Monte Carlo study of the fcc Blume-Capel model

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(Received 21 March 1980)

We have used a Monte Carlo method to study the face-centered-cubic (fcc) Blume-Capel model: $\mathcal{H} = -J \sum_{\langle ij \rangle} S_{iz} S_{jz} + \Delta \sum_i S_{iz}^2 + H \sum_i S_{iz}$, where $S = 1$ and the sum $\langle ij \rangle$ is over the $q = 12$ nearest neighbors. We have traced out the Δ-T phase boundary and have found a tricritical point at $kT_t/qJ = 0.256 \pm 0.004$. The tricritical behavior is consistent with the classical behavior of the Riedel-Wegner Gaussian fixed point. We have also traced out the tricritical "wings" in Δ-T-H space and have found their critical behavior to be consistent with three-dimensional Ising exponents.

I. INTRODUCTION

Beginning with Griffiths's observation[1] that the change in the order of a phase transition along the phase boundary could be due to the intersection of three lines of critical points in a full three-dimensional thermodynamic space (at a tricritical point), extensive attention has been given to tricritical behavior in a variety of physical systems[2–5] and simple theoretical models.[6–19] In particular, Riedel and Wegner[6] used renormalization-group theory to show that the tricritical behavior of a three-dimensional Gaussian model is described by mean-field (classical) exponents with logarithmic corrections for the order parameter. (This result was further clarified by application of the Ginzburg criterion.[7]) This study neither showed the location of the phase boundaries nor did it indicate whether or not similar behavior should occur in other models. Results of several numerical studies (series expansions[10] and Monte Carlo[9]) showed that the simple cubic Ising metamagnet and next-nearest-neighbor (NNN) antiferromagnet both fit the Riedel-Wegner mean-field picture as predicted by another renormalization-group study.[11] The numerical work indicated, however, that computational difficulties were substantial (finite-size effects in the Monte Carlo studies and the effects of crossover on series of limited length) and that care must be exercised in applying these methods. Blume, Emery, and Griffiths[8] (BEG) studied the tricritical behavior of an $S = 1$ Ising model using mean-field theory. This work has recently been extended to models with higher spin dimensionality using renormalization-group techniques.[16,17] Extensive series expansions[12,15] have been derived and analyzed for the Blume-Capel model (a special case of the BEG model) on an fcc (face-centered-cubic) lattice. The most detailed study by Saul *et al.*[12] is particularly significant since it includes a detailed analysis of both high- and low-temperature series. Substantial effort was devoted to analyzing the free energy and its derivatives as obtained from the series in order to distinguish between a first- and a second-order transition. Even so, some features of the results are still ambiguous. More recently a position space renormalization-group method[19] was applied to this model, but we shall see that the results are not promising. In this paper we shall present results of a Monte Carlo study[20] of the Blume-Capel model. We believe that the results of our study will not only provide new information about the properties of the Blume-Capel model but will also provide an independent assessment of the suitability of present series expansion and real-space renormalization-group methods for studies of multicritical behavior. Details of the model and method will be presented in the next section. In Sec. III we present our results regarding critical, tricritical, and wing-critical behavior. In Sec. IV we summarize and conclude.

II. MODEL AND METHOD

The Hamiltonian for the Blume-Capel model[13,14] is defined as

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_{iz} S_{jz} + \Delta \sum_i S_{iz}^2 + H \sum_i S_{iz} \quad , \tag{1}$$

where the ferromagnetic exchange J acts only between the q nearest-neighbor pairs of $S = 1$ spins, where in the case of the fcc lattice $q = 12$. Mean-field theory[8] has shown that for $J > 0$ the ground state is ferromagnetic and is separated from the disordered state by a 2nd-order phase transition for a wide range of the chemical potential (single-ion splitting) Δ. A tricritical point is found to lie at $\Delta_t/qJ = 2 \ln \frac{2}{3}$, $kT_t/qJ = \frac{1}{3}$, while for $\Delta/qJ > 0.5$ the system does not order. Since the ordered state is ferromagnetic, the order parameter m is the spontaneous magnetization and the conjugate ordering field is the magnetic field H. In this model the quadrupole moment $X = 1 - \langle S_z^2 \rangle$ is the "nonordering" parameter and its conjugate field is Δ. The quantity X is the spin analog of the fractional ^{3}He concentration in ^{3}He-^{4}He mixtures. (This situation should perhaps be contrasted with antiferromagnets which show tricritical points where the staggered magnetization is the order parameter and the conjugate field is the staggered magnetic field. The magnetization and uniform magnetic field are then the corresponding "nonordering" quantities.)

