \leqslant L \leqslant 20$. Results for the probability distribution, $P_L(q)$, of the spin-glass order parameter are analyzed by finite-size scaling. Data for $T \geqslant 1.2$ are consistent with a conventional phase transition at $T_c = 1.2^{+0.1}_{-0.2}$, with exponents $\nu = 1.3 \pm 0.3$ and $\eta = -0.3 \pm 0.2$. However, results at lower temperature indicate marginal behavior and suggest that the lower critical dimensional is close to three.

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Despite extensive studies, the question whether a spin-glass transition occurs in three dimensions ($d=3$) has remained controversial. Several careful measurements[1] of the nonlinear susceptibility for Heisenberg systems have been interpreted as strong evidence for a nonzero transition temperature, T_c, though they may also[2] be consistent with $T_c = 0$. However, apart from some early real-space renormalization results,[3] calculations for Ising spin-glass models in zero magnetic field have led[4] to the conclusion that the lower critical dimension (LCD), below which no transition occurs at finite temperature, is $d_L = 4$. (In pure systems, the LCD for Ising spins is known to be lower than that for Heisenberg spins.) Very recently, though, Bray and Moore[5] and McMillian[6] have studied the scaling of defect energies with size for small samples for the Ising spin-glass with Gaussian nearest-neighbor bonds in zero field at $T=0$. They conclude that T_c is finite in $d=3$, while $T_c = 0$ for $d=2$ in agreement with earlier work.[7] Extending their calculation to finite temperatures they estimate T_c (in units of the standard deviation of the bond distribution) and *one* of the exponents, ν, as follows: $T_c = 0.83 \pm 0.08$, $\nu = 3.3 \pm 0.6$ for $2 \leqslant L \leqslant 4$ (Ref. 5); $T_c = 1.0 \pm 0.2$, $\nu = 1.8 \pm 0.5$ for $3 \leqslant L \leqslant 6$ (Ref. 6). Preliminary results on a large ($L=64$) lattice for the $\pm J$ Ising model (see below) down to $T = 1.4$ indicated the possibility of an incipient transition.[8]

Here we investigate the possibility of a spin-glass transition by Monte Carlo simulations of the $d=3$ Ising model with a symmetric $\pm J$ distribution. We cover a wide range ($3 \leqslant L \leqslant 20$) and larger sizes than in Refs. 5 and 6, and are able to determine *two* independent exponents from which all others can be evaluated by means of scaling relations.

Our main conclusions are as follows. A finite-size scaling[9] fit to the data with $T \geqslant 1.2$ (in units of the nearest-neighbor coupling) yields a conventional transition at $T_c = 1.2^{+0.1}_{-0.2}$. The correlation length exponent, ν, is estimated to be $\nu = 1.3 \pm 0.3$ while η, which describes the decay of correlations at T_c, is found to be $\eta = -0.3 \pm 0.2$. However, our results for $1.0 \leqslant T \leqslant 1.2$ indicate a more marginal behavior and suggest that the LCD is close to three.

The Hamiltonian for our system is

$$H = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j, \tag{1}$$

where $S_i = \pm 1$, the sites are on a $L \times L \times L$ simple cubic lattice, and the J_{ij} are independent random nearest-neighbor interactions with a probability distribution

$$P(J_{ij}) = [\delta(J_{ij}-1) + \delta(J_{ij}+1)]/2. \tag{2}$$

Periodic boundary conditions are imposed. Most of the simulations have been performed on the distributed array processor at Queen Mary College, London. The program updates 13.5 million spins per second for L of the form 2^m ($m = 2,3,4,\ldots$) and up to about 9.5 million for the other even sizes. Some data have also been obtained from the Cray 1S at the University of London Computer Centre (ULCC). Between 100 and 1000 samples were averaged over for each datum point, depending on size and temperature.

