Universality and tricritical behavior of three-dimensional Ising models with two- and four-spin interactions

O. G. Mouritsen*
Department of Physics, University of British Columbia, Vancouver, British Columbia V6T 1W5, Canada

S. J. Knak Jensen*
Department of Chemistry, University of California, Los Angeles, California 90024

B. Frank
Department of Physics, Concordia University, Montreal, Province of Quebec H3G 1M8, Canada
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The Monte Carlo technique is applied to a study of the phase transitions and the critical behavior of the spin-$\frac{1}{2}$ Ising model on an fcc lattice with mixtures of two- (J_2) and four- (J_4) spin interactions. In the limit $J_2=0$ the model exhibits a first-order transition. The transition remains of first order for $J_4/J_2 \gtrsim \frac{1}{2}$, but a crossover to continuous transitions is found around $J_4/J_2 \approx \frac{1}{4}-\frac{1}{2}$ indicating that the model exhibits tricritical behavior. A modified mean-field theory is presented leading to an approximate description of the tricritical behavior in agreement with the Monte Carlo calculations. In the region of continuous transitions, $0 \leq J_4/J_2 \lesssim \frac{1}{4}$, the critical exponent β pertaining to the order parameter derived from the Monte Carlo data retains the Ising value, in accordance with the universality hypothesis. Our findings show that the four-spin interactions do not lead to nonuniversal critical behavior, contrary to the conclusions made by Griffiths and Wood from a series analysis.

I. INTRODUCTION

The universality hypothesis for systems undergoing continuous phase transitions predicts that the critical exponents are independent of variations of linear parameters in the Hamiltonian, provided that the symmetry of the order parameter and the spatial dimension remain unchanged. This prediction is supported by a considerable body of theoretical and experimental evidence. Systems not covered by this prediction are those fulfilling the Kadanoff-Wegner criterion for nonuniversality,[1] of which the exactly solvable two-dimensional Baxter model[1,2] is a celebrated example. Certain two-dimensional Ising models with pair interactions are also expected to display nonuniversal critical behavior.[3] No three-dimensional system is definitely known to exhibit critical behavior in conflict with the universality hypothesis. However, a series analysis by Griffiths and Wood (GW)[4–6] of three-dimensional Ising models on cubic lattices with pair- and multispin (three-spin and four-spin) interactions has suggested these systems as possible candidates, although they do not fulfill the Kadanoff-Wegner criterion.[6] The results of GW are at variance with renormalization-group predictions.[7,8] Obviously, it is therefore of importance to investigate, by an independent approach, the critical properties of the three-dimensional models studied by GW.

In this paper we report the results of a numerical calculation and a modified mean-field calculation of the critical properties for a spin-$\frac{1}{2}$ Ising model on an fcc lattice with two- and four-spin (quartet) interactions described by the Hamiltonian

$$H = -J_2 \sum_{\{i,j\}} \sigma_i \sigma_j - J_4 \sum_{\{i,j,k,l\}} \sigma_i \sigma_j \sigma_k \sigma_l \ , \qquad (1.1)$$

J_2 and $J_4 > 0$ are coupling parameters, and $\sigma_i = \pm 1$ is the Ising spin variable at the ith lattice site. The sums in Eq. (1.1) comprise all nearest-neighbor bonds $\{i,j\}$ and all elementary tetrahedra $\{i,j,k,l\}$ formed by nearest-neighbor bonds of the fcc lattice. Our numerical calculation is based on the Monte Carlo (MC) method. This method appears well suited to investigate the dependence on J_4/J_2 of the phase transitions and the critical behavior of this model as no additional assumptions need be introduced into the calculation scheme when including the four-spin term. It should be noted that our realization of the MC method is free of assumptions except for those introduced through the use of finite lattices and finite ensembles in the calculation of averages; moreover, the dependence of the results on these assumptions may readily be determined.