Monte Carlo studies were carried out on this model using $L \times L \times L$ fcc lattices with periodic boundary conditions. (Since there are 4 atoms per unit cell the total number of sites is $N = 4L^3$.) The method used has been described in detail elsewhere[21,22] and we shall only outline it here. A "spin-flip" Monte Carlo method was used in which the probability P of a successful spin flip is given by

$$P = \begin{cases} e^{-\epsilon/kT} & \text{if } \epsilon > 0 \ , \\ 1 & \text{if } \epsilon \leq 0 \ , \end{cases} \tag{2}$$

where ϵ is the energy involved in the change of the state of the spin. (Since this is a 3-state model the possible "new" state was chosen randomly before each spin-flip trial.) Lattice sizes considered varied from $L = 4$ to 10. Typically 100–200 Monte Carlo steps per spin (MCS) were discarded and 500–2000 MCS were retained for computing averages. All data points were computed at least twice using different starting configurations. No systematic differences were observed except at the low-temperature first-order phase boundary where distinct hysteresis (metastability) indicated that the transition was first order.

The size dependence of the thermodynamic quantities was interpreted using finite-size scaling theory.[23] Finite-size scaling theory has been successfully used to interpret Monte Carlo data for simple magnetic models in zero magnetic field[9,21] and near-field-induced phase transitions.[24] The maximum in the specific heat is defined as the "pseudocritical" temperature T_c^L. The corresponding infinite lattice critical temperature T_c is given by

$$T_c = T_c^L + aL^{-1/\nu} \ , \tag{3}$$

where ν is the exponent associated with the divergence of the correlation length in the infinite lattice. Similarly the magnetization m, ordering susceptibility χ^+, etc., in the finite system are expected to depend upon the scaled variable $x = tL^{1/\nu}$ where $t = |1 - T/T_c|$:

$$m = L^{-\beta/\nu} f(x) \rightarrow Bt^{\beta}, \quad \text{as } t \rightarrow 0, \ x \rightarrow \infty \ , \tag{4a}$$

$$\chi^+ T = L^{\gamma/\nu} g(x) \rightarrow Ct^{-\gamma}, \quad \text{as } t \rightarrow 0, \ x \rightarrow \infty \ . \tag{4b}$$

Both the "quality" of the scaling of the data and the asymptotic, large-X behavior then provide a test of the estimates.

III. RESULTS

A. Phase boundaries in the Δ-T plane

Data were taken along a number of paths of constant Δ sweeping the temperature both up and down. For all $\Delta/12J < 0.471$ the results were qualitatively the same. Typical data, for $\Delta/12J = 0.4393$, are shown in Fig. 1 (this particular value was chosen because it was identical to a value of Δ_c obtained in the series study of Saul *et al.*[12]). Both the internal energy E and nonorder parameter X increase smoothly and continuously with increasing temperature with very small finite-size effects except near the inflection point which marks the transition. The order parameter m decreases smoothly and rapidly near T_c and shows a finite-size "tail" at high temperature. Both the specific heat C/R and ordering (ferromagnetic) susceptibility χ^+ show sharp peaks whose magnitude and location are clearly affected by finite lattice size. Estimates for $T_c^L(\Delta)$ were obtained by examination of the data, such as those shown in Fig. 1, and then extrapolated to the infinite lattice $T_c(\Delta)$ using the finite-size scaling relation in Eq. (3). For all paths which cross the phase boundary at $\Delta/12J \lesssim 0.4393$ our results agree well with the series expansion values. For example, for $\Delta = 0$ we find $kT_c/12J = 0.570 \pm 0.005$ as compared with the series estimate 0.5684 ± 0.0010. For $\Delta/12J > 0.4393$ we find small but systematic differences. The resultant phase boundary bends over rather rapidly and paths of constant Δ become almost tangent to it. For this reason additional data were obtained by sweeping Δ along paths of constant temperature. Data taken at low temperatures show distinct hysteresis indicative of a first-order transition. As the temperature is increased the hysteresis decreases until it disappears at the tricritical point (see Fig. 2). We estimate that $kT_t/12J = 0.256 \pm 0.002$, $\Delta_t/12J = 0.471 \pm 0.004$ for an infinite lattice. The phase boundary is shown in Fig. 3. Our estimate differs slightly from the series value of $kT_t/12J = 0.2615 \pm 0.0070$, $\Delta_t/12J = 0.4715 \pm 0.0100$ although the two agree within "experimental" error. The data show that the phase boundary is quite smooth near T_t. A small "dip" appeared to be present in the small lattice data but was much less pronounced in our estimated infinite lattice critical curve. A slight depression does appear in the series expansion data but may be due, at least in part, to the uncertainty in the location of the second-order portion of the phase boundary near T_t. Therefore, if a "dip" does occur, such as the one reported[25] for the two-dimensional Blume-Capel model, it must be quite shallow. Mean-field theory yields a phase boundary which is systematically high in temperature. The mean-field tricritical point lies close to the correct value of Δ although the value of T_t is about 30% too high. The curve obtained from a position-

