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Fluctuation-induced first-order transition in a bcc Ising model with competing interactions

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We study the simple system of $(S = \frac{1}{2})$ Ising spins on a bcc lattice with ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor exchange. Particular emphasis is placed on the region of competition between ferromagnetic and antiferromagnetic ordering of the second kind $[AF(2)]$. Renormalization-group ϵ -expansion methods along with Monte Carlo analysis leads to the suggestion that the mean-field bicritical phase diagram becomes, with the inclusion of fluctuations, a critical-end-point diagram,

I. INTRODUCTION

Renormalization-group calculations, especially those using ϵ -expansion techniques,¹ have proven very useful in predicting the general features of the critical behavior of complex systems. Even when complete analytic solutions (to a given order in ϵ) are absent, information on the structure of the phase diagram may be obtained from the renormalization trajectories; On the other hand, Monte Carlo tech $niques²$ allow one to obtain high-accuracy numerical results for the phase diagrams of specific models in the physical parameter space.

The present work was undertaken to study the phase diagram of a simple system with competing interactions and place particular emphasis on the fluctuation-induced modifications of mean-field predictions. We have chosen the specific case of an dictions. We have chosen the specific case of an $(S = \frac{1}{2})$ Ising model on a bcc lattice with nearest- and next-nearest-neighbor interactions $(J_1$ and J_2 , respectively).³ Our analysis involves both an ϵ expansion, which is an extrapolation from four dimensions, and Monte Carlo methods. As pointed out recently by Jensen et $al.$,⁴ it is of particular interest to check on ϵ -expansion predictions extrapolated to $d = 3$ when they involve the possibility of fluctuation-induced first-order transitions. In the present case the renormalization-group and Monte Carlo methods effectively complement one another.

Figure 1 shows schematically six simple possibilities for the phase diagram; the mean-field result⁵ is included in Fig. 1(a). The nature of the phases labeled F (ferromagnetic) and AF(2) (antiferromagnetic type II) will be discussed in Sec. II.

Our analysis indicates that fluctuations apparently drive the transition between the paramagnetic and antiferromagnetic type-II phases first order. This

changes the mean-field bicritical diagram $[Fig. 1(a)]$ to a critical end point suggested in Figs. $1(c)$ or $1(f)$. As noted below, the renormalization-group approach does not lead to a completely unambiguous prediction. This is due to the incomplete analysis of the role played by irrelevant variables, which appear in

FIG. 1. Six simple possibilities for the phase diagram (temperature vs $p = |J_2|/J_1$) near the region where the ordering changes from ferromagnetic to $AF(2)$. Figure 1(a) corresponds to a mean-field theory prediction. The dashed lines represent first-order transitions and the solid lines continuous. transitions.

the construction of the renormalization-group Hamiltonian, in determining local features of the phase diagram. The consistency of the Monte Carlo results along with a global viewpoint allow the construction of a phase diagram for all J_1 and J_2 with reasonable confidence.

We emphasize that it is the consistency of the two techniques, renormalization-group and Monte Carlo, which provides the confidence in the final results. Each of the methods has its own weaknesses and ambiguities. When fluctuation-induced first-order transitions are suspected, high-temperature series⁶ alone are of limited utility, and mean-field and related arguments⁷are of no help. Real-space renormalization-group calculations could provide additional support.

The organization of the remainder of this paper is as follows. Section II introduces the model and presents the results of mean-field theory. Section III contains a brief summary of the e-expansion calculations, while the Monte Carlo results and a concluding summary are presented in Secs. IV and V, respectively. Some details of the ϵ -expansion calculations are relegated to the Appendix.

II. MODEL

Figure 2 shows a body-centered-cubic lattice; a given spin has eight nearest neighbors, and the cube edge is denoted by a. The lattice is divided into four sublattices, as indicated in Fig. 2.

