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Tricritical exponents and crossover behavior of a next-nearest-neighbor Ising antiferromagnet*

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Monte Carlo data for a simple cubic Ising antiferromagnet with nearest- and next-nearest-neighbor interactions reveal asymptotic tricritical behavior of the order parameter which is mean-field-like modified by logarithmic corrections and high-temperature susceptibilities which are mean-field-like without corrections, in agreement with renormalization-group calculations. Crossover between tricritical and critical behavior is observed in the temperature variation of the order parameter and high-temperature susceptibility.

I. INTRODUCTION

Theoretical studies by Riedel and Wegner[1,2] showed that the tricritical behavior of a three-dimensional ($d=3$) system with a Gaussian fixed point should be described by mean-field-like exponents modified in some cases by logarithmic corrections. Although subsequent numerical work on the $d=3$ Blume-Capel model[3,4] found mean-field exponents (but was unable to decide the question of logarithmic corrections), studies on Ising antiferromagnets have yielded rather contradictory results. Early Monte Carlo[5] and series-expansion[6] investigations of a simple cubic Ising antiferromagnet with nearest-neighbor (nn) and next-nearest-neighbor (nnn) coupling suggested that the tricritical behavior was *not* mean-field-like. However, similar studies on a simple cubic metamagnet[7,8] indicated that the exponents were indeed, at least in part, mean-field-like. Nelson and Fisher[9] later showed, using renormalization-group theory, that both of these latter antiferromagnetic models should have the same tricritical behavior as the Riedel-Wegner model.

The results of previous numerical work on the nnn model were not really definitive for several reasons. The Monte Carlo studies[5] were made on lattices of limited size and did not include an analysis of finite-size effects. Also, only high-temperature series expansions were available,[6] and although a very careful analysis was made, the determinations of both T_t and the exponents were not totally unambiguous. In fact, Wortis, Harbus, and Stanley[10] later showed that by shifting T_t to a lower temperature and using a standard ratio analysis, one could alter the high-temperature susceptibility exponents to make them compatible with mean-field values.

We have extended our investigation to larger lattices with the identical interactions considered by Harbus and Stanley in hopes of resolving the controversy. We present here results obtained for a system of $s=\frac{1}{2}$ Ising spins arrayed on $N\times N\times N$ simple cubic lattices with periodic boundary conditions and

$$\mathcal{H} = J_{\rm nn} \sum_{\substack{(ij)\\ \text{nn pairs}}} \sigma_i\sigma_j + J_{\rm nnn} \sum_{\substack{(ik)\\ \text{nnn pairs}}} \sigma_i\sigma_k + \mu H \sum_i \sigma_i , \tag{1}$$

where $\sigma_i, \sigma_j, \sigma_k = \pm 1$, $J_{\rm nn} = +1$ (antiferromagnetic), $J_{\rm nnn} = -\frac{1}{2}$ (ferromagnetic), and H is a uniform magnetic field. Lattices with $6 \leqslant N \leqslant 20$ were studied so that finite size effects could be determined and accounted for in the analysis of the critical and tricritical behavior. A minimum of 2000 Monte Carlo steps/spin was generated for each data point and each point was taken at least twice from different starting configurations. Complete details of the calculational method have already been given elsewhere.[11]

II. RESULTS AND DISCUSSION

The determination of the location (H_t, T_t) of the tricritical point is clearly crucial to the investigation of the tricritical behavior of this model. The temperature and field dependence of the mag-

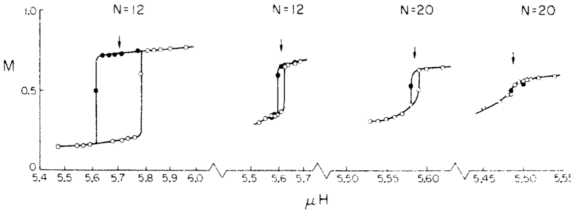

FIG. 1. Magnetization vs magnetic field for several temperatures near $T_t = 6.10$. Open circles are for increasing field, closed circles are for decreasing field. Note the change in the scale for the field between (b) and (c).