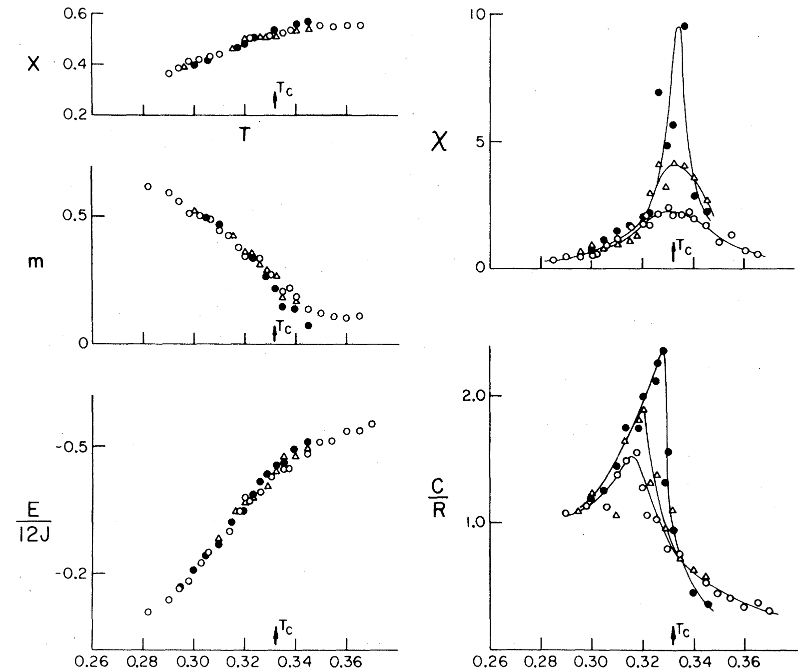

FIG. 1. Temperature dependence of various thermodyamic properties along a path of $\Delta/12J = 0.4393$ for $L = 6$, ○; $L = 8$, Δ; and $L = 10$, ●.

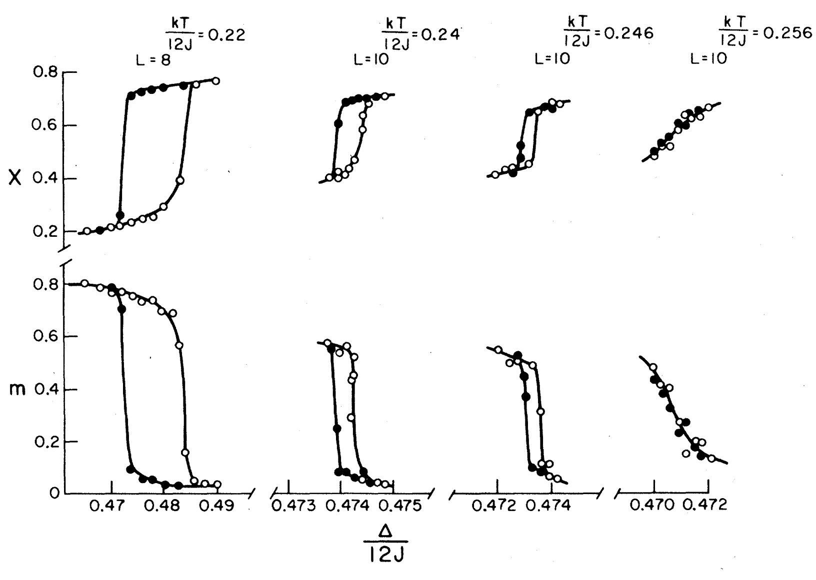

FIG. 2. Variation of the order parameter, m, and nonorder parameter, X, with Δ along paths of constant temperature. Data taken for increasing Δ are shown by open circles and data for decreasing Δ by closed circles.