With nearest-neighbor (nn) interaction J_1 and next-nearest-neighbor (nnn) interaction J_2 (we use the convention that a positive J is ferromagnetic), the reduced Hamiltonian

$$
\overline{H}_{\text{int}} = -\beta H_{\text{int}} = -H_{\text{int}}/k_B T
$$

is given by

$$
\overline{H}_{\text{int}} = \frac{1}{2} \sum_{RR'} K(R,R') s(R) s(R') \quad , \tag{2.1}
$$

FIG. 2. Body-centered-cubic lattice divided into four face-centered cubic sublattices.

where

$$
K(R, R') = \begin{cases} K_1 = J_1/k_B T & \text{if } R, R' \text{ nn} \\ K_2 = J_2/k_B T & \text{if } R, R' \text{ nin} \\ 0 & \text{otherwise} \end{cases}
$$
 (2.2)

Standard mean-field theory' shows that there are three kinds of sublattice ordering that the system can support depending on the relative signs and magnitudes of the exchange constants J_1 and J_2 . Denoting the order on the *i* th sublattice by M_i the possibilities are

(i)
$$
M_1 = M_2 = M_3 = M_4
$$
 (F) ,
\n(ii) $M_1 = -M_2 = M_3 = -M_4$ [AF(1)] , (2.3)
\n(iii) $M_1 = -M_3$; $M_2 = -M_4$ [AF(2)] .

The first possibility obviously corresponds to ferromagnetism (F). The ordering described by the second line is customarily termed antiferromagnetic ordering of the first kind $[AF(1)]$ and corresponds to the state in which each spin has its eight nearest neighbors antiparallel and its six next-nearest neighbors parallel. The third line describes a twofold degenerate (depending on whether $M_1 = \pm M_2$) antiferromagnetic ordering termed antiferromagnetic ordering of the second kind $[AF(2)]$. This arrangement can be simply described as two interpenetrating simple cubic lattices, each antiferromagnetically ordered.⁵

The kind of low-temperature ordering which occurs for a given (J_1,J_2) is shown in Fig. 3. Mean-field theory further predicts that for any (J_1,J_2) increasing the temperature causes the system to undergo a continuous transition to a disordered state.

FIG. 3. Mean-field magnetic ordering phase diagram in the J_1-J_2 plane for the bcc lattice. For any given J_1 and J_2 mean-field theory predicts, that on increasing the temperature, there is a continuous transition between the ordered state and the disordered state.

III. e EXPANSION

Our e-expansion treatment follows the lines developed for discussing layered metamagnets.⁸ As usual,¹ we take the $s(R)$ to be continuous classical variables subject to spin-weighting factors $\exp[-w(s)]$ with $w(s) = \frac{1}{2}s^2 + fs^4 + \dots$. The essential step is then to introduce four spin fields $S_{\alpha}(q)$, $S_{\mathbf{a}}(q)$, $S_{\mathbf{v}}(q)$, and $S_{\mathbf{a}}(q)$,

$$
S_{\alpha}(q) = \frac{1}{2} [s_1(q) + s_2(q) + s_3(q) + s_4(q)] ,
$$

\n
$$
S_{\beta}(q) = \frac{1}{2} [s_1(q) - s_2(q) + s_3(q) - s_4(q)] ,
$$

\n
$$
S_{\gamma}(q) = \frac{1}{2} [s_1(q) - s_2(q) - s_3(q) + s_4(q)] ,
$$

\n
$$
S_{\delta}(q) = \frac{1}{2} [s_1(q) + s_2(q) - s_3(q) - s_4(q)] ,
$$
 (3.1)

with

$$
s_i(q) = \sum_{R \in i} e^{i \vec{q} \cdot \vec{R}} s_i(R); \quad i = 1, 2, 3, 4 \quad . \tag{3.2}
$$

where 1, 2, 3, and 4 label the four interpenetrating sublattices into which the lattice is decomposed (Fig. 2). The wave vectors run over a reduced Brillouin zone corresponding to a superlattice. This construction allows one to make a ready analysis of the ordering effects associated with competition between the four sublattices. The variables $S_{\alpha}(q)$, $S_{\beta}(q)$, $S_{\gamma}(q)$, and $S_{\delta}(q)$ diagonalize [neglecting higher-order nondiagonal terms of order $(q³)$] the *quadratic* parts of the reduced Hamiltonian

$$
\overline{H} = \overline{H}_{int} - \sum_{R} w(s(R)) \quad . \tag{3.3}
$$

The weight function $w(s)$ introduces quartic coupling among the $S_a(q)$, $a = \alpha$, β , γ , δ .

