# Critical Behavior of Three-Dimensional Ising Spin-Glass Model

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First results of massive Monte Carlo simulations of the $d=3$ Ising spin-glass with $\pm J$ bond distribution, performed on a fast special-purpose computer, are presented. A qualitative change in the behavior of the system and best fits for the spin-glass correlation length and relaxation time favor an equilibrium phase transition at $T_c/J \approx 1.2$.

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In this Letter we address the problem of the existence of a genuine phase transition in the three-dimensional Ising spin-glass model. There has been no generally accepted theoretical prediction for the lower-critical dimension (LCD).[1] After a period of controversy, however, recent experiments favor a transition picture.[2] In this situation an insight into the behavior of the $d=3$ spin-glass could be provided by numerical methods. This approach has faced major difficulties: The randomness of the system calls for fairly large lattice sizes, and large relaxation times require an enormous amount of computation to achieve equilibrium and sample adequately the configurations in the Monte Carlo (MC) simulations. Earlier numerical analysis of the $d=3$ Ising spin-glass included transfer-matrix (TM) calculations,[3] and conventional MC work. The TM method could be applied only to very small lattices of size $4\times4\times L$ ($L \leqslant 10$), too small to describe correctly the development of spin-glass ordering. Previous large MC simulations[4–6] could achieve equilibrium only at high temperatures ($T/J \geqslant 1.55$), and therefore could be interpreted ambiguously, either in favor of $T_c=0$ freezing,[4,5] or of a finite $T_c$ transition.[4,6] More recently finite-size scaling for "defect energies" for small lattices by Bray and Moore[7] ($2^3$–$4^3$) and McMillan[8] ($2^3$–$6^3$) has been interpreted as an indication that $T_c \approx J$ in $d=3$. It is doubtful, however, that such small systems are already in the scaling regime.

Here we present new Monte Carlo data from simulations which exceed the previous ones by several orders of magnitude. We conclude that spin-glasses exhibit an equilibrium phase transition in $d=3$. Our result is based on (1) a qualitative change in the behavior of the system at $T/J \approx 1.2$; (2) the best fit for the correlation length $\xi$, i.e., $\xi \propto |T-T_c|^{-\nu}$, and the best fit for the relaxation time $\tau$, i.e., $\tau \propto |T-T_c|^{-z\nu}$.

The model is defined by the nearest-neighbor Ising Hamiltonian

$$H = -\sum_{x,x'} J_{xx'} S_x S_{x'} - \sum_x h_x S_x \tag{1}$$

with random interactions $J_{xx'}$ distributed independently on each lattice bond with probability $\frac{1}{2}$ for discrete values $+J$ and $-J$. A simple cubic lattice with periodic boundary conditions is used, and we discuss the case of zero magnetic fields. The time-dependent local magnetizations

$$m_x(\Delta t) = (\Delta t)^{-1} \int_0^{\Delta t} dt' \langle S_x(t') \rangle, \tag{2}$$

the average correlation function

$$G(r) = V^{-1} \sum_x \langle S_x S_{x+r} \rangle^2, \tag{3}$$

and dynamic correlation function

$$q(t) = V^{-1} \sum_x \langle S_x(0) S_x(t) \rangle \tag{4}$$

have been directly measured. It has been found that for $32^3$ and $64^3$ lattices the differences in measurements on lattices with distinct bond realizations do not significantly exceed the sampling errors on a single lattice; therefore a systematic study of spatial correlations was performed on one $32^3$ lattice, and dynamic correlations were recorded systematically for one $32^3$ and one $64^3$ lattice. Several $16^3$ lattices were examined to understand qualitatively the finite-size effects.

We began simulations with random initial configurations at high temperature $T=5$ (we set $J=1$). Each series of measurements at a fixed $T$ was performed for a time much longer than the longest relaxation time, and was followed by slow cooling to a slightly lower temperature.

We know that the simulations exhausted all time scales from the fact that the equilibrium time correlation function $q(t)$ completely decays to zero—after averaging over 20 to 200 "histories" [repetitions of the measurement (4)]. Even at lowest temperatures, $1.25 \geqslant T \geqslant 1.10$, we do observe complete reversals of the ordered lattice; i.e., even below $T_c$ we can observe the decay of $q(t)$ to zero for a finite lattice. Summarizing, our simulations were very well equilibrated and we certainly deal with equilibrium values in our work. We analyze the development of spin-glass ordering as follows:

(1) We have observed directly the ordering of the $32^3$ lattices at $T \approx 1.25$ in several ways. First, we have verified that the long-time relaxation at this and lower temperatures proceeds often via rigid, coherent reversals of the entire lattice (by inspection of the local magnetizations). Second, we find that at $T < 1.20$ the

 

correlation function (3) quickly decays to a constant value at longer distance (see Fig. 1). Third, at $T=1.25$ and a little below we observe a dramatic change in the probability distribution $P(m_x)$. Above this temperature the distribution is Gaussian-like and shrinks *continuously* to a delta function as time increases. Below $T=1.25$ the distribution stays flat until we reach the time scale of complete lattice reversals. Figure 2 shows $P(m_x)$ for these two typical cases.