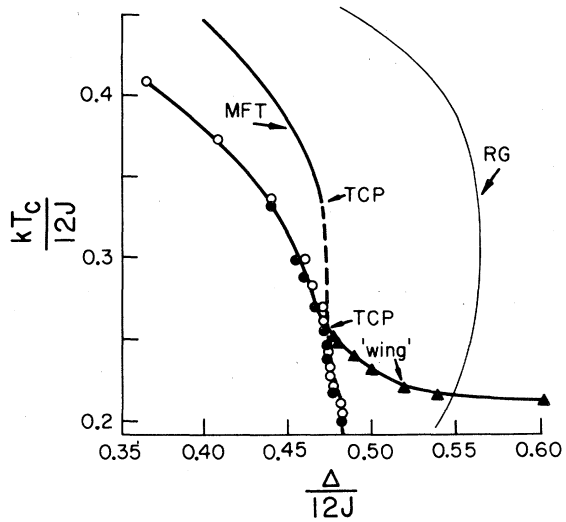

FIG. 3. Phase diagram in the Δ-T plane. Monte Carlo results, ●; series estimates, ○. The projection of the wing boundary on the Δ-T plane is shown by filled triangles. The predictions of mean-field theory (MFT) (Ref. 8) and position-space renormalization-group (RG) theory (Ref. 19) are shown by labeled curves. The solid curves are estimates for the location of the second-order phase boundary, the dashed lines are first-order phase boundaries.

space renormalization-group study[19] is obviously in serious error. The general analysis of the series is quite complex, particularly near the tricritical point. Saul *et al.*[12] looked directly at the free energies of the ordered and disordered phases in order to locate the phase boundary. This procedure yielded only a slight uncertainty in the critical point in the Δ-T plane for each path, but the ambiguity in the phase diagram in the X-T plane was quite large. In Fig. 4 we plot our

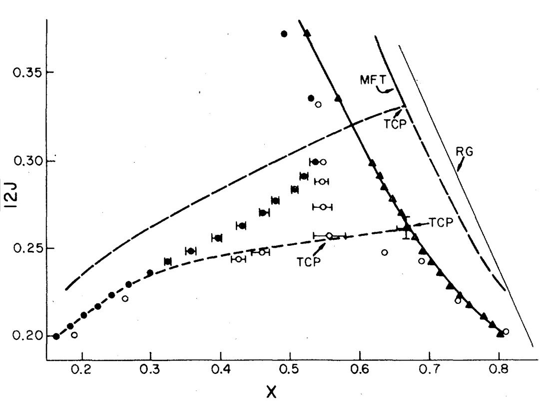

FIG. 4. Phase boundary in the X-T plane. Monte Carlo results are shown by open circles. High-temperature and low-temperature-series estimates are ▲ and ●, respectively. The predictions of mean-field theory (MFT) (Ref. 8) and position-space renormalization-group (RG) theory (Ref. 19) are shown by labeled curves.

values along with the series results for the X-T phase diagram. Our results show that neither the high-temperature nor low-temperature series correctly locate the critical value(s) of X just above (below) T_t. As expected, mean-field theory yields systematically incorrect results. The position-space renormalization-group study[19] yielded results which are substantially worse than those predicted by mean-field theory; in fact, the predicted tricritical point and coexistence region do not even appear on scale in Fig. 4.

B. Tricritical behavior

The asymptotic critical behavior along the second-order portion of the phase boundary was described by three-dimensional Ising exponents as expected. Near the tricritical point, however, crossover between critical and tricritical behavior was observed. This is demonstrated in the order parameter data in Fig. 5. Extensive data were taken along the path $\Delta/kT = 1.84$ which essentially passes through the tricritical point roughly perpendicular to the phase boundary. Along this "tricritical path" there is no evidence of Ising critical behavior. The order parameter data are consistent with tricritical behavior which is classical with logarithmic corrections