A standard momentum shell integration scheme' produces the recursion relations. The only technical point is the introduction of distinct spin rescaling factors c_{α} , c_{β} , c_{γ} , and c_{δ} for the corresponding spin components. The c 's are chosen to keep the coefficents of $q^2|S_q(q)|^2$ in the renormalized Hamiltonian equal to unity (in magnitude). Some terms in \overline{H} can be .easily eliminated. For example, if one is studying the transition between ferromagnetic and AF(2) ordering $(2J_1 \approx -3J_2; J_2 < 0)$, the β mode [which corresponds to $AF(1)$ ordering] is noncritical and can be explicitly integrated out of the problem. The resulting reduced Hamiltonian contains no terms with β dependence and may be written to quartic order schematically as

$$
\overline{H}_{\text{red}} = -\int d^d R \left\{ \frac{1}{2} \left[r_\alpha S_\alpha^2 + |\nabla S_\alpha|^2 + r_\gamma (S_\gamma^2 + S_\delta^2) + |\nabla S_\gamma|^2 + |\nabla S_\delta|^2 \right] + u_1 (S_\gamma^4 + S_\delta^4) + u_2 S_\alpha^4 + u_3 S_\gamma^2 S_\delta^2 + u_4 S_\alpha^2 (S_\gamma^2 + S_\delta^2) \right\} \tag{3.4}
$$

The symmetry of the Hamiltonian shows the degeneracy of the γ and δ modes [the two AF(2) modes]. This degeneracy leads to the condition that $u_3 = 6u_1$ in the starting Hamiltonian (3.3), which exact symmetry, however, is broken while obtaining the reduced renormalized Hamiltonian, so that the condition

$$
u_3 \approx 6u_1 \qquad (3.5) \qquad \overline{H}_{II} = -\int d^d R \; \left(\frac{1}{2}\right)
$$

is now appropriate in Eq. (3.4).

Renormalization-group differential recursion relations are now constructed to $O(\epsilon)$ using standard techniques.¹ Carrying out the usual procedure on Eq. (3.4) results in a new renormalized effective Hamiltonian. In the region with the ferromagnetic ordering one finds that the AF(2) modes are noncritical and can be integrated out of the problem. This results in an effective Hamiltonian taking the form

$$
\overline{H}_f = -\int d^d R \left[\frac{1}{2} (r_1 S_\alpha^2 + |\nabla S_\alpha|^2) + u_2^{\prime} S_\alpha^4 \right] \quad . \tag{3.6}
$$

This is the well-known $n = 1$ Hamiltonian which exhibits a continuous transition with Ising exponents when' $u'_2 > 0$, but further admits the possibility of a first-order line terminating at a classical tricritical point.⁹ We find that starting from the physical Hamiltonian, u_2 continues to be positive giving the expectation that the transition from the ferromagnetic to the paramagnetic state is continuous and has Ising exponents.

A similar approach on the $AF(2)$ side of the phase diagram (provided the ferro mode is noncritical) leads to an effective Hamiltonian

$$
\overline{H}_{II} = -\int d^d R \left\{ \frac{1}{2} \left[r_2 (S_y^2 + S_\delta^2) + |\nabla S_y|^2 + |\nabla S_\delta|^2 \right] + u_1' (S_y^4 + S_\delta^4) + u_3' S_y^2 S_\delta^2 \right\} .
$$
 (3.7)

Hamiltonians of this form have been analyzed by Aharony⁹ and Rudnick¹⁰ for various fixed points and their relative stabilities. The line $u_3' = 6u_1'$ separates two domains in the (u'_1, u'_3) plane. For $u'_1 > 0$ and u'_3 < 6u'₁, the $n = 2$ isotropic fixed point is stable, whereas for $u'_3 > 6u'_1$, the transition becomes one of first order. The line $u_3' = 6u_1'$ contains an Ising-like fixed point (which thus corresponds to a nonclassical tricritical point) that one flows into, if and only if one starts exactly on the line $u'_3 = 6u'_1$ with $u'_1 > 0$. The degeneracy in our Hamiltonian for the γ and δ modes was such that we started with $u_3^0 = 6u_1^0$. However this exact symmetry is broken on integrating out the irrelevant α and β modes.

The effect of the full recursion relations is to make

 u_3 > 6u₁, so that the transition becomes first order in the neighborhood of the transition region between ferromagnetic and AF(2) ordering. Numerical iteration of the recursion relations in the $AF(2)$ region results in u_1 rapidly going to zero and then becoming negative. This suggests that the bicritical point predicted by mean-field theories^{5,7} and indicated by high-temperature series analysis (see below) should be in fact a critical end point $[Fig. 1(c)]$. A further prediction of the renormalization-group analysis^{9,10} is that on going deeper into the $AF(2)$ region (by increasing $|J_2|$, if the transition becomes continuous Fig. 1(f)], it will be characterized by $n = 2$ exponent with an Ising-like nonclassical tricritical point.^{9,10} The above analysis holds for the $AF(1)-AF(2)$ transition also, as the symmetry of the Hamiltonian is unchanged on letting J_1 go to $-J_1$.