For the model in Eq. (1.1) the series analysis by

GW[6] leads to exponents varying continuously with the ratio J_4/J_2 for $J_4/J_2 \gtrsim \frac{1}{2}$. This result is based on the assumption that the phase transition of the model is *continuous* for all values of J_4/J_2. In a previous paper[9] we have shown that the model in the pure quartet limit, $J_2=0$, exhibits only one phase transition which is of *first order*. The transition temperature differs from that of the Onsager solution, implying that the pure quartet model is likely not to possess a self-dual property as claimed by Wood[10] and by GW.[4] The calculations to be presented in this paper demonstrate that the phase transition remains of first order for large values of J_4/J_2, but a *crossover to continuous phase transitions* is found for $J_4/J_2 \simeq \frac{1}{4}-\frac{1}{2}$ indicating that the model exhibits *tricritical behavior*. In the region of continuous transitions, $0 \leq J_4/J_2 \lesssim \frac{1}{4}$, the critical exponent β pertaining to the order parameter has the Ising value, in agreement with the universality hypothesis. Our results therefore resolve the discrepancy between the results of GW and the predictions of the universality hypothesis, revealing the alleged dependence of the exponents on the value of J_4/J_2 to be an artifact of series analysis carried out in terms of power-law singularities in a regime of first-order transitions.

In Sec. II we present the results of the MC calculations of the order parameter and the internal energy as functions of the coupling ratio J_4/J_2 and the temperature. It is described in some detail how MC calculations may be applied to determine first-order phase transitions. From the order-parameter data we extract the exponent β for various values of J_4/J_2. The transition temperature as a function of J_4/J_2 is compared with the transition temperature obtained from the series analysis by GW[6] and from calculations based on the Frank-Mitran theory.[11–13] In Sec. III we present a modified mean-field theory which leads to a prediction of the transition temperatures and the tricritical point. Section IV contains a brief discussion of our results in the context of universality.

II. MONTE CARLO CALCULATIONS

A. Computational method and detection of first-order phase transitions

The MC method as an importance-sampling technique currently constitutes a useful standard tool in statistical mechanics.[14] Our implementation of the technique and the criteria of convergence are described in detail in Ref. 15.

The model described by the Hamiltonian in Eq. (1.1) is arrayed on an fcc lattice with N lattice points. The fcc lattice is represented by two equivalent interpenetrating sublattices. Each sublattice is a tetragonally distorted simple cubic lattice with L^3 lattice sites subject to periodic boundary conditions of the toroidal type. An Ising-spin variable $\sigma_i = \pm 1$ is associated with each lattice point. We have calculated the internal energy per spin $E(T) = \langle H \rangle / N$ and the ferromagnetic order parameter (the bulk magnetization per spin)

$$m(T) = N^{-1}\left\langle \left| \sum_{i=1}^{N} \sigma_i \right| \right\rangle \ . \tag{2.1}$$

In addition, we have determined the corresponding fluctuation quantities, i.e., the heat capacity $C(T)$ and the bulk susceptibility $\chi(T)$. The calculations are performed on lattices with $L=6$, 10, 18, and 20. Our results to be presented in Secs. II B and II C are based on statistics corresponding to 500–1000 MCS/S outside transition regions and to 2000–3000 MCS/S in transition regions (MCS/S≡ Monte Carlo steps per site).

In this paper we deal with systems which may exhibit first-order transitions. First-order transitions in MC simulations are signaled by the appearance of metastable states (which may be long-lived), and therefore special precautions have to be taken when calculating ensemble averages in the transition region. Detection of metastable states is facilitated by calculating coarse-grained averages[15] and distribution functions[16,17] of $E(T)$ and $m(T)$. The coarse-grained averages, which are averages over a small number of systems of the ensemble, make it possible to follow the relaxation towards a stable or a metastable state of the system. The distribution functions, which give the frequency of occurrence of a given energy and order in the systems comprising the ensemble, also reveal the various stable and metastable states and are particularly useful in evaluating the actual average energy and order associated with a short-lived metastable state.

In MC calculations on finite systems the occurrence of metastabilities—and thereby first-order transitions—is indicated by one or more of the following observations: (i) the coarse-grained averages display a characteristic two-step relaxation process,[18] first showing relaxation towards a metastable state and then eventually towards the stable equilibrium state. In some cases this two-step process may be followed by additional relaxation processes leading to (ii) successive shifts between the stable state and a metastable state.[16,17,19] Often it is not possible within reasonable computer time to determine which state is the stable one, and the system therefore effectively behaves in the simulations as though it were bistable; and (iii) hysteresis is displayed in $E(T)$ and $m(T)$ when these are calculated for increasing and decreasing series of temperatures.