netization, internal energy, and specific heat can all be used to locate the phase boundary quite accurately. In addition, near the tricritical point isothermal magnetization (nonordering density) data were used to determine the changeover of the transition from first order to second order as indicated by the disappearance of hysteresis between the data taken at increasing and decreasing field.[12] Data for several different temperatures are shown in Fig. 1. Note the change in scale between Figs. 1(b) and 1(c). Using the results of all the isothermal sweeps for $N=20$ we find $kT_t = 6.05 \pm 0.05$. Data taken on lattices of different sizes show that finite lattice size tends to "smear out" the transition and eliminate hysteresis. This effect becomes more pronounced as the lattice size decreases and the "effective" tricritical temperature (at which hysteresis first occurs) is depressed. We estimate for an infinite lattice $kT_t = 6.10 \pm 0.10$ and $h_t = \mu H_t/kT_t = 0.90 \pm 0.02$. This value of T_t is intermediate between the early series estimate[6] ($kT_t = 6.4 \pm 0.1$) and the early Monte Carlo value for $N=12$ ($kT_t \simeq 6.0$). This value is slightly above the estimate ($kT_t = 5.88 \pm 0.02$) suggested[10] by a reanalysis of the series expansions in which T_t was chosen so that the asymptotic behavior of the ratios was consistent with mean-field exponents. The phase boundary (Fig. 2) shows no depression near T_t as found for the Blume-Capel model.[3] The deviation between the series estimates[6] and the Monte Carlo values begins well above T_t and increases with decreasing temperature.

Data were taken near the second-order phase boundary along paths of constant $h = H/T$ (as in the series expansion studies). The observed behavior of the order parameter (staggered magnetization) is shown in Fig. 3 for a range of h between $h=0$ and $h=h_t$. In zero field the critical behavior is well described by the $d=3$ nn-Ising-model exponent $\beta_c = 0.31$. For small $\epsilon = |1 - T/T_c|$ the effect of finite lattice size is quite important. Below $\epsilon = 5 \times 10^{-3}$ even the values for $N=20$ are "rounded" so as to lie above the infinite lattice value. In terms of the finite size scaling variable[13] $x = \epsilon N^{1/\nu}$, the data for $x \lesssim 0.3$ are affected by finite size rounding. Use of smaller lattice data without correction would clearly lead to an incorrect low estimate of the exponent. The critical region extends to relatively large $\epsilon \lesssim 0.2$, because of the stabilizing effect of the ferromagnetic nnn interaction. (A similar increase in the size of the critical region was found for the nnn square lattice).

As h increases (see Fig. 3), the asymptotic critical exponent remains *unchanged* as predicted by Universality) but the *size* of the critical region

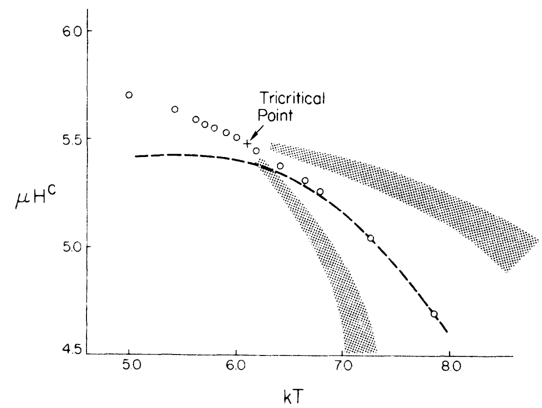

FIG. 2. Phase boundary near the tricritical point. The dashed line gives the series expansion result and the open circles are Monte Carlo data points. The shaded regions give a semiquantitative indication of the crossover regions for $T > T_t$ as determined from the order-parameter and high-temperature χ_{stg} data.