One quantity of interest is the spin-glass susceptibility χ_{SG}, defined by

$$\chi_{SG} = L^{-d} \sum_{ij} \langle \langle S_i S_j \rangle_T^2 \rangle_J; \tag{3}$$

$\langle \cdots \rangle_T$ denotes a statistical mechanics average for a given set of J_{ij} and $\langle \cdots \rangle_J$ is a bond average. Above T_c, χ_{SG} for an infinite system varies as $(T-T_c)^{-\gamma}$ with $\gamma = (2-\eta)\nu$. χ_{SG} is calculated in two different ways as follows. The first t_0 Monte Carlo steps per spin are used for equilibration and averaging is carried out during the next t_0 steps. By simulation of two sets of spins, $S_i^{(1)}$ and $S_i^{(2)}$, with the same set of bonds and no coupling between them, our first estimate of χ_{SG} is from χ_{SG}^a where

$$\chi_{SG}^a = \frac{1}{L^d t_0} \left\langle \sum_{t=1}^{t_0} \left[\sum_i S_i^{(1)}(t+t_0) S_i^{(2)}(t+t_0) \right]^2 \right\rangle_J. \tag{4}$$

The two sets of spins are prepared in uncorrelated states at the initial time so χ_{SG}^a approaches χ_{SG} from *below* if t_0 is shorter than the necessary equilibration time. We also calculate the four-spin–correlation function

$$\chi_{SG}(t)=L^{-d}\langle[\sum_i S_i(t_0)S_i(t_0+t)]^2\rangle_J, \quad (5)$$

and our second estimate, χ_{SG}^b, is given by $\chi_{SG}^b=\chi_{SG}(t_0)$, which, we find approaches χ_{SG} from *above* if t_0 is not long enough. A run was only accepted if the two estimates of χ_{SG} agreed. Our longest runs were for $t_0=220\,000$.

It is useful to study the probability distribution of the projection of the spin configurations in the two sets, defined by

$$P_L(q)=\frac{1}{t_0}\sum_{t=1}^{t_0}\langle\delta(q-Q(t))\rangle_J, \quad (6)$$

where

$$Q(t)=L^{-d}\sum_i S_i^{(1)}(t_0-t)S_i^{(2)}(t_0+t). \quad (7)$$

Clearly, from Eq. (4), $\chi_{SG}=L^d\langle q^2\rangle$ where $\langle\cdots\rangle$ indicates an average over $P_L(q)$. [As $L\to\infty$, above T_c, $P_L(q)$ becomes a Gaussian of width $L^{-d/2}$, so that χ_{SG} is independent of L, while below T_c, $P_L(q)\to P(q)$, the distribution of overlaps between different "thermodynamic phases," which plays an important role in mean-field theory.[10]] According to finite-size scaling[9] $P_L(q)$ can be written as

$$P_L(q)=L^{\beta/\nu}\bar{P}(qL^{\beta/\nu},L^{1/\nu}(T-T_c)), \quad (8)$$

where β is the order parameter exponent, and from hyperscaling, $\beta/\nu=(d-2+\eta)/2$. Consequently, the finite-size scaling form for χ_{SG} is

$$\chi_{SG}=L^{2-\eta}\bar{\chi}(L^{1/\nu}(T-T_c)). \quad (9)$$

Data for χ_{SG} are shown in Fig. 1. In principle, by analyzing these results according to Eq. (9), one may obtain T_c, η, and ν. However, it is more practical to deal with ratios of moments of $P_L(q)$, such that the scaling form involves fewer parameters. One such

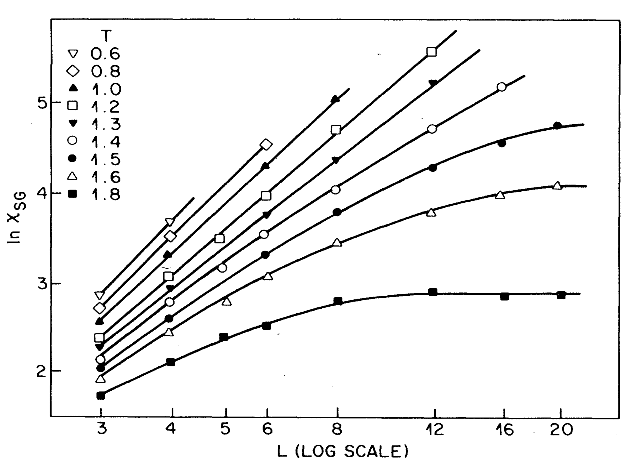


FIG. 1. χ_{SG} versus L on a log-log plot.