(2) The scaling of correlations, $G(r) \sim \xi^{-d+2-\eta} g(r/\xi)$, which is well satisfied, together with comparison to correlations on a $16^3$ lattice show that finite-size effects become appreciable at distances close to half the lattice size, which are discarded. The phenomenological three-parameter fit

$$G(r) = C\{[\exp(-r/\xi)]/r^x\} \tag{5}$$

works well for $2.0 \geq T \geq 1.325$ on a $32^3$ lattice. Best error-weighted least squares fits for all temperatures together give $C=0.56 \pm 0.04$, and $x=1.07 \pm 0.07$. Error estimates for the correlation length $\xi(T)$ are predominantly due to the fitting uncertainty. At $T=1.325$, $\xi$ is about 10 lattice spacings, which explains the breakdown of the above fitting procedure. In this work we do not include a complete finite-size scaling analysis which requires a substantial amount of additional data and is therefore beyond the scope of this report.

In Fig. 1 we plot $r^{1+\eta}G(r)$ vs $r/\xi$. The data lie on a universal curve if the exponent $\eta \approx 0$. $T=1.10$ (below $T_c$) lies on a different branch. For $T=1.10$, $G(r)$ tends to a constant at large distances, which must be subtracted in order to apply a fit analogous to (5), this time with $x$ close to 0.5—in agreement with our qualitative picture of a transition.

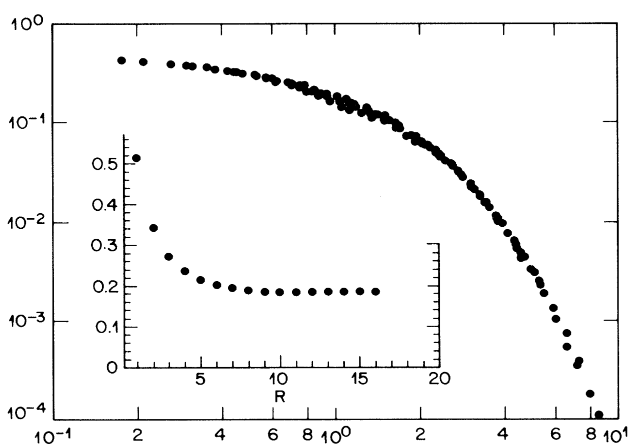


FIG. 1. Scaling plot $r^{d-2+\eta}G(r)$ vs $r/\xi$ ($\eta \approx 0$). Universal curve for $1.325 \lesssim T \lesssim 1.80$, and $32^3$ lattice. Data for $T \lesssim 1.20$ lie on a different branch. Inset: $G(r)$ vs $r$ for $T=1.10$.

The growth of $\xi(T)$ is very well described by the power law $\xi \sim C|T-T_c|^{-\nu}$, with $C=1.00 \pm 0.04$, $T_c=1.20 \pm 0.05$, and $\nu=1.2 \pm 0.1$. The attempt to fit the power law with $T_c=0$ shows large systematic deviations from the data, with least-squares $\chi^2$ 2 orders of magnitude larger, and we rule out this possibility (see Fig. 3).

We also try the fit appropriate for the lower critical dimension, with $\xi(T) \sim a\exp(b/T^\sigma)$. We find that this function provides a fit to the data which is quite good, with the exponent $\sigma=3.6 \pm 0.2$, and constants $a=0.74 \pm 0.05$ and $b=7.4 \pm 0.3$. We note that for the nonrandom Ising model at LCD this exponent is equal to 1.

