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Monte Carlo simulation of the fcc antiferromagnetic Ising model

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Monte Carlo methods are employed to measure the internal energy, sublattice magnetization, and spin-spin correlation function of the fcc antiferromagnetic Ising model as a function of temperature. The internal energy of both the ordered and disordered phases is fitted by appropriate series expansions, and the free energy is obtained analytically from the series. The ordering transition is seen to be of first order with a transition temperature of 1.736 ± 0.001 in units of the nearest-neighbor coupling J. These results are compared with earlier approximations of the model, in particular, the low-temperature series expansion and the Kikuchi tetrahedron approximation, and other Monte Carlo results. The spin-spin correlation function was measured in the disordered phase up to eight lattice spacings in the [100] direction. The correlation length at the transition is found to be $\sim 2.5a$. The behavior of the correlation length is approximately mean-field-like.

I. INTRODUCTION

There has been considerable effort expended recently toward understanding the behavior of the order-disorder transition in CuAu. The fcc antiferromagnetic Ising model is particularly relevent to this understanding. Recent work includes extension of the Kikuchi cluster variation method to large clusters,[1-3] extension of the low-temperature series expansion to five terms,[4] and Monte Carlo measurements in the neighborhood of the transition.[5-8] This paper presents the thermodynamic functions of the model determined from Monte Carlo measurements. In addition the spin-spin correlation function has been measured yielding correlation lengths in the disordered phase.

The Ising model of interest is defined by the Hamiltonian

$$H = J \sum_{\langle ij \rangle} \sigma_i \sigma_j \ ,$$

where $J > 0$, $\sigma_i = \pm 1$, and the sum is over nearest neighbors of the fcc lattice. This is the zero-field nearest-neighbor antiferromagnetic Ising model. We wish to know the free energy of this model for temperatures near the order-disorder transition. The Monte Carlo method allows us to measure the internal energy of the model over a wide range of temperatures. Then we can calculate the free energy from a basic thermodynamic relation.

In practice the internal energy data are fitted to a power series in the temperature and the free energy is calculated analytically from the power series. The free energy of the ordered phase and the disordered phase are calculated separately. The first-order phase transition occurs at the temperature at which the free energies of the two phases are equal. This method is similar to one employed by Binder[8] on the next-neighbor fcc antiferromagnetic Ising model in nonzero magnetic field.

Sections II and III describe the determination of the free energy of the ordered and disordered phases, respectively. The correlation function fitting procedure is described in Sec. IV. Section V describes the Monte Carlo procedure. The results are presented in Sec. VI.

II. FREE ENERGY OF THE ORDERED PHASE

Slawny[9] and MacKenzie and Young[4] have shown that the free energy of this model in the low-temperature limit is given by the free energy of the β phase. The β phase (defined by Danielian[10,11]) at $T=0$ is a ground state of maximum symmetry and consists of two spin-up and two spin-down cubic sublattices of the fcc lattice. (An fcc lattice with lattice constant a may be formed from four cubic sublattices of lattice constant a.) This phase is equivalent to L_{10} ordering and, more specifically, the structure of CuAuI.

The free energy per spin $F_{\rm LT}$ of the β phase in the low-temperature (LT) limit is given by the series expansion

$$-\beta F_{\rm LT} = -\beta E_0 + \sum_i a_i x^{i+1} \ ,$$

where $x = \exp(-4\beta J)$, $\beta = 1/k_B T$, and $E_0 = -2J$ is the ground-state energy per spin. The first five coefficients have been calculated.[4]

The internal energy per spin U may be determined from the thermodynamic relation

$$U = \frac{\partial(\beta F)}{\partial \beta} \ ,$$

yielding the low-temperature–series form

$$U_{\rm LT} = E_0 + 4J \sum_i b_i (i+1) x^{i+1} \ .$$

We have measured the internal energy of this system via Monte Carlo methods over the temperature range $T = 1.00J - 1.76J$ and find that the low-temperature series expansion and the Monte Carlo measurements disagree for temperatures greater than $\sim 1.3J$. The internal energy data are fitted to a series of the form

$$U_{\rm fit} = E_0 + 4J \sum_i b_i (i+1) x^{i+1} \ .$$

The series is integrated from $T = J$ to obtain the free energy

$$-\beta F_{\rm fit} = -\beta E_0 + \sum_i b_i x^{i+1} + \text{const} \ .$$

The constant is evaluated by setting $F_{\rm fit}(T=J) = F_{\rm LT}(T=J)$.

