[9] J. Kanamori and K. Yosida, Progr. Theoret. Phys. (Kyoto) 14, 423 (1955).

[10] Previous treatments of the problem did not treat the anisotropy interaction correctly and therefore differ in the $D\cos^2\theta$ term; see Ref. 5.

[11] R. Loudon, Advan. Phys. 17, 243 (1968).

[12] An alternate approximation by Y. L. Wang and H. B. Callen [J. Phys. Chem. Solids 25, 1459 (1964)] gives essentially the same result at the zone edge, with $2SD$ replaced by $(2S-1)D$.

[13] F. Keffer, Phys. Rev. 87, 608 (1952).

[14] J. M. Ziman, Proc. Phys. Soc. (London) A65, 540 (1952).

[15] At general points of the Brillouin zone these terms cause a splitting of the magnon energies.

[16] G. G. Low, in *Inelastic Scattering of Neutrons* (International Atomic Energy Agency, Vienna, 1965), p. 453.

[17] R. Loudon and P. Pincus, Phys. Rev. 132, 673 (1963).

[18] The energy must be averaged over a whole cycle, and it is assumed that the magnon is still located on a single sublattice. This is equivalent to neglecting the D, E, F, and G lattice sums, which cause elliptical precession and the mixing of the two sublattice modes.

[19] G. Heller and H. A. Kramers, Proc. Roy. Akad. Sci. (Amsterdam) 37, 378 (1934).

[20] M. F. Thorpe, J. Appl. Phys. 41, 892 (1970).

[21] J. B. Parkinson, J. Phys. C 4, 498 (1971).

[22] J. H. Van Vleck, J. Phys. Radium 12, 262 (1951).

[23] M. Tinkham, Proc. Roy. Soc. (London) A236, 535 (1956); A236, 549 (1956).

[24] M. R. Brown, B. A. Coles, J. Owen, and R. W. Stevens, Phys. Rev. Letters 7, 246 (1961).

[25] T. Bernstein, Ph.D. thesis (MIT, 1971) (unpublished).

[26] O. Nikotin, P. A. Lingard, and O. W. Dietrich, J. Phys. C 2, 1168 (1969).

[27] M. Griffel and J. W. Stout, J. Am. Chem. Soc. 72, 4351 (1950).

[28] Discussions of the spin orientations above the SFT can be found in Ref. 5; also in R. S. Meltzer and L. L. Lohr, Jr., J. Chem. Phys. 49, 541 (1968); C. R. Abeledo, R. B. Frankel, A. Misetich, and N. A. Blum, J. Appl. Phys. 42, 1723 (1971).

[29] P. A. Fleury, in *Proceedings of the International Conference on Light Scattering in Solids*, edited by M. Balkanski (Flammarion, Paris, 1971).

[30] P. A. Fleury (private communication).

PHYSICAL REVIEW B VOLUME 6, NUMBER 3 1 AUGUST 1972

Equation of State near the Critical Point. I. Calculation of the Scaling Function for $S=\frac{1}{2}$ and $S=\infty$ Heisenberg Models Using High-Temperature Series Expansions*

Sava Milošević† and H. Eugene Stanley‡

Physics Department, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

(Received 3 January 1972)

In recent years there have been many measurements of the scaling-law equation of state for different materials, and the "scaling function" so obtained has generally been fit by an empirical equation involving the selection of several adjustable parameters. We propose a method for calculating, directly from high-temperature series expansions, the function $h(x)$ that determines the scaling-law equation of state $H=M^\delta h(x)$. Previously, $h(x)$ has been calculated only for the $S=\frac{1}{2}$ Ising model, but the method is not generalizable to the case of the Heisenberg model because it relies upon the use of low-temperature expansions as well, and these are not known for the Heisenberg model. First we calculate $h(x)$ for the Ising model (bcc, fcc, and simple cubic lattices) in order to assess the utility and credibility of our method. Our Ising model $h(x)$ agrees well with the previous calculation that used both high- and low-temperature expansions. Next we calculate $h(x)$ in its entire region of definition for the $S=\frac{1}{2}$ Heisenberg model (fcc and bcc lattices) and the $S=\infty$ Heisenberg models (fcc lattice), where S denotes the spin quantum number. The accuracy of our resulting expressions is limited by the finite number of known terms in the corresponding high-temperature series expansions, but it is generally of the order of a few percent. In Paper II the scaling functions calculated here are compared with experiment and with the predictions of the universality hypothesis.

I. INTRODUCTION AND OUTLINE OF PRESENT WORK

The static scaling hypothesis[1–4] predicts the following form for the equation of state near the critical point:

$$H(\epsilon, M)=M^\delta h(\epsilon/M^{1/\beta}) \quad (M\geq 0)\,, \tag{1.1}$$

where H, ϵ, and M denote, respectively, the singular parts of the magnetic field divided by kT_c/μ (μ being the magnetic moment per spin), the reduced temperature $(T-T_c)/T_c$, and the magnetization divided by its saturation value as $T\to 0$ or $H\to\infty$. The critical-point exponents δ and β are defined by the asymptotic relations $H\sim M^\delta$ when $\epsilon=0$, and $M\sim(-\epsilon)^\beta$ when $H=0$. The relation (1.1) is assumed to be valid in the one-phase region close to the critical point, which implies that the thermodynamic variables ϵ and M should be *small* quantities. The form of the function $h(x)$ is not specified by the static scaling hypothesis, although it has certain well-defined characteristics,[4] some of which are outlined in Appendix A.

Experimental investigations on ferromagnetic conductors,[5–7] insulators,[8,9] semiconductors,[10] and alloys[11] confirmed the assumption of Eq. (1.1) that the "scaled field" H/M^{δ} appears to be some function of only the "scaled temperature" $\epsilon/M^{1/\beta}$. We call this function $h(x)$ the scaling function.

Given that Eq. (1.1) appears to be experimentally verified, it is of interest to obtain a theoretical expression for the scaling function $h(x)$. The first proposals[6,8,12] for the function $h(x)$ were strictly phenomenological with numerous "adjustable parameters" chosen such as to afford a plausible fit to the experimental data. Somewhat more theoretically motivated were the parametric representations of the equation of state,[13,14] and other reformulations of the basic scaling hypothesis that have recently been put forward.[15–18] However, these introduce new unspecified functions and parameters, and thus diminish possibilities of some kind of approximate calculation.

The first theoretical calculation of the scaling function $h(x)$ was carried out for the simplest of model systems, the Ising model, by Gaunt and Domb.[19] Their calculation utilized information provided by high-temperature *and low-temperature* series expansions. Since for most other model Hamiltonians (e.g., the Heisenberg model), low-temperature series are impractical to obtain, any attempt to furnish a straightforward generalization of the Gaunt-Domb technique would appear to be futile.

It is the purpose of this work to present a method for calculation of the scaling function $h(x)$ which requires the knowledge of high-temperature expansions only. In Sec. II the appropriate formulation of the static scaling hypothesis is outlined, and for the sake of illustration and assessment of our method, a calculation for the Ising model is presented. In Secs. III and IV we proceed to apply our method to the $S=\frac{1}{2}$ and $S=\infty$ Heisenberg ferromagnets, respectively. In Paper II,[20] we discuss the dependence of $h(x)$ upon the form of the model Hamiltonian, and we examine the question of whether the scaling function depends upon lattice structure and spin quantum number (according to the universality hypothesis it should not). We also compare in II the calculated scaling functions with experimental data on insulating ferromagnets ($CrBr_3$, EuO) and other materials.

II. METHOD OF CALCULATING SCALING FUNCTIONS FROM HIGH-TEMPERATURE EXPANSIONS AND APPLICATION TO ISING MODEL

A. Method of Calculating Scaling Functions

Our method of calculating the scaling function $h(x)$ was discovered after consideration of a recent formulation of the scaling hypothesis that involves the concept of generalized homogeneous functions.[21–23] By definition, a function $f(x, y)$ is a generalized homogeneous function if there exist two numbers a, b, such that for all positive values of λ, the relation

$$f(\lambda^a x,\ \lambda^b y) = \lambda^p f(x, y) \tag{2.1}$$

is satisfied, where the exponent p is called the "scaling power" of the function $f(x, y)$ (one can choose $p=1$ by redefining $a \to a/p$ and $b \to b/p$). The reader can verify by inspection that the scaling hypothesis in the form of Eq. (1.1) implies that $H(\epsilon, M)$ is a generalized homogeneous function *in the critical region*, since there exist two numbers, $a[=1/\beta(\delta+1)]$ and $b[=1/(\delta+1)]$, such that for all positive λ, one has

$$H(\lambda^{1/\beta(\delta+1)}\epsilon,\ \lambda^{1/(\delta+1)}M) = \lambda^{\delta/(\delta+1)} H(\epsilon, M)\ . \tag{2.2}$$

Conversely, if we assume that $H(\epsilon, M)$ is a generalized homogeneous function, then we can derive Eq. (1.1) by setting $\lambda \equiv (1/M)^{\delta+1}$ in (2.2) with the result

$$H(\epsilon, M)/M^{\delta} = H(\epsilon/M^{1/\beta}, 1) = h(\epsilon/M^{1/\beta})\ . \tag{2.3}$$

Therefore the scaling function $h(x)$ is seen by (2.3) to be identical to the function $H(x, 1)$.

However, if $H(\epsilon, M)$ is not the *singular* part of the magnetic field, then the last result is not a complete truth since the arguments of $H(\epsilon/M^{1/\beta}, 1)$ are not always small quantities, as they should be in order that values of H are germane to the critical region. That is, if $H = H_{\text{sing}} + H_{\text{nonsing}}$, then by definition $H \cong H_{\text{sing}}$ near the critical point. Hence, if we stay very near the critical point we can simply consider H, but if we do not manage to stay near the critical point we must "sort out" H_{sing} and H_{nonsing} in order to consider H_{sing} only. Since there is no way of doing this sorting out, we must choose arguments of H such that we are always near the critical point, i.e., such that always $H \cong H_{\text{sing}}$.

