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Critical behavior of the three-dimensional Ising spin glass

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The three-dimensional nearest-neighbor Ising spin-glass model with Gaussian bonds ($\langle J^2\rangle = 1$) is studied numerically using the "large-cell" renormalization group. Estimates for the critical coupling and the thermal exponent are $K_c = 1/T_c = 1.2 \pm 0.1$ and $y_t = 1/\nu = 0.30 \pm 0.05$, respectively.

The question of whether a three-dimensional spin glass with short-ranged interactions can exhibit a phase transition is a long-standing one. Until recently the theoretical consensus, based on high-temperature series,[1] exact transfer-matrix studies[2] and expansions around mean-field theory[3] was that the "lower critical dimension" d^* for spin glasses is probably four. This consensus has been weakened, however, by recent numerical work[4–7] suggesting the existence of a transition in the three-dimensional Ising spin glass. In Ref. 4, referred to as I, the "defect energies" of finite systems were used to infer the flow of the distribution of coupling constants at zero temperature under a transformation of the length scale. This is essentially a realization of the "large-cell renormalization group" (LCRG)[8] for Ising spin glasses. It was found that the system scales towards weak coupling for dimension $d = 2$, but towards strong coupling for $d = 3$, implying a phase transition for Ising glasses for $d = 3$ but not for $d = 2$. Identical conclusions were reached by McMillan,[5] whose "domain-wall renormalization group" is a variant of the LCRG.

In this Rapid Communication the LCRG is extended to finite temperatures in order to estimate the critical temperature T_c and the thermal exponent $y_t (= 1/\nu$, where ν is the correlation length exponent) for Ising spin glasses in three dimensions. The Hamiltonian is

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

where the nearest-neighbor couplings $\{J_{ij}\}$ are independent random variables drawn from a Gaussian distribution of unit width ($\langle J_{ij}^2\rangle = 1$), and the spins are located at the sites of a simple cubic lattice. In the LCRG a new distribution of couplings, appropriate to length scale L, is derived by computing the "defect free energies" for an ensemble of blocks of linear dimension L. The basic geometry is illustrated in Fig. 1. Periodic boundary conditions are imposed in the y and z directions. The spins on the two free boundaries are fixed either all up ($\uparrow\uparrow$) or up on one boundary and down on the other ($\uparrow\downarrow$). (This is "gauge equivalent" to the boundary conditions described in I, where the boundary spins are fixed randomly.)

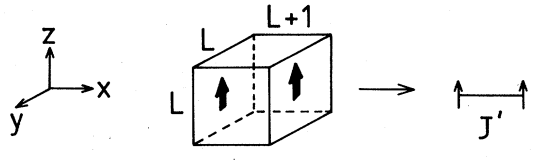

FIG. 1. Basic cell for the large-cell renormalization-group transformation.

The coupling across the block is mediated by the $L^2 \times (L-1)$ interior spins. The renormalized coupling K' for this particular sample, at a particular temperature T, is given by

$$K' = J'/T = (\tfrac{1}{2})\ln(Z_{\uparrow\uparrow}/Z_{\uparrow\downarrow}),$$

$$Z_{\uparrow\uparrow(\uparrow\downarrow)} = \mathrm{Tr}_{\uparrow\uparrow(\uparrow\downarrow)} \exp\left(\sum_{\langle i,j\rangle} K_{ij} S_i S_j\right) \ .$$

