Stability of the tricritical point in a three-dimensional next-nearest-neighbor Ising antiferromagnet: A Monte Carlo simulation

H. J. Herrmann and D. P. Landau*
HLRZ, Forschungszentrum Jülich, Postfach 1913, D-5170 Jülich, Germany
and Center for Simulational Physics, University of Georgia, Athens, Georgia 30602
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We investigate via Monte Carlo simulations the multicritical behavior of Ising antiferromagnets in three dimensions. Even for ratios between the intrasublattice and intersublattice couplings as small as $R=0.05$, we find tricritical behavior and no evidence for a decomposition into a critical end point and a double critical end point as predicted by mean-field theories.

INTRODUCTION

Highly anisotropic antiferromagnets with multiple interactions—one between sublattices and another within each sublattice—have magnetic-field-induced phase boundaries that are second order for a range of field and temperature and are first order at very low temperature; the phase transition is generally believed to exhibit tricritical behavior at the point where the order of the transition changes. Existing experimental work[1] has confirmed this picture.

Mean-field calculations—performed as early as 1959 by Motizuki[2]—predict that below a given ratio R of the intra- to intersublattice coupling the tricritical point transforms into two end points of critical lines. This situation is sketched in Fig. 1, where the phase diagram is given as a function of the temperature T, the magnetic field H, and the "staggered" magnetic field h. The usual scenario is the one shown in Fig. 1(a) where three critical lines join at the tricritical point t and the three sheets of first-order transitions that are limited by these critical lines intersect at one (dashed) line of first-order transition that ends at the tricritical point T_t. The unusual situation predicted by mean-field theory to occur at small ratios R of coupling constants is shown in Fig. 1(b). The two symmetric critical lines that go into the direction of the staggered field still join in one point, the double critical end point (DCE), at which the (dashed) line of first-order transitions ends and where all the three sheets meet. The third critical line, however, ends at a different point, the critical end point (CE), which lies on the line of first-order transitions in the H-T plane.

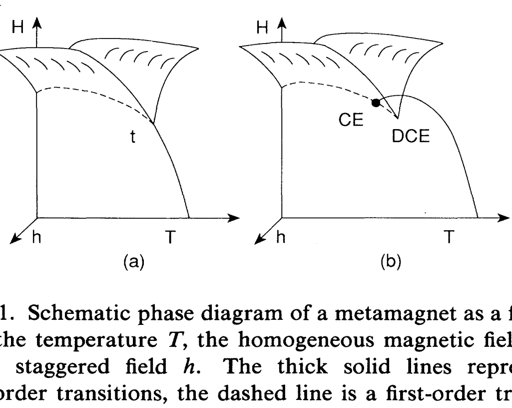

FIG. 1. Schematic phase diagram of a metamagnet as a function of the temperature T, the homogeneous magnetic field H, and the staggered field h. The thick solid lines represent second-order transitions, the dashed line is a first-order transition, and the special points are explained in the text.

Although the situation described in Fig. 1(b) has never been observed experimentally, theoretical and simulational efforts to find such behavior have continued. Mean-field theories have been refined[3] and reviewed in much detail in Ref. 4, in particular for the antiferromagnet Ising model with next-nearest-neighbor (NNN) interactions. This model has also been investigated in two dimensions by a Monte Carlo renormalization group[5] (MCRG) and transfer matrix techniques[6] and while the first technique gave no indication for the decomposition of the tricritical point, the transfer matrix calculations failed to reproduce tricritical behavior at very small ratios R. (This may well have been due to the limited strip widths which could be studied.) In three dimensions an MCRG study[7] of various metamagnetic models including the NNN antiferromagnet yielded results which were inconsistent with the mean-field scenario.

Other models that within the context of mean-field theory show the existence of multicritical points and the subsequent decomposition of Fig. 1(b) are the Ising random-field model[8] and the antiferromagnetic Blume Capel model.[9] The latter was also studied via Monte Carlo simulations and while in two dimensions only tricritical behavior was found,[10] recent three-dimensional results[11] gave clear evidence for the decomposition into a CE and a DCE.