III. FREE ENERGY OF THE DISORDERED PHASE

The free energy of the disordered phase is determined in a manner similar to that for the ordered phase. The high-temperature series expansion of Sykes[12] is of the form

$$-\beta F_{\mathrm{HT}} = \ln(2) + 6\ln[\cosh(K)] + \sum_i a_i [\tanh(K)]^i \ ,$$

where HT denotes high temperature, and

$$U_{\mathrm{HT}}/J = 6\tanh(K) + \sum_i b_i [\tanh(K)]^i \ ,$$

where $K = -\beta J$ and $b_i = (i+1)a_{i+1} - (i-1)a_{i-1}$. Coefficients have been calculated up to a_{14}.[12]

The measured internal energy agrees with this expansion only for temperatures greater than $20J$. Therefore, we have made measurements over the temperature range $1.74J$–$50J$ and fitted the data to

$$U_{\mathrm{fit}}/J = 6\tanh(K) - \sum_i d_i [\tanh(K)]^i \ .$$

Upon integration we have

$$-\beta F_{\mathrm{fit}} = 6\ln[\cosh(K)] + \sum_i c_i [\tanh(K)]^i - \mathrm{const} \ ,$$

where $d_i = (i+1)c_{i+1} - (i-1)c_{i-1}$ and the constant is determined by setting $F_{\mathrm{fit}}(T = 50J) = F_{\mathrm{HT}}(T = 50J)$.

IV. SPIN-SPIN CORRELATIONS

The spin-spin correlation function has been measured in the disordered phase for spins separated along the [100] axis by distances up to $8a$. The correlation function may be written as

$$G(R,T) = \frac{D(R/\xi_T)}{R^{1+\eta_T}} \ ,$$

where ξ_T is the correlation length. The form of the function $D(R/\xi_T)$ is chosen so as to correctly describe the large-R behavior. We write

$$D(R/\xi_T) = \sum_{k=1}^{3} D_k e^{-kR/\xi_T} \ .$$

All of the correlation data are fitted to $G(RT)$ simultaneously, yielding $\xi(T)$, $\eta(T)$, and the scaled function $D(x)$.

V. MONTE CARLO METHOD

The Monte Carlo method is performed on the fcc nearest-neighbor antiferromagnetic Ising model. The lattice consists of four cubic sublattices each containing $16\times16\times16$ sites for a total of 16 384 sites. The boundary conditions applied to each sublattice are skew periodic, i.e., periodic along the x and z axes and periodic but shifted by $a\hat{x}$ along the y axis. The initial condition of the lattice is either the ordered β phase or the disordered phase depending upon the phase to be measured.

A combination of bit logic and an array processor allows the processing of many sites essentially simultaneously. Thus it is necessary to find sets of sites upon which Monte Carlo dynamics may be legitimately performed simultaneously. For the fcc lattice, the four cubic sublattices are such sets. The Metropolis spin-flip method[13] is employed to update the state of every site in a given sublattice. Each of the sublattices is updated in turn so that after four steps all of the sites of the lattice have been updated once; i.e., one Monte Carlo step per site (MCS). At this point, the internal energy, sublattice magnetization, and spin-spin correlations are measured. At each temperature the first 500 MCS are discarded to ensure equilibration. Then the measured values are averaged over 2000 MCS. For the spin-spin correlations, 20 sets of 1000 MCS were averaged after discarding the first 1000 MCS.

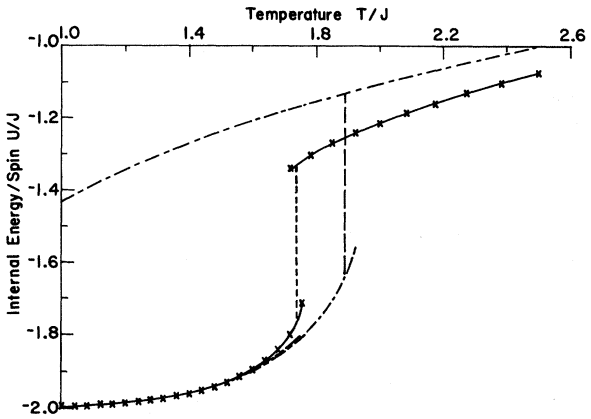

FIG. 1. Internal energy per spin of the nearest-neighbor fcc Ising antiferromagnetic in zero field plotted vs temperature. ×, Monte Carlo data; ——, series expansion fit to data; – – –, Monte Carlo transition; – – – –, low-temperature series expansion; – – –, Kikuchi tetrahedron approximation; — —, Kikuchi transition.