Here, the $K_{ij} = J_{ij}/T$ are the coupling constants in the block and the trace is over the $L^2(L-1)$ interior spins for the boundary conditions ($\uparrow\uparrow$ or $\uparrow\downarrow$) indicated. Hence, J' is one-half of the free-energy difference between $\uparrow\downarrow$ and $\uparrow\uparrow$ boundary conditions, i.e., one-half of the defect free energy for the block. This procedure is repeated for a large number of independently generated samples in order to build up a distribution $P_L(K')$ of coupling constants at length scale L. The spin traces are computed exactly using the transfer-matrix technique.[2] This requires of order 2^{L^2} operations per sample, and storage for an array of 2^{L^2} elements, limiting the sample size to $L \leq 4$. The computations are repeated, using a new set of samples, for each new temperature T. The number of samples used per temperature point was 600 000 for $L = 2$, 30 000 for $L = 3$, and 1600 for $L = 4$. As a measure of the effective coupling K_L at a given temperature we adopt the rms value $K_L = \langle K'^2\rangle_L^{1/2}$, where the average $\langle\ \rangle_L$ is over all samples of linear dimension L. The function $K_L(K)$, where $K = 1/T$ is the rms value of K_{ij} for the bare distribution, defines the "cell-to-bond" RG transformation for the LCRG.[8] The implicit equation $K_L(K) = K_{L'}(K)$ defines the cell-to-cell transformation between cell sizes L and L'.[8] [Note that the cell-to-bond RG is the special case $L' = 1$ of the cell-to-cell RG: for $L = 1$ the system reduces to a single bond, giving $K_1(K) = K$].

A subset of the data in the range $0.7 < K \leq 1.4$ is presented in Fig. 2. The error bars shown on the $L = 4$ data are statistical noise due to finite sampling; for $L = 2, 3$ the errors are smaller than the sizes of the points. Estimates for the critical coupling $K_c (= 1/T_c)$ and the thermal exponent $y_t (= 1/\nu)$ for given L and L' are obtained from the fixed point K^* of the RG transformation and from the derivatives at the fixed point, in the usual way:

$$K_L(K^*) = K_{L'}(K^*) \ ,$$

$$K_c^{L,L'} = K^* \ ,$$

$$y_t^{L,L'} = \ln[K_L'(K^*)/K_{L'}'(K^*)]/\ln(L/L') \ ,$$

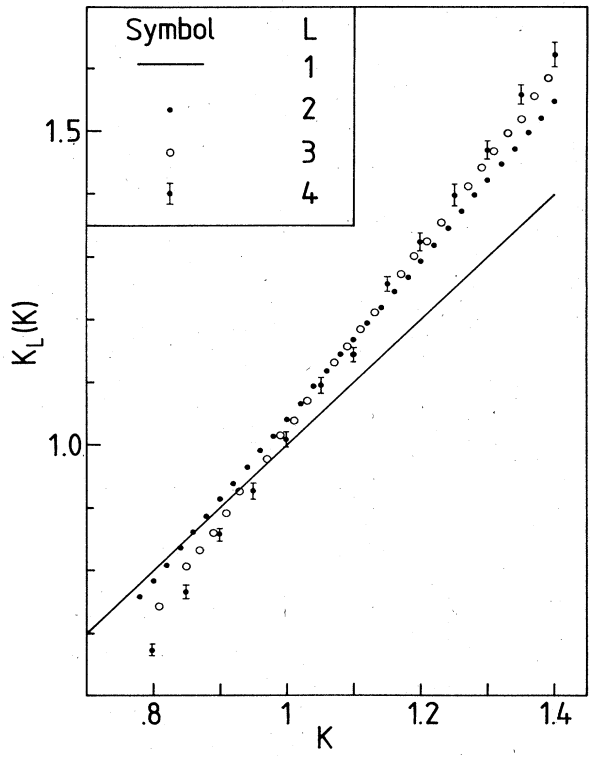

FIG. 2. LCRG transformation functions $K_L(K)$ for $1 \leq L \leq 4$. About half of the $L = 3$ data has been omitted for the sake of clarity.

where $K_L'(K)$ indicates the derivative dK_L/dK. The functions $K_L(K)$ were obtained by least-squares fitting of parabolas to the data points. (Fitting higher-order polynomials gave no significant improvement in the fits.) Results for $K_c^{L,L'}$ and $y_t^{L,L'}$ for $1 \leq L' < L \leq 4$, are presented in Table I.