The purpose of this short paper is to present high-quality Monte Carlo data that convincingly exclude the decomposition of the NNN antiferromagnetic Ising model for $R>0.05$ in three dimensions. In the next section we describe the model and the method, we then briefly describe our results, and in the last section we discuss our findings.

MODELS AND METHODS

We consider Ising spins $\sigma_i=\pm1$ on the simple cubic lattice. The system is divided into two interpenetrating sublattices having a ferromagnetic intrasublattice coupling J' and an antiferromagnetic intersublattice coupling

J between the spins. (According to mean-field theory it is only the ratio $R=q'J'/qJ$, where q' is the number of NNN and q is the number of NN neighbors, between the total strength of the two couplings which determines the phase diagram.) The Hamiltonian of this next-nearest-neighbor antiferromagnet (NNNAF) is then

$$\mathcal{H}=J\sum_{\mathrm{NN}}\sigma_i\sigma_j-J'\sum_{\mathrm{NNN}}\sigma_i\sigma_j-H\sum_i\sigma_i\ , \tag{1}$$

where the first sum goes over all six nearest neighbors and the second sum over all twelve next-nearest neighbors of the simple cubic lattice, J, $J'>0$, and H is a homogeneous field. Nearest neighbors belong to different sublattices while next-nearest neighbors belong to the same sublattice. Various studies have been carried out for this model before[12-14] and for $R=1$ the tricritical point was located at $(kT_t/J,H_t)=(6.1,4.9)$.

The mean-field predictions for this model[3,4] are the following: For $R>\frac{3}{5}$ one expects tricritical behavior as shown in Fig. 1a and the tricritical point has mean field exponents $\alpha_t=\frac{1}{2}$, $\beta_t=\frac{1}{4}$, $\gamma_t=1$, and $\lambda_t=\frac{1}{2}$. The order parameter which scales with β_t is the staggered magnetization. Since the upper critical dimension for tricritical points is $d=3$ one expects, in fact, additional logarithmic corrections[15] which may be either multiplicative or additive, depending on the quantity. For $0<R<\frac{3}{5}$ mean-field theory predicts the situation shown in Fig. 1(b) where the CE and DCE have mean-field critical exponents. We suspect that if Fig. 1(b) is qualitatively correct in three dimensions, both the CE and the DCE probably show usual three-dimensional critical behavior, i.e., exponents $\alpha\approx0.11$, $\beta\approx0.32$, and $\gamma\approx1.24$. At $R=\frac{3}{5}$ mean field predicts a fourth-order critical point with exponents $\alpha_4=\frac{2}{3}$, $\beta_4=\frac{1}{6}$, and $\gamma_4=1$.

Using the standard Metropolis Monte Carlo algorithm we simulated lattices of linear sizes L ranging from $L=10$ to $L=61$. Small systems were studied using periodic boundary conditions on an IBM 3090 while data for larger systems were obtained on a Cray-YMP. In the second case the system was stored on the computer as a one-dimensional array and therefore helical boundary conditions were used in two directions and periodic boundary conditions in the third direction. The configurations were thermalized over 500 to 5000 MC steps per site starting either from a ferromagnetic or an antiferromagnetic initial configuration. We averaged over up to 500 configurations separated by 20 to 50 MC steps per site. We measured the magnetization $M=N^{-1}\sum_i\sigma_i$, the staggered magnetization $m=N^{-1}(\sum_{i\,\mathrm{even}}\sigma_i-\sum_{i\,\mathrm{odd}}\sigma_i)$ and the two corresponding susceptibilities χ_M and χ_m calculated from the fluctuations of M and m.