In the case of (ii) with a high shift-frequency the distribution functions are necessary in order to

separate close-lying states and to evaluate the properties of these states. In the calculations reported in this paper our statistics are sufficient to determine the positions of the peaks in the distribution functions but not their relative intensities. We are therefore unable to give a very accurate determination of the equilibrium phase-transition temperature in the case of first-order transitions associated with metastabilities which occur in an extended temperature range. In that case, and in the case of a broad hysteresis curve, we estimate the equilibrium transition temperature by using an equal-area rule.

B. Phase transitions and tricritical behavior

In this section we present the MC results for the temperature dependence of $E(T)$ and $m(T)$ and use the results to determine the phase diagram spanned by the temperature and the coupling ratio J_4/J_2.

Figure 1 shows the internal energy as a function of temperature for various values of J_4/J_2. The figure also includes the result for the pure quartet limit,[9] $J_2=0$. The figure demonstrates that the system for $J_4/J_2 \gtrsim \frac{1}{2}$ undergoes a *first-order* phase transition associated with a discontinuity in the internal energy. The first-order nature of the transition is deduced from the observations (i)–(iii) listed in Sec. II A. For decreasing values of J_4/J_2 the discontinuity in E decreases, and eventually for $J_4/J_2 \lesssim \frac{1}{4}$ it disappears. For $J_4/J_2 \lesssim \frac{1}{4}$ we make none of the observations (i)–(iii), and conclude that the phase transition in this region is *continuous*. Thus the model possesses a *tricritical point* somewhere in the region $\frac{1}{4} < J_4/J_2 < \frac{1}{2}$.

A more detailed picture of $E(T)$ close to the tricritical point is shown in Fig. 2 which gives an enlargement of the $E(T)$ curves in Fig. 1 for $J_4/J_2=\frac{1}{4}$ and $\frac{1}{2}$. In addition, Fig. 2 displays the finite-size dependence of the results by giving $E(T)$ for various values of N. For $J_4/J_2=\frac{1}{4}$ the results for $N=2000$ and 11 664 are identical within the uncertainties and therefore represent the thermodynamic limit. There is no evidence of metastable states, and the energy curve is smooth and continuous within the data-point density. For $J_4/J_2=\frac{1}{2}$ the figure shows a region of coexistence for the ordered and the paramagnetic phase. For increasing values of N the width of the coexistence region shrinks, exposing more clearly the discontinuity of $E(T)$ at the transition.

The ferromagnetic order parameter $m(T)$ as a function of temperature is given in Fig. 3 for the same values of J_4/J_2 as in Fig. 1. The behavior of $m(T)$ agrees with our finding of a tricritical point in the interval $\frac{1}{4} < J_4/J_2 < \frac{1}{2}$. A finite-size analysis similar to that given in Fig. 2 for $E(T)$ shows for $J_4/J_2=\frac{1}{4}$ that $m(T)$ remains continuous for increasing values of N. The $E(T)$ curves presented in Figs. 1 and 2 are more useful in locating the tricritical point, because $E(T)$ is expected to be less affected by finite-size effects than $m(T)$. A remark is in order on the pure quartet case, where the high degeneracy of the ground state[9] makes it impossible to determine from the MC calculations the actual finite-size order on the high-temperature branch of the $m(T)$ curve. As explained in Ref. 9 the high-temperature values of $m(T)$ for $J_2=0$ in Fig. 3 are underestimates of the actual order in the finite lattice.