(3) In order to characterize the average thermal relaxation time $\tau(T)$ we use the representation of $q(t)$ in terms of a distribution of normally relaxing modes:

$$q(t) = \int_0^\infty d\tau\, P(\tau) e^{-t/\tau}, \qquad \tau = \int_0^\infty d\tau'\, P(\tau')\tau' = \int_0^\infty dt\, q(t). \tag{6}$$

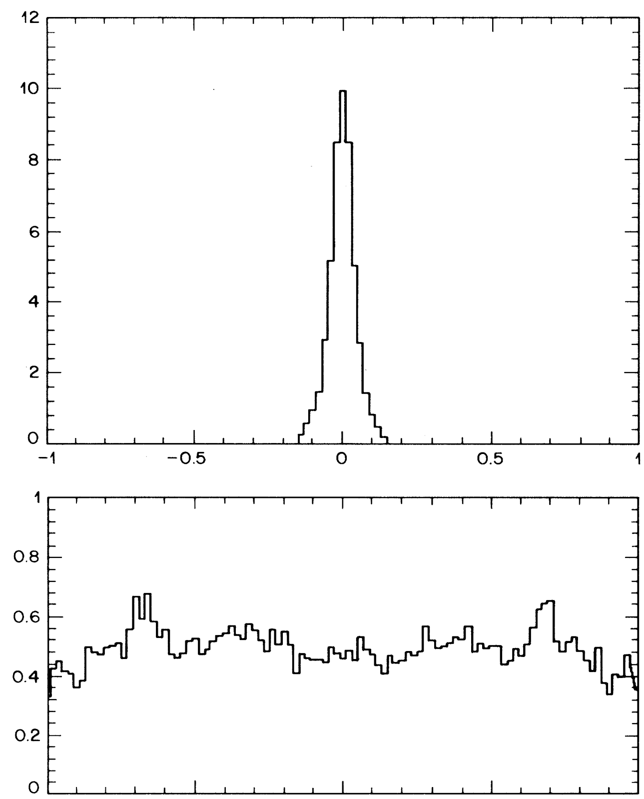


FIG. 2. Typical histograms of local magnetic moments: top, at $T=1.45$, after $11.4\times10^6$ Monte Carlo steps and 2784 measurements, the variance $q=(1/v)\sum\langle S_x\rangle^2=0.002$; bottom, at $T=1.10$, $32.6\times10^6$ Monte Carlo steps and 3984 measurements with $q=0.323$.

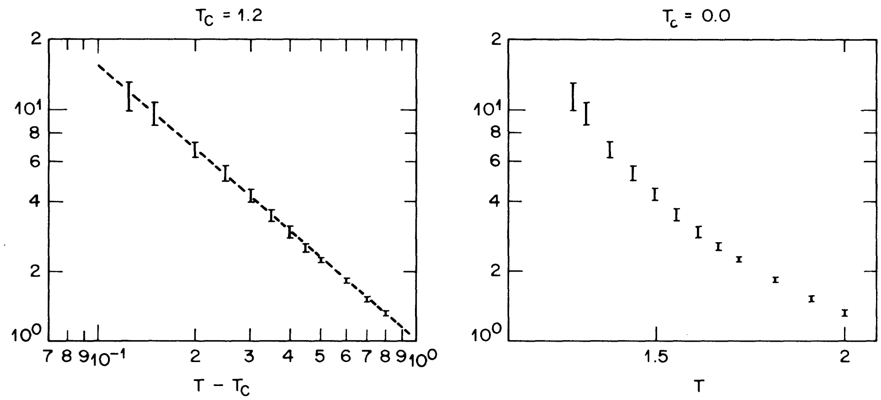


FIG. 3. Temperature dependence of the correlation length $\xi(T)$. If $T_c=0$, the data should lie on a straight line in the right plot, following Ref. 5.

Rapid increase of relaxation times at low $T$ is very well described by the critical slowing down $\tau(T) \sim C_\tau |T-T_c|^{-z\nu} \sim \xi^z$ when the fitted values are $C_\tau = 4.5 \pm 0.5$, $T_c = 1.20 \pm 0.05$, and $z\nu = 6 \pm 1$, giving a large dynamic exponent $z \approx 5$ (Fig. 4). It is noted that the best fit for $T_c$ gives here essentially the same value as from the correlation length.

Another three-parameter fitting function, $\tau \sim a_\tau \times \exp(b_\tau / T^\sigma)$, which should characterize the decay of correlations at LCD with the same exponent $\sigma$ as the correlation length and which appears also in the hypothesis of $T_c = 0$ freezing,[5] can also be fitted to the data quite well (Fig. 4). It yields $\sigma = 4.5 \pm 0.3$, $a_\tau = 4.5 \pm 1$, $b_\tau = 74 \pm 5$ in some disagreement with the analogous fit to $\xi(T)$. Another often-tried relaxation-time fit is the Vogel-Fulcher law,[9] $\tau = \tau_0 \exp[\Delta F/(T-T_0)]$. The fitted values of the "freezing" temperature lie about $T_0 \sim 0.9$. We believe this is accidental, and deviations are expected at still lower temperatures.