At temperatures near the transition, finite-size effects become important. Binder[14] indicates that the internal energy scales as

$$U_L = U_\infty + Ae^{-L/b\xi_T} \ ,$$

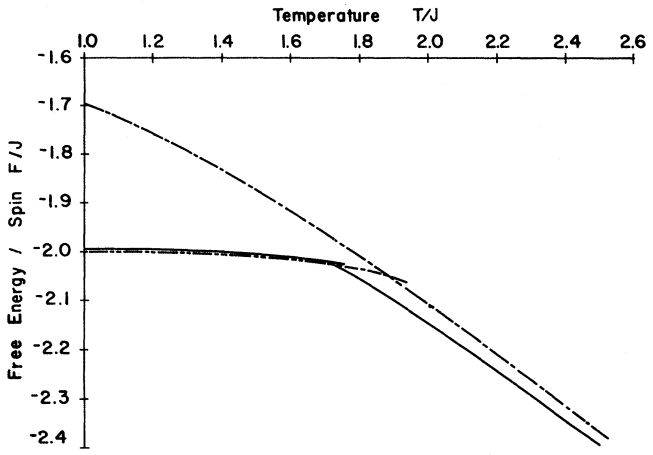

FIG. 2. Free energy per spin of the nearest-neighbor fcc Ising antiferromagnet in zero field plotted vs temperature. Results of the Kikuchi method, low-temperature series expansion, and the current Monte Carlo method for the low-temperature phase are indistinguishable at this scale. ——, analytic function from data; – – – –, low-temperature series expansion; – – –, Kikuchi tetrahedron approximation.

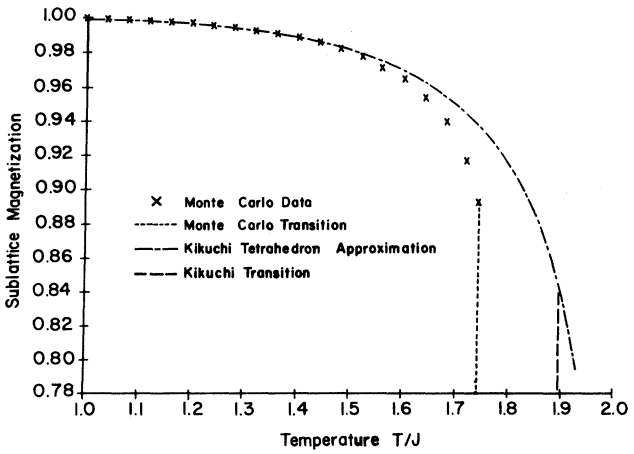

FIG. 3. Sublattice magnetization of the nearest-neighbor Ising antiferromagnet in zero field plotted vs temperature. ×, Monte Carlo data; ----, Monte Carlo transition; – – –, Kikuchi tetrahedron approximation; – – –, Kikuchi transition.

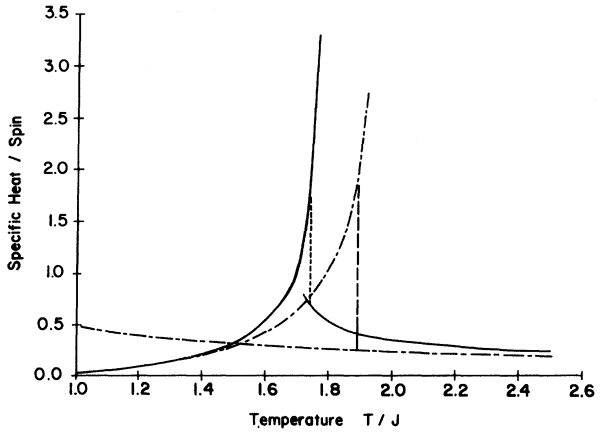

FIG. 5. Specific heat per spin of the nearest-neighbor Ising antiferromagnet in zero field plotted vs temperature. ——, analytic function from data; ----, Monte Carlo transition; – – –, Kikuchi tetrahedron approximation; – – –, Kikuchi transition.

where U_L is the internal energy measured on a lattice of linear dimension L, U_∞ is the internal energy in the thermodynamic limit, and A and b are scaling factors to be determined. For $T/J = 1.8$, using $L = 12$, 16, 24, and 32, the scaling factors were found to be $A \sim -0.24$ and $b \sim 1.25$. (Here we used our value of $\xi_{T=1.8} \sim 2.3a$.) Therefore, in order to determine the transition temperature to within $T/J \sim 0.001$, it is necessary and sufficient to use $L = 32$ whenever $\xi_T > 1.6a$. This occurs in the region $1.6 \leq T/J \leq 2.0$. For these temperatures, the internal energy was averaged over 900 MCS after discarding 100 MCS on an $L = 32$ lattice.