$$m = B_t(t \ln t)^{1/4} \tag{5}$$

as predicted by renormalization-group theory. The

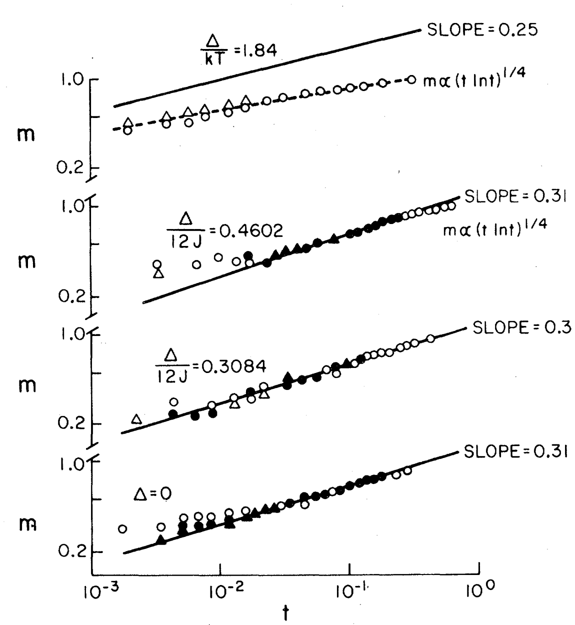

FIG. 5. Critical and tricritical behavior of the order parameters. $t = |1 - T/T_c|$. $\Delta/kT = 1.84$ is the tricritical path. Data are for $L = 4$, ○; $L = 6$, ●; $L = 8$, ▲; $L = 10$, Δ.

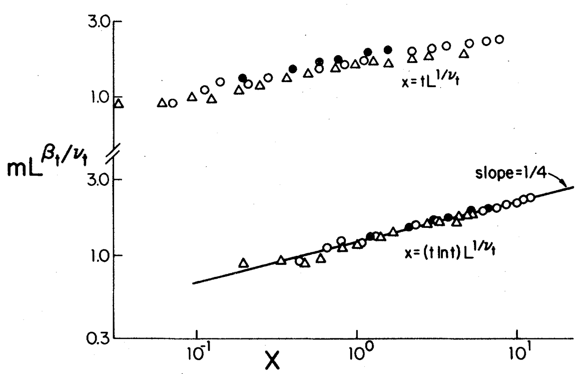

FIG. 6. Finite-size scaling behavior of the order parameter along the tricritical path $\Delta/kT = 1.84$ with $\beta_t = \frac{1}{4}$, $\nu_t = \frac{1}{2}$, $t = |1 - T/T_t|$. Data are for $L = 6$, ○; $L = 8$, Δ; $L = 10$, ●.

significance of the logarithmic correction is demonstrated in the finite-size scaling plot shown in Fig. 6. If we ignore the logarithmic term the data do not collapse onto a single curve, but they scale very nicely if the logarithmic term is included. The high-temperature susceptibilities were also analyzed along the "tricritical path" assuming tricritical behavior of the form

$$\chi^+ T = C_t t'^{-\gamma} \ , \tag{6a}$$

$$\chi T = \tilde{C}_t t'^{-\lambda} \ , \tag{6b}$$

where χ^+ is the ordering susceptibility and χ is the nonordering susceptibility. The ordering susceptibility data (see Fig. 7) are consistent with Eq. (6a) with the classical exponent $\gamma = 1.0$ and $C_t = 0.23 \pm 0.02$. This value for the tricritical amplitude C_t is in good

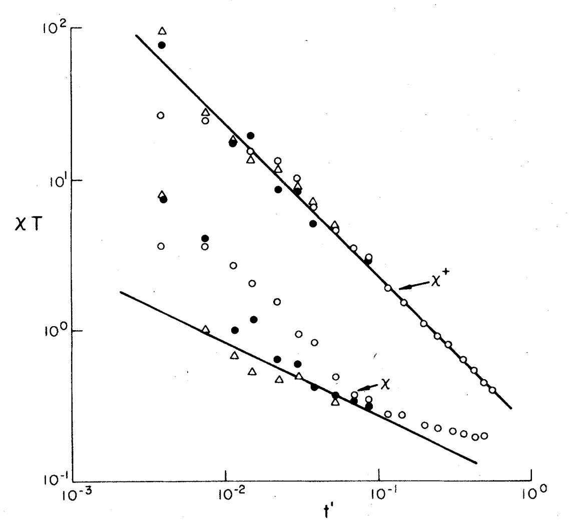

FIG. 7. Tricritical behavior of the high-temperature ordering susceptibility χ^+, and nonordering susceptibility χ. Data are for $L = 4$, ○; $L = 6$, ●; $L = 10$, Δ, $t' = |1 - T_t/T|$.