quantity is

$$g=(3-\langle q^4\rangle/\langle q^2\rangle^2)/2 \quad (10)$$

defined so that $0\leqslant g\leqslant 1$, and above T_c, $g\to 0$ as $L\to\infty$. g has the finite-size scaling form

$$g=\bar{g}(L^{1/\nu}(T-T_c)) \quad (11)$$

with *no* power of L multiplying $\bar{g}$. To our knowledge, g has not been used before in finite-size scaling analyses of spin-glasses, though an analogous quantity involving ratios of the moments of the magnetization distribution has proved very successful for ferromagnetic systems.[11] For conventional transitions with long-range order below T_c, curves of g vs T for various L intersect at T_c (since g is independent of L at $T=T_c$), and ratios of the slopes of the different curves at T_c may be used to determine ν. We have tested the usefulness of g for spin-glasses by applying it to the infinite-range Sherrington-Kirkpatrick (SK) model,[12] which has a mean-field transition at $T_c=1$. Figure 2(a) shows the results for various number of spins, $N=32$, 128, and 512 (N plays the role of lattice size), obtained on the ULCC Cray-1S. Although there are some corrections to finite-size scaling for this range of sizes (as evidenced by the noncoincidence of the intersection points), the curves *do* all intersect, and errors in both T_c and ν are no more than 10% (and as low as 3% in T_c from intersection of the two larger sizes). A similar accuracy would be entirely acceptable for the three-dimensional (3D) spin-glass.

Our data for g in $d=3$ are shown in Fig. 2(b). From the high-temperature phase, the curves for $4\leqslant L\leqslant 12$ all come together at $T=1.2$, implying a phase transition, and all data above $T=1.2$ scale well with $T_c=1.2$ and an exponent $\nu=1.4$, as shown in Fig. 2(c). In fact, the whole distribution $P_L(q)$ appears to have a size-independent shape at $T=1.2$ (Fig. 3), with the scale of q varying as $L^{\beta/\nu}$ with $\beta/\nu=0.36$ (so that $\eta=-0.28$), just as expected at T_c (see Eq. 8). Thus our results for $T\geqslant 1.2$ are consistent with a conventional transition with finite exponents at $T_c=1.2$. Further, the nonlinear susceptibility exponent γ, if we use $\gamma=(2-\eta)\nu$, is $\gamma\simeq 3.2$, which agrees well with several experimental determinations[1] (perhaps by coincidence; see, however, Kotliar and Sompolinsky[13]).

However, unlike the SK model and other systems displaying a conventional phase transition, the data for g in Fig. 2(b) do not fan out below $T=1.2$, where we can equilibrate sizes $L\leqslant 8$. This could occur if the scaling function were very flat for $T<T_c$ (so that size dependence, though present, is small and lost in the statistical fluctuations). Such a scenario is not borne out by the variation of g below $T=1.2$ [Fig. 2(b)], and the data do not scale well below $T=1.2$ [see Fig, 2(c)], except with much larger values of ν than for $T>1.2$. Such behavior would appear consistent with

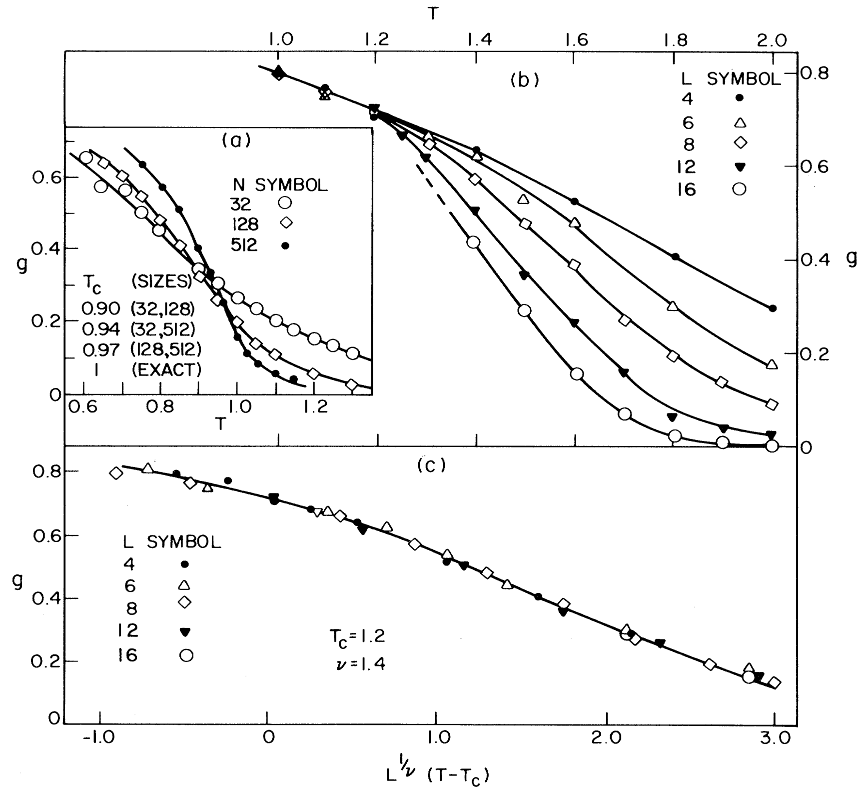
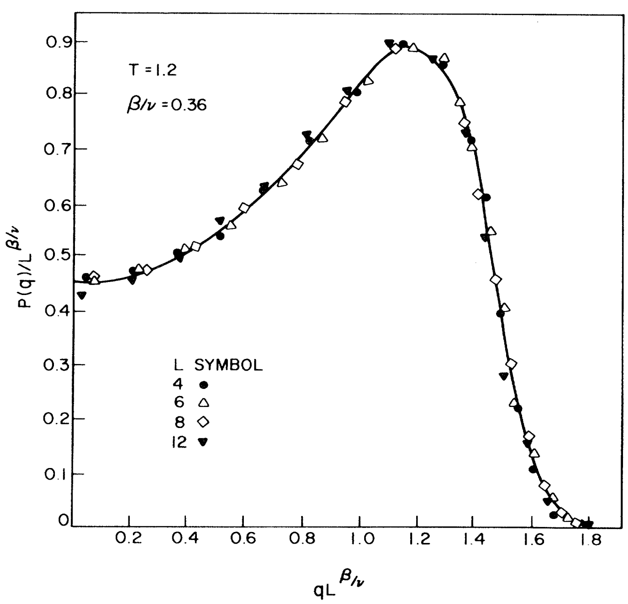