The transition temperatures in the various cases are determined as follows: In the case of continuous transitions the transition temperature T_c (the critical temperature) is determined as the temperature where the heat capacity attains its maximum. Equivalently,

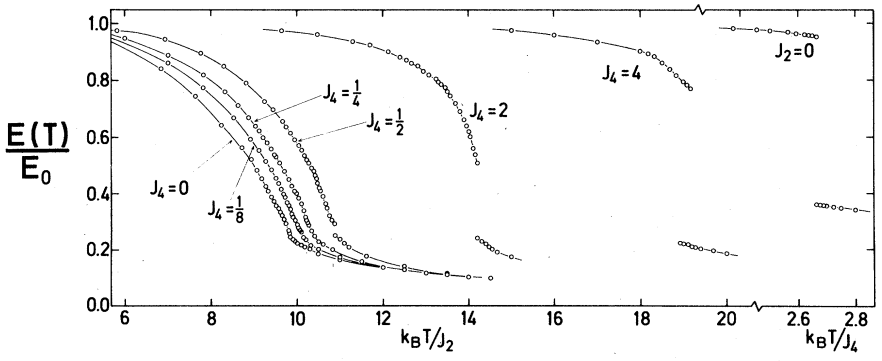

FIG. 1. Normalized internal energy $E(T)/E_0$ as a function of temperature for various values of the coupling constants J_2 and J_4. E_0 is the energy of the ground state. The data are obtained from Monte Carlo calculations on systems with $N=2000$ spins, except in the case $J_4=4$ where the system contains $N=432$ spins.

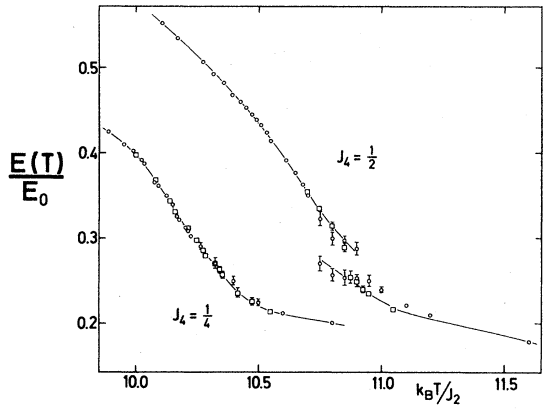

FIG. 2. Temperature dependence of the normalized internal energy $E(T)/E_0$ in the tricritical region. J_4 is the four-spin coupling constant, and J_2 is the two-spin coupling constant. E_0 is the energy of the ground state. The data are obtained from Monte Carlo calculations on systems with N spins. ○: $N=2000$ for both values of J_4; □: $N=11\,664$ for $J_4=\frac{1}{4}$ and $N=16\,000$ for $J_4=\frac{1}{2}$.

we may obtain T_c from the position of the maximum of the susceptibility. For finite lattices these two estimates normally differ slightly. In this investigation we are not interested in providing an accurate estimate of T_c, and consequently we have not performed a full finite-size analysis.[20] Instead we give T_c^{MC} with error limits expected to cover the thermodynamic limit. In the case of first-order transitions T_c^{MC} is derived using a simple equal-area rule.

Our results for T_c^{MC} are given in Table I which also includes the transition temperatures T_c^{GW} derived by GW[6] from an analysis of the low-temperature series for the order parameter. The series, which extend to order $[\exp(-4J/k_BT)]^{12}$, are analyzed in terms of a simple power-law singularity assuming that the transition is continuous for all values of J_4/J_2. Comparison of T_c^{MC} and T_c^{GW} reveals the following trends: for $J_4/J_2 \lesssim \frac{1}{4}$, T_c^{MC} and T_c^{GW} agree within the error limits; for $J_4/J_2 \gtrsim \frac{1}{2}$, T_c^{GW} lies increasingly below T_c^{MC} (excepting the limit $J_2=0$). These trends are in accord with our finding of a tricritical point in the interval $\frac{1}{4} < J_4/J_2 < \frac{1}{2}$, implying that the assumption made in the series analysis breaks down above $J_4/J_2 \sim \frac{1}{2}$. It is well known from series studies of models exhibiting first-order phase transitions that analysis in terms of power-law singularities is likely to lead to unreliable estimates of T_c. In Table I we have also included transition temperatures T_c^F derived by Frank.[13] (The transition temperatures obtained from a related approach by Mitran[11] are not included as this approach has recently been shown not to be self-consistent.[12]) The theory by Frank seems applicable to continuous as well as to first-order transitions.[13] The table shows that T_c^F lies systematically above T_c^{MC} and the deviation increases with increasing values of $J_4/J_2 < \infty$.