In the limit $L \to \infty$ all LCRG estimates should converge to the exact result. The problem is how to extrapolate from the rather small values of L available here. Finite-size scaling suggests[9] that the sequence $y_t^{L,1}$ converges only logarithmically, $y_t^{L,1} - y_t^{\infty,1} \sim (\ln L)^{-1}$, while the sequence $K_c^{L,1}$ converges as $K_c^{L,1} - K_c^{\infty,1} \sim L^{-y_t}$. Accelerated convergence should be obtained by comparing successive cell sizes,[8] i.e., by using the sequences $y_t^{L,L-1}, K_c^{L,L-1}$. Unfortunately, due to the statistical noise in the data, the uncertainties on $y_t^{L,L-1}, K_c^{L,L-1}$ are larger than those on $y_t^{L,1}, K_c^{L,1}$, as is evident from Table I. Taking account of all the data, we estimate

$$K_c = 1.2 \pm 0.1 \ , \tag{1}$$

$$y_t = 0.30 \pm 0.05 \ . \tag{2}$$

The value of K_c is comparable to that obtained by McMillan (Ref. 5), $K_c = 1.0 \pm 0.2$. Comparison with the K_c obtained by Ogielski and Morgenstern[6] (OM) and Bhatt and Young[7] (BY) is not meaningful, as these authors used the $\pm J$ model which has a different K_c, but is expected to have the same y_t.

The value of ν implied by (2), $\nu = y_t^{-1} = 3.3 \pm 0.6$ is, however, significantly larger than the value obtained by McMillan[5] ($\nu = 1.8 \pm 0.5$), OM ($\nu = 1.12 \pm 0.12$) or BY ($\nu = 1.3 \pm 0.3$). The reason for the discrepancy is not clear. McMillan's domain-wall RG (DWRG) is similar in spirit to the LCRG except that the effective coupling J' is obtained from the free-energy difference between a system with fully periodic boundary conditions and the same system with antiperiodic boundary conditions in one direction. McMillan uses Monte Carlo simulation rather than transfer matrices to find J', and uses fewer systems (≤ 1000) per temperature point. Thus, while McMillan's data cover a wide range of L ($3 \leq L \leq 6$), the errors on the individual data points must be considerably larger than in the present work. The results of OM and BY are both based on Monte Carlo simulation, OM inferring values of T_c and ν from a direct computation of the spin-glass correlation function, BY combining a computation of the spin-glass susceptibility with a finite-size scaling analysis for systems with linear dimension $L \leq 20$.

In an attempt to understand the discrepancy between our result for ν and those of OM and BY we have also applied the LCRG to the $\pm J$ model (defined by $P(J_{ij}) = \frac{1}{2} \times [\delta(J_{ij} - J) + \delta(J_{ij} + J)]$). The results are less consistent for this model due to significant "even-odd" effects which are not present for the Gaussian model. Nevertheless, the data do suggest that the transition temperature for $\pm J$ model is somewhat lower than the value $T_c/J = 1.22 \pm 0.4$ quoted by OM. The estimates for $K_c \equiv J/T_c$ obtained from the 2/1, 3/1, 4/1, 3/2, 4/2, 4/3 RG transformations are 0.62, 0.70, 0.75, 0.99, 0.93, 0.90, respectively. As a result of even-odd effects, this sequence is nonmonotonic, in contrast to the equivalent sequence for the Gaussian model (Table I), but does suggest an extrapolated K_c somewhat larger than the OM value 0.82. Fitting the OM data for the correlation length with a smaller T_c would necessarily give a larger value of ν.[10] Unfortunately the direct estimates for $y_t = 1/\nu$ obtained from the LCRG for the $\pm J$ model have large fluctuations due to the even-odd effects.

In conclusion, the large-cell method has been applied to the three-dimensional Ising spin glass. The critical exponent ν is found to be significantly larger than that obtained by other methods using Monte Carlo simulations. The present method has the advantage that the spin traces are carried out exactly, whereas Monte Carlo methods have potential equilibration problems and statistical noise due to finite simulation times in addition to that associated with sample averaging. The only limitation of the present method is the restriction to relatively small cells.

TABLE I. LCRG estimates for K_c and y_t.

L/L'	2/1	3/1	4/1	3/2	4/2	4/3
K_c	0.852 ± 0.001	0.947 ± 0.002	0.986 ± 0.006	1.097 ± 0.005	1.105 ± 0.015	1.12 ± 0.04
y_t	0.364 ± 0.003	0.347 ± 0.004	0.342 ± 0.014	0.32 ± 0.01	0.31 ± 0.03	0.29 ± 0.07

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