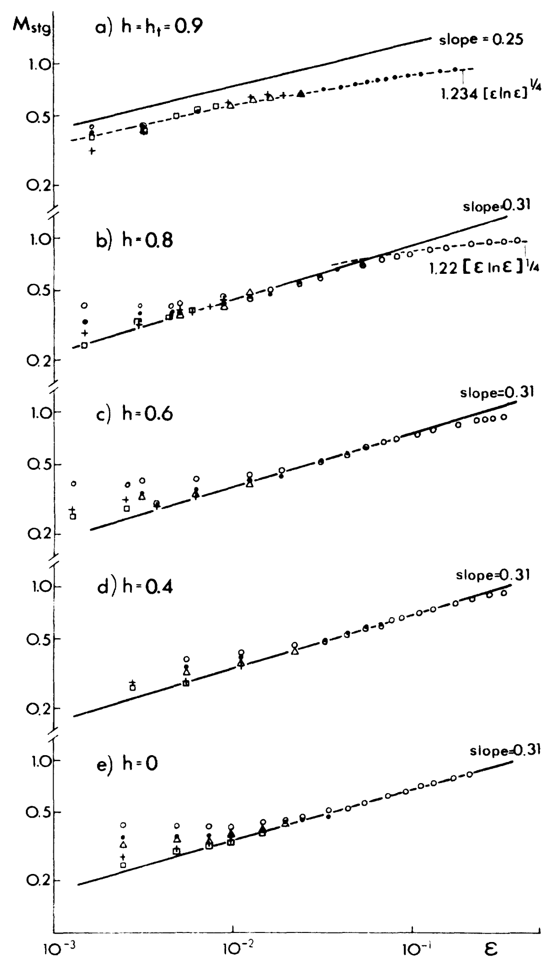

FIG. 3. Order-parameter data: $N=6$, ○; $N=8$, ●; $N=10$, △; $N=14$, +; and $N=20$, □.

shrinks. For $h=0.6$ this effect has become dramatic although the deviation from the critical form is surprisingly gentle. For $h=h_t$ there is no evidence of any critical region, but the data are also *not* consistent with the mean field prediction of $\beta=\frac{1}{4}$. However, by including the multiplicative logarithmic correction suggested by Wegner and Riedel[2] so that

$$M_{stg} \alpha (\epsilon \ln \epsilon)^{1/4}, \tag{2}$$

we can fit the data over the entire temperature range! The curvature in Fig. 3(a) is sufficiently small that over a limited range the behavior could be mistaken for a simple power law with a spuriously low exponent $\beta \approx 0.17$. For h slightly below h_t, see Fig. 3(b), the data for large ϵ are well described by the tricritical form in Eq. (2) and separated from the asymptotic *critical* behavior by a *crossover* region. For $h \lesssim 0.6$ the tricritical region is quite narrow and is obscured by the crossover.

Besides the changeover in exponent as $h=h_t$, there is a dramatic reduction in the finite size "rounding." Since rounding occurs when the scaling variable $x=\epsilon N^{1/\nu}$ becomes small, this suggests that ν decreases as $h \approx h_t$. This is consistent with crossover to the mean field value $\nu_t=\frac{1}{2}$ which is less than $\nu_c=0.64$.

The high-temperature ordering (staggered) and disordering (ferromagnetic) susceptibilities are shown in Figs. 4 and 5 for paths of constant h. For $h=0.4$, the asymptotic critical behavior in χ_{stg} is well described by the $d=3$ Ising exponent $\gamma=1.25$. Here too, finite size effects are pronounced and even for $N=20$, rounding occurs for $\epsilon \lesssim 5\times10^{-3}$. For larger h [see Fig. 4(b)] the crossover from tricritical behavior with $\gamma=1$ at large ϵ to critical behavior with $\gamma=1.25$ for small ϵ becomes clear. When $h=h_t$, the ordering susceptibility is well described over the entire range by $\gamma_t=1.0$! This indicates that the amplitude of the *additive* logarithmic correction predicted by Wegner and Riedel[2] is quite small.