We now address the question whether there exists a tricritical point as in Fig. 1(f) for the specific case of nn and nnn interactions only. Note that when $J_1 = 0$, the bcc lattice decomposes into two decoupled, interpenetrating simple cubic lattices each having only nearest-neighbor interactions; hence one has a continuous transition with Ising exponents. Furthermore it appears that the crossover exponent associated with J_1 is less than unity indicating that the XY or firstorder lines terminating at the Ising-like point $|J_1| = 0$ come in smoothly. (Recall there is complete symmetry in $J_1 \rightarrow -J_1$). There seems to be no reason for a first-order transition separating the two ordered phases at $J_1 = 0 \pm$. Hence a bicritical phase diagram does not seem likely in the region of $J_1 = 0$. It seems most reasonable, then, to associate the multicritical point at $J_1 = 0$ $(J_2$ fixed) with the nonclassical tricritical point with Ising exponents mentioned above.

The renormalization-group treatment strongly suggests the critical end point shown in Figs. 1(c) and 1(f) and it further suggests that for large $|J_2|/J_1$ the transition is of first order, It does not rule out the possibility of an even number of tricritical points involved with the transition to the AF(2) state. This does not seem very 'likely, but we have not dealt carefully with the specific features of the model and have not allowed for the possibility of irrelevant variables modifying local features of the phase boundaries.

One must consider how weak further-neighbor interactions might modify the conclusions. We assume that the same diagonalization scheme is valid, i.e., we consider interactions in a regime which does not introduce the necessity of more complicated sublattice decompositions. Those interactions which couple the two simple cubic sublattices (even at $J_1 = 0$) result in making the transition first order at $J_1 = 0$ in the AF(2) region $(J_2 < 0)$. The multicritical point formerly at $J_1 = 0$ moves off to a finite value of J_1 depending on the strength of the new interactions. The usual qualifications concerning the effect of irrelevant variables must again be made.

If the $AF(2)$ symmetry is broken, that is, the quadratic term in Eq. (3.4) is modified to read $r_{\gamma}(1+g)S_{\gamma}^2 + r_{\gamma}(1-g)S_6^2$ with $|g| > g_0$, a continuous transition results.¹¹ However, simple perturbations of physical Hamiltonian (2.1) do not lead to distortions necessary to break the degeneracy of the two $AF(2)$ modes.

In the first-order $AF(2)$ region we can determine the ordered-phase free energy^{10,12} using a generalization of the analysis developed by Rudnick¹⁰ for $n = 2$ systems. This allows a mapping out of the firstorder line and estimation of the order-parameter discontinuities in the vicinity of the critical end point. Some details are sketched in the Appendix. As expected one finds no interesting crossover behavior in the vicinity of the critical end point.

IV. MONTE CARLO RESULTS

Monte Carlo data on finite-size lattices were obtained by using a basic computer code developed by Landau $¹³$ in a different context. The program, writ-</sup> ten in FORTRAN, required about 175μ secs per spin trial (including the time needed for averages) on a DEC 1099. Most of the data were taken for $N \times N \times N$ lattices with $N = 6$, 10, and 14 with periodic boundary conditions.

In a typical "run" for a given point in the phase plane, 2000 passes through the lattice (2000 "Monte Carlo steps") were used to obtain the appropriate thermodynamic quantities. Such runs were repeated up to four times in important regions of the phase diagram, thereby yielding up to four data points for the thermodynamic functions. Typically, starting from an equilibrium configuration, about 200 Monte Carlo

FIG. 4. Monte Carlo estimate for the specific heat vs temperature for a $14 \times 14 \times 14$ lattice with $J_1 = +0.5$ and $J_2 = -0.3325$ indicating characteristic behavior associated with a continuous transition.

steps were discarded in allowing the lattice to attain equilibrium at a nearby point in the phase space. In detecting hysteresis in the vicinity of a first-order boundary (see below) runs of the length noted above were used; the spacing between successive temperatures was generally the same as indicated in the typical specific-heat run shown in Fig. 4.

