Domain-wall renormalization-group study of the three-dimensional random Ising model at finite temperature

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The three-dimensional random Ising model with a Gaussian distribution of nearest-neighbor interactions is studied for the pure spin-glass case where the average interaction vanishes. The distribution of domain-wall free energies at finite temperature is calculated with the use of the Metropolis Monte Carlo algorithm for finite lattices. A renormalization-group transformation is set up which preserves the domain-wall free-energy distribution when the lattice parameter is changed. The spin-glass transition temperature is found to be $T_g=(1.0\pm0.2)\tilde{J}$ where $\tilde{J}$ is the variance of the Gaussian interaction distribution. The thermal exponent is $\nu=1.8\pm0.5$ and the heat-capacity exponent is $\alpha=-3.4\pm1.5$. The heat capacity exhibits a rounded peak at higher temperatures.

I. INTRODUCTION

In a previous paper[1] the domain-wall renormalization-group (DWRG) method[2] has been applied to the three-dimensional random Ising model in the strong-coupling regime. A Monte Carlo—quench algorithm was used to calculate the variance of the distribution of domain-wall energies at zero temperature. It was found that the model iterates toward strong coupling and therefore exhibits a spin-glass phase transition at nonzero temperature. Bray and Moore,[3] using similar methods, have independently reached the same conclusion. In this paper we study the model at finite temperature using the same DWRG method but with the Metropolis Monte Carlo algorithm to calculate the variance of the domain-wall free-energy distribution.

II. NUMERICAL METHODS

The model is the cubic, nearest-neighbor Ising model with a Gaussian distribution of interactions with zero mean and variance $\tilde{J}$. The DWRG method requires that one be able to calculate the variance of the distribution of domain-wall free energies for finite lattices. A cubic lattice of n^3 sites with periodic boundary conditions is used; introduction of antiperiodic boundary conditions in one direction inserts a domain wall. The energy of the domain wall for a particular configuration of interactions is

$$E_n(T)=E_n^a(T)-E_n^p(T)\ , \tag{1}$$

where $E_n^a(T)$ and $E_n^p(T)$ are the thermodynamic energy of the finite lattice with periodic (p) or antiperiodic (a) boundary conditions. We calculate the thermodynamic energies using the Metropolis Monte Carlo method[4] with Glauber dynamics.[5] The calculation is repeated for N configurations of interactions; this yields N samples of the domain-wall energy from which we estimate the variance $\tilde{E}_n(T)$ of the energy distribution. We perform the Monte Carlo average over M updates per spin and there are thermal fluctuations of the energies due to the finite averaging time. The variance $\tilde{E}_n(T)$ squared converges as $1/M$ and we fit this form to the variance squared for finite M and extrapolate M to infinity. In this way we find the variance of the domain-wall energy distribution for temperatures $T\geq0.7\tilde{J}$; we use 1000 interaction configurations for $n=3$—5 and 100 configurations for $n=6$. We then use the thermodynamic relationship between energy and free energy to find the variance of the domain-wall free-energy distribution versus temperature. We also use the Monte Carlo—quench algorithm[1] to find $\tilde{E}_n(0)$ for the same set of interaction configurations. This establishes the temperature dependence of the free-energy variance with sufficient accuracy; a larger number of interaction configurations was used in the earlier work at zero temperature and we use that data to scale the present data to provide a more accurate absolute magnitude for the free-energy variance.

III. RESULTS

The DWRG method compares two systems, the first with n^3 sites, lattice parameter a, length $L=na$ and Hamiltonian parameter $\tilde{J}$, and the second with $(n')^3$ sites, lattice parameter $a'>a$, length $L=n'a'$, and Hamiltonian parameter $\tilde{J}'$. The variances of the domain-wall free energies are required to be equal,

$$\tilde{W}_{n'}(\tilde{J}',T)=\tilde{W}_n(\tilde{J},T)\ , \tag{2}$$

at the same temperature T and (2) is the implicit recursion relation relating $\tilde{J}'$ to $\tilde{J}$ for a lattice-parameter change from a to a'.