C. Critical exponent β

We now investigate the critical behavior of the order parameter in the region of continuous transitions, $J_4/J_2 \lesssim \frac{1}{4}$, by analyzing the MC data in terms of a simple power law

$$m(T) \simeq Bt^{\beta}, \quad t \equiv (T_c - T)/T_c \ , \tag{2.2}$$

β is the critical exponent and B is the critical amplitude. In the analysis we have put $T_c = T_c^{GW}$, as we expect the series estimate of T_c to be more accurate than T_c^{MC} in the case of a continuous transition.

In Fig. 4 is presented a log-log plot of $m(T)$ versus the reduced temperature t for $J_4/J_2=0$, $\frac{1}{8}$, and $\frac{1}{4}$.

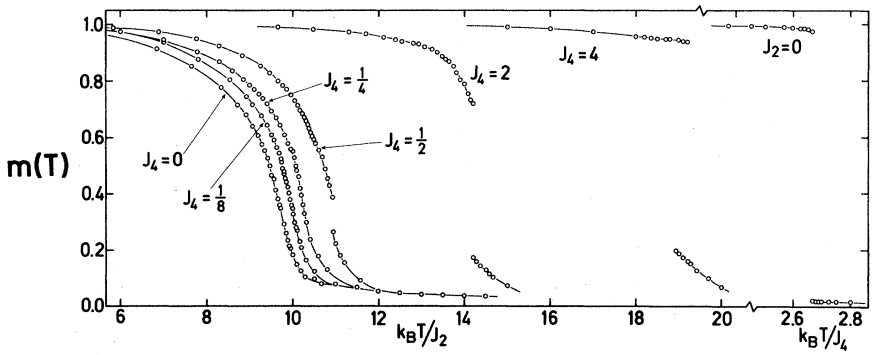

FIG. 3. Ferromagnetic order parameter $m(T)$, Eq. (2.1), as a function of temperature for various values of the coupling constants J_2 and J_4. The data are obtained from Monte Carlo calculations on systems with $N=2000$ spins, except in the case $J_4=4$ where the system contains $N=432$ spins.

TABLE I. Transition temperatures for the model in Eq. (1.1) for various values of the coupling ratio J_4/J_2. T_c^{MC} is the transition temperature obtained from Monte Carlo calculations on systems with N spins. T_c^{GW} is the transition temperature derived from series analysis. T_c^{F} is the transition temperature obtained from the theory of Frank. All temperatures are in units of J_2/k_B, except for the case $J_4/J_2=\infty$ where the temperatures are in units of J_4/k_B.

J_4/J_2	T_c^{MC}	T_c^{GW}	T_c^{F}	N
0	9.75 ± 0.05	9.7920[a]	9.7920[b]	2×18^3
$\frac{1}{8}$	9.95 ± 0.05	10.02[c]	10.15[d]	2×18^3
$\frac{1}{4}$	10.25 ± 0.05	10.27 ± 0.06[c]	10.51[d]	2×18^3
$\frac{1}{2}$	10.86 ± 0.05	10.61 ± 0.08[c]	11.22[d]	2×20^3
2	14.28 ± 0.10	13.78 ± 0.06[c]	15.51[d]	2×10^3
4	18.95 ± 0.15		21.23[d]	2×6^3
∞	2.66 ± 0.01	2.79 ± 0.01[c]	2.86[d]	2×10^3

[a]Reference 21.
[b]The value of T_c (pair) in Eq. (3.18) is taken from the series analysis of Ref. 21.
[c]Reference 6.
[d]Values derived from Eq. (3.18).