To overcome this difficulty, we can return to Eq. (2.2) and set $\lambda = (c/M)^{\delta+1}$, where the number c may (*in principle* at least) be chosen arbitrarily small. With this choice, Eq. (2.3) is replaced by

$$c^{\delta} H(\epsilon, M)/M^{\delta} = H(\epsilon c^{1/\beta}/M^{1/\beta}, c) = c^{\delta} h(\epsilon/M^{1/\beta})\ , \tag{2.4}$$

and the scaling function $h(x)$ is now determined by the equation

$$h(x) = H(x c^{1/\beta}, c)/c^{\delta}\ . \tag{2.5}$$

That is, if we knew the function $H(\epsilon, M)$, then $h(x)$ could be obtained by replacing the variables ϵ and M by $xc^{1/\beta}$ and c, respectively.

Unfortunately, for all but the most unrealistic model Hamiltonians (such as the one-dimensional Ising model and the Curie-Weiss model or "mean-field theory"), all that we know about the function $H(\epsilon, M)$ is a finite number of terms in a series expansion. Hence in order to obtain a reliable estimate for $H(\epsilon, M)$ we must extrapolate the regular behavior of these terms using, e.g., the technique of Padé approximants (PA's).[24,25]

In order to demonstrate the utility of our calculational method, we begin with a calculation of the scaling function for the Ising model.

B. Calculation of Scaling Function for Ising Model

As mentioned in Sec. I, Gaunt and Domb[19] have calculated the scaling function $h(x)$ for the two- and three-dimensional ($d = 2, 3$) Ising models utilizing both high- and low-temperature series expansions. In this section we obtain an expression for $h(x)$ that requires for its calculation only high-temperature series expansions. The appropriate high-temperature expansions have been obtained by Gaunt and Baker[26] in connection with their calculation of $M(T, H=0)$, the spontaneous magnetization or "phase boundary." These expansions have the form

$$H(\epsilon, M) = (\epsilon+1)\tanh^{-1}[M\tau(M, v)] , \qquad (2.6)$$

where

$$\tau(M, v) \equiv \sum_{n=0}^{\infty} \psi_n(M)v^n \cong \sum_{n=0}^{L} \psi_n(M)v^n . \qquad (2.7)$$

Here $\psi_n(M)$ are polynomials in M^2 of degree n,

$$v \equiv \tanh(J/kT) \equiv \tanh[K_c/(\epsilon+1)] , \qquad (2.8)$$

$K_c \equiv J/kT_c$, k is the Boltzmann constant, and J is the exchange parameter in the Ising Hamiltonian ($J > 0$). Only a limited number (L) of polynomials $\psi_n(M)$ could be calculated,[26] the number L being equal to 8, 12, and 12 for the fcc, bcc, and simple cubic (sc) lattices, respectively. Hence Eq. (2.7) truncated at order L is not expected to describe the behavior of $H(\epsilon, M)$ in the critical region unless it can be approximated by some closed-form expression that represents an extrapolation beyond order L.

According to Eq. (2.5), to obtain the scaling function $h(x)$ we must set $M = c$ in Eqs. (2.6) and (2.7), where c is a small positive constant. Formally, this procedure is similar to a problem encountered by Gaunt and Baker in a different context,[26] and we shall therefore follow their approach here. Specifically, we shall assume that the function $\tau(M=c, v)$ in (2.7) vanishes at the phase boundary with the power-law form

$$\tau(c, v) \cong \sum_{n=0}^{L} \psi_n(c)v^n \cong (v_0 - v)^q f(v) , \qquad (2.9)$$

where v_0, q, and $f(v)$ are to be estimated by the method of PA's. Thus one first must find v_0 and q by considering PA's to $(d/dv)[\ln\tau(c, v)]$, and afterwards $f(v)$ can be determined by studying the product $(v_0 - v)^{-q}\tau(c, v)$.

Gaunt and Baker[26] noted that the series (2.9) was not sufficiently lengthy for reliable estimates for v_0 and q to be obtained unless c was inside the interval $0.6 \lesssim c \lesssim 0.975$. Since the smaller the value of c, the larger the region of x where the relation (2.5) is satisfied, we shall choose $c = 0.6$ for our further analysis. For the Ising-model analysis we shall consider first the bcc lattice. Table I contains poles and residues of the PA's to $(d/dv) \times [\ln\tau(0.6, v)]$; these correspond, respectively, to the numbers v_0 and q of Eq. (2.9). We estimate[27] from Table I that $v_0 = 0.1658$ and $q = 1.076$. Then we form PA's to the function $f(v)$ of Eq. (2.9); these PA's were found to be consistent up to five decimal places. We therefore, almost arbitrarily, chose the [4, 4] PA, and Eq. (2.9) becomes

$$\tau(0.6, v) = \left(1 - \frac{v}{0.1658}\right)^{1.076} \times \frac{1 - 4.566v + 5.406v^2 + 5.842v^3 + 0.3907v^4}{1 - 5.936v + 17.603v^2 - 37.098v^3 + 25.811v^4} . \qquad (2.10)$$

If we now combine Eqs. (2.10), (2.9), and (2.6), we can obtain from (2.5) an approximate expression for $h(x)$ that depends upon the exponents β and δ. If we use the generally accepted estimates $\beta \cong \frac{5}{16}$ and $\delta \cong 5$, then we finally obtain for $h(x)$ the small-x expression

$$h(x) \cong h_1(x) = [(0.195x+1)/0.07776]\tanh^{-1}[0.6\tau, \tilde{v})] , \qquad (2.11a)$$

where $\tau(0.6, \tilde{v})$ is given by (2.10) and $\tilde{v} \equiv \tanh[0.15743/(0.195x+1)]$.

It is important to emphasize that the expression of Eq. (2.11a) for $h_1(x)$ is not expected to be accurate for very large values of x. For example, if $x = 1.6$ and $\beta = \frac{5}{16}$, then the first argument of $H(\epsilon, M)$ in Eq. (2.5) is given by $xc^{1/\beta} = 0.312$, which is hardly of the order of ϵ in the critical region. Hence we must expect (2.11a) to fail for values of x larger than about unity. This is the reason we use subscript 1 in Eq. (2.11a), reserving the notation $h_2(x)$ for an expression for large x.

Since $x \equiv \epsilon/M^{1/\beta}$ [cf. Eq. (1.1)], positive x corresponds to $T > T_c$ and it turns out that we can also calculate $h(x)$ for *large* x directly from high-temperature expansions. The method has, in fact, been carefully explained by Gaunt and Domb[19] (cf. also Sec. III C). Thus[28] we find the following expression for $h(x)$, valid at large x:

$$h_2(x) = x^\gamma \, \frac{1.0097 + 1.0189x^{-2\beta} + 0.4945x^{-4\beta} + 0.1696x^{-6\beta}}{1 + 0.4388x^{-2\beta}} , \qquad (2.11b)$$

where $\gamma = 1.25$ and $\beta = \frac{5}{16}$. This expression differs only very slightly from the fifth expression of Ref. 19, and the difference is probably caused by the rounding off of results at different stages of the calculation.

At $x \cong 1$, the large-x expression of Eq. (2.11b) for $h_2(x)$ overlaps the small-x expression of Eq. (2.11a) for $h_1(x)$ (within an accuracy of about 1%). Hence our order-of-magnitude estimate presented above for the domain of validity of $h_1(x)$ was indeed fairly reasonable.

C. Comparison with Results of Gaunt and Domb

We have shown above that, using high-temperature expansions *exclusively*, we can obtain two expressions that represent the scaling function of the Ising model in its whole region of definition: $h(x) \equiv h_1(x)$ for $x \lesssim 1$, while $h(x) \equiv h_2(x)$ for $x \gtrsim 1$ [Eqs. (2.11a) and (2.11b), respectively]. On the other hand, Gaunt and Domb[19] derived *five* different expressions for five different domains of x. Their first four expressions were obtained using "low-temperature" expansions,[29] and they cover the same domain of x as does Eq. (2.11a) for $h_1(x)$, while their fifth expression for large x coincides with our Eq. (2.11b) for $h_2(x)$. Therefore we make comparison only between our $h_1(x)$ and the four "low-temperature" expressions of Ref. 19.

A few words of caution should be spoken in advance. First, $h_1(x)$ can be as accurate as the determination of the phase boundary from the series (2.6) (cf. Fig. 1). This determination is limited in accuracy owing to the fact that high-temperature expansions, at least those of finite length as in

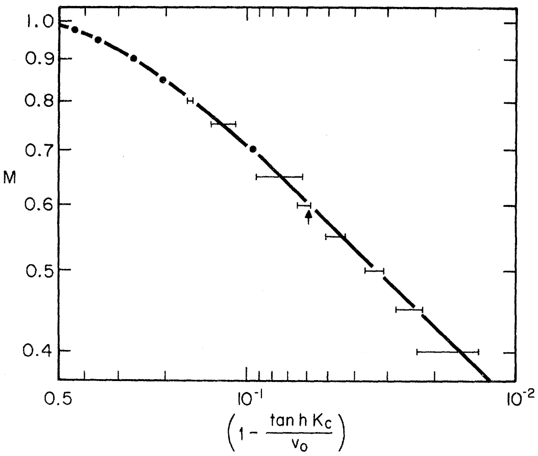

FIG. 1. Log-log plot of the phase boundary of the Ising model for the bcc lattice. This curve, similar to Fig. 5 of Ref. 26, is based upon calculations in Ref. 29 using exact low-temperature series expansions. The horizontal lines represent the confidence limits that follow from high-temperature-expansion calculations of the corresponding values of v_0 (Ref. 26). The arrow indicates *our* estimation of v_0, for $M = 0.6$, obtained from Table I.