We now use standard renormalization-group arguments together with (2) to find the fixed point and the thermal exponent. We find the critical temperature to be $T_g=(1.0\pm0.2)\tilde{J}$ and the thermal exponent to be $\nu=1.8\pm0.5$. The uncertainties arise primarily from the

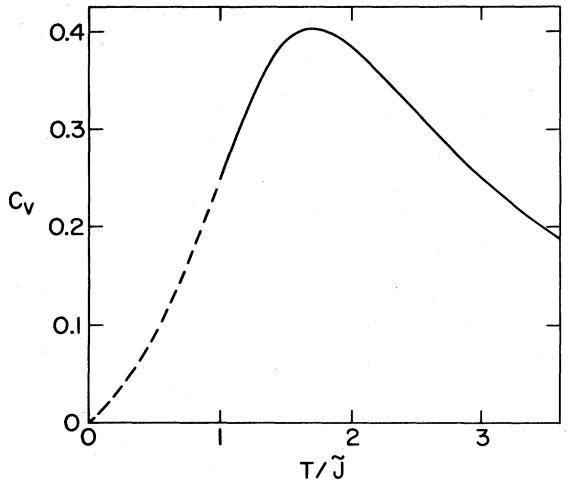

FIG. 1. The heat capacity versus temperature for the random Ising model with 5^3 sites as obtained from the Monte Carlo simulation. The dashed portion of the curve at low temperature is obtained by interpolation as described in the text.

uncertainties in the zero-temperature data rather than from the finite-temperature corrections. The heat-capacity exponent is $\alpha=2-3$, $\nu=-3.4\pm1.5$.

The heat capacity C_V from the Monte Carlo simulation is shown in Fig. 1 for the 5^3 lattice. For $T>\tilde{J}$ the heat capacity is found by differentiating the thermodynamic energy. The accuracy of the Monte Carlo data deteriorates below $T=\tilde{J}$ as the relaxation times become long. We estimate the heat capacity for $0<T<\tilde{J}$ in the following way. We fit the energy difference between zero temperature and $T=\tilde{J}$ as well as the heat capacity at $T=\tilde{J}$ using the expression $C_V=AT+BT^2$; we find $A\cong0.1/\tilde{J}$ and $B\cong0.15/\tilde{J}^2$. This region is shown as the dashed line in Fig. 1. The random Ising-model heat capacity is qualitatively similar to the heat capacity of $Cu_{1-x}Mn_x$ measured by Fogle, Ho, and Phillips.[6] However, the random Ising-model heat-capacity peak is sharper than that for $Cu_{1-x}Mn_x$ and falls off more rapidly at high temperature. The ratio of the glass temperature to the temperature of the heat-capacity peak is 0.6 for the random Ising model with six nearest neighbors and 0.7 for $Cu_{1-x}Mn_x$.[7]

IV. CONCLUSIONS

We conclude that the three-dimensional random Ising model exhibits a spin-glass phase transition at a temperature somewhat below the temperature of the heat-capacity peak with a very weak thermodynamic singularity. From the arguments presented in the scaling theory[8] and the very small zero-temperature eigenvalue,[2] we conclude, however, that the de Almeida—Thouless transition[9] is a glass transition, not a phase transition.

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[1]W. L. McMillan, Phys. Rev. B **30**, 476 (1984).
[2]W. L. McMillan (unpublished).
[3]A. J. Bray and M. A. Moore (unpublished).
[4]N. Metropolis, A. W. Rosenbluth, M. N. Metropolis, A. H. Teller, and E. Teller, J. Phys. Chem. **21**, 1087 (1953).
[5]R. J. Glauber, J. Math. Phys. **4**, 294 (1963).
[6]W. H. Fogle, J. C. Ho, and N. E. Phillips, J. Phys. (Paris) Colloq. **39**, C6-901 (1978).
[7]D. L. Martin, Phys. Rev. B **21**, 1902 (1980).
[8]W. L. McMillan, J. Phys. C (to be published).
[9]J. R. L. de Almeida and D. J. Thouless, J. Phys. A **11**, 983 (1978).