FIG. 2. (a) $g=[3-\langle q^4\rangle/\langle q^2\rangle^2]/2$ vs T for the SK infinite-ranged model for $N=32$, 128 and 512 spins. $0\leqslant g\leqslant 1$ and $g\rightarrow 0$ for $T>T_c=1$ as $N\rightarrow\infty$. Estimating T_c by intersection of curves gives results shown. (b) g for the short-range $3d$ spin-glass. At $T=1.2$, g is independent of size L (for $L=4,6,8,12$) and remains independent of L ($L=4,6,8$) at $T=1.1$ and 1.0. (c) Scaling plot for g (see Eq. 11) with $\nu=1.4$, which works well for $T\geqslant 1.2$, but systematic deviations are seen for $T<1.2$.

a $T_c=0$, but with an exponentially diverging correlation length[14] as $T\rightarrow 0$, so that curves for g approach each other exponentially fast at low temperatures. This occurs at an LCD (e.g., 2D Heisenberg and 1D Ising ferromagnets). However, one would then have to explain the apparent consistency with a $T_c\simeq 1.2$ [in particular, the insensitivity of the intersection point in Fig. 2(b) to size], as well as the much larger variation of g with T than with L below $T=1.2$ [Fig. 2(a)].

A different but rather natural interpretation is that the system at every temperature $T\leqslant 1.2$ is close to criticality which would, in turn, also imply an LCD close to $d=3$. In fact our results are qualitatively of the form one would expect if there is a phase transition at a finite temperature, but with no long-range order below T_c, as occurs for the 2D XY ferromagnet.[15]

McMillan's value of $\nu=1.8\pm 0.5$ is consistent with our fit to the $T\geqslant 1.2$ data. However, Bray and Moore's value of 3.3 ± 0.6 is much larger, which may be related to the near marginal behavior we observe at lower T. Results of recent extensive Monte Carlo simulations on the $\pm J$ model by Ogielski and Morgenstern[16] on large sizes $L=32$ and 64, received since this manuscript was submitted, also favor a conventional



FIG> 3. $P_L(q)/L^{\beta/\nu}$ vs $qL^{\beta/\nu}$ at $T=1.2$ with $\beta/\nu=0.36$. Data lie on a single scaling distribution, as expected if $T=1.2$ is a critical point (see Eq. 8).

transition with $T_c = 1.2 \pm 0.1$, $\nu = 1.2 \pm 0.1$ and $\eta \simeq 0$ mainly on the basis of $T > T_c$ data, which is compatible with our $T \geqslant 1.2$ results, but we find somewhat different behavior at lower T. Clearly it would be desirable to have results on larger sizes for temperatures $T \leqslant 1.2$, to further investigate the possibility that $d = 3$ is close to the LCD of the Ising spin-glass.

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