Specific-heat values were determined from the fluctuations in internal energy and were used to determine T_c for the para-ferro transition. As has been mentioned, a typical run is shown in Fig. 4, The scatter is not surprising considering the small range of temperatures (close to T_c) studied and can be reduced by making longer runs. However, our intention in doing the Monte Carlo computations was not to make a very accurate numerical analysis of this specific model but rather to complement the ϵ expansion calculations. Finite-size scaling¹⁴ analysis was used to determine $T_c(\infty)$. An example is shown in Fig. 5. Figure 6 shows a typical plot of the ferromagnetic order parameter versus $|T - T_c(\infty)|$. The critical exponent β is given by the slope of the log-log plot and is found to be about $\frac{1}{3}$, consistent with the accepted Ising value¹⁵ of $\beta \approx 0.31 - 0.33$. Such behavior was found along the ferro-para boundary with no sign of any hysteresis effects. These observations are consistent with expectations of a continuous transition between the paramagnetic and ferromagnetic phases based on ideas of universality and indicated by the renormalization-group analysis discussed previously.

A first-order transition is signaled by hysteresis and by discontinuous jumps in the internal energy and order parameter. Clear evidence for a first-order transition was found for the boundary separating the ferromagnetic and AF(2) ordered phases as suggested, for example, by Figs. $1(c)$ and $1(f)$. This hysteresis clearly persisted to the boundary separating the *paramagnetic* and $AF(2)$ phases leading to the

FIG. 5. Finite-size scaling plot for $T_c(N)$ for the ferropara transition with $v = 0.64$. The values of N used are 4, 6, 10, and 14. $J_1 = 0.5$ and $J_2 = -0.3325$.

FIG. 6. Log-log plot of the ferromagnetic order, M_f , vs $T_c(\infty) - T$ for $J_1 = 0.500$ and $J_2 = -0.3325$. $T_c(\infty) = 1.115$. The error bars are roughly the size of the points themselves. The exponent β is found from the slope of the straight line through the data to be about 0.33.

conclusion of a critical end point as shown in Figs. $1(c)$ and $1(f)$. However, moving out along the para-AF(2) boundary, the hysteresis weakened suggesting that a tricritical point might appear as sketched in Fig. 1(c).

To provide further information on these possibilities we considered relaxation to equilibrium in more detail. As has been discussed by Landau and Binder¹⁶ further evidence for a first-order transition is provided by observation of a two-step relaxation process (presumably due to the presence of metastable states) on either quenching to slightly below the transition temperature from high temperatures or

FIG. 7. (a) Relaxation plot of the AF(2) order M_{II} for $J_1 = 0.500$, $J_2 = -0.375$ indicating the characteristic two-step process of a first-order transition. A $18 \times 18 \times 18$ lattice was used and the relaxation to equilibrium studied after quenching to just below the transition temperature from an initial high-temperature equilibrium state. (b) Similar relaxation plot of the ferromagnetic order M_f for $J_1 = 0.500$, $J_2 = -0.100$ where the transition is continuous to a ferromagnetic state. Note the difference in scale.

FIG. 8. Phase diagram from the Monte Carlo analysis in the neighborhood of the suggested critical end point. The dashed lines indicate a first-order transition whereas the solid line represents a continuous transition.

a sudden heating to slightly above the transition temperature from low temperatures. Since in this process the full thermodynamic structure is not needed, we were able to deal with slightly larger lattices. A typical two-step relaxation for the para-AF(2) transition is shown in Fig. 7 along with a smooth relaxation indicative of a continuous transition found for the para-ferro boundary.

Figure 8 shows the summarized phase diagram for the bcc as determined by the Monte Carlo analysis. We find the results in qualitative agreement with the predictions of the ϵ -expansion calculation. In particular, at least near the mean-field bicritical point, the transition is found to be first order in the AF(2) region.

V. DISCUSSION

We have reported the results of our analysis of a model of Ising spins on a bcc lattice with competing nn and nnn exchange interactions using both renormalization-group e-expansion and Monte Carlo methods. We have presented evidence that, near the mean-field bicritical point, the para-AF(2) transition is first-order. Preliminary high-temperature series analysis,⁶ assuming a continuous transition between the AF(2) and paramagnetic phases, yielded fairly regular estimates' for critical temperatures. Series coefficients for the AF(2) susceptibility were used and transition temperatures were estimated using and transition temperatures were estimated using
Padé approximant analysis.¹⁷ More recent series ana-
lyses have been reported by Plischke and Oitmaa.¹⁸ lyses have been reported by Plischke and Oitmaa.