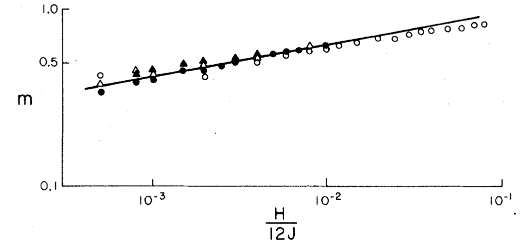

FIG. 8. Field dependence of the order parameter along the tricritical isotherm $kT/12J = 0.256$. Data are for $L = 4$, ○; $L = 6$, ●; $L = 8$, ▲; $L = 10$, Δ.

agreement with the (more precise) series estimate of 0.241 ± 0.001. Finite-size effects are much more important for the nonordering susceptibility (see Fig. 7). The large L data are consistent with Eq. (6b) with the classical exponent $\lambda = \frac{1}{2}$ and $\tilde{C}_t = 0.09$. Our estimate for $\tilde{C}_t$ is much less than the series value of $\tilde{C}_t = 0.50$. The only possible explanation that we can offer is that the region of asymptotic behavior could be $t' < 0.01$ and that the "fit" shown in Fig. 7 is therefore not appropriate.

In Fig. 8 we analyze the field dependence of the magnetization along the tricritical isotherm

$$m = D_t H^{1/\delta_t} \ . \tag{7}$$

The data (Fig. 8) are well fitted by Eq. (7) with $\delta_t = 5.0$ and $D_t = 1.0 \pm 0.2$. For comparison the series expansion yielded $\delta_t = 5.2 \pm 0.5$ and $D_t = 1.1$.

In Fig. 9 we analyze the Δ dependence of the nonordering parameter along the "tricritical path" $\Delta/kT = 1.84$:

$$X = X_t \pm d t^{\omega_t} \ . \tag{8}$$

The asymptotic behavior is consistent with the classical value $\omega_t = \frac{1}{2}$ with $d = 1.5 \pm 0.2$ as compared with the series estimate of 2.1.

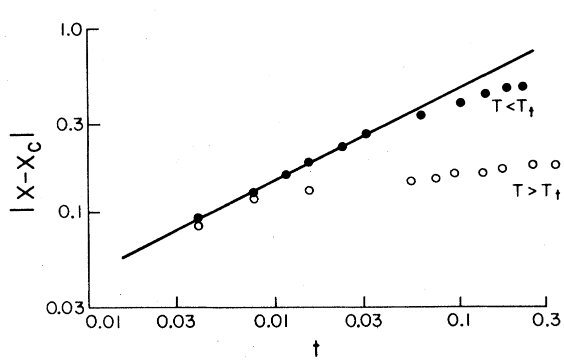

FIG. 9. Tricritical behavior of the nonorder parameter along the tricritical path $\Delta/kT = 1.84$, $t = |1 - T/T_t|$.

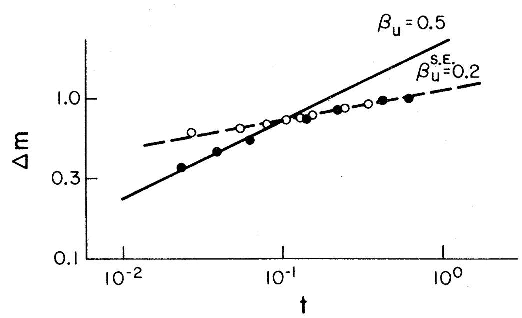

FIG. 10. Temperature dependence of the discontinuity in the order parameter across the first-order phase boundary, $t=|1-T/T_t|$. Open circles show series expansion results, closed circles are Monte Carlo values.

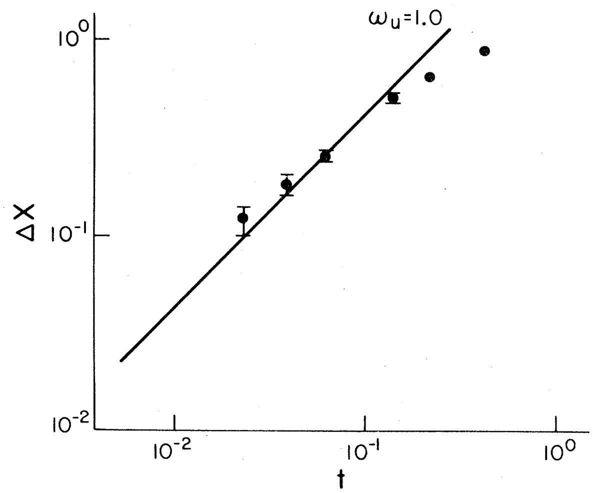

FIG. 11. Temperature dependence of the discontinuity in the nonorder parameter across the first-order phase boundary, $t=|1-T/T_t|$.