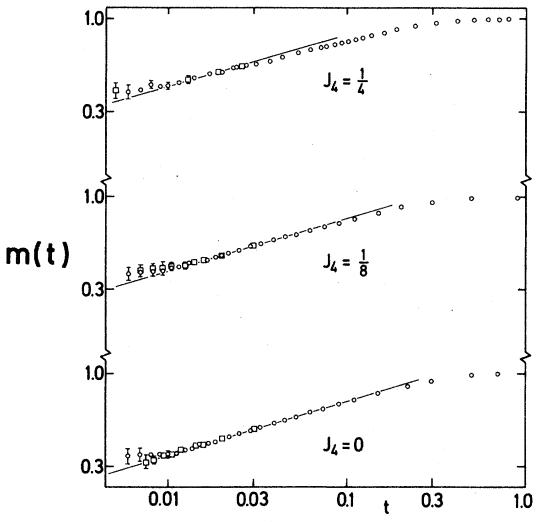

FIG. 4. Log-Log plot of the ferromagnetic order parameter $m(t)$ vs the reduced temperature $t=(T_c-T)/T_c$ for values of the four-spin coupling constant J_4 leading to continuous transitions. The critical temperature T_c is the one derived from series analysis. The data for $m(t)$ are obtained from Monte Carlo calculations on systems with $N=2000$ spins (○), and $N=11\,664$ spins (□). The solid lines represent the power law $m(T)\sim t^{\beta}$, Eq. (2.3), with $\beta=0.31$.

Comparing MC data for two different lattice sizes, $N=2000$ and 11 664, we conclude that our data to a good approximation represent the thermodynamic limit for $t\gtrsim0.008$ for all three values of J_4/J_2. For $J_4=0$, Fig. 4 shows that the data satisfy the asymptotic critical form, Eq. (2.2), for $t\lesssim0.2$ with critical parameters

$$\beta=0.310\pm0.015,\quad B=1.45\pm0.05\ , \tag{2.3}$$

which are consistent with the respective series estimates,[22] $\beta=0.312\pm0.005$ and $B=1.487\pm0.002$. For increasing values of J_4/J_2 Fig. 4 shows that the asymptotic slopes, i.e., β, remain unchanged, but the amplitude B increases and the critical region described by Eq. (2.3) shrinks. The shrinking is caused by crossover to the tricritical point. However, we consider our data to be too far from the tricritical point to sustain a detailed analysis of $m(t)$ in terms of a power law with multiplicative logarithmic corrections.[23]

III. MODIFIED MEAN-FIELD THEORY

The results of the previous section may be understood in terms of mean-field theory suitably modified to take account of third-order correlations. The need for such a modification arises from the failure of or-

dinary mean-field theory to agree quantitatively with the tricritical value of the coupling ratio, $(J_4/J_2)_t$, inferred from the MC calculations and even qualitatively to account for the variation of the transition temperature with J_4/J_2. Ordinary mean-field theory (MFT) implies the equation

$$m = \tanh[(12J_2 m + 8J_4 m^3)/k_B T] \ ,$$

which leads to the prediction of a tricritical point for $(J_4/J_2)_t = 0.5$, and transition temperatures which are independent of J_4/J_2. The modification is made on the basis of a generalization[13] of the Frank-Mitran theory[11,12] for the Ising ferromagnet with pair and quartet interactions in the immediate vicinity of the phase transition. It will be seen that the modified mean-field theory predicts a value of $(J_4/J_2)_t$ which is in good agreement with the MC results.

We start with a summary of the relevant parts of the Frank-Mitran theory. We consider the Hamiltonian

$$\tilde{H} = H + H_a \tag{3.1}$$

where H is the Hamiltonian in Eq. (1.1), written as

$$H = -(1/2!)\sum_{i,j} J_{ij}\sigma_i\sigma_j - (1/4!)\sum_{i,j,k,r} J_{ijkr}\sigma_i\sigma_j\sigma_k\sigma_r \ . \tag{3.2}$$

The lattice-site summations are now unrestricted, and H_a is an added Hamiltonian similar to that used in the work of Griffiths[24]

$$H_a = \sum_{j;m,n} \lambda^j_{mn}(O_j)^m(P_j)^n \tag{3.3}$$

$$(m,n = 0,1,2,\ \ldots,\ m+n \text{ odd})$$

with

$$P_i = O_i + Q_i \ , \tag{3.4a}$$

$$O_i = \sum_j J_{ij}\sigma_j \ , \tag{3.4b}$$

$$Q_i = (1/3!)\sum_{j,k,r} J_{ijkr}\sigma_j\sigma_k\sigma_r \ , \tag{3.4c}$$

where the coefficients λ^j_{mn} are to vanish at the end of the calculation.