Our own Pade approximant analysis on the series of Lambeth et al.⁶ for the $AF(2)$ region produced associated values of γ slightly *lower* than the accepted Ising values¹⁵ of \sim 1.25. It is worth recalling that according to renormalization-group analysis, if the transition is continuous, XY exponents are expected, i.e., $\gamma \approx 1.31$. The values of T_c obtained from the series expansions are consistently lower than the values of transition temperature obtained by Monte. Carlo methods. This suggests that the series are extrapolated "right through" the first-order transition. When a first-order transition is expected, high- and lowtemperature series expansions must both be used. Even then, as pointed out by Saul, Wortis, and Stauffer,¹⁹ the method is not without difficulties

To conclude, the present evidence suggests that the mean-field phase diagram of Fig. $1(a)$ is modified by fluctuations to the form suggested schematically in Fig. $1(c)$. The numerical results suggest the phase diagram of Fig. 8 for the specific model (2.1). The renormalization-group analysis is not completely unambiguous, since we have not investigated the full dependence of the phase boundaries on the irrelevant variables. Nor have we used "model dependences" of the renormalization-group fields on the physical parameters J_1 , J_2 , and T. Hence it is not possible to rule out completely one or more second-order regions for the para- $AF(2)$ transitions as indicated schematically in Fig. 1(f). Renormalization-group analysis then predicts unambiguously that XY exponents occur in the continuous regions and Ising-like nonclassical tricritical points separate the first-order and second-order regions. The addition of weak furtherneighbor interactions does not affect the general conclusions.

The work reported here provides an additional example of the complex behavior that can result from rather simple models with competing interactions. Furthermore, the complementary nature of the two techniques, Monte Carlo and renormalization-group ϵ -expansion, has been demonstrated in a problem which probes the strengths and weaknesses of each.

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APPENDIX

In this Appendix we sketch further results for the behavior in the vicinity of the critical end point of Figs. $1(c)$ and $1(f)$. The recursion relations for Eq. (3.4) can be written down according to the usual prescriptions.⁹ The procedures of Rudnick and Nelson¹³ and particularly Rudnick¹⁰ are followed closely. The equations describing the "critical manifolds" are

$$
t_{\gamma}(l) \approx t_{\gamma}(0) \exp\left[\int_0^l [2 - Au_1(l') - Au_3(l')/6] \, dl'\right] \tag{A1}
$$

with a similar form for $t_{\alpha}(l)$ involving just $[2 - Au_2(l')]$ in the exponential. Here $A = 3/2\pi^2$. The line of continuous transitions for the ferromagnetic phase is given by $t_{\alpha}(0) = 0$, which in principle determines $T_c(p)$. Following Rudnick¹⁰ we make the ansatz that the first-order line is given by the equation $t_{\nu}(l^*) = O(\epsilon) > 0$, with an appropriately chosen l^* .

The nature of the critical end point can then be understood as follows: On the ferro side, the γ and δ modes can be integrated out since t_y is $O(\epsilon)$ (hence effectively noncritical), and an effective renormalized one-component (the α mode) Hamiltonian which shows normal critical behavior characteristic of an Ising transition at $t_{\alpha} = 0$ is obtained. This describes the second-order line separating the ferro and paramagnetic regions.

On the other hand, on the AF(2) side, the γ and δ modes can again be integrated out $[t_v=O(\epsilon)]$, but the α mode does not go critical as it did on the ferromagnetic side. This is so, because, before the mode can go critical, there is a crossing of free energies of the paramagnetic and AF(2) phases and a first-order transition takes place.

This implies that the critical end point is relatively

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- ¹K. G. Wilson and J. Kogut, Phys. Rep. 12 C , 75 (1974); M. E. Fisher, Rev. Mod. Phys. 46, 597 (1974); A. Aharony, in Phase Transitions and Critical Phenomena, edited by C. Domb and M. S. Green (Academic, Ne York, 1976), Vol. 6.
- ²See, for example, K. Binder, Adv. Phys. 23, 917 (1974); D. P. Landau, in Magnetism and Magnetic Materials-1973, edited by C. D. Graham, Jr., and J.J. Rhyne, AIP Conf. Proc. No. 18 (AIP, New York, 1974), p. 819.

uninteresting compared to bicritical or tricritical points, where approaching multicriticality implies crossover effects to a new kind of critical behavior. In the present case, on moving up in temperature in the ferro region infinitesimally close to the coexistence curve for ferro and AF(2) ordering, a normal Ising transition without any interesting crossover effects is observed.