VI. RESULTS AND DISCUSSION

The measured internal energy is plotted in Fig. 1. The internal energies of the low-temperature series expansion and the Kikuchi tetrahedron approximation are included for comparison. Figure 2 presents the calculated free energy along with the low-temperature series expansion and Kikuchi tetrahedron approximation free energies. The first-order phase transition occurs at $K_B T/J = 1.736 \pm 0.001$ compared with the Kikuchi[15] result of 1.89. Using Monte Carlo data, Phani *et al.*[6] report a transition at $K_B T/J \sim 1.76$. Our studies indicate that this is most likely the superheating point of the β phase and not the first-order transition.

The sublattice magnetization of the β phase is plotted in Fig. 3 along with the Kikuchi tetrahedron result. Finally, the entropy and specific heat are shown in Figs. 4 and 5, respectively.

The failure of both the low-temperature series expansion and the Kikuchi method is understood in terms of the correlation length which is shown in Fig. 6. Both methods rely on clusters of "length" less than a. Even for $T/J > 3$,

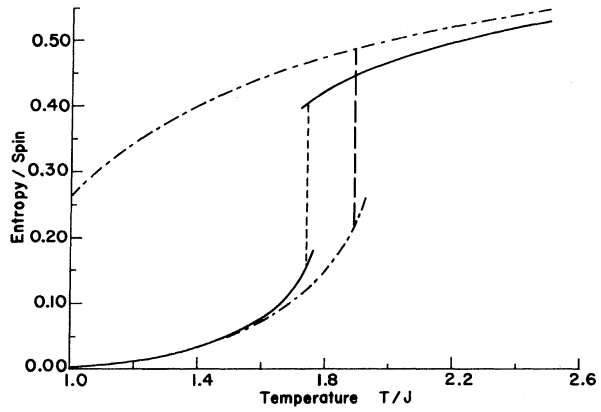

FIG. 4. Lattice entropy per spin of the nearest-neighbor Ising antiferromagnet in zero field plotted vs temperature. ——, analytical function from data; ----, Monte Carlo transition; — - —, Kikuchi tetrahedron approximation; — —, Kikuchi transition.

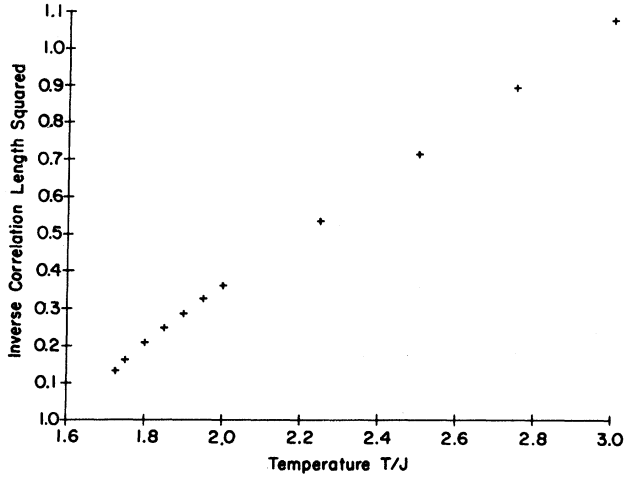

FIG. 6. Inverse correlation length squared for the disordered phase in units of $1/a^2$ plotted vs temperature.

the correlation length is greater than a, and therefore clusters exist which are too large for either method. It is not reasonable to expect that adding a few more terms to either of the methods will result in significant improvement.

It is presently assumed that there exists a multicritical point when a next-nearest-neighbor coupling is added to this model. The multicriticality should drive the upper critical dimension below $d=3$. Therefore mean-field behavior is warranted in the neighborhood of the multicritical point. Our correlation-length measurements (see Fig. 6) are carried out at a zero value of the next-nearest-neighbor coupling. However, for temperatures greater than the measured first-order transition temperature, the correlation length exhibits mean-field temperature dependence as follows:

$$\xi_T \sim (T - T_c)^{-0.5}, \quad T_c \sim 1.5J \ .$$

Work is in progress to measure the correlation length in the immediate neighborhood of the multicritical point.

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