The nonordering susceptibility diverges much more slowly than does the ordering susceptibility and the data analysis is consequently less precise. Nonetheless one can say with some certainty that for low h (see Fig. 5) the asymptotic critical behavior has the form $\chi=C\epsilon^{-\lambda}$ with $\lambda=\alpha=\frac{1}{8}$. For $h=h_t$, the divergence is stronger and, except for deviations for very small ϵ, is well described by the mean-field value $\lambda_t=\frac{1}{2}$. The finite size rounds and broadens the susceptibility peak so that the initial deviation from the infinite lattice curve is in the opposite direction from that found for the ordering susceptibility. Here too, it appears that correction terms are small although the uncer-

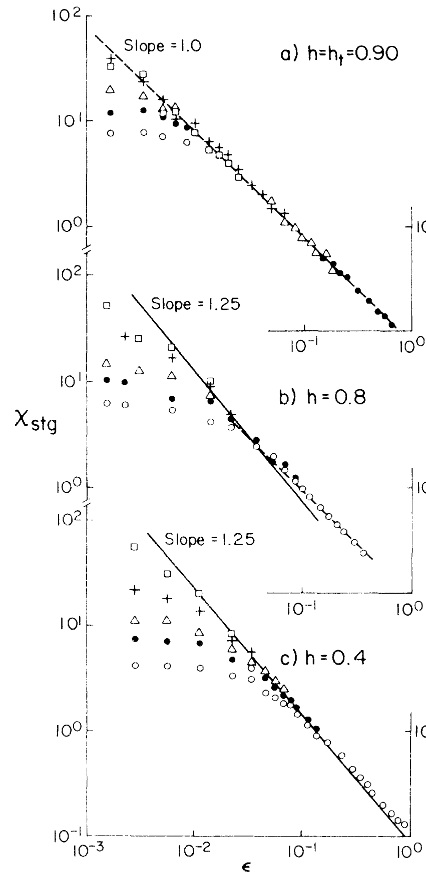

FIG 4. High-temperature-ordering susceptibility data: data points are for $N=6$, ○; $N=8$, ●; $N=10$, △; $N=14$, +; and $N=20$, □.

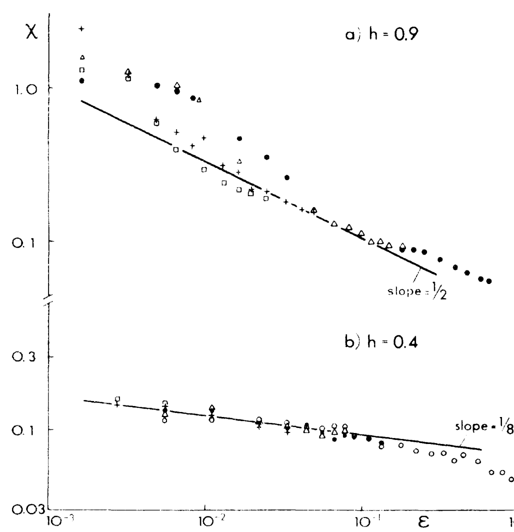

FIG. 5. High-temperature-nonordering susceptibility data: data points are for $N=6$, ○; $N=8$, ●; $N=10$, △; $N=14$, +; and $N=20$, □.

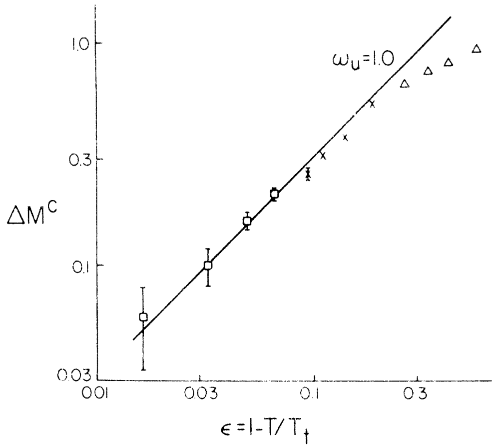

FIG. 6. Temperature dependence of the discontinuity in the magnetization at the phase boundary as T_t is approached from below: $N=10$, △; $N=12$, ×; $N=20$, □.