The present picture is consistent with the fact that on going deeper into the AF(2) region (by making $|J_2|$ large), $t_{\alpha} > O(\epsilon)$, and the α mode can be integrated out immediately leading to an effective $n = 2$ Hamiltonian (3.7). This Hamiltonian, however, is such that the stable fixed point is not accessible and the transition therefore is first order.

Following the techniques developed in Refs. 10 and 13, free energies in the ordered phase can be readily constructed. The coexistence curve between the paramagnetic and $AF(2)$ phases and the jump in the AF(2) order parameter can hence be obtained. At the critical end point one finds,

$$
t_{\gamma}(l^*; t_{\alpha} = 0) = (8\pi^2)^{-1}(1+z^2)h(z)u_3(l^*) \quad , \quad (A2)
$$

where $z = u_4(l^*)/u_3(l^*)$ and

$$
h(z) = \left(\frac{1}{2}\right) \exp\left(-\frac{1}{2} - \frac{2}{1+z^2} \ln z\right) \tag{A3}
$$

This is consistent with the above ansatz. The parameter l^* is chosen such that $u_1(l^*) = 0$, i.e., the renormalized Hamiltonian, neglecting $O(s^6)$ terms, is about to go unstable. Hence z remains of order unity. If, on the other hand, a fixed point is approached, the transition becomes continuous. We have determined, by numerically following the renormalization trajectories, that in the vicinity of the mean-field bicritical point, the trajectories indeed flow unstable. A similar analysis is possible for small $t_{\alpha} > 0$ allowing a mapping of the first-order line.

Considering the complexity of Rudnick's¹⁰ solution with only two coupled fourth-order fields, we have not attempted further analysis. Numerical integration of the recursion relations along with analytic expressions for the free energy allow further information to be extracted.

³It can be shown that very weak distant-neighbor interactions do not qualitatively change the nature of the phase diagram. For a discussion, see Sec. III of this paper.

- 4S. J. Knak Jensen, 0. G. Mouritsen, and Per Bak (unpublished).
- ⁵J. S. Smart, *Effective Field Theories of Magnetism* (Saunders, Philadelphia, 1966). See Also S. Katsura and S. Fujimori, J. Phys. C 7, 2S06 (1974).
- D. N. Lambeth, G. Paul, and H. E. Stanley (unpublshed); we wish to thank H. E, Stanley for sending us the series coefficients and the unpublished results.

 $\ddot{}$

- 7'M. E. Lines, Phys. Rev. 135, A1336 (1964); R. A. Tahir-Kheli, H. B. Callen, and H. Jarrett, J. Phys. Chem. Solids 27, 23 (1966).
- $8D. R.$ Nelson and M. E. Fisher, Phys. Rev. B 11 , 1030 (1975); 12, 263 (1975).
- 9See, for example, A. Aharony, Ref. 1.
- 10 J.Rudnick, Phys. Rev. B 18, 1406 (1978).
- $¹¹$ The effects of such symmetry-breaking fields in another</sup> context have been studied by E. Domany, D. Mukamel, and M. E. Fisher, Phys. Rev. B 15, 5432 (1977).
- ¹²J. Rudnick and D. R. Nelson, Phys. Rev. B 13 , 2208 (1976).
- 13 A description of the code may be found in D. P. Landau, Phys. Rev. B 13, 2997 (1976).
- ¹⁴See, for example, M. E. Fisher, in Critical Phenomena,

edited by M. S. Green (Academic, New York, 1971), p. 1. ¹⁵See, for example, C. Domb, in Phase Transitions and CriticaI Phenomena, edited by C. Domb and M. S. Green

(Academic, New York, 1974), Vol. 3; see also J. C. LeGuillou and J. Zinn-Justin, Phys. Rev. Lett. 39, 95 (1977), and references cited therein.

- $16D$. P. Landau and K. Binder, Phys. Rev. B 17, 2328 (1978).
- ¹⁷See, for example, M. E. Fisher, Rep. Prog. Phys. 30, 615 (1967).
- ¹⁸M. Plischke and J. Oitmaa, Phys. Rev. B 19, 487 (1979).
- ¹⁹D. M. Saul, M. Wortis, and D. Stauffer, Phys. Rev. B 9, 4964 (1974).