It is seen that on the basis of fitting the data at higher temperatures $1.30 \leqslant T \leqslant 1.80$ above it is rather hard to distinguish the power-law divergences from the LCD fit with $\sigma \sim 4$. However, we remind that ultimately the LCD fitting is inconsistent with the observed decay of $G(r)$ to a constant for $T < 1.20$, which implies that $\xi(T)$ has to decrease again in the ordered phase.

Summarizing, we have found that with the best Monte Carlo data currently available, the development of long-range order in three-dimensional Ising spin-glass model can be well explained by an equilibrium phase transition at finite $T_c$. Neither the freezing, nor the LCD picture provides a consistent description of our simulations. A detailed discussion will be presented elsewhere.

After the release of this report, we have received a report by R. N. Bhatt and A. P. Young,[10] where similar estimates of $T_c$ and the exponents for this model have been obtained from finite-size scaling analysis done for smaller lattices.

The simulations presented here were done on a very fast special-purpose computer, designed and built at AT&T Bell Laboratories by J. H. Condon and A. T.

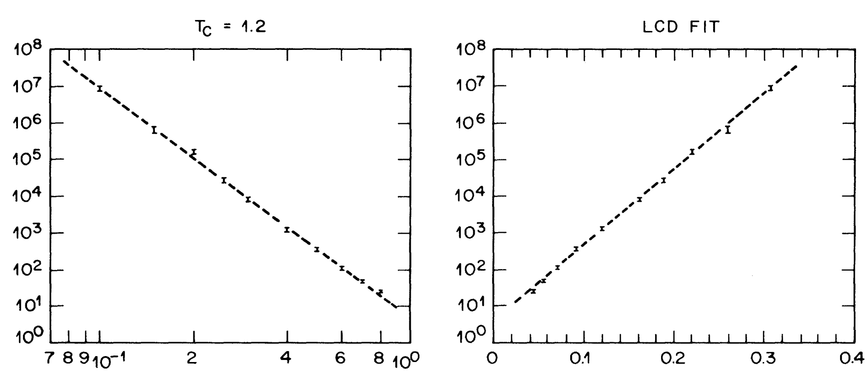


FIG. 4. Growth of average relaxation time $\tau(T)$, interpreted as critical slowing down (left), and as LCD exponential growth (right), for a $64^3$ lattice.

Ogielski. This machine executes the MC heat-bath algorithm, faster than the Cray-1 supercomputer, on a variety of random Ising spin systems (spin-glasses, random fields, bond or site dilution, etc.) and can be programmed in the C language to perform any kind of measurements.

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[1]P. W. Anderson, J. Appl. Phys. **49**, 1599 (1978); R. Fisch and A. B. Harris, Phys. Rev. Lett **38**, 785 (1977); A. J. Bray and M. A. Moore, Phys. Rev. Lett. **41**, 1068 (1978); H. Sompolinsky and A. Zippelius, in *Heidelberg Colloquium on Spin-Glasses,* edited by J. L. Van Hemmen and I. Morgenstern (Springer-Verlag, Berlin, 1983).

[2]C. A. M. Mulder, A. J. van Duynveldt, and J. A. Mydosh, Phys. Rev. B **23**, 1384 (1981); N. Bontemps, J. C. Rivoal, M. Billardon, J. Rajchenbach, and J. Ferre, J. Appl. Phys. **52**, 1760 (1981); A. P. Malozemoff and Y. Imry, Phys. Rev. B **24**, 489 (1981); L. Lundgren, P. Svedlindh, and O. Beckman, Phys. Rev. B **26**, 3990 (1982).

[3]I. Morgenstern and K. Binder, Z. Phys. B **39**, 227 (1980).

[4]A. P. Young, in *Heidelberg Colloquium on Spin-Glasses,* edited by J. L. Van Hemmen and I. Morgenstern (Springer-Verlag, Berlin, 1983).

[5]K. Binder and A. P. Young, Phys. Rev. B **29**, 2864 (1984).

[6]A. P. Young, J. Phys. C **17**, L517 (1984).

[7]A. J. Bray and M. A. Moore, J. Phys. C **17**, L463 (1984).

[8]W. F. McMillan, Phys. Rev. B **30**, 476 (1984).

[9]H. Vogel, Physik. Z. **22**, 645 (1921); G. S. Fulcher, J. Am. Ceram. Soc. **8**, 339 (1925).

[10]R. N. Bhatt and A. P. Young, preceding Letter [Phys. Rev. Lett. **54**, 924 (1985)].