Fifth International Colloquium on Magnetic Thin Films, Hakone, Japan, April, 1972 (unpublished), p. D5-1.

[8]H. E. Bömmel and K. Dransfeld, Phys. Rev. Lett. **3**, 83 (1959).

[9]M. Pomerantz, Phys. Rev. Lett. **7**, 312 (1961).

[10]M. F. Lewis, T. G. Phillips, and H. M. Rosenberg, Phys. Lett. **1**, 198 (1962).

[11]M. H. Seavey, Jr., IEEE Trans. Ultrason. Eng. **10**, 49 (1963); Proc. IEEE **53**, 1387 (1965).

[12]P. E. Wigen, W. I. Dobrov, and M. R. Shanabarger, Phys. Rev. 14, A1827 (1965).

[13]J. H. Collins, D. A. Wilson, and F. A. Pizzarello, J. Appl. Phys. **40**, 1201 (1969); J. H. Collins (private communication).

[14]C. Kittel, Phys. Rev. **110**, 1295 (1958).

[15]It is more appropriate to define $\omega_0\tau_m$ as $(1/|\eta|)\{[H_0(H_0+4\pi M_0\sin^2\theta)]^{1/2}/(H_0+2\pi M_0\sin^2\theta)\}$, for then $1/\tau_m$ is directly proportional to the frequency linewidth of the uniform-precession mode defined by Eq. (11) of I. For K-band frequencies, however, the term in the brackets does not deviate very much from unity (1 at $\theta=0$ and 0.94 at $\theta=90°$).

[16]Note that the dispersion relations contain the square of the magnetoelastic constant. See Eqs. (41) and (56) of I.

[17]G. V. Skrotskii and L. V. Kurbatov, in *Ferromagnetic Resonance*, edited by S. V. Vonsovskii (Pergamon, Oxford, England, 1966).

[18]C. Vittoria, R. C. Barker, and A. Yelon, Phys. Rev. Lett. **19**, 792 (1967).

[19]Y. J. Liu, R. C. Barker, and A. Yelon (unpublished data).

[20]S. Levy and R. Truell, Rev. Mod. Phys. **25**, 140 (1953).

[21]B. Luthi (private communication).

[22]T. Kobayashi, R. C. Barker, J. L. Bleustein, and A. Yelon, Letters Appl. Eng. Sci. (to be published).

PHYSICAL REVIEW B VOLUME 7, NUMBER 7 1 APRIL 1973

Monte Carlo Calculation of the Scaling Equation of State for the Classical Heisenberg Ferromagnet

K. Binder*
IBM Zurich Research Laboratory, 8803 *Rüschlikon, Switzerland*

H. Müller-Krumbhaar
Physikdepartment E14, *Technische Universität München, D* 8046 *Garching, West Germany*

(Received 5 September 1972)

Using a Monte Carlo procedure with a self-consistent-field boundary condition, the magnetization of a simple cubic classical Heisenberg ferromagnet with nearest-neighbor interactions only is calculated. For reduced temperatures and reduced fields in the range $0.02 \leqslant |T/T_c - 1|$, $H/J \leqslant 0.5$ the data of this computer experiment can be described in terms of the "effective" critical exponents $0.31 \leqslant \beta \leqslant 0.35$, $1.33 \leqslant \gamma \leqslant 1.39$, and $4.9 \leqslant \delta \leqslant 5.3$. Although the present data are not very close to the critical point they do obey the homogeneity requirement and determine the scaling function rather precisely. This function agrees very well with the scaling function for the face-centered-cubic classical Heisenberg magnet derived recently by Miloševič and Stanley using high-temperature–series-expansion techniques. This agreement supports their hypothesis that neither critical exponents nor the scaling function depend on the lattice structure in the Heisenberg model.

I. INTRODUCTION

Considerable effort has been devoted to derive the critical properties of three-dimensional Heisenberg ferromagnets.[1–26] Most of this research uses high-temperature–series-expansion techniques,[27] which yield direct information about the exponents γ, ν, η, and α. Making use of the scaling assumptions[28] one can then draw more conclusions also about the exponents β and δ. A more direct result concerning β has been derived by Stephenson and Wood[17] in the case of an fcc classical Heisenberg lattice. Inverting the series for the free energy in a magnetic field[16] these authors find $\beta = 0.38 \pm 0.03$. The series for other lattices and other values of spin turned out to be too irregular to yield very precise results.[18]

More recently, other estimates for the critical exponents have been given using the Wilson $\epsilon = 4-d$ expansion technique[24,25] and also using approximate renormalization-group recursion relations.[26] Apart from the values of critical exponents, temperatures, and amplitudes, one is also interested in the homogeneous function determining the scaling equation of state.[28–30] An important question is whether this function is independent of "irrelevant" features of the system (e.g., lattice structure or value of spin) as conjectured by the hypothesis of universality.[31,32] So far, this function has been calculated for the fcc lattice only in both the $S=\frac{1}{2}$ and $S=\infty$ cases by Miloševič and Stanley.[23] For the bcc lattice the scaling function has been given only in the $S=\frac{1}{2}$ case,[23] and no scaling functions have been available for the simple cubic (sc) lattice. This scaling function has also been calculated using the renormalization-group techniques.[33] Another interesting question concerns the regime of validity of this asymptotic description in terms of critical properties and the magnitude of the corrections to the scaling behavior.[34–41]

Bearing in mind all these problems it seems worthwhile applying techniques which could yield additional information about the thermodynamics of Heisenberg magnets near their critical point. Rough estimates of exponents and other critical properties have been obtained by generalizing the Monte Carlo sampling technique of Metropolis *et al.*[42] to the classical Heisenberg magnet.[43,44] However, the critical behavior is somewhat obscured by the pronounced finite size-rounding phenomenon,[45] which itself demands careful attention using this method,[46,47] and is a serious hindrance in making statements about infinite systems. Quite recently, it has been shown[48] that the use of a self-consistent-field boundary condition reduces the finite size effects to a very great extent. This method is also used in the present paper to derive the critical exponents and amplitudes of the sc classical Heisenberg magnet as well as the scaling function.

In Sec. II we give a short outline of the method (for a more detailed justification see Ref. 48, where some computational remarks are also given) and in Sec. III we discuss the numerical values of the critical exponents and the low-temperature susceptibility. In Sec. IV we analyze the scaling behavior and compare it with the Milošević–Stanley function. Section V contains our conclusions and also a few remarks about the corrections to scaling.

II. "SELF-CONSISTENT" MONTE CARLO METHOD

In the conventional Monte Carlo method[42,49,50] one considers a finite system, usually with periodic boundary conditions. With the help of random numbers one generates a Markov chain of points in the configurational space of the system. For the transition from state i to state j one uses a transition probability p_{ij} satisfying a detailed balance condition[42,49,50]

$$U_i p_{ij} = U_j p_{ji} , \tag{1}$$

with the canonical distribution $U_i \propto e^{-E_i/k_B T}$, where E_i is the energy of the system in state i. In the limit where the number of configurations M tends to infinity, it can be shown[49] that the canonical expectation value $\langle A\rangle$ of an observable A_i is given by an average over the Markov chain,

$$\langle A\rangle \sim \frac{1}{M}\sum_{i=1}^{M} A_i . \tag{2}$$

This average is a "time average" of the stochastic model whose dynamics are governed by Eq. (1). It is equal to the phase average since the method is ergodic by construction.[49] The general hope is[49] that one can already estimate $\langle A\rangle$ with reasonable accuracy from Markov chains with rather short length M. This method can be applied to the classical Heisenberg magnet, but one has to deal with two difficulties when making predictions about the critical behavior. The first difficulty is that one observes near T_C a "critical slowing down of convergence" which can be understood if the model is interpreted dynamically[51] in analogy to the stochastic Ising model.[52] It has been shown[51] that near T_C the error in the magnetization m,

$$m \equiv \langle m_z\rangle = \left\langle \frac{1}{N}\sum_{i=1}^{N} S_i^z \right\rangle , \tag{3}$$

increases like the susceptibility. Therefore in order to obtain a good accuracy the number of Monte Carlo steps per spin, $n = M/N$, must get very large,

$$n \gg \chi/\chi_0 , \tag{4}$$

where χ_0 denotes the susceptibility of a system of N noninteracting spins. The hope that not too large n might be sufficient is not justified for $N\to\infty$ and $t = |T/T_C - 1| \to 0$ since $\chi \propto t^{-\gamma} \to \infty$.

The second difficulty is that finite systems cannot exhibit singularities[45] and, therefore, the critical anomalies are smeared out.[45–47] Furthermore, we have $\langle m_z\rangle \equiv 0$ for the Heisenberg model in zero magnetic field and $m_{\rm rms} = \langle m^2\rangle^{1/2}$ has to be taken as an estimate for the spontaneous magnetization.[43,44] It is easy to see that $m_{\rm rms} \sim N^{-1/2}$ even for $1/T\to 0$, while near T_C, $m_{\rm rms} \sim N^{-1/6}$ in three-dimensional systems.[46,48] In the general case one has strong rounding effects if the linear dimension of the system $N^{1/d}$ [53] equals the correlation length[45] $\xi(t) \propto \xi_0 |t|^{-\nu}$. Since $\xi_0 \approx 1$,[53] we have rounding for

$$N^{1/d} \approx \xi_0 |t|^{-1/\nu} \to |t| \lesssim N^{-1/3\nu} \approx N^{-1/2} . \tag{5}$$

The difficulty $\langle m_z\rangle \equiv 0$ may be removed by applying a suitable effective field h acting on the spins at the surface of the system as a boundary condition instead of the periodicity condition.[54] This field defines the $+z$ direction and its magnitude is chosen by a consistency condition

$$\langle m_z\rangle_{\rm surface} = \langle m_z\rangle_{\rm bulk} , \tag{6}$$

where we define ($N_{\rm surface} + N_{\rm bulk} = N$)

$$\langle m_z\rangle_{\rm surface} = \frac{1}{N_{\rm surface}} \left\langle \sum_{i \text{ on surf.}} S_i^z \right\rangle , \qquad \langle m_z\rangle_{\rm bulk} = \frac{1}{N_{\rm bulk}} \left\langle \sum_{i \text{ in bulk}} S_i^z \right\rangle . \tag{7}$$

This condition, Eq. (6), is a generalization of the consistency condition of Bethe's[55] improvement of the mean-field approximation. Since neither $\langle m_z\rangle$ nor h is known at the beginning of the calculation, h has to be determined self-consistently by an iterative process for each of the parameter values J/kT and H/J.[56] This method does not yield the usual rounding but a well-defined critical point[48] which agrees very well with the value of T_C predicted by the series expansion.[8] In a sense this method is a systematic generalization of mean-field theory, and general arguments can be given[48] that very near T_C the wrong mean-field behavior must occur again. Therefore, one might assume at first sight that the range of temperatures where the method is unreliable is again given by Eq. (5), and nothing has been gained in comparison with the periodic boundary condition. In fact, this criterion, Eq. (5), is somewhat too pessimistic, as can be seen considering $N \to 1$, i.e., proceeding to the limiting case of the Bethe and mean-field approximations. These are known to give reasonably accurate results for[57] $|t| > 1/Z$ where Z is the coordination number of the lattice, while the above criterion, Eq. (5), would require $|t| > 1$. One might conjecture that the present method is accurate as long as one has

$$\xi(tZ) \lesssim N^{1/d}, \qquad \xi(t) \propto |t|^{-\nu_d} \quad \text{for } t \to 0. \tag{8}$$

This estimate seems to be supported by numerical studies[48] varying N in the range $64 \leq N \leq 4096$.

From Eqs. (4), (5), and (8) we recognize the advantage of this "self-consistent" Monte Carlo (SMC) method compared to the periodic Monte Carlo (PMC) method. On the average, about six iterations are used to adjust the effective field. To approximate the infinite system in both cases to the same extent, the size of the system is $N_{\text{PMC}} = Z^{\nu_d d} N$. Thus we get, for the total number of configurations,

$$M_{\text{SMC}} \approx 6Nn, \qquad M_{\text{PMC}} \approx Z^{\nu_d d} Nn. \tag{9}$$

The gain factor in computing time is thus roughly $\frac{1}{6} Z^{\nu_d d}$. This is a large number for three-dimensional systems.[58-60]

In the present investigation we used $N = 512$, $n > 10^4$, and various temperatures and magnetic fields. The calculation was performed on the IBM 370/155 computer of the IBM Zurich Research Laboratory. In Table I we give the data for the magnetization and compare the error estimates derived from the statistical analysis of the data with the theoretical estimate based on the study of the dynamical correlations of the model.[51] Both the order of magnitude and the trend as functions of H/J and $|T - T_C|/T_C$ of the experimental and theoretical error estimates are in reasonable agreement. In spite of the large n there are considerable errors near T_C, demonstrating the "critical slowing down" mentioned above. It is this fact which prevents us from choosing a larger N and trying to get nearer to T_C.

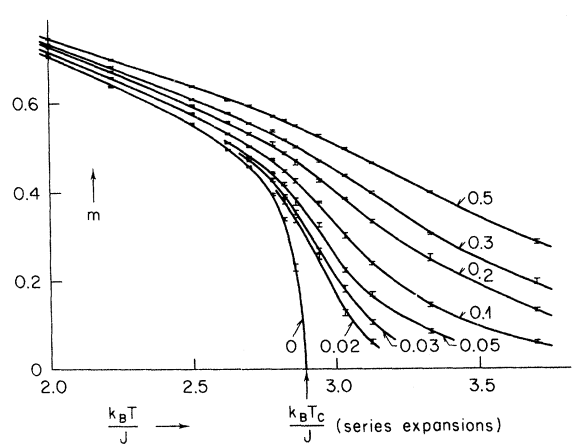

FIG. 1. Magnetization m (saturation value $m = 1$) plotted vs temperature, for various magnetic fields H/J.

III. CRITICAL EXPONENTS OF CLASSICAL HEISENBERG MODEL

In Fig. 1 we plot the magnetization versus the temperature for various fields. From these results one immediately gets the magnetic phase boundary and the magnetic isotherm, which are given on a log-log plot in Fig. 2. Replotting the magnetization versus the field one can find the susceptibilities by graphical differentiation.[61] The initial slope of the m-vs-H/J curves then determines the zero-field susceptibility. While this procedure is straightforward for T/T_C it is very questionable below T_C. From spin-wave theories[62] one expects that not only will the transverse susceptibility diverge below T_C but also the longitudinal susceptibility, since the expected behavior of the magnetization in a field is[62]

$$m(t, H/J) = m_0(t) + m_1(t)(H/J)^{0.5} + \cdots, \quad t < 0 \tag{10a}$$

with[62]

$$m_0(t) = 1 - 1.516(kT/12J) - 1.0(kT/12J)^2 - \cdots. \tag{10b}$$

Plotting m vs $(H/J)^{1/2}$, one does not see this behavior, but this may be due to the fact that the magnetic fields chosen are not small enough. It is important to note that the asymptotic decay laws of the correlation functions in zero and nonzero field are different; the decay is exponential for $H \neq 0$ but according to a power p for $H = 0$.[63] Following Halperin and Hohenberg[63] we may define correlation lengths ξ_H, ξ by

$$\langle S_0^z S_R^z \rangle \propto e^{-R/\xi_H}/R, \qquad R \to \infty, \quad H \neq 0 \tag{11a}$$

$$\langle S_0^z S_R^z \rangle \propto m_0^2(t)(\xi/R)^p, \quad R \to \infty, \quad H = 0. \tag{11b}$$

Note that $\xi_H(H=0) \neq \xi$; in fact we have $\xi_H(H \to 0) \to \infty$ at any $T < T_C$. In order to have consistency both with scaling and with the square-root singularity of χ according to Eq. (10a), the following relation is conjectured[63] ($\xi_H \gg \xi$):

$$\xi_H^2 \approx [t^{\beta\delta}(H/J)^{-1}]\,\xi^2 . \qquad (11c)$$

Our data belong to the region $t^{\beta\delta}(H/J)^{-1} \lesssim 1$, however, and $\xi_H \lesssim \xi$. This would explain the absence[63] of any indication of a divergent susceptibility. It is not useful to consider fields H/J which are considerably smaller than the ones used, since as $\xi_H \gg N^{1/d}$ the susceptibility is rounded off to mean-field-like behavior. According to Eq. (11) our "extrapolated" susceptibility $\bar{\chi}$ is then a measure of ξ^2 and in this restricted sense it can be useful to plot it in Fig. 2. However, we cannot make really conclusive statements about the divergence of χ below T_C at $H=0$.[64]

In Fig. 2 we found it convenient to normalize $\chi = \partial m/\partial H$ above T_C with $\chi_0 = \frac{1}{3}J/k_BT$ and below T_C with the asymptotic result of the mean-field theory,

$$\chi_{\mathrm{MF}}(T\to 0) \sim \frac{1}{9}\,\frac{k_BT}{J}\left(\frac{J}{k_BT_C}\right)^2_{\mathrm{MF}} = \frac{1}{144}\,\frac{k_BT}{J} . \qquad (12)$$

From Fig. 2 we now estimate "effective" critical exponents and amplitudes,

$$m \sim 1.03\,(-t)^{0.31}, \qquad m \sim 0.61\,(H/J)^{1/5.3} \qquad (13)$$

and

$$\chi/\chi_0 \sim 0.97 t^{-1.36}, \qquad \bar{\chi}/\chi_{\mathrm{MF}} \sim 0.90\,(-t)^{-1.36} . \qquad (14)$$

The high-temperature value $J/k_BT_C = 0.3458$ was used in Eqs. (13) and (14) and in Fig. 2. This description has been taken for temperatures $|t|$ and fields H/J in the range $0.02 < |t|$, $H/J < 0.2$, but even for larger $|t|$ and H/J the deviations from this behavior (dashed curves in Fig. 2) are not significant. The question now arises whether these data have been derived close enough to the critical point to be interpreted in terms of critical exponents. In experiments one takes, rather arbitrarily in most cases, $|t| \lesssim 0.01$ (or, in very few cases, $|t| \lesssim 0.1$) to define the "critical region." The reason for this choice is that for larger $|t|$ rather large deviations from the critical behavior are observed. In some cases the mean-field exponents apply in this region. This behavior may be due to the existence of "irrelevant" parameters.[65–68] Such parameters are not included in our model Hamiltonian, and therefore a region with significant deviations from the critical behavior due to such parameters[65] is absent in our case. Another argument is that for $|t| \lesssim 1/z$, mean-field theory breaks down[57,69] and therefore in this region critical behavior should be observed. A similar limit is given by $|t| < |T_C - T_C^{\mathrm{MF}}|/T_C^{\mathrm{MF}}$, which is nearly 0.3 in our case. Note that this quantity will be nearly one order of magnitude smaller in most experimental situations. According to this latter argument essentially all of our data should show the critical behavior, since $k_BT_C^{\mathrm{MF}}/J = 4.0$. A simple physical condition for the critical behavior is $\xi(t)$

TABLE I. Magnetization m of the sc classical Heisenberg ferromagnet. The number of configurations per spin n is given in units of 10^4, and the observed error Δm^e and the calculated error Δm^t are given in units of 10^{-3} (and then rounded to integers).

H/J →	0.00			0.02				0.03				0.05			
J/K_BT	m	Δm^e	n	m	Δm^e	Δm^t	n	m	Δm^e	Δm^t	n	m	Δm^e	Δm^t	n
0.800	0.838	1	1		...				...				...		
0.600	0.766	1	2		...				...				...		
0.500	0.704	2	2		...				...				...		
0.450	0.638	2	3		...				...				...		
0.400	0.555	2	2		...				...				...		
0.380	0.495	2	3		...				...			0.513	2	2	4
0.370	0.458	2	2		...			0.471	2	2	6	0.479	2	2	5
0.360	0.395	2	2		...			0.428	5	6	1	0.444	1	2	10
0.355	0.339	3	2	0.380	7	8	3	0.389	3	5	4	0.417	4	3	4
0.350	0.230	7	3	0.338	6	9	7	0.354	5	7	5	0.379	9	4	6
0.340		...		0.254	6	9	13	0.267	6	8	3	0.327	5	4	7
0.330	0.0		2	0.128	7	10	6	0.181	8	10	4	0.223	5	5	4
0.320	0.0		1	0.062	5	7	8	0.107	6	10	4	0.170	6	8	4
0.300	0.0		1		...				...			0.085	5	7	3
0.270	0.0		1		...				...				...		

H/J →	0.10				0.20				0.30				0.50			
J/K_BT	m	Δm^e	Δm^t	n	m	Δm^e	Δm^t	n	m	Δm^e	Δm^t	n	m	Δm^e	Δm^t	n
0.800	0.841	1	1	1	0.843	1	1	1								
0.600	0.773	1	1	2	0.779	1	1	2					0.795	1	1	2
0.500	0.713	2	1	1	0.725	1	1	1	0.731	1	1	1	0.746	1	1	1
0.450	0.657	2	1	1	0.672	1	1	1	0.682	1	1	1	0.700	2	1	1
0.400	0.579	3	2	1	0.595	3	2	1	0.610	2	2	1	0.640	1	1	1
0.380	0.533	2	2	2	0.559	3	2	1	0.579	3	2	1	0.608	2	1	1
0.370	0.503	2	2	2	0.532	4	2	1	0.556	1	1	2	0.595	2	1	1
0.360	0.474	2	2	4	0.509	4	3	1	0.538	2	2	1	0.569	2	2	1
0.355	0.448	3	3	2	0.487	2	2	2	0.518	1	1	2	0.563	1	1	4
0.350	0.426	5	3	3	0.469	6	3	1	0.502	2	2	3	0.549	2	2	2
0.340	0.377	2	3	3	0.425	4	3	1	0.471	2	2	2	0.527	3	2	1
0.330	0.303	7	6	1	0.385	2	1	5	0.438	2	2	2	0.498	2	2	2
0.320	0.239	4	7	1	0.335	4	5	1	0.400	2	2	2	0.468	2	2	2
0.300	0.145	5	7	1	0.253	7	5	1	0.306	2	3	2	0.399	2	2	2
0.270	0.059	4	6	1	0.133	4	5	1	0.196	7	5	1	0.285	5	3	2

$\gg 1$, which is true for at least part of our data.

The second question is to what extent the results summarized in Fig. 2 and Eqs. (13) and (14) are invalidated by the finite size of our system. This question has been studied by varying the system size N,[48] and only a very small effect attributable to the finite size of the system was found. For example, for $N=4096$ instead of $N=512$ the magnetization was consistently slightly smaller, the effect being roughly equivalent to a small shift of the critical temperature of the finite system to higher temperatures compared to the value of T_C of the infinite system.[8] The largest shift being compatible with the data of Ref. 48 and the present data is about $\delta T/T_C \approx 0.5\%$, which would decrease δ to about 5.1 and increase β to about 0.33. Note that we are rather limited in such "fitting T_C" procedures since in the high-temperature region χ agrees with the high-temperature formula of Ritchie and Fisher[22] ($K=2J/k_BT$),

$$\frac{\chi}{\chi_0}=\left(1-\frac{T_C}{T}\right)^{-1.375}\frac{1+0.62369K-0.37657K^2+0.18076K^3+0.13052K^4}{1+0.61183K-0.27988K^2+0.21222K^3+0.12206K^4}, \tag{15}$$

numerically very closely on the *absolute* temperature scale (see Fig. 2). Any substantial shift of T_C to higher T tends to destroy this good agreement, decreases γ, and increases γ'.

In view of all these uncertainties we take as a final estimate for the exponents

$$0.31 \le \beta \le 0.35, \quad 1.33 \le \gamma, \quad \gamma' \le 1.39, \quad 4.9 \le \delta \le 5.3. \tag{16}$$

Within the given accuracy, the scaling law[12,28] $\gamma=\beta(\delta-1)$ is fully satisfied. We compare our result [Eq. (16)] with various other estimates in Table II. In most cases, the series expansions apply to the fcc lattice only, since the sc-lattice series behave less regularly. The entry "series/numerical" denotes the method of Stephenson and Wood[17] inverting the series for the free energy in a magnetic field[16] to derive numerical values for the magnetization for $T<T_C$. Their estimate for β is the only direct series estimate for this exponent in the case of the classical Heisenberg magnet; it exhibits the most pronounced deviation from our result. These Padé approximations for the magnetiza-

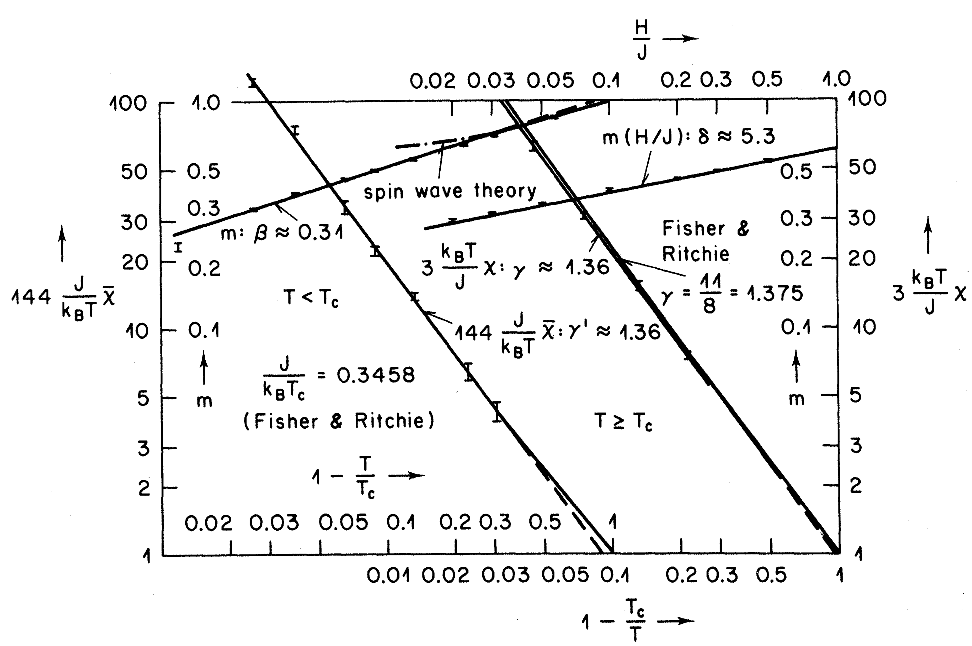

FIG. 2. Log-log plot of the magnetization and the susceptibility, displaying the various exponents. The left-hand part of the figure refers to $T<T_C$ and the right-hand part to $T>T_C$ [we used the T_C of the series expansions (Ref. 22)]. The magnetic phase boundary (curve marked by $m:\beta\simeq 0.31$) is compared to the spin-wave prediction (dashed-dotted curve), both plotted vs $1-T/T_C$. This part of the figure also contains the "extrapolated" susceptibility [curve marked by $144\,(J/k_BT)\,\bar{\chi}:\gamma\approx 1.36$]. In the right-hand part of the figure the magnetic isotherm is plotted vs H/J [curve marked by $m(H/J):\delta\approx 5.3$]. This part of the figure also contains the susceptibility, which is plotted vs $1-T_C/T$ [curve marked by $3(k_BT/J)\,\chi:\gamma\approx 1.36$], and which is compared to the high-temperature series prediction by Fisher and Ritchie (Ref. 22).

tion must be evaluated numerically for $T < T_C$ and plotted logarithmically versus $T_C - T$ as we do with our data, since their analytic exponent is $\frac{1}{2}$.[18,70] Thus both methods suffer basically from similar objections and we do not have a conclusive explanation for this discrepancy. The estimates according to Wilson's ϵ expansion[71] are taken from the formulas[24] ($\epsilon = 4 - d$, classical Heisenberg model)

$$\gamma = 1 + \tfrac{5}{22}\,\epsilon + \tfrac{635}{5324}\,\epsilon^2 + o(\epsilon^3),$$
$$\eta = \tfrac{5}{242}\,\epsilon^2 + \tfrac{2155}{117128}\,\epsilon^3 + o(\epsilon^4), \qquad (17)$$

which give, combined with the scaling laws,[12,28] the relations

$$\beta = \tfrac{1}{2} - \tfrac{3}{22}\,\epsilon + \tfrac{35}{2662}\,\epsilon^2 + o(\epsilon^3),$$
$$\delta = 3 + \epsilon + \tfrac{111}{242}\,\epsilon^2 + o(\epsilon^3). \qquad (18)$$

These exponents of our calculation agree quite reasonably with all the other estimates. Our rather high value of δ, however, introduces a slight difficulty with the scaling law involving the dimensionality[12]

$$\eta = 2 - d\gamma/(\gamma + 2\beta), \qquad (19)$$

since then η turns out to be slightly negative ($\eta \cong -0.015$) contrary to the direct estimates.[22,24] This difficulty is similar to the Ising model where $\beta = \frac{5}{16}$ and $\delta = 5$,[12] which lead to $\eta = 0$, contrary to the direct estimates $\eta \cong 0.04$,[24,72] or 0.05.[22] This difficulty would not exist if we took instead of Eq. (13) the corresponding exact inequality[73] $\eta \geq 2 - d\gamma/(\gamma + 2\beta) \cong -0.015$. From series expansions only one direct estimate of δ is available for the case of $S = \frac{1}{2}$ and the fcc lattice.[18] The method meets some difficulties[74]; however, it proves conclusively $\delta \leq 5.6$. The final estimate of Baker *et al.*[18] is $\delta = 5.0 \pm 0.2$, which agrees reasonably with our result [Eq. (16)]. The most recent scaling estimates are $\delta = 4.9 \pm 0.4$[21] and $\delta = 4.8 \pm 0.3$.[22]

Concluding this section about the critical exponents we see from Table II that the uncertainty in their values is larger than for the Ising model. We do not claim that the accuracy of the present calculation exceeds previous treatments, but it has been stressed[75] that it is very important to have several methods to estimate the exponents to avoid systematic errors as far as possible.

IV. SCALING BEHAVIOR OF MAGNETIZATION

In our treatment so far we have only used the results for $H/J = 0$ or $|t| = 0$, respectively. It is also interesting to use the results for both H/J and $|t| \neq 0$, to see whether they can be described in terms of a homogeneous function.[29] For this purpose we plot in Fig. 3 the reduced magnetization $y = m(H/J)^{-1/6}$ vs the reduced temperature, raised to the power β, $x = |t|^{\beta}(H/J)^{-1/6}$.[76] If the homo-

TABLE II. Critical exponents of the Heisenberg model. In the case of series expansions only direct estimates and no scaling estimates are shown.

Method	Ref.	Lattice	Spin quantum number	Exponents η	ν	γ	β	δ	2Δ
Series	3	fcc	∞	...	...	1.33	...	...	...
Series	9	sc, bcc, fcc	∞	...	...	1.38 ± 0.02	...	...	...
Series	11	sc, bcc, fcc	$\frac{1}{2}$	...	...	1.43 ± 0.01	...	...	3.63 ± 0.03
Series	13	sc, bcc, fcc	∞	...	...	1.38 ± 0.02	...	...	...
Series	14	fcc	∞	$0 < \eta < 0.07$	0.70 ± 0.01	1.375 ± 0.002	...	...	...
Series	16	fcc	∞	...	...	...	...	...	3.45 ± 0.05
Series	20	sc, bcc, fcc	$\frac{1}{2}$	...	...	1.36 ± 0.04	...	...	3.50 ± 0.20
Series	21	fcc	∞	...	0.717 ± 0.007	1.405 ± 0.02	...	...	3.54 ± 0.03
Series	22	sc, bcc, fcc	general	0.043 ± 0.014	0.703 ± 0.01	$1.375 \pm^{0.02}_{0.01}$	...	...	...
Series/numerical	17	fcc	∞	...	...	...	0.38 ± 0.03	...	...
Series/numerical	18	fcc	$\frac{1}{2}$	...	...	...	0.35 ± 0.05	5.0 ± 0.2	...
Wilson/ϵ recursion	26	...	∞	0	...	1.356	...	...	...
Wilson/ϵ expansion	24	...	∞	0.039	0.684	1.347	0.377	4.46	...
Monte Carlo	present work	sc	∞	...	...	1.36 ± 0.03	0.33 ± 0.02	5.1 ± 0.2	...

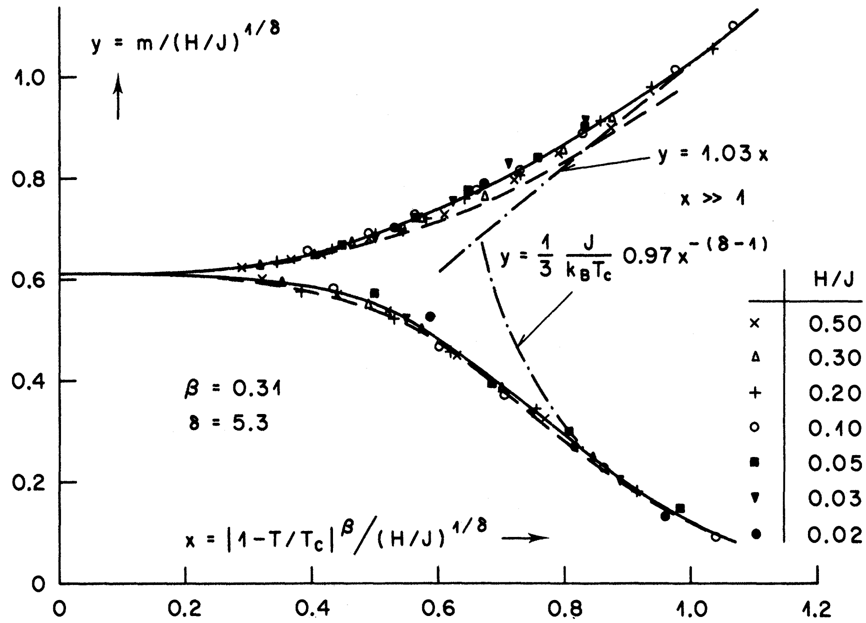

FIG. 3. Scaling function $y=f(x)$ for the sc classical Heisenberg ferromagnet using the exponents β and δ of the Monte Carlo calculation. The dash-dotted curves represent the asymptotic behavior for $x \gg 1$. The dashed curve is the scaling function of Miloševič and Stanley (Ref. 23) normalized to the same amplitudes of the critical isotherm and susceptibility χ.

geneity assumption is correct even for temperatures and fields not very close to T_C, all the data points should now fit a single curve $y \equiv f(x)$. Figure 3 shows that this is indeed correct. The small scatter of points still present is fully accounted for by the statistical errors quoted in Table I.[77] For small $x \ll 1$, we have $f(x) \equiv m(H/J)^{-1/\delta} \approx 0.61$ as expected from Eq. (13), while for large $x \gg 1$ the asymptotic expressions are $f(x) \approx 1.03x$ on the ferromagnetic branch [Eq. (13)] and $f(x) \approx \chi_0^{-1} \times 0.97 x^{-(\delta-1)}$ on the paramagnetic branch [Eq. (14)]. From Fig. 3 we see that these asymptotic descriptions actually hold down to $x \cong 1$. From this fact it is also clear that the scaling function is unaffected by the uncertainty in the low-temperature susceptibility, since the coefficients b_1, b_2 of the higher-order terms in the asymptotic expansion

$$y = f(x) \approx 1.03x + b_1 x^{1-\delta/2} + b_2 x^{1-\delta} + \cdots, \quad x \gg 1 \qquad (20)$$

must be very small. The term with exponent $1-\frac{1}{2}\delta$ leads to a contribution to the magnetization proportional to $H^{1/2}$, while the next term is proportional to H. According to spin-wave theory[62] both contributions should be present.

Using series expansions for the fcc lattice[16,18] Miloševič and Stanley[23] derived, with the help of the scaling hypothesis, the result for the scaling function ($S=\infty$),

$$H(t, m) = 0.8K_c\left(1 - \frac{z}{0.1577}\right)^{1.33} \times \frac{3 - 22.169z + 23.71z^2 + 9.512z^3}{1 - 7.823z + 10.745z^2 + 1.697z^3}, \qquad (21)$$

where $K_c = J/k_BT_c = 0.1573$ and z is related to m and $x' = t/m^{1/\beta}$ by the expressions

$$z = K_c(x'm^{1/\beta} + 1)^{-1}, \qquad m(x'm^{1/\beta} + 1) = 0.8\ \mathrm{K}. \qquad (22)$$

Adjusting the amplitudes at $x=1$ and $x \gg 1$ (para-

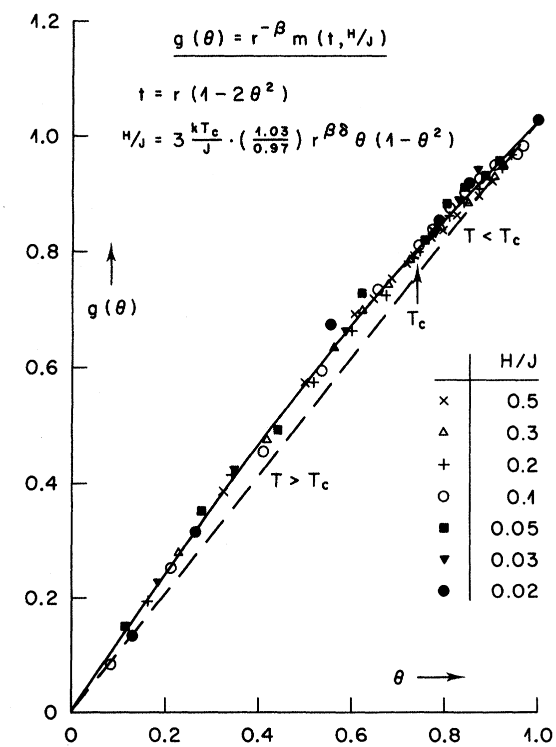

FIG. 4. Plot of the function $g(\theta)$ vs θ in the Schofield (Ref. 78) paramagnetic representation of the equation of state. The exponents and critical amplitudes are taken from Eqs. (13) and (14).

magnetic branch) this function is included in Fig. 3 (dashed curve), showing striking agreement with our result! The small deviations which are still present should not be taken seriously since Milošević and Stanley[23] consider the possibility that the error of their function could be as large as 10%, and the uncertainties in our method also amount to several percent. Figure 3 demonstrates the important result that the scaling functions of the classical Heisenberg model are lattice independent at least to the quoted accuracy. This property has been conjectured from the universality arguments.[23,31,32] Furthermore, Fig. 3 is not very sensitive to the choice of the critical exponents in the range given in Eq. (16) as long as T_C is shifted appropriately.

As a second way of showing the scaling properties of our result we use the Schofield parametric representation[78] in Fig. 4. In this representation the scaling function is nearly linear, but in our case the deviations from linearity are somewhat larger than in the experiment on $CrBr_3$.[78] Note, however, that the exponents of $CrBr_3$ are[78] $\gamma = 1.215 \pm 0.015$, $\beta = 0.368 \pm 0.005$, which are neither the Heisenberg nor the Ising values. If we choose in the Schofield transformation [H/J and t are transformed to the new variables r, θ, $t = r(1 - b^2\theta^2)$] the constant

$$b^2 = (\delta - 3)/(\delta - 1)(1 - 2\beta)$$

instead of $b^2 = 2$ as in Ref. 78 and Fig. 4, as suggested for the linear model,[79] the linearity of the curve is only slightly improved.

V. CONCLUSIONS

From Figs. 3 and 4 it is evident that any deviations from scaling are numerically negligible if we choose the critical exponents and T_C as suggested by our results [Fig. 2 and Eq. (16)]. The corrections to the scaling equation of state for larger $|t|$ and H/J are small and masked by the statistical errors. If we use our data together with the estimates of the series expansion, e.g., $\gamma = 1.37$, $\beta = 0.36$, $\delta = 4.8$, and $J/k_B T_C = 0.3458$, then we get considerable deviations from scaling, however, as shown in Fig. 5, which is the analog of Fig. 3 with other exponents but the same T_C. In this case, considerable correction terms would evidently be necessary, since now the various magnetic fields yield definitely different curves,[80] even if we treat T_C as an adjustable parameter. It is the uncertainty concerning the precise values of the critical exponents which prevents us from making further statements on this question of correction terms.[34-42]

Summarizing our discussion we can say we have calculated the critical properties of the sc classical Heisenberg ferromagnet with an accuracy comparable to the series-expansion method[1-22] and the ϵ-expansion method.[24-26] As far as previous treatments are available, we get a reasonable agreement. The scaling function can be calculated rather unambiguously, and it agrees with the fcc scaling function of Milošević and Stanley.[23] This fact supports one aspect of the universality hypothesis, namely, that the scaling functions should be lattice

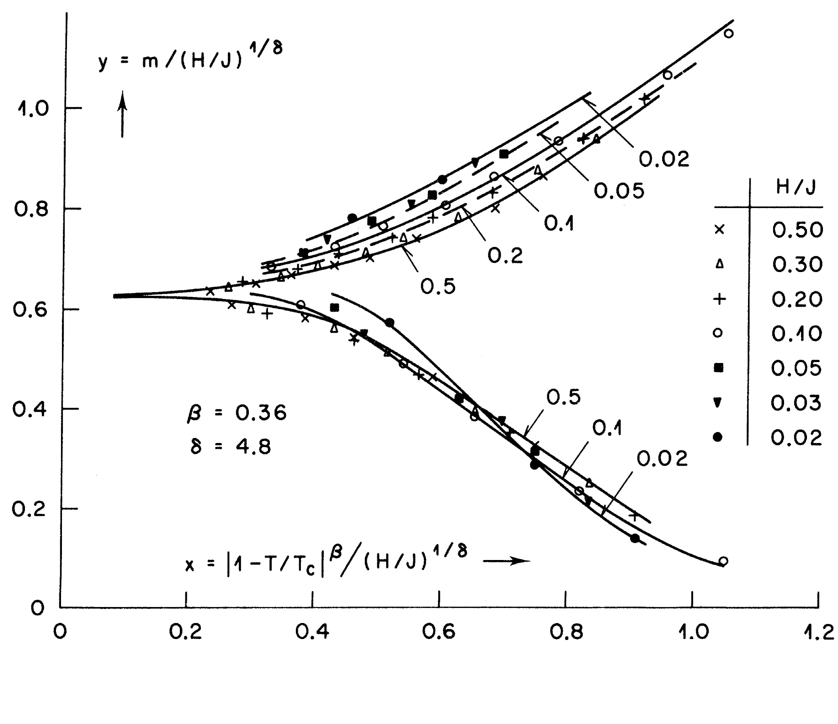

FIG. 5. Scaling plot $y = f(x)$ as in Fig. 3, but with the exponents β and δ of the series expansions.

independent. Deriving these results we did not need to make any *a priori* scaling assumptions as in some of the other methods.[23-26] The main advantage of our method is the fact that other parameters could be included in the Hamiltonian without great difficulty, so that further applications seem rather straightforward.

ACKNOWLEDGMENTS

The authors express their gratitude to Dr. P. C. Hohenberg for helpful and valuable comments. They are also indebted to Dr. T. Schneider and Dr. E. Stoll for discussions, and to the latter also for advice on the computer.

---

*IBM Postdoctoral Fellow. Permanent address: Physikdepartment E14, Technische Universität München, D 8046 Garching, West Germany.

[1]G. S. Rushbrooke and P. J. Wood, Mol. Phys. 1, 257 (1958).

[2]C. Domb, Adv. Phys. 9, 149 (1960).

[3]C. Domb and M. F. Sykes, Phys. Rev. 128, 168 (1962).

[4]G. S. Rushbrooke and P. J. Wood, Mol. Phys. 6, 409 (1963).

[5]J. Gammel, W. Marshall, and L. Morgan, Proc. Roy. Soc. (London) 275, 257 (1963).

[6]G. A. Baker, H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Letters 20, 146 (1966).

[7]H. E. Stanley and T. A. Kaplan, Phys. Rev. Letters 16, 981 (1966).

[8]P. J. Wood and G. S. Rushbrooke, Phys. Rev. Letters 17, 307 (1966).

[9]G. S. Joyce and R. G. Bowers, Proc. Phys. Soc. (London) 89, 776 (1966).

[10]H. E. Stanley, Phys. Rev. 158, 537 (1967); 158, 546 (1967).

[11]G. A. Baker, H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Rev. 164, 800 (1967).

[12]M. E. Fisher, Rept. Progr. Phys. 30, 615 (1967).

[13]D. Jasnow and M. Wortis, Phys. Rev. 176, 739 (1968).

[14]R. G. Bowers and M. E. Woolf, Phys. Rev. 177, 917 (1969).

[15]H. E. Stanley, J. Appl. Phys. 40, 1546 (1969).

[16]R. L. Stephenson and P. J. Wood, Phys. Rev. 173, 478 (1968).

[17]R. L. Stephenson and P. J. Wood, J. Phys. C 3, 90 (1970).

[18]G. A. Baker, J. Eve, and G. S. Rushbrooke, Phys. Rev. B 2, 706 (1970).

[19]C. Domb, Adv. Phys. 19, 339 (1970).

[20]M. H. Lee and H. E. Stanley, Phys. Rev. B 4, 1613 (1971).

[21]M. Ferer, M. A. Moore, and M. Wortis, Phys. Rev. B 4, 3954 (1971); B 4, 3964 (1971).

[22]D. S. Ritchie and M. E. Fisher, Phys. Rev. B 5, 2668 (1972).

[23]S. Milošević and H. E. Stanley, Phys. Rev. B 5, 2536 (1972); Phys. Rev. B 6, 986 (1972); B 6, 1002 (1972).

[24]K. G. Wilson, Phys. Rev. Letters 28, 548 (1972).

[25]F. J. Wegner, Phys. Rev. B 6, 1891 (1972).

[26]M. K. Grover, L. P. Kadanoff, and F. J. Wegner (unpublished).

[27]W. Opechowski, Physica 4, 181 (1937); 6, 1112 (1938).

[28]L. P. Kadanoff, W. Götze, D. Hamblen, R. Hecht, E. A. S. Lewis, V. V. Palciauskas, M. Rayl, J. Swift, D. Aspnes, and J. Kane, Rev. Mod. Phys. 39, 395 (1967).

[29]B. Widom, J. Chem. Phys. 43, 3898 (1965).

[30]R. B. Griffiths, Phys. Rev. 153, 176 (1967).

[31]L. P. Kadanoff, in *Proceedings of the* 1970 *Enrico Fermi Summer School on Critical Phenomena, Villa Monastero, Varenna sul Lago di Como, Italy* (Academic, New York, 1971).

[32]P. G. Watson, J. Phys. C 2, 1883 (1969), J. Phys. C 2, 2158 (1969).

[33]E. Brezin, D. J. Wallace, and K. G. Wilson (unpublished).

[34]C. Domb, in Ref. 31; C. Domb and D. S. Gaunt, J. Phys. (Paris) 31, Cl-345 (1971).

[35]D. S. Gaunt and G. A. Baker, Phys. Rev. B 1, 1184 (1970).

[36]D. C. Hemmer and G. Stell, Phys. Rev. Letters 24, 1284 (1970).

[37]M. S. Green, M. J. Cooper, and J. M. H. Levelt Sengers, Phys. Rev. Letters 26, 492 (1971).

[38]D. Stauffer, C. S. Kiang, G. H. Walker, O. P. Puri, J. D. Wise, Jr., and E. M. Patterson, Phys. Letters 35A, 172 (1971).

[39]N. D. Mermin and J. J. Rehr, Phys. Rev. Letters 26, 1155 (1971).

[40]F. J. Wegner, Phys. Rev. B 5, 4529 (1972).

[41]T. Schneider, G. Srinivasan, and E. Stoll, Helv. Phys. Acta 45, 629 (1972).

[42]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953).

[43]K. Binder and H. Rauch, Z. Physik 219, 201 (1969).

[44]R. E. Watson, M. Blume, and G. H. Vineyard, Phys. Rev. 181, 811 (1969).

[45]A. E. Ferdinand and M. E. Fisher, Phys. Rev. 185, 832 (1969).

[46]K. Binder, H. Rauch, and V. Wildpaner, J. Phys. Chem. Solids 31, 391 (1970).

[47]K. Binder, Phys. Status Solidi (b) 46, 567 (1971).

[48]H. Müller-Krumbhaar and K. Binder, Z. Phys. 254, 269 (1972).

[49]L. D. Fosdick, in *Methods in Computational Physics* (Academic, New York, 1963), Vol. 1, p. 245.

[50]W. W. Wood, in *Physics of Simple Liquids* (North-Holland, Amsterdam, 1968), Chap. 5.

[51]H. Müller-Krumbhaar and K. Binder, J. Stat. Phys. (to be published).

[52]R. J. Glauber, J. Math. Phys. 4, 294 (1963).

[53]We measure all lengths in units of the lattice spacing. The dimensionality of the system is denoted by d.

[54]K. Binder, Phys. Letters 30A, 273 (1969).

[55]H. Bethe, Proc. Roy. Soc. (London) A 150, 552 (1935).

[56]We measure the applied magnetic field H in units of the exchange constant J.

[57]R. Brout, *Phase Transitions* (Benjamin, New York, 1965).

[58]Essentially no advantage would be obtained in the case of, for example, the two-dimensional Ising model, where the PMC method is indeed suitable to yield satisfactory results (Refs. 59 and 60). Our SMC method is further restricted to cases where no ambiguity is present about the existence and nature of the order parameter. For further remarks about the justification and applicability of the SMC method see Ref. 48.

[59]N. Ogita, A. Ueda, T. Matsubara, H. Matsuda, and F. Yowezawa, J. Phys. Soc. Japan 26, S145 (1969).

[60]E. Stoll and T. Schneider, Phys. Rev. A 6, 429 (1972).

[61]Because of this inaccurate procedure the error bars shown for the susceptibilities χ in Fig. 2 are considerably larger than for the phase boundary of magnetic isotherm. We do not give any estimate for the zero-field susceptibilities at $J/K_BT=0.34$ and $J/K_BT=0.35$, where no sufficiently low fields have been calculated. For these temperatures a finite size effect is expected as it occurs for the spontaneous magnetization and thus they should not be included for the estimate of the zero-field susceptibility exponent.

[62]V. G. Vaks, A. I. Larkin, S. A. Pikin, Zh. Eksp. Teor. Fiz. 53, 281 (1967) [Sov. Phys. JETP 26, 188 (1968)]; Zh. Eksp. Teor. Fiz. 53, 1029 (1969) [Sov. Phys. JETP 26, 647 (1968)]; F. Schwabl and K. H. Michel, Phys. Rev. B 2, 189 (1970).

[63]P. C. Hohenberg (private communication); B. I. Halperin and P. C. Hohenberg, Phys. Rev. 177, 952 (1969).

[64]The series expansions are also inconclusive on this question, see Ref. 18.

[65]Such "irrelevant" parameters are, for example, nonzero exchange constants with next-nearest neighbors. Recent series expansions for the Ising model (Ref. 66) show that these parameters do indeed obscure the critical behavior, so that one cannot obtained reliable estimates for the exponents, if Padé approximants for rather short series are analyzed. A similar behavior occurs in the case of the susceptibility at the surface of an Ising half-space, if the exchange constant at the surface is smaller than in the bulk (Ref. 67). Such situations should be described in such a way that very close to T_C the true exponent dominates, while futher from T_C other "effective" exponents apply, and the position of the crossover between these exponents is related to the magnitude of the "irrelevant" parameters (Ref. 68).

[66]G. Paul and H. E. Stanley, Phys. Rev. B 5, 3715 (1972).

[67]K. Binder and P. C. Hohenberg, Phys. Rev. B 6, 3461 (1972).

[68]E. Riedel and F. J. Wegner, Z. Phys. 225, 195 (1969).

[69]This fact can be demonstrated with our data only if we plot them versus $|t_{MF}| = |T - T_c^{MF}|/T_c^{MF}$ instead of t. We denote the coordination number by Z. If there is exchange with more than only the nearest neighbors, Z has the meaning of some weighted coordination number.

[70]This feature is a consequence of deriving low-temperature properties from a high-temperature series by these special procedures described in Refs. 16–18. One does not have this difficulty in the Ising case where true low-temperature series are available.

[71]K. G. Wilson and M. E. Fisher, Phys. Rev. Letters 28, 240 (1972).

[72]M. A. Moore, D. Jasnow, and M. Wortis, Phys. Rev. Letters 22, 940 (1969).

[72]M. E. Fisher, Phys. Rev. 180, 594 (1969).

[74]See Table VIII and Fig. 3 of Ref. 18.

[75]G. Paul and H. E. Stanley, Phys. Rev. B 5, 2578 (1972).

[76]These variables have been chosen in order to display the data points in the figure most distinctly. Of course it is straightforward to transform to the Griffiths (Ref. 30) function $h(x')$.

[77]The statistical errors of Fig. 1 are enhanced in Fig. 3 by a factor $(H/J)^{-1/6}$ which is always larger than 1.

[78]P. Schofield, Phys. Rev. Letters 22, 606 (1969); J. T. Ho and J. D. Litster, Phys. Rev. Letters 22, 603 (1969).

[79]P. Schofield, J. D. Litster, and J. T. Ho, Phys. Rev. Letters 23, 1098 (1969).

[80]Neglecting the systematic nature of the "scatter" the average function would be again very close to the scaling function of Fig. 3, which therefore is essentially unaffected by the uncertainty of the exponents. This observation agrees with some remarks of Milošević and Stanley (Footnote 15 in Ref. 23).

PHYSICAL REVIEW B VOLUME 7, NUMBER 7 1 APRIL 1973

Calculation of Pressure and Temperature Dependence of the hfs Interactions in FeF_2

D. M. Silva†

Physics Department, University of Washington, Seattle, Washington 98105

(Received 27 April 1972)

The temperature and pressure dependence of the hyperfine magnetic field in ferrous fluoride is determined by diagonalizing the appropriate crystal-field Hamiltonian self-consistently with the expectation value of the operator S_z. The results of this calculation are in good agreement with experimental data for $P=0$. Attention is also given to the temperature and pressure dependence of the nuclear quadrupole splitting associated with $^{57}Fe^{2+}$.

INTRODUCTION

The effective magnetic field at the nucleus of the iron ion in FeF_2 has been determined experimentally,[1] being found to decrease monotonically from a zero-temperature value of − 329 kOe, with the antiferromagnetic transition temperature (Néel temperature) determined to be approximately