For $\lambda^j_{mn} = 0$, one has the exact equation for the order parameter

$$m \equiv \langle\sigma_i\rangle = \langle\tanh\beta P_i\rangle, \quad \beta = 1/k_B T \tag{3.5}$$

derived most easily by the method of Suzuki,[25] where the thermal averages $\langle\cdots\rangle$ are in terms of the basic Hamiltonian H. Reverting now to the full Hamiltonian $\tilde{H}$, and going to the limit $\lambda^j_{mn} \to 0$, $T \to T_c$, the assumption is made that the thermal averages of the same odd powers of P_i and O_i approach zero in the same way

$$\langle(P_i)^{2r+1}\rangle = B_{2r+2}\langle(O_i)^{2r+1}\rangle \ , \tag{3.6}$$

$$r = 0,1,2,\ \ldots \ ,$$

where the B_{2r+2} may be functions of λ^j_{mn} and β, assumed to be analytic in the above limit.

It may then be shown directly that

$$\langle(P_i)^n\rangle = (B_2)^n\langle(O_i)^n\rangle, \quad n = 1,2,\ \ldots \ , \tag{3.7}$$

where, using Eq. (3.4)

$$B_2 = \langle O_i P_i\rangle/\langle(O_i)^2\rangle = 1 + 4a_2 J_4/J_2 \ . \tag{3.8}$$

An approximate, self-consistent calculation[13] of a_2 for the fcc lattice yields

$$a_2 = 0.073 \tag{3.9}$$

(independent of J_4 and J_2). Using Eq. (3.7), Eq. (3.5) may then be written, for $\lambda^j_{mn} \to 0$ and $T \to T_c$, as

$$m = \langle\tanh\beta B_2 O_i\rangle \ . \tag{3.10}$$

It is noted that in the limit $J_4 = 0$, Eq. (3.10) is exact.

We are now in a position to set out and modify ordinary mean-field theory. For the pure pair-interaction case, $B_2 = 1$, one ordinarily takes the thermal averages in Eq. (3.10) inside the hyperbolic tangent, to write

$$m = \tanh\beta\langle O_i\rangle \ . \tag{3.11}$$

This is equivalent to a complete decoupling of the multispin correlation functions. Similarly, in the pair-quartet case, the first stage of an MFT would be to write Eq. (3.5) as [using Eq. (3.4a)]

$$m = \tanh\beta(\langle O_i\rangle + \langle Q_i\rangle) \ . \tag{3.12}$$

To remain within the spirit of the MFT one would completely decouple the spins inside $\langle Q_i\rangle$, writing

$$m = \tanh\beta\left[\langle O_i\rangle + (1/3!)\sum_{j,k,r} J_{ijkr}\langle\sigma_j\rangle\langle\sigma_k\rangle\langle\sigma_r\rangle\right] \ . \tag{3.13}$$

The value of $(J_4/J_2)_t$ obtained from Eq. (3.13) is 0.5, a value approximately 25% higher than the Monte Carlo result.

Now Frank-Mitran theory, as outlined above, provides a guide for the modification of and improvement over Eq. (3.13). Taking the thermal average inside the hyperbolic tangent in Eq. (3.10), which itself has validity only in the limit $T \to T_c^-$, one obtains

to $O(m)$ within the tanh,

$$m = \tanh\beta B_2 \langle O_i \rangle \ . \tag{3.14}$$

The contribution of each spin in Eq. (3.14) to the molecular field is seen to be effectively obtained from the ordinary MFT, Eq. (3.13), by replacing m by $B_2 m$ to order m within the tanh. The ansatz is now made that to higher orders in m also, one proceeds from Eq. (3.13) to the modified equation by replacing m by $B_2 m$ everywhere inside the tanh. The result is, for the fcc lattice,

$$m = \tanh\beta(12J_2 B_2 m + 8J_4 B_2^3 m^3) \ . \tag{3.15}$$

The tricritical point, located from $d^2\beta/dm^2 = 0$, is given, using Eq. (3.8), by

$$4J_4/J_2 = 2(1 + 4a_2 J_4/J_2)^{-2}, \quad T = T_t \ , \tag{3.16}$$

so that, with Eq. (3.9),

$$(J_4/J_2)_t = 0.401 \ . \tag{3.17}$$

This value of the tricritical coupling ratio is consistent with the MC data of Sec. II.