We have also analyzed the discontinuities in the ordering and nonordering densities along the first-order phase boundary. As the tricritical point is approached from the low-temperature side the discontinuities should behave like

$$\Delta m = b t^{\beta_u} \quad , \tag{9a}$$

$$\Delta X = q t^{\omega_u} \quad , \tag{9b}$$

where $t=(1-T/T_t)$. The data for Δm, shown in Fig. 10, agree well with the series values well below T_t but decrease much more rapidly near T_t. In the region of small t where the asymptotic form [Eq. (9a)] is expected to hold, our data are well fitted by Eq. (9a) with $\beta_u=\frac{1}{2}$ and $b=2.2\pm0.2$. Since the series expansion estimate for Δm does not go to zero at T_t (see Fig. 4) we must also regard the estimates for very small t as suspect. The data for ΔX (see Fig. 11) are also consistent with Eq. (9b) with $\omega_u=1$ and $q=3.9\pm0.3$. The relatively large errors in these data, for both Δm and ΔX, would clearly make it impossible to exclude nonclassical exponents. Furthermore, we cannot draw any conclusions regarding logarithmic corrections.

C. "Wing" boundaries

Griffiths[1] pointed out that the phase diagram for a tricritical system such as the Blume-Capel model consists of three thermodynamic sheets in the full Δ-H-T parameter space. The phase transitions which are observed upon crossing these sheets are first order; however, each surface is bounded by a line of second-order critical end points. The phase boundary to one surface, described in Sec. III A, is in the Δ-T plane; the other two surfaces or "wings" extend out symmetrically into the $\pm H$ directions. The intersection of the three lines of critical end points is the tricritical point. In order to map out the wing boundary we studied the behavior of the system at fixed temperature by either varying H with Δ held fixed or keeping H constant and sweeping Δ. Pronounced hysteresis was observed in both the other parameter and nonordering parameter when the wing surface was crossed far from the line of critical end points. The wing phase boundary was then determined by observing the disappearance of hysteresis. The projection of the wing boundary onto the Δ-T plane is shown in Fig. 3 and onto the H-T plane in Fig. 12. Scaling theory can be used to predict[26] the shape of the wing critical line as it approaches the tricritical point

$$k(T_t-T_c)=aH_c^{\rho} \tag{10}$$

with $\rho=\frac{2}{5}$. In Fig. 13 we show a log-log plot of $(T_t-$

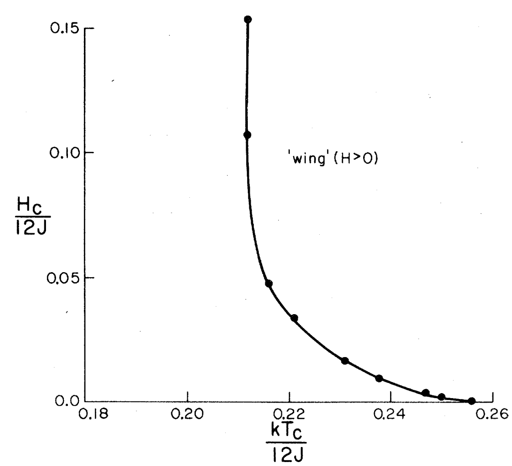

FIG. 12. Projection of the wing boundary on the H-T plane.

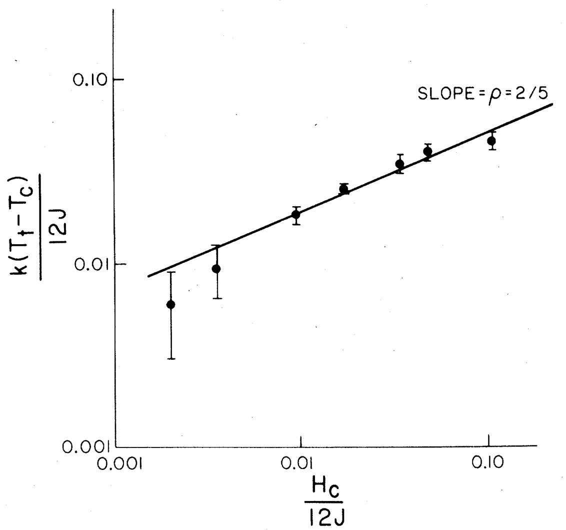

FIG. 13. Behavior of the wing boundary as the tricritical point is approached.