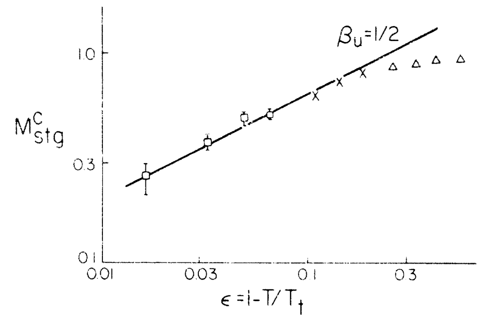

FIG. 7. Temperature dependence of the discontinuity in the order parameter at the phase boundary as T_t is approached from below: $N=10$, △; $N=12$, ×; $N=20$, □.

tainty is much greater than for the ordering susceptibility.

The results suggest that the region of ϵ which is dominated by some sort of critical phenomena remains approximately constant along the phase boundary although the path must come quite close to the tricritical point to allow separation of tricritical from crossover behavior. Otherwise any analysis is likely to lead to spurious exponents. The difficulties connected with further series expansions due to crossover effects should not be underestimated. If series are not sufficiently long, they will provide information about the crossover region but not the true asymptotic exponents. Examples are the series estimates[6,10] for γ and λ along $h=0.84$: $\gamma=1.1$, $\lambda=0.25$. It is possible that the series were just sufficiently long to measure a $\gamma_{\text{effective}}$ which lies between $\gamma_t=1.0$ and $\gamma_c=1.25$ and $\lambda_{\text{effective}}$ between $\lambda_t=0.5$ and $\lambda_c=0.125$. The analysis of the low-temperature order-parameter series would be further complicated by the logarithmic corrections which can easily lead to a spurious exponent estimate.[14]

The exponents which we have just examined describe the tricritical behavior as T_t is approached along a path which is *not* tangent to the critical field curve at (H_t, T_t). In addition, we have studied the behavior of the ordering *and* nonordering densities *along* the first-order phase boundary. The discontinuity in the critical magnetization ΔM_c (nonordering parameter) along the critical field curve as T_t is approached from below should disappear as

$$\Delta M^c \propto \epsilon^{\omega_u}, \tag{3}$$

where the mean-field value is $\omega_u=1$. The Monte Carlo data, plotted in Fig. 6, are clearly consistent with the mean field estimate although the relatively large error bars associated with the determination of ΔM^c make any precise independent estimate impossible. Similarly, the discontinuity in the order parameter M^c_{stg} ($M_{\text{stg}}=0$ in the paramagnetic state) should vary as

$$M^c_{\text{stg}} \propto \epsilon^{\beta_u}, \tag{4}$$

where $\beta_u=\frac{1}{2}$. Here too, the data (see Fig. 7) support the mean field prediction. In both cases, the data are too imprecise to allow us to pass judgement on the possible existence of logarithmic corrections.

III. SUMMARY AND CONCLUSION

In summary, our data provide "experimental" verification that the simple cubic Ising antiferromagnet with nnn interactions does have mean-field tricritical exponents (with logarithmic corrections for β). The crossover between tricritical and critical behavior is observable along a considerable length of the phase boundary and for a range of ϵ which is readily accessible in experimental studies of real systems. Together with recent results on the fcc Blume-Capel model,[3,4] these results suggest that the Universality class for static tricritical behavior may be the same as for static critical behavior.

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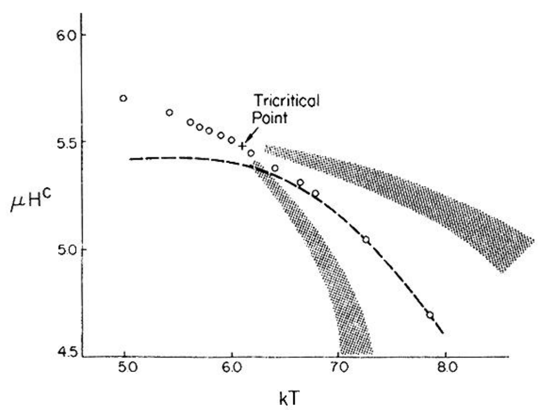

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