RESULTS

By varying the homogeneous field H on lines of constant temperature we studied the phase transitions of the NN AF for three values of R: 0.5, 0.1938, and 0.05. (The value 0.1938 is special only in that one of the generalizations of the NNN AF studied in Ref. 7 had this unusual ratio.) The resultant phase diagrams are shown in Fig. 2. The transition points were localized by measuring the order parameter m and the homogeneous magnetization M during multiple field sweeps: on one hand increasing H starting with an antiferromagnetic initial configuration and on the other hand decreasing H starting with a ferromagnetic initial configuration. At sufficiently low temperatures strong asymmetric hysteresis is observed characterizing first-order transitions (circles in Fig. 2). The error bars in Fig. 2 in fact show the width of the hysteresis. As the temperature increases the jumps of M and m at this first-order transition decrease. For $R=0.5$ the jump in M decreases linearly while for $R=0.05$ the behavior is clearly nonlinear. The temperature at which the jump seemed to vanish gave us a first guess for the location of the tricritical point. The second-order transitions are shown by crosses in Fig. 2. Note that in none of the phase diagrams of Fig. 2 do we see indications of a splitting into two transition lines as one would expect from the mean-field prediction. Note that mean-field theory predicts that the separation between the critical end point and double critical end-point temperatures is not small: over 5% for $R=0.5$ and 50% for $R=0.05$. It therefore seems likely that only tricritical behavior is present in all of the three figures.

it is also interesting to note that the slope of the transition line in the tricritical region varies substantially for the different values of R considered. While for $R=0.5$ the transition line has negative slope the tricritical region

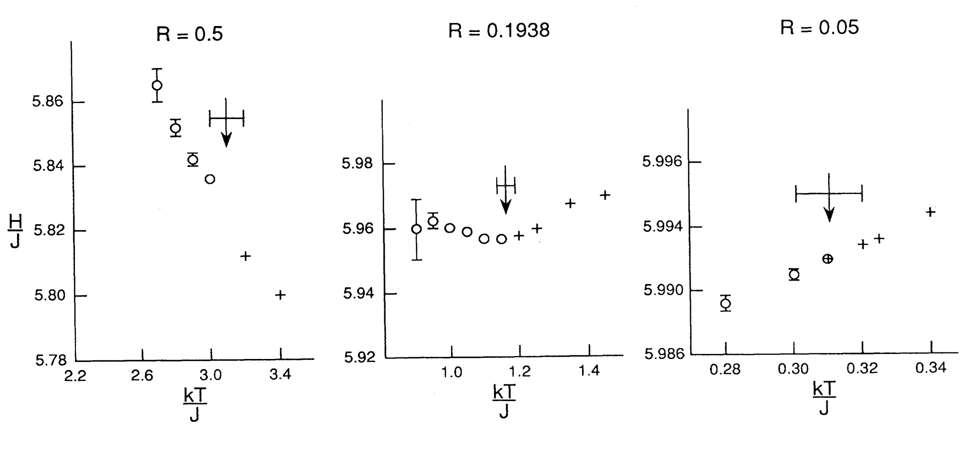

FIG. 2. Phase diagrams in the H-T plane (the staggered field is zero) for three values of R. Circles are first-order transitions and crosses second-order transitions. The arrow indicates the position of the tricritical point. Note that the axis in the three plots have different scales.

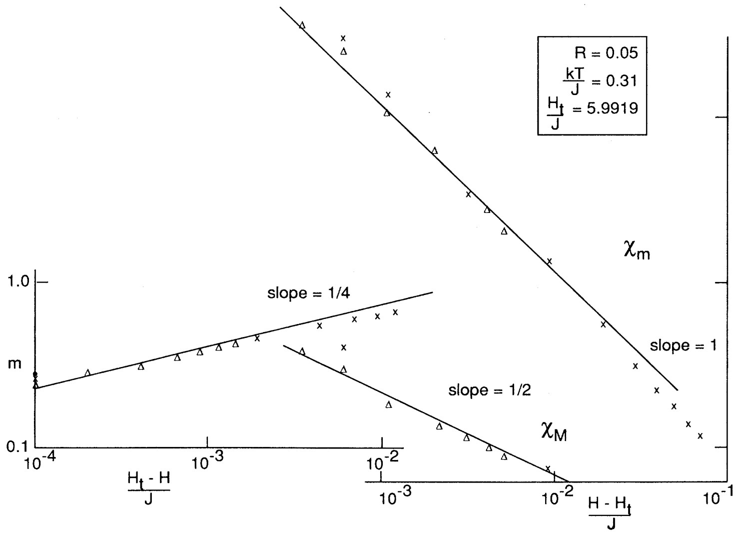

FIG. 3. Log-log plot of the order parameter m and the two susceptibilities χ_m and χ_M as a function of $|H-H_t|$ for $kT_t/J=0.31$, $H_t/J=5.9919$, and $R=0.05$ for two different lattice sizes $L=61$ (triangles) and $L=41$ (crosses). The full lines are guides to the eye of slope $\frac{1}{4}$ for m, of slope -1 for χ_m, and of slope $-\frac{1}{2}$ for χ_M.

just lies within a dip of the line for $T=0.1938$ and for $R=0.05$ the line has a very weak positive slope. (Note that the resolution of the H axis in the third figure is higher than for the other two.)

To further test the conclusion that only tricritical behavior is present, we focused on the smallest ratio of couplings, namely $R=0.05$, since according to mean field it is the most likely candidate for a decomposition into a CE and a DCE. By monitoring the maximum of the ordering susceptibility χ_m for sizes $L=31$, 41, and 61 we located the tricritical point more precisely and found $(kT_t/J, H_t/J)=(0.31, 5.9919)$ (see arrows and error bars in Fig. 2) and studied the critical behavior associated with this point. In the log-log plot of Fig. 3 we examine the data for the staggered magnetization m, the ordering (staggered) susceptibility χ_m and the nonordering (uniform) susceptibility χ_M. All three quantities show power-law behavior only quite near T_t. Below H_t the order parameter m in Fig. 3 lies on a straight line over 1.5 orders of magnitude with an exponent close to $\beta_t=\frac{1}{4}$, i.e. the tricritical value and is definitely smaller than the Ising critical value of ≈ 0.32. The data for the ordering susceptibility χ_m are slightly curved and seem asymptotically to have a slope $\gamma_t=1$ which is the tricritical exponent. Clearly the absolute value of the slope is less than the Ising critical value of 1.24. The curvature in the data away from H_t is likely to be a consequence of logarithmic corrections predicted to occur for tricritical points in three dimensions.[15] The uniform susceptibility has an exponent close to $\lambda_t=\frac{1}{2}$ again consistent with tricritical behavior. The analysis of the critical exponents therefore clearly characterizes a tricritical point thus supporting our previous conclusions.

SUMMARY AND DISCUSSION

We have found that in three dimensions the Ising antiferromagnet with next-nearest-neighbor ferromagnetic interactions has tricritical behavior for quite small intrasublattice coupling, i.e., $R \geq 0.05$. Our Monte Carlo simulations were able to resolve the tricritical region with a precision of 3% in temperature and 0.01% in the homogeneous field. Even if our estimates for the locations of the tricritical points were very slightly in error, data obtained along a path which eventually intersects either the first-order line or the critical line should still show tricritical behavior outside a narrow crossover region. We think that it is, therefore, rather unlikely that the tricritical point decomposes into a critical end point and a double critical end point as predicted by mean-field theory for any value of R. We can, of course, not exclude the possibility that a decomposition of the transition line occurs for even smaller R, but we think that this is very unlikely. In particular, although we might expect that the fluctuations in our model might modify the special R value with respect to the mean field value, it is difficult to see how the reduction could be over an order of magnitude, particularly when the mean-field predictions for the tricritical behavior are relatively intact. Our result is particularly perplexing in light of the recent Monte Carlo study of Ref. 11 which gave convincing evidence for a decomposition of the tricritical point in the antiferromagnetic Blume Capel model in three dimensions. It would certainly be interesting to use Monte Carlo methods to investigate other models which have this same predicted behavior according to mean-field theory, like the layered metamagnet[4] or the random-field Ising model.[8]

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*Permanent address: Center for Simulational Physics, The University of Georgia, Athens, GA 30602.

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