T_c) vs H_c. Our data are consistent with the theoretical prediction, although the relatively large error bars associated with the location of the critical end points make any independent estimate for ρ quite inaccurate. We have also studied the critical behavior along the wing boundary. In Figs. 14 and 15 we show an analysis of the order parameter and high-temperature susceptibility for $\Delta/12J = 0.60$. The order parameter follows the usual power law

$$m = Bt^{\beta} \tag{11}$$

with $\beta = 0.32 \pm 0.02$ and $B = 1.34$. For comparison we note that along the $H = 0$ phase boundary

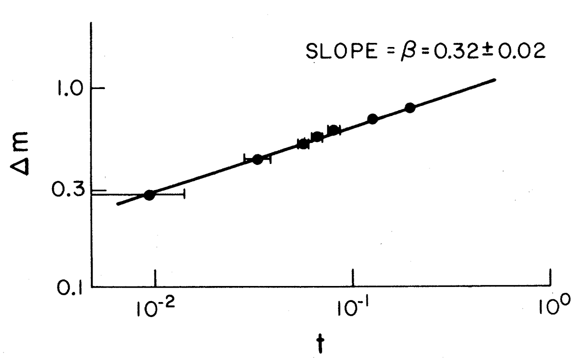

FIG. 14. Wing critical behavior for $\Delta/12J = 0.60$. Data are for $L = 10$, $t = |1 - T/T_c|$.

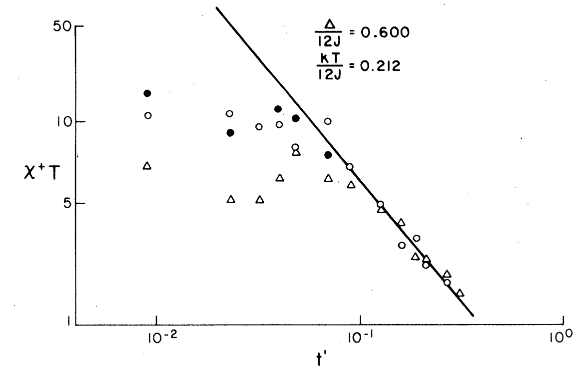

FIG. 15. High-temperature ordering susceptibility data as the wing boundary is approached along $\Delta/12J = 0.60$; $L = 4$, Δ; $L = 6$, ○; $L = 10$, ●; $t' = |1 - T_c/T|$.

$\beta = 0.31$ with $B = 1.36$ for $\Delta = 0$, and for $\Delta = -\infty$, $B = 1.49$. The high-temperature susceptibility obeys a simple power law

$$\chi^+ T = Ct'^{-\gamma} \tag{12}$$

with $\gamma = 1.2 \pm 0.1$ and $C = 0.30$. For $\Delta = 0$, $C = 0.56$ and for $\Delta = -\infty$, $C = 0.97$. Since the $\Delta/12J = 0.6$ wing critical point is not really very far from the tricritical point we regard the amplitudes obtained for the wing critical behavior as quite similar to those obtained along the "usual" critical line.

IV. SUMMARY AND CONCLUSION

We have studied the behavior of the fcc Blume-Capel model in the full Δ-H-T space. Our estimate for the location of the phase boundary in the Δ-T plane agree closely with that obtained by series expansions. We find tricritical behavior which is mean-field-like with logarithmic corrections in the case of the order parameter. In addition the tricritical amplitudes obtained generally agree with those obtained from series expansions. These results show that, in spite of some ambiguity in the nonorder parameter, a series study can be quite accurate provided both high- *and* low-temperature series are available. We have also traced out the "wing" boundaries. Our data are consistent with wing critical exponents which are the same as normal three-dimensional Ising exponents.

ACKNOWLEDGMENTS

This research was supported in part by the National Science Foundation. We wish to thank Dr. M. Novotny for helpful comments and suggestions.

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