(2.7), are not the best source of information near the phase boundary. We have used no specific values of critical-point exponents or critical amplitudes in calculating $h_1(x)$. However, these critical parameters were utilized by Gaunt and Domb in their construction of $h(x)$, thereby fixing certain values of $h(x)$ in advance. For instance, if we combine (2.8) and (2.9) with the *independent* esti-

TABLE I. Poles and residues of the PA's to $(d/dv)[\ln\tau(0.6, v)]$ [see Eq. (2.9)]. N and D, respectively, denote the order of the numerator and denominator of the PA. At each PA the upper number corresponds to v_0, while the number in brackets approximates q of Eq. (2.9). Here CZ ("competing zero") means that the PA erroneously predicts that $\tau(0.6, v)$ has two zeros, one below T_c and the other above T_c.

$D \backslash N$	2	3	4	5	6	7	8	9
2	0.1847 (1.6788)	0.1601 (0.8770)	0.1638 (1.0052)	0.1692 (1.3012)	0.1665 (1.1215)	CZ	0.1658 (1.0767)	0.1658 (1.0804)
3	0.1669 (1.1288)	0.1662 (1.1016)	0.1662 (1.1015)	0.1661 (1.0973)	0.1661 (1.0954)	0.1659 (1.0868)	0.1658 (1.0816)	
4	0.1649 (1.0330)	0.1662 (1.1014)	0.1662 (1.1016)	0.1660 (1.0939)	CZ	0.1658 (1.0758)		
5	0.1662 (1.1033)	0.1661 (1.0973)	0.1660 (1.0911)	CZ	CZ			
6	CZ	0.1660 (1.0930)	CZ	CZ				
7	0.1661 (1.0949)	0.1658 (1.0688)	CZ					
8	CZ	CZ						
9	0.1658 (1.0794)							

TABLE II. Values of $h(0)$ of the Ising model (the bcc lattice) obtained by using different PA's (different rows of the table) to the function $f(v)$, Eq. (2.9), and by choosing different estimates (different columns) of the exponent q.

Padé $[N,D]$	A ($q=1.076$)	B ($q=1.08$)	C ($q=1$)	D $q=1.076$ $\delta=4.8$
[3,3]	0.3812	0.3807	0.3911	0.3442
[4,3]	0.3819	0.3812	0.3906	0.3448
[5,3]	0.3819	0.3812	0.3889	0.3448
[6,3]	0.3819	0.3813	0.3874	0.3448
[3,4]	0.3819	0.3812	0.3906	0.3448
[4,4]	0.3819	0.3813	0.3914	0.3448
[5,4]	0.3819	0.3813	0.3769	0.3448
[6,4]	0.3819	0.3811	0.3856	0.3448
[3,5]	0.3819	0.3813	0.3899	0.3448
[4,5]	0.3819	0.3814	0.3812	0.3448
[5,5]	0.3819	0.3812	0.3868	0.3449
[6,5]	0.3830	0.3820	0.3842	0.3448
[3,6]	0.3819	0.3813	0.3888	0.3448
[4,6]	0.3819	0.3812	0.3863	0.3448
[5,6]	0.3819	0.3801	0.3846	0.3448
[6,6]	0.3819	0.3817	0.3830	0.3448

mate[28,30] $B=1.5056$ [where B is defined by $M=B(-\epsilon)^{\beta}$] and $M=0.6$, then we find $v_0=0.16466$. Our conclusion from Table I was $v_0\cong 0.1658$, a value 0.69% larger. The effect of this discrepancy is that the Gaunt-Domb function $h(x)$ vanishes at $x=-x_0=-B^{-1/\beta}=-0.27$, whereas Table I implies that $h(x)=0$ when $x=-0.30$.

A second cautionary note concerns the effect of different estimates of q upon the result in Eq. (2.11a). Table II provides values of $h_1(0)$ obtained from expressions *fully* analogous to Eq. (2.11a), only constructed with different PA's to the function $f(v)$ of Eq. (2.9). Column A is constructed using $q=1.076$, column B uses $q=1.08$, while column C uses the Gaunt and Baker prediction $q=1$.[26,27]

The reader will note in column A the rather striking consistency between different PA's [as is typical for other values of $h_1(x)$ as well]. It is noticeable from column B that this consistency is weakened when one takes a sort of average estimate, $q=1.08$, from Table I for q. From column C we see that the consistency gets still worse when one takes $q=1$ (of course, this lack of consistency does not disprove the Gaunt-Baker conjecture that $q=1$).[26,27]

More significant, perhaps, is that all these values for $h_1(0)$ are about 10% different from the value $h(0)=0.345$ that was estimated[31] as the amplitude of the critical isotherm [$H=h(0)M^{\delta}$ from Eq. (1.1)] and was utilized in the construction of the Gaunt-Domb[19] scaling function. That this 10% discrepancy is due to the shortness of the high-temperature expansions (2.9) is supported by the following argument. The critical-point exponent δ is estimated by conventional methods (involving the use of "high-field"[29] series expansions) to have a value *exceedingly* close to 5.[31] However, when Gaunt and Baker[26] decided to test their *high-temperature* expansion methods by estimating δ, they were able to come up with the much *less* precise estimate $\delta=5.0\pm 0.2$. Presumably if considerably more terms were known in the basic high-temperature series, the confidence limits placed on this estimate could be reduced. Correspondingly, we decided to calculate $h(x)$ using a range of values of δ between 4.8 and 5.2. When we did this, we found that the agreement with the Gaunt-Domb $h(x)$ is considerably improved if we allow δ to decrease below 5. For example, we show in column D of Table II the values of $h_1(0)$ for the choice $\delta=4.8$, and we note that they agree with the value $h(0)=0.345$.[19,31] Thus we conclude that our method for calculating $h_1(x)$ is no less accurate than the analogous method for determining the phase boundary.[26]

Considerably better agreement with the Gaunt-Domb scaling function is obtained if we compare not plots of $h(x)$ vs x but rather follow Refs. 19 and 12 and plot $h(x)/h(0)$ vs $(x+x_0)/x_0$. There are many reasons for this kind of plotting. First, any comparison with experimental data is most plausibly achieved with such "normalized" plots (see Paper II). Second, for the purposes of such a normalized plot, *we do not need knowledge of the numerical values of the critical-point exponents β and δ*. This is because of our method of calculating $h_1(x)$ [cf. Eq. (2.5)]; β becomes irrelevant because of the identity

$$(xc^{1/\beta}+x_0c^{1/\beta})/x_0c^{1/\beta}=(x+x_0)/x_0 \tag{2.12}$$

and δ becomes irrelevant because c^{δ} would be canceled by taking the ratio $h_1(x)/h_1(0)$. In this way errors implied by possibly inaccurate estimates of β and δ are eliminated.

Table III presents this kind of comparison between normalized values of $h_1(x)$ using expression (2.11a) and the four corresponding "low-temperature" expressions of Gaunt and Domb.[19] It is evident that the discrepancy is much smaller than 10%, and moreover it appears in regions of x where Gaunt and Domb claimed only about 10% accuracy for their own calculation. Therefore we feel that our results (and theirs) for the normalized function $h_1(x)/h_1(0)$ are accurate to, at worst, 10%, and might be considerably better.

D. Calculation of Ising-Model Scaling Function for fcc and sc Lattices

We have also calculated expressions for $h_1(x)$ for the fcc and sc lattices, and these are given in Appendix B.

TABLE III. Comparison of the normalized scaling function $h(x)/h(0)$ as it is calculated in this work by using the *high-temperature* series expansion (see column 2) with the results for the same function obtained in Ref. 19 by using *low-temperature* (Ref. 29) series expansions (see column 3).

$(x+x_0)/x_0$	$h_1(x)/h_1(0)$	$h(x)/h(0)$
0.25	0.224	0.231
0.50	0.473	0.471
0.75	0.733	0.733
1.25	1.27	1.27
1.50	1.55	1.55
1.75	1.83	1.83
2.00	2.12	2.11
2.25	2.41	2.40
2.50	2.70	2.69
2.75	3.00	2.99
3.00	3.29	3.28
3.25	3.59	3.59
3.50	3.89	3.89
3.75	4.20	4.20
4.00	4.50	4.52
4.25	4.81	4.84
4.50	5.11	5.16

For both lattices the precision in determining the phase boundary (i.e., in determining v_0 and q) was *worse* than for the bcc lattice. In the case of the fcc lattice, this is because fewer terms in the series (2.7) were known ($L=8$); in the case of the sc lattice, the 12 known terms were less convergent than in the bcc case. We used $c=0.64$ for the fcc calculation and $c=0.70$ for the sc calculation.

One might get the impression that the constant c is rather arbitrarily chosen. The fcc and bcc lattices, however, have similar phase boundaries, so that the value $M=0.64$ for the fcc lattice lies as much in the critical region as does the value $M=0.60$ for the bcc lattice. Moreover, the sc lattice has a steeper phase boundary, and it turns out that $M=0.70$ for the sc lattice corresponds to about the same reduced temperature as does $M=0.60$ for the bcc lattice.[28,30]

A detailed consideration of the possible dependence of the scaling function on lattice structure is presented in Paper II.

III. CALCULATION OF SCALING FUNCTION FOR $S=\frac{1}{2}$ HEISENBERG MODEL

In this section we utilize the technique illustrated in Sec. II for the Ising model to calculate for the first time the scaling function of the $S=\frac{1}{2}$ Heisenberg model, with Hamiltonian

$$\mathcal{H}=-\tfrac{1}{2}J\sum_{\langle ij\rangle}\vec{\sigma}^{(i)}\cdot\vec{\sigma}^{(j)}-kT_cH\sum_{i=1}^{N}\sigma_3^{(i)}\ . \tag{3.1}$$

Here $\vec{\sigma}^{(i)}$ and $\vec{\sigma}^{(j)}$ are the Pauli spin operators at the nearest-neighbor pair of sites $\langle i,j\rangle$, H is the external magnetic field divided by KT_c/μ (to make it dimensionless), and σ_3 is the component of $\vec{\sigma}$ parallel to the field $\vec{\mathrm{H}}$.