We have now presented a theory which predicts tricritical behavior in qualitative agreement with MC calculations. While the above theory is fairly successful in its prediction of the tricritical coupling ratio, it is less so in its quantitative determination of the transition temperatures. The latter deviate from the predictions of series analysis, MC calculations, and Frank-Mitran theory, by roughly 25% for all values of J_4/J_2. This is not surprising, in that $(J_4/J_2)_t$ is dependent on the relative way in which the m and m^3 terms enter whatever function is on the right-hand side of Eq. (3.15), while T_c depends sensitively on the coefficient of m in this equation. However, the linearity between T_c and J_4/J_2

$$T_c(\text{pair-quartet}) = B_2 T_c(\text{pair}) \tag{3.18}$$

remains as in Frank-Mitran theory. This linearity is supported by the present MC data, with a MC value of $a_2 = 0.068$. The within-10% agreement between this value and that of Eq. (3.9) is regarded as satisfactory. To devise a theory which leads to accurate values for both T_t and $(J_4/J_2)_t$, one might look for a way to modify Frank-Mitran theory in the light of ordinary MFT, rather than the reverse as was done here.

IV. SUMMARY AND DISCUSSION ON UNIVERSALITY

We have studied the phase transitions and the critical behavior of a three-dimensional Ising model with mixtures of ferromagnetic two-spin (J_2) and four-spin (J_4) interactions. The model does not fulfill the Kadanoff-Wegner criterion for nonuniversality as it does not contain a marginal operator which transforms under change of length scale R as R^{-d}, where d is the spatial dimension. The critical exponents are therefore expected to be independent of the values of the model parameter J_4/J_2. Our calculations reveal a tricritical point and show that in the region of continuous transitions the critical exponent β retains the Ising value, in agreement with the universality hypothesis. Our results remove a puzzle which has persisted for quite some time in the literature of phase transitions, brought about by the evidence reported from series analysis[6] in favor of nonuniversal critical behavior for this model. Moreover, our results are in accordance with renormalization-group calculations[7,8] which predict a crossover to first-order transitions when a fourth-order interaction parameter becomes sufficiently large.

The results presented in this paper were obtained for a model including four-spin interactions on an fcc lattice. We believe, however, that the interpretation of the series results in light of the encountered tricritical behavior may in some cases apply to other lattices and other types of multispin interactions. Griffiths and Wood[6] (GW) concluded from a series analysis that the spin-$\frac{1}{2}$ Ising model on a bcc lattice with ferromagnetic two-spin and four-spin interactions exhibits nonuniversal critical behavior for all values of $J_4/J_2 \gtrsim 0$. We interpret this as evidence for crossover to first-order phase transitions for even a very small admixture of four-spin interactions. Similarly, GW[5,6] from series analysis of spin-$\frac{1}{2}$ Ising models on fcc and bcc lattices with ferromagnetic two-spin and three-spin (J_3) interactions found that the exponents vary with J_3/J_2 for all values of J_3/J_2 investigated. As shown by Monte Carlo calculations in Ref. 9, the phase transition for the fcc lattice in the pure three-spin interaction limit is of first order. It seems reasonable to interpret the series results as evidence for first-order phase transitions down to very small values of J_3/J_2. It would be of interest to investigate whether the transition is of first order for arbitrarily small values of J_3/J_2. If this is the case, it may have important implications for the description by lattice-gas models of simple fluids where three-body interactions are known to play an important role.[26]

Finally, we wish to comment on the usefulness of mean-field predictions for phase transitions of Ising models with mixtures of two-spin and multispin interactions involving clusters of $p > 2$ spins. In general it can be shown that simple mean-field theory in any dimension predicts a tricritical point for mixtures of ferromagnetic two-spin and p-spin interactions. For p even the tricritical point appears for a finite value of J_p/J_2, and for p odd the tricritical point coalesces with the $J_p = 0$ axis. These predictions are in qualitative agreement with the Monte Carlo results presented in this paper and with our interpretation of the series results by GW for various three-dimen-

sional models. For two-dimensional models, however, the mean-field predictions may well be even qualitatively incorrect.[27]

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*On leave of absence from Department of Physical Chemistry, Aarhus University, Denmark.

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