A. Calculation of $h_1(x)$ for Small Values of x

Baker, Eve, and Rushbrooke[32] have calculated high-temperature series expansions for the Hamiltonian (3.1) that are analogous to the Ising-model series of Eq. (2.7):

$$H(\epsilon,M)=(\epsilon+1)\tanh^{-1}[Mg(M,z)]\ , \tag{3.2}$$

where

$$g(M,z)\equiv\sum_{n=0}^{\infty}(2^{-n}/n!)P_n(M)z^n\cong\sum_{n=0}^{L}(2^{-n}/n!)P_n(M)z^n\ . \tag{3.3}$$

Here $P_n(M)$ are polynomials in M^2 of degree n,

$$z\equiv K_c/(\epsilon+1)\ , \tag{3.4}$$

$K_c=J/kT_c$, and $L=8$ for all three lattices (fcc, bcc, and sc).

Again, we assume that the one-phase region is analytic (see Refs. 33 and 34), and we assume that, in analogy with (2.9), the function $g(M,z)$ for fixed $M=c$ vanishes at the phase boundary as

$$g(c,z)\cong 1+\sum_{n=1}^{L}(2^{-n}/n!)P_n(c)z^n\cong(z_0-z)^q\phi(z)\ . \tag{3.5}$$

We first consider the fcc lattice. The PA analysis of $(d/dz)\ln g(c,z)$ provides relatively reliable results for z_0 and q, providing c is in the range $0.4\le c\le 0.85$.[32] For the reasons discussed in Sec. II, we will choose the smallest possible value, $c=0.4$. The PA's for z_0 and q are somewhat less consistent (cf. Table IV) than in the Ising case (Table I). Our estimates are essentially the same as those of Ref. 32, $z_0=0.255\,26$ and $q=1.29$.

The PA's to the function $\phi(z)$ of Eq. (3.5) were next formed. They were found to be quite consistent, and we chose the [3, 3] approximant as representative. The corresponding closed-form expression for $g(0.4,z)$ is, from (3.5),

$$g(0.4,z)=\left(1-\frac{z}{0.25526}\right)^{1.29}\times\frac{1+3.789z+1.671z^2+3.612z^3}{1+3.775z+4.622z^2+14.397z^3}\ . \tag{3.6}$$

Substituting Eq. (3.6) into Eq. (3.2) and using Eq. (2.5), we obtain the following expression for the scaling function $h(x)$ of the $S=\frac{1}{2}$ Heisenberg model:

$$h_1(x)=\frac{(0.4)^{1/\beta}x+1}{(0.4)^{\delta}}\tanh^{-1}[0.4g(0.4,\tilde{z})]\ , \tag{3.7a}$$

where

TABLE IV. Poles (the upper numbers) and residues (the numbers in brackets) which correspond to z_0 and q, respectively, of PA's to $(d/dz)[\ln g(0.4, z)]$ [cf. Eq. (3.5)]. c.c. denotes that the corresponding prediction is a pair of complex conjugates.

D\N	1	2	3	4	5	6
1	0.33967 (2.977)	0.27670 (1.609)	0.22846 (0.748)	0.25084 (1.193)	0.26554 (1.679)	0.26015 (1.455)
2	0.29396 (2.016)	0.18033 (1.894)	0.24343 (1.007)	c.c.	0.26158 (1.518)	
3	0.25496 (1.281)	0.25518 (1.286)	0.25601 (1.307)	0.25757 (1.356)		
4	0.25519 (1.286)	0.25488 (1.280)	0.25394 (1.270)			
5	0.25599 (1.306)	0.25397 (1.271)				
6	0.25782 (1.367)					

$$\tilde{z} \equiv 0.2492/[(0.4)^{1/\beta}x+1] . \tag{3.7b}$$

Again we must emphasize that Eq. (3.7a) is valid for small x.[27] In order to obtain an expression for large x we use the Gaunt-Domb method which is quite sensitive to the estimated values of the critical-point exponents γ and Δ. Here γ denotes the critical-point exponent that describes the divergence of the zero-field isothermal susceptibility ($\chi_T \sim \epsilon^{-\gamma}$), while the "gap exponent" Δ describes the divergences of the higher-order derivatives of the magnetization with respect to field H, when $H=0$ and $T \to T_c^+$. Thus in our construction of $h(x)$ two separate groups of exponents are necessary: We need β and δ to get $h_1(x)$ for small x and we need γ and Δ to get $h_2(x)$ for large x.

However, if we accept the scaling hypothesis, we cannot choose these four exponents independently: As noted above, they are related by the scaling relations[1-4, 21]

$$\Delta = \beta + \gamma , \tag{3.8a}$$

$$\beta\delta = \beta + \gamma . \tag{3.8b}$$

Therefore, in writing Eqs. (3.7a) and (3.7b), we have not expressed the values of $(0.4)^{1/\beta}$ and $(0.4)^{\delta}$, since there is now an alternative to choose either $\beta = 0.35$ and $\delta = 5$ (as in Ref. 32), or to take $\beta = 0.385$ and $\delta = 4.71$, which are obtained by combining earlier but presumably more accurate estimates[35] $\gamma = 1.43$ and $2\Delta = 3.63$ together with the scaling relations (3.8a) and (3.8b).[36] For reasons to be explained later, we shall choose $\gamma = 1.43$, $2\Delta = 3.63$, $\beta = 0.385$, and $\delta = 4.71$, a set of exponents that satisfies the scaling relations.[37]

B. Asymptotic Behavior of Derivatives of Magnetization with Respect to Field

One can show[4] (cf. Appendix A) that if the scaling hypothesis, Eq. (1.1), is to be valid near the critical isochore ($M=0$, $T > T_c$), then it follows from usual thermodynamic assumptions that the function $h(x)$ should have the large-x series expansion

$$h(x) = \sum_{n=1}^{\infty} \eta_n x^{\beta(\delta+1-2n)} , \tag{3.9}$$

valid when x exceeds some finite constant R (i.e., $R \le x \le \infty$).

On the other hand, Domb and Hunter[2] obtained the same result, Eq. (3.9), following a different method, and their calculation provided a clue for the actual calculation of the coefficients η_n. One first assumes that successive higher-order field derivatives of the magnetization, evaluated at $H=0$, have singularities as $T \to T_c^+$ that are related to one another by a constant "gap" index,

$$\left(\frac{\partial^{2r-1}M}{\partial H^{2r-1}}\right)_{H=0} \cong A_{2r-1}\,\epsilon^{-\gamma-2(r-1)\Delta} \quad (r = 1, 2, \ldots) . \tag{3.10}$$

The "gap exponent" Δ defined in (3.10) is related to the exponents β, γ, and δ by Eqs. (3.8a) and (3.8b); note that (3.10) reduces for $r=1$ to the zero-field isothermal susceptibility χ_T, so that the "amplitude" A_1 is simply the susceptibility amplitude.

If one now substitutes the asymptotic behavior, Eq. (3.10), into the Taylor series expansion of $M(\epsilon, H)$ about $H=0$,

$$M(\epsilon, H) = \sum_{r=1}^{\infty} \left(\frac{\partial^{2r-1}M}{\partial H^{2r-1}}\right)_{H=0} \frac{H^{2r-1}}{(2r-1)!} , \tag{3.11}$$

then one can obtain a simple relation between the coefficients η_n in (3.9) and the coefficients A_{2r-1} in (3.10) by reverting the series (3.11) (see Appendix C for the details of this procedure). Therefore, it is necessary to know the amplitudes A_{2r-1} in order to obtain the coefficients η_n in the large-

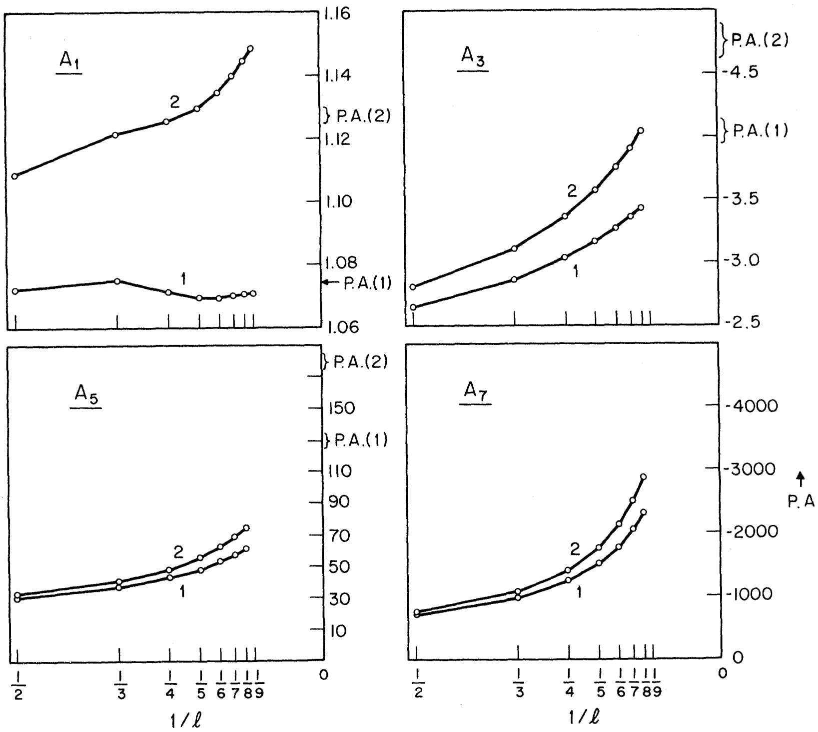

FIG. 2. Plot of the sequences (3.15). Estimates of the amplitudes A_{2r-1} can be obtained by extrapolating the curves until they intersect with the line $1/l=0$ ($l\to\infty$). The curvy brackets, labeled with PA, show the estimates of A_{2r-1} that follow from the PA's (see Table V). Curves numbered 1 correspond to the critical-point exponents $\gamma=1.43$ and $2\Delta=3.63$, whereas those numbered 2 correspond to the choice $\gamma=1.40$ and $2\Delta=3.50$.

x expansion of $h(x)$ [Eq. (3.9)].

The only amplitude A_{2r-1} before evaluated[35] for the $S=\frac{1}{2}$ Heisenberg model is the susceptibility amplitude A_1. Therefore we calculated the higher-order amplitudes from the series expansion[35]

$$M(\epsilon, H)=\sum_{n=1}^{\infty} F_{2n}(\epsilon)(\epsilon+1)^{2n-1}\frac{H^{2n-1}}{(2n-1)!}, \qquad (3.12)$$

where

$$F_{2n}(\epsilon)=\sum_{l=0}^{\infty} a_{2n,l}\left(\frac{K_c}{\epsilon+1}\right)^l \qquad (3.13)$$

and the coefficients $a_{2n,l}$ are derived in Ref. 35. From (3.12) it follows that

$$\left(\frac{\partial^{2r-1}M}{\partial H^{2r-1}}\right)_{H=0}=(\epsilon+1)^{2r-1}F_{2r}(\epsilon)\ . \qquad (3.14)$$

Equations (3.13) and (3.14) imply that the amplitude A_{2r-1} of Eq. (3.10) can be obtained in either of two fashions: (i) by estimating the $l\to\infty$ limit of the sequence

$$A_{2r-1}^{(l)}\equiv(-1)^l a_{2n,l}K_c^l\Big/\binom{-\gamma-2(r-1)\Delta}{l}, \qquad (3.15)$$

or (ii) by evaluating the residues of the PA's to the function

$$[F_{2r}(\epsilon)]^{1/[\gamma+2(r-1)\Delta]}\cong(A_{2r-1})^{1/[\gamma+2(r-1)\Delta]}\epsilon^{-1}\ . \qquad (3.16)$$

Methods (i) and (ii) are the conventional techniques used for obtaining amplitudes.[38]

Only series of the form of (3.13) with $r=1$, 2, 3, and 4 are known,[35] and therefore only the four amplitudes A_1, A_3, A_5, and A_7 can be estimated. As is clear from Eqs. (3.15) and (3.16), the values of the amplitudes A_{2r-1} depend strongly upon the estimates used for γ and Δ. Following the considerations discussed at the end of Sec. III A, we shall try the two choices ($\gamma=1.40$, $2\Delta=3.50$) and ($\gamma=1.43$, $2\Delta=3.63$).

In Figs. 2(a)–2(d) we have plotted against $1/l$ for $r=1$, 2, 3, and 4, respectively, the known number of terms in the sequence $A_{2r-1}^{(l)}$, defined in Eq. (3.15). For each value of r, plots for *both* sets of exponents (γ, Δ) are shown; however, only one value for K_c was used—the estimate $K_c\cong0.2492$ of Ref. 35.

Similarly, in Tables V(a)–V(d) we show the PA's to the function of Eq. (3.16) for $r=1$, 2, 3, and 4, respectively, and again we show the predictions for each of the two possible sets of exponents (γ, Δ).

We see from Fig. 2 that the set $\gamma=1.43$, $2\Delta=3.63$ causes less curvature in the sequences $A_{2r-1}^{(l)}$ than the other set. We also see from Table V that the PA's are somewhat more consistent when we use this set of the critical-point exponents. Hence, the amplitudes A_{2r-1} can be determined more reliably for $\gamma=1.43$, $2\Delta=3.63$ than for $\gamma=1.40$, $2\Delta=3.50$. In fact, for the first set we find $A_1=1.072\pm0.002$, $A_3=-4.05^{+0.09}_{-0.08}$, and $A_5=130.0^{+3.0}_{-5.0}$.

TABLE V. Residues of PA's to the functions $F_{2r}(\epsilon)$ of Eq. (3.14). The amplitudes A_1, A_3, A_5, and A_7 follow, respectively, from the (a), (b), (c), and (d) parts of the Table, by using the formula $A_{2r-1} \cong \lambda$ (residue/$K_c)^{\gamma+2(r-1)\Delta}$, where λ is 1, -2, 16, and 272, correspondingly. Two possible choices of the critical-point exponents, ($\gamma=1.43$, $2\Delta=3.63$) and ($\gamma=1.40$, $2\Delta=3.50$), are considered (cf. text). The dots appear at those places where the corresponding Padé predictions are unrealistic.

(a)

D\N	2	3	4	5	6	7
			$\gamma=1.43$			
2	0.274	0.272	0.249	0.259	0.259	0.266
3	0.265	0.261	0.261	0.262	0.262	
4	0.262	0.261	0.261	0.262		
5	0.261	0.262	0.262			
6	0.262	0.262				
7	0.262					
			$\gamma=1.40$			
2	0.279	0.276	0.258	0.267	0.267	0.281
3	0.270	0.268	0.269	0.271	0.271	
4	0.268	0.269	0.267	0.272		
5	0.269	0.267	0.271			
6	0.271	0.272				
7	0.272					

(b)

D\N	2	3	4	5	6	7
			$\gamma=1.43$, $2\Delta=3.63$			
2	0.302	0.306	0.283	0.426	0.282	
3	0.307	0.297	0.285	0.282		
4	0.273	0.287	0.290			
5	0.285	0.292				
6	0.281					
			$\gamma=1.40$, $2\Delta=3.50$			
2	0.310	0.310	0.296	⋯	0.294	
3	0.312	0.302	0.299	0.293		
4	0.288	0.299	0.301			
5	0.298	0.306				
6	0.289					

(c)

D\N	2	3	4	5	6	7
			$\gamma=1.43$, $2\Delta=3.63$			
2	0.350	0.295	0.379	0.215	0.237	
3	0.314	0.328	0.318	0.318		
4	0.332	0.321	0.318			
5	0.312	0.318				
6	0.320					
			$\gamma=1.40$, $2\Delta=3.50$			
2	0.352	0.305	0.390	0.231	0.726	
3	0.319	0.335	0.329	0.332		
4	0.343	0.330	0.331			
5	0.323	0.331				
6	0.337					

(d)

D\N	2	3	4	5	6	7
			$\gamma=1.43$, $2\Delta=3.63$			
2	0.497	⋯	⋯	⋯	⋯	
3	0.296	0.373	0.291	0.505		
4	0.442	0.326	0.348			
5	0.258	0.356				
6						
			$\gamma=1.40$, $2\Delta=3.50$			
2	0.491	⋯	⋯	⋯	⋯	
3	0.295	0.376	0.303	0.513		
4	0.466	0.331	0.356			
5	0.263	0.369				
6	⋯					

On the other hand, for $\gamma=1.40$ and $2\Delta=3.50$ we estimate $A_1=1.127\pm0.004$, $A_3=-4.7^{+0.3}_{-0.5}$, and $A_5=178.0\pm5.0$ using only predictions of PA's. For either set of exponents, we see from Fig. 2(d) and Table V (d) that all estimates of A_7 are extremely erratic and unreliable so that we shall not use this amplitude in the calculation of $h_2(x)$ that follows.

We will calculate $h_2(x)$, first for the set $\gamma=1.43$, $2\Delta=3.63$ (since this set corresponds to more reliable estimates for the amplitudes) and second, for the set $\gamma=1.40$, $2\Delta=3.63$. We shall find that although the amplitudes A_{2r-1} (for the two sets of exponents) differ quite considerably in magnitude, the resulting large-x expressions for the scaling functions are very similar, the discrepancy being within 1% for the range $x \lesssim 2$. For larger x, the discrepancy increases, but for all x within the range corresponding to usual experimental values ($x \lesssim 10^3$) we find that the discrepancy never exceeds about 10%.[39]

C. Calculation of $h_2(x)$ for Large Values of x

From the considerations of Sec. III B it follows that the first three terms of the expansion (3.11) for $M(\epsilon, H)$ may be estimated fairly reliably for the set of exponents $\gamma=1.43$, $2\Delta=3.63$, with the result that

$$M(\epsilon, H) = 1.072\epsilon^{-\gamma}H - 4.05\epsilon^{-\gamma-2\Delta}(H^3/3!) + 130\epsilon^{-\gamma-4\Delta}(H^5/5!) + \cdots . \qquad (3.17)$$

From Eqs. (C2) and (C8) of Appendix C we can obtain from (3.17) the first three coefficients η_n in the expansion (3.9) for $h_2(x)$,

$$h_2(x) = 0.9328x^{\gamma} + 0.5111\,x^{\gamma-2\beta} + 0.1263\,x^{\gamma-4\beta} + \cdots , \qquad (3.18)$$

where we have eliminated the exponent δ in (3.9) in favor of the exponent γ by using the scaling relation $\beta(\delta+1)=2\beta+\gamma$ [Eq. (3.8b)]. In our final result, (3.18), the coefficients η_n decrease in reliability with order n because the process of series reversion (cf. Appendix C and Ref. 19) increases the uncertainty of the higher-order coefficients. This is not serious, for the higher-order coefficients in (3.18) do not influence the numerical values of $h_2(x)$ for large x nearly as much as do the lower-order coefficients.

The knowledge of only three terms in the series expansion (3.18) is certainly a disadvantage, but owing to its presumably fast convergence it is not disastrous. In fact, we found that numerical values of $h_2(x)$ were almost the same if we simply truncated the series (3.18) at the three calculated terms, or if we formed the "[1, 1] PA" to (3.18) (this is the only PA possible for three terms),

$$h_2(x) = x^\gamma \frac{0.9328 + 0.2805x^{-2\beta}}{1 - 0.2472x^{-2\beta}} . \qquad (3.19)$$

Equation (3.19) for the large-x expression $h_2(x)$ matches perfectly with Eq. (3.7) for the small-x expression $h_1(x)$; the region of overlap extends from $x = 1.2$ to $x = 1.5$, within which the discrepancy between the two expressions is never larger than about 1%. {Of course, when we consider matching $h_1(x)$ and $h_2(x)$, we have to use the exponents $\beta = 0.385$ and $\delta = 4.71$ in evaluating $h_1(x)$ [cf. Eq. (3.7a)], since Eq. (3.19) for $h_2(x)$ has been calculated *only* for the corresponding values $\gamma = 1.43$ and $2\Delta = 3.63$.}[39]

In summary, then, we have found that in the case of the $S = \frac{1}{2}$ Heisenberg model, just as in the case of the Ising model, *two* expressions are sufficient to represent the scaling function $h(x)$ over its entire range of definition, $-x_0 \leq x \leq \infty$; $h(x) = h_1(x)$ for $x \lesssim 1.25$ and $h(x) = h_2(x)$ for $x \gtrsim 1.25$, where $h_1(x)$ and $h_2(x)$ are given in Eqs. (3.7a) and (3.19), respectively.

Comparison of the calculated $h(x)$ with experimental results on ferromagnetic systems is presented in Paper II.

D. Calculation of Scaling Function for Other Cubic Lattices

The above calculations are for the fcc lattice. For the bcc lattice we have also obtained an analogous expression for $h_1(x)$, and it is given in Appendix B. However, for the sc lattice we could not calculate a satisfactory expression for $h_1(x)$ because it was impossible to determine z_0 and q in Eq. (3.5) with sufficient accuracy. In fact, the same obstacle prevented a complete determination of the phase boundary for this lattice.[32]

Numerical comparison of the scaling functions for the fcc and bcc lattices will be studied in Paper II.

IV. CALCULATION OF SCALING FUNCTION FOR CLASSICAL HEISENBERG MODEL ($S = \infty$)

The classical ($S = \infty$) Heisenberg model is no less interesting than the $S = \frac{1}{2}$ Heisenberg model, either from an experimental or from a theoretical point of view. In fact, according to the (unproved) universality hypothesis, critical-point exponents are *independent* of spin quantum number S. However, even for those properties which may depend on spin, the $S = \infty$ Heisenberg model is probably no worse an approximation than the $S = \frac{1}{2}$ Heisenberg model[21,40] for the Heisenberg magnets $CrBr_3(S = \frac{3}{2})$ and EuO ($S = \frac{7}{2}$). Therefore in this section we calculate the scaling function $h(x)$ for the classical Heisenberg model, described by the Hamiltonian

$$\mathcal{H} = -2J \sum_{\langle ij \rangle} \vec{S}^{(i)} \cdot \vec{S}^{(j)} - kT_c H \sum_{i=1}^{N} S_3^{(i)} , \qquad (4.1)$$

where $\vec{S}^{(i)}$ and $\vec{S}^{(j)}$ are unit vectors ("classical spins") at the nearest-neighbor pair of sites $\langle ij \rangle$ of a lattice, while the other variables are defined following Eq. (3.1). In contrast to Eq. (3.1), the exchange parameter is now labeled $2J$ rather than $\frac{1}{2}J$; the present convention was adopted to conform with that of the workers who calculated the series that we are about to use.[41]

A. Two Different Approaches to the Phase Boundary

For the purpose of calculating the magnetic phase boundary for the classical Heisenberg model, Stephenson and Wood[41,42] generated the following high-temperature series expansion for the fcc lattice:

$$H(\epsilon, M) \cong M(\epsilon + 1) \sum_{n=0}^{9} B_n(y) \left(\frac{K_c}{\epsilon + 1}\right)^n , \qquad (4.2)$$

where B_n is a polynomial of order n in the variable

$$y \equiv M(\epsilon + 1)/K_c . \qquad (4.3)$$

In the present case, we cannot follow strictly the procedure applied previously to obtain the function $h(x)$. For if we were to follow Eq. (2.5), fixing $M = \text{const} \equiv c$ in Eq. (4.2), and rearranging the series in terms of increasing powers of $K_c/(\epsilon + 1) \equiv J/kT$, then we would obtain a series

$$H(\epsilon, c) \cong \sum_{n=0} S_n(c) \left(\frac{K_c}{\epsilon + 1}\right)^n , \qquad (4.4)$$

whose coefficients $S_n(c)$ are *not* known exactly. Rather, $S_n(c)$ are infinite series in the variable c, and only a few terms are known for each value of n. Therefore the coefficients $S_n(c)$ are not known accurately so that if we attempted to obtain an approximate closed-form expression for (4.4), it would be exceedingly inaccurate.

Therefore we return to Eq. (4.2) and fix $y \equiv \text{const} \equiv a$, which is more suitable[42] since the quantities

$B_n(y)$ are *polynomials* in the variable y (rather than infinite series) and hence for fixed $y=a$ they become precisely known numbers. In this case, instead of Eq. (4.4) we obtain *two* coupled equations,

$$H(\epsilon, M) \cong M(\epsilon+1)\sum_{n=0}^{9} B_n(a)\left(\frac{K_c}{\epsilon+1}\right)^n , \tag{4.5a}$$

$$M(\epsilon+1)/K_c = a . \tag{4.5b}$$

To obtain the scaling function $h(x)$ we *begin* as in Secs. II and III. First we assume that the summation of Eq. (4.5a) vanishes at the phase boundary in the form [cf. Eqs. (2.9) and (3.5)]

$$\sum_{n=0}^{9} B_n(a)z^n \cong (z_0 - z)^q \phi_\infty(z) , \tag{4.6}$$

where $z \equiv K_c/(\epsilon+1) \equiv J/kT$ as before. We must choose the constant a in the range $0.8 < a < 3$. (For $a > 3$, PA's do not give consistent predictions[42] for z_0 and q, while for $a < 0.8$, z_0 is of the order of K_c and thus available techniques are not sufficient for a precise estimation of z_0.) Since we wish both ϵ and M to be in the critical region, it follows from (4.5b) that we should choose a as small as possible and, accordingly, we choose $a = 0.8$.

Next we seek to estimate the numbers z_0 and q that appear in Eq. (4.6) by studying, respectively, the poles and residues of PA's to the logarithmic derivative of (4.6), $(d/dz)\ln[\sum_{n=0}^{9} B_n(0.8)z^n]$. The consistency of the PA's thus obtained (cf. Table VI) is superior to the consistency in the corresponding tables for the Ising model (Table I) and the $S=\frac{1}{2}$ Heisenberg model (Table IV). The fact that the consistency is slightly weakened at the last diagonal of Table VI does not cause us alarm and might even have a simple explanation.[43] From Table VI we infer that $z_0 = 0.1577$ and $q = 1.33$. We then formed PA's to the function $(1 - z/z_0)^{-q}\sum_0^9 B_n(0.8)z^n$ [cf. Eq. (4.6)], and choosing the [3, 3] PA as representative, we obtain, on subsituting Eqs. (4.6) into (4.5a),

$$H(\epsilon, M) = M(\epsilon+1)\left(1 - \frac{z}{0.1577}\right)^{1.33} \times \frac{3 - 22.169z + 23.71z^2 + 9.51z^3}{1 - 7.823z + 10.745z^2 + 1.697z^3} , \tag{4.7a}$$

where ϵ and M are restricted to those values that satisfy (4.5b) with $a = 0.8$:

$$M(\epsilon+1) = 0.8K_c . \tag{4.7b}$$

Next we apply Eq. (2.5) and we obtain from Eqs. (4.7a) and (4.7b) an expression for the scaling function $h(x)$ that is in the form of two coupled equations:

$$h(x) = \frac{0.8K_c}{c^\delta}\left(1 - \frac{\tilde{z}}{0.1577}\right)^{1.33} \times \frac{3 - 22.169\tilde{z} + 23.71\tilde{z}^2 + 9.512\tilde{z}^3}{1 - 7.823\tilde{z} + 10.745\tilde{z}^2 + 1.697\tilde{z}^3} , \tag{4.8a}$$

$$c(xc^{1/\beta} + 1) = 0.8K_c , \tag{4.8b}$$

where $\tilde{z}$ denotes $K_c/(xc^{1/\beta}+1)$ as in the $S=\frac{1}{2}$ case.[27]

The coupling between Eqs. (4.8a) and (4.8b) essentially means that in order to calculate $h(x)$ at some particular value of x, one first has to find the corresponding value of c from Eq. (4.8b). It follows from (4.8b) that large values of x imply small values of c. But according to the discussion that followed Eq. (2.5), it is very important to have c small; indeed, *the fact that c decreases when x increases leads to Eq.* (4.8a) *being a valid*

TABLE VI. Poles (the upper numbers) and residues (the numbers in brackets) which correspond to z_0 and q, respectively, of PA's to $(d/dz)[\ln(\sum_0^9 B_n(0.8)z^n)]$ [cf. Eq. (4.6)].

D \ N	1	2	3	4	5	6	7
1	0.1563 (1.284)	0.1569 (1.299)	0.1574 (1.315)	0.1576 (1.324)	0.1576 (1.326)	0.1579 (1.345)	0.1575 (1.317)
2	0.1570 (1.303)	0.1591 (1.446)	0.1577 (1.332)	0.1577 (1.328)	0.1576 (1.323)	0.1578 (1.333)	
3	0.1624 (2.328)	0.1578 (1.334)	0.1576 (1.323)	0.1577 (1.331)	0.1582 (1.383)		
4	0.1577 (1.331)	0.1576 (1.327)	0.1577 (1.334)	0.1579 (1.342)			
5	0.1577 (1.328)	0.1577 (1.331)	0.1579 (1.343)				
6	0.1576 (1.323)	0.1585 (1.417)					
7	0.1578 (1.335)						

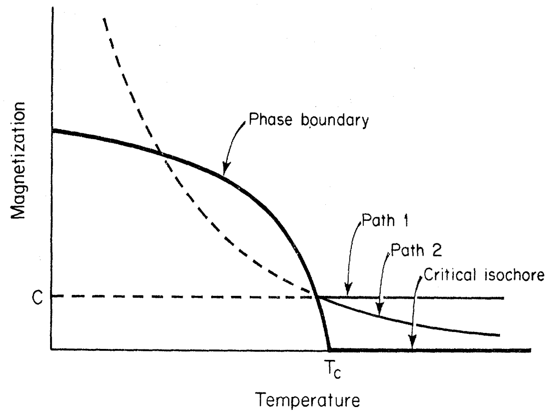

FIG. 3. Two ways of approaching the phase boundary by the high-temperature expansion of the magnetic field $H(\epsilon, M)$. The path labeled 1 is used in the Ising and $S=\frac{1}{2}$ Heisenberg model cases, Eqs. (2.7) and (3.2), whereas path 2 is used in the case of the $S=\infty$ Heisenberg model, Eq. (4.5a) (cf. also Refs. 26, 32, and 42).

expression for large x as well as for small x [and this is why we do not place a subscript 1 on $h(x)$ in (4.8a)].

The meaning of the last sentence is graphically illustrated in Fig. 3, which shows the two paths of approach to the phase boundary utilized by the high-temperature expansions used in this work. In the case of the Ising and $S=\frac{1}{2}$ Heisenberg models, the phase boundary is approached along paths of the type labeled "path 1" in Fig. 3 (c fixed). In the case of the classical Heisenberg model, we approach the phase boundary along the hyperbolic path labeled "path 2" (a fixed). Therefore when we apply Eq. (2.5) to the Ising and $S=\frac{1}{2}$ Heisenberg models, we in fact use the H function given on path 1, while in the $S=\infty$ Heisenberg model, the H function on path 2 has been used. When x increases, c remains constant for path 1 and decreases for path 2. Therefore, although expressions (2.11a) and (3.7a) for the Ising and $S=\frac{1}{2}$ Heisenberg models cease to be valid at large x, we might expect that the corresponding expression (4.8a) for the $S=\infty$ Heisenberg model will be valid for very large x.

Consistent with the expectation that (4.8a) be valid for large x is the following observation. Expansion (3.9), from which the large-x expressions for the Ising and $S=\frac{1}{2}$ Heisenberg models were obtained, was necessary in order to obtain $h(x)$ for large $x \equiv \epsilon/M^{1/\beta}$, corresponding to the region near the "critical isochore" ($M=0$, $T>T_c$). From Fig. 3 we see that this region is not probed by path 1, but is probed by path 2. Thus it is reasonable to expect that for the $S=\infty$ Heisenberg model it will not be necessary to appeal to a critical-isochore expansion of the form (3.9) in order to obtain $h(x)$ for large x.

B. Possible Sets of Critical-Point Exponents

The derivation of the expression (4.8) for the scaling function $h(x)$ of the $S=\infty$ Heisenberg model, like expressions (2.11a) and (3.7a) for $h_1(x)$ for the Ising and $S=\frac{1}{2}$ Heisenberg models, respectively, is independent of a particular choice of critical-point exponents β, δ, and inverse critical temperature $K_c \equiv J/kT_c$. As in the case of the $S=\frac{1}{2}$ Heisenberg model, current estimates of critical-point exponents are sufficiently imprecise that we feel obligated to try all three possibilities that have been recently proposed.

(i) Stephenson and Wood[41,42] have proposed $\beta=0.38\pm0.03$ and they have not challenged the earlier estimates[44] for γ ($\gamma\cong1.38$). Hence by using the scaling relation (3.8b), it follows that $\delta=4.63$. These exponents are consistent with $K_c=0.1573$.

(ii) Using longer series for the zero-field isothermal susceptibility and using higher-order moments of the two-spin correlation function as well, Ferer, Moore, and Wortis[45] estimated $\gamma=1.405\pm0.02$, $2\Delta=3.54\pm0.03$, $\alpha=-0.14\pm0.06$, and $K_c=0.15747$ from which they obtain, on using the scaling relations $\alpha+2\beta+\gamma=2$ and (3.8), the estimates $\beta=0.373\pm0.014$ and $\delta=4.9\pm0.4$.

(iii) From the hypothesis that critical-point exponents vary with spin dimensionality D according to a simple "bilinear form" (ratio of first-order polynomials in D), Stanley and Betts[46] propose $\alpha=-\frac{1}{10}$, $\beta=\frac{7}{20}=0.35$, $\gamma=\frac{7}{5}=1.40$, $\delta=5$, and $2\Delta=\frac{7}{2}=3.5$.

We have calculated $h(x)$ from Eq. (4.8) using all three possibilities—(i), (ii), and (iii). Table VII shows for each possibility values of x_0 and $h(0)$, where x_0 is defined by the relation $h(-x_0)=0$, i.e., the domain of definition of $h(x)$ is $-x_0\leq x<\infty$. From Eqs. (4.5a) and (4.5b), x_0 is seen to be given by the expression

$$x_0=(1-K_c/z_0)/(az_0)^{1/\beta}, \quad (4.9)$$

and $z_0=0.1577$ as mentioned above. We note from Table VII that each of the three possible sets of exponents leads to markedly different values for

TABLE VII. Values of $h(0)$ and x_0 for the classical Heisenberg model obtained by using Eqs. (4.8) and (4.9) and three different sets of estimates of the critical-point exponents [cf. text; we made the estimate $K_c=0.1575$ for the third choice by studying PA's to $(\chi_T)^{1/1.40}$, where χ_T is the zero-field susceptibility].

	$\beta=0.38$, $\delta=4.63$, $K_c=0.1573$	$\beta=0.373$, $\delta=4.9$, $K_c=0.15747$	$\beta=0.35$, $\delta=5$, $K_c=0.1575$
x_0	0.589	0.375	0.470
$h(0)$	2.13	1.78	1.82

x_0 and $h(0)$.[47] This is not surprising since the critical temperature is not the same for all three sets of exponents and a very small change in critical temperature leads to a very large change in the amplitudes $h(0)$ of the critical isotherm and $B=1/x_0^\beta$ for the coexistence curve [cf. also Eq. (4.9)].

However, when we compare normalized plots of $h(x)/h(0)$ *versus* $(x+x_0)/x_0$, all three sets of exponents produce curves that are in agreement within 1% for all x less than about 100; at extremely large x, the function $h(x)$ varies as x^γ [cf. Eq. (3.9) or (3.18)] (since γ is not the same for all three choices, the normalized functions will differ). However, this difference is quite small, e.g., even for $x=1000$, the discrepancy is only about 8%.

In summary, then, since normalized plots are used in all practical applications (as in comparison with experimental data—cf. Paper II), it does not matter much which set of exponents one chooses. However, since the Stephenson-Wood values, set (i), were obtained from expansion (4.2), as was (4.8), we shall use set (i) in actual comparisons with experiment to be carried out in Paper II.[48]

The $h(x)$ functions calculated in this work have very recently been cast into the parametric representation of the equation of state by Karo and Krasnow (their work will be reported in a future publication).

ACKNOWLEDGMENTS

Our debt is great to Gerald Paul for extensive discussions and invaluable advice. We also wish to thank George A. Baker, Jr., Alex Hankey, Pierre C. Hohenberg, and M. Howard Lee for helpful discussions. David Gaunt and Richard Krasnow very kindly read the manuscript, and their comments will hopefully improve the clarity of the present work.

APPENDIX A: CERTAIN PROPERTIES OF THE SCALING FUNCTION $h(x)$

Here we review those general properties of the scaling function $h(x)$ that are used in the present work; these properties are mainly consequences of the basic scaling hypothesis (2.5) and of "common assumptions"[4] about the thermodynamic variables magnetic field H and magnetization M.

(i) We begin by writing (2.5) in the form

$$h(x)=H/|M|^\delta = H(\epsilon c^{1/\beta}/|M|^{1/\beta},\ (\mathrm{sgn}M)c)/c^\delta \tag{A1}$$

in order to allow for both positive *and* negative M. If we restrict M to being nonnegative, it follows that H is nonnegative and hence that $h(x)$ is nonnegative. Actually, since in the one-phase region H is zero only on the phase boundary, it follows that for nonnegative M, $h(x)$ is always *positive* except at the single point $-x_0$ for which $h(-x_0)=0$. This point corresponds to a portion of the phase boundary which lies in the critical region. Since $x\equiv\epsilon/M^{1/\beta}$, and $M\equiv B(-\epsilon)^\beta$ on the phase boundary, it follows that

$$x_0=B^{-1/\beta}. \tag{A2}$$

(ii) Assuming[21] that $H(\epsilon, M)$ is a monotonic nondecreasing function of ϵ for fixed M, we can see from (A1) that $h(x)$ is also a monotonic nondecreasing function.

(iii) Analyticity of $H(\epsilon, M)$ in the one-phase region implies that $h(x)$ is an analytic function for all $x\geq -x_0$. However, careful consideration should be given to the region of very large x, i.e., close to the "critical isochore" $M=0$, $\epsilon>0$. For very small M, analyticity of H requires that the expansion

$$H(\epsilon, M)=\sum_{n=1}^{\infty} f_n(\epsilon)M^{2n-1} \tag{A3}$$

be convergent for $|M|$ less than some positive number $\mathfrak{M}(\epsilon)$. However, (A1) combined with (A3) requires a particular form of the functions $f_n(\epsilon)$ and, by implication, a specific expansion of $h(x)$ for large x. Specifically, we find on applying the scaling hypothesis (A1) to the expansion (A3) that

$$\epsilon^{\beta\delta}x^{-\beta\delta}H(xc^{1/\beta}, c)=c^\delta \sum_{n=1}^{\infty} f_n(\epsilon)\epsilon^{(2n-1)\beta}x^{-(2n-1)\beta}. \tag{A4}$$

Equation (A4) multiplied with $\epsilon^{-\beta\delta}$ can be true only if

$$f_n(\epsilon)=\eta_n\epsilon^{\beta(\delta+1-2n)}. \tag{A5}$$

Thus for large x, Eq. (A3) becomes

$$H(xc^{1/\beta}, c)=c^\delta\sum_{n=1}^{\infty}\eta_n x^{\beta(\delta+1-2n)}. \tag{A6}$$

Combining (A6) and (A1) results in the expression reproduced as Eq. (3.9) in the text,

$$h(x)=\sum_{n=1}^{\infty}\eta_n x^{\beta(\delta+1-2n)}. \tag{A7}$$

Now the initial series (A3), afforded by the analyticity of H, is convergent for a given ϵ providing M is sufficiently *small;* therefore (A7) is convergent with the proviso that $x[\equiv\epsilon/M^{1/\beta}]$ is sufficiently *large*, i.e., in the range $R\leq x<\infty$, where R is some positive constant. We cannot predetermine the value of R in general, nor even for the specific cases under consideration. Fortunately, it turned out that R was sufficiently small ($R\cong 1$) for both the Ising and $S=\frac{1}{2}$ Heisenberg models (cf. Secs. II B and III C, respectively) that our expansions for $h_2(x)$, based upon Eq. (A7), extended to sufficiently small values of x "overlapped" smoothly with the small-x expressions derived for $h_1(x)$.

The scaling functions for the $S=\frac{1}{2}$ Ising and Heisenberg models vary as x^γ for large x in accordance with (A7), but the scaling function of Eq. (4.8) for the $S=\infty$ Heisenberg model can be seen to vary as $x^{(1+\gamma)/(1+\beta)}$. This discrepancy means that (4.8) cannot be valid for *arbitrarily* large x, but in practice the discrepancy is manifest only for extremely large x ($x \gtrsim 10^7$).

We conclude with a remark concerning one particular value of $h(x)$, namely, $h(0)$. It is evident from (A1) that $h(0)$ is the amplitude of the critical isotherm $H=h(0)M^\delta$. Hence we might expect that it would play a special role in our analysis. Indeed, following Gaunt and Domb[19] we chose to compare our calculated scaling functions with experimental data and with each other by making plots of $h(x)/h(0)$ vs $(x+x_0)/x_0$, where x_0 is related to the coexistence curve amplitude B by Eq. (A2). In fact, normalization by $h(0)$ (the critical amplitude) might appear to be more judicious than normalization by $h(1)$,[49] especially since Betts, Guttmann, and Joyce[17] have recently made a plausible argument for how the critical amplitudes correspond to very specific characteristics of a given system.

APPENDIX B: EXPRESSIONS FOR THE SCALING FUNCTION $h(x)$ OF ISING MODEL FOR fcc AND sc LATTICES AND OF $S=\frac{1}{2}$ HEISENBERG MODEL FOR THE bcc LATTICE

1. Ising Model

Calculations of $h_1(x)$ in the case of the Ising model are based on the series (2.6), where the necessary coefficients of the polynomials $\psi_n(M)$ were obtained in Ref. 26 for $n=1, 2, \ldots, L$, and L is equal to 8 and 12 for the fcc and sc lattices, respectively. Details of the calculations are analogous to the bcc lattice (cf. Sec. II) and here we present only the results. Thus for the fcc lattice we obtain[27]

$$h_1(x)=\{[x(0.64)^{1/\beta}+1]/(0.64)^\delta\} \times \tanh^{-1}[0.64\tau_f(0.64, u)], \qquad \text{(B1)}$$

where

$$\tau_f(0.64, u)=\left(1-\frac{u}{0.1102}\right)^{1.0771} \times \frac{1-5.4432u+12.194u^2-23.296u^3}{1-8.1315u+41.835u^2-121.68u^3+122.28u^4} \qquad \text{(B2)}$$

and $u \equiv \tanh\{0.1021/[x(0.64)^{1/\beta}+1]\}$.

Similarly, we find for the sc lattice

$$h_1(x)=\{[x(0.7)^{1/\beta}+1]/(0.7)^\delta\}\tanh^{-1}[0.7\tau_s(0.7, u)], \qquad \text{(B3)}$$

where

$$\tau_s(0.7, u)=\left(1-\frac{u}{0.239}\right)^{1.065} \times \frac{1-3.3757u+1.0923u^2-2.9041u^3}{1-4.7718u+9.5748u^2-15.399u^3} \qquad \text{(B4)}$$

and $u=\tanh\{0.2217/[x(0.7)^{1/\beta}+1]\}$. In derivation of both (B1) and (B3) no specific values for β and δ were used, but in using these expressions one may assume the commonly accepted values[21] $\beta=\frac{5}{16}$ and $\delta=5$.

These two expressions cannot be expected to be adequate for $x \gtrsim 1$, just as our $h_1(x)$ expression in Eq. (2.11a) for the bcc lattice was found to fail for $x \gtrsim 1$. In fact, the series analogous to (2.7) is less convergent in the sc lattice case; in the case of the fcc lattice $L=8$ instead of 12, as for the bcc and sc lattices. Both facts imply that (B1) and (B3) are not as accurate as Eq. (2.11a), which is caused by a corresponding weaker precision in locating the phase boundaries.

The corresponding large-x functions $h_2(x)$ were not calculated.

2. $S=\frac{1}{2}$ Heisenberg Model

For the $S=\frac{1}{2}$ Heisenberg model for the bcc lattice we find[27]

$$h_1(x)=\{[(0.55)^{1/\beta}x+1]/(0.55)^\delta\} \times \tanh^{-1}[0.55g_{\text{bcc}}(0.55, 2)], \qquad \text{(B5)}$$

where $z \equiv 0.3973/[(0.55)^{1/\beta}x+1]$ and

$$g_{\text{bcc}}(0.55, 2)=\left(1-\frac{z}{0.430}\right)^{1.32} \times \frac{1-0.0696z-1.1591z^2-1.5507z^3}{1-0.3492z+0.2296z^2-2.3247z^3-1.1641z^4}. \qquad \text{(B6)}$$

Again, we did not have to specify β and δ in calculating (B5) and (B6), so that one can use both choices $\beta=0.35$ and $\delta=5$ or $\beta=0.385$ and $\delta=4.71$ (cf. Sec. III A). As far as the validity of (B5) is concerned it cannot be more accurate than Eq. (3.7) for the fcc lattice and hence we also expect (B5) to break down for $x \gtrsim 1$. We did not calculate a large-x expression for $h_2(x)$ for the bcc lattice.

APPENDIX C: REVERSION OF SERIES EXPANSION OF THE SCALING FUNCTION $h(x)$ FOR LARGE x

Here we will show that from the series (3.11) and assumption (3.10) (Sec. III B) one can get expansion (3.9) of the scaling function $h(x)$, with the coefficients η_n expressed in terms of the amplitudes A_{2r-1}. Relations (3.10) and (3.11) yield

$$M=\sum_{r=1} a_{2r-1}\epsilon^{-\gamma-2(r-1)\Delta} H^{2r-1}, \qquad \text{(C1)}$$

where the abbreviated notation

$$a_{2r-1} \equiv A_{2r-1}/(2r-1)! \qquad \text{(C2)}$$

has been used. Using the scaling relations $\gamma+\beta=\beta\delta$ and $\Delta=\beta\delta$, Eq. (C1) can be transformed into

$$M=\sum_{r=1} a_{2r-1}\epsilon^{\beta-(2r-1)\beta\delta} H^{2r-1} , \tag{C3}$$

and further

$$\frac{M}{\epsilon^{\beta}}=\sum_{r=1} a_{2r-1} \frac{M^{(2r-1)\delta}}{\epsilon^{(2r-1)\beta\delta}} \frac{H^{2r-1}}{M^{(2r-1)\delta}} , \tag{C4}$$

or, more conveniently,

$$\left(\frac{\epsilon}{M^{1/\beta}}\right)^{-\beta}=\sum_{r=1} a_{2r-1}\left(\frac{\epsilon}{M^{1/\beta}}\right)^{-(2r-1)\beta\delta}\left(\frac{H}{M^{\delta}}\right)^{2r-1} . \tag{C5}$$

This form is suitable for introducing the scaled variables $x\equiv\epsilon/M^{1/\beta}$ and $y\equiv H/M^{\delta}$. Hence

$$x^{-\beta}=\sum_{r=1} a_{2r-1}(y/x^{\beta\delta})^{2r-1} . \tag{C6}$$

On the other hand, the series expansion (3.9) states

$$y/x^{\beta\delta}=\sum_{n=1} \eta_n x^{-(2n-1)\beta} , \tag{C7}$$

i.e., $y/x^{\beta\delta}$ appears as a function of $x^{-\beta}$, whereas (C6) expresses the inverse function. Therefore, one can get η_n from a_{2r-1} and vice versa, by the series-reversion method. Since estimation of a_{2r-1} is more reliable, one usually obtains η_n from a_{2r-1}.

Inserting (C7) into (C6) and identifying coefficients of the equal powers of $x^{-\beta}$ on both sides of the resulting identity, the following expressions for the first few coefficients can be obtained:

$$\eta_1=1/a_1 , \tag{C8a}$$

$$\eta_2=-a_3/a_1^4 , \tag{C8b}$$

$$\eta_3=(3a_3^2-a_1a_5)/a_1^7 . \tag{C8c}$$

The higher-order coefficients can be obtained in a similar way, but we quote here only as many as are necessary to obtain Eq. (3.18) from (3.17).

---

*Work forms a portion of a Ph.D. thesis submitted to the MIT Physics Department by Sava Milošević. A preliminary report of portions of the present work appears in S. Milošević and H. E. Stanley, Phys. Rev. B 5, 2526 (1972).

†On leave of absence from the Institute of Physics, Belgrade, Yugoslavia.

‡Work supported by the NSF, under Grant No. GP-15428.

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

[2]C. Domb and D. L. Hunter, Proc. Phys. Soc. (London) 86, 1147 (1965).

[3]L. P. Kadanoff, Physics 2, 263 (1966); A. Z. Patashinskii and V. L. Pokrovski, Zh. Eksperim. i Teor. Fiz. 50, 439 (1966) [Sov. Phys. JETP 23, 292 (1966)].

[4]R. B. Griffiths, Phys. Rev. 158, 176 (1967).

[5]J. S. Kouvel and D. S. Rodbell, Phys. Rev. Letters 18, 215 (1967).

[6]A. Arrott and J. E. Noakes, Phys. Rev. Letters 19, 786 (1967).

[7]J. S. Kouvel and J. B. Comly, Phys. Rev. Letters 20, 1237 (1968).

[8]J. T. Ho and J. D. Litster, Phys. Rev. Letters 22, 603 (1969).

[9]K. Miyatani, J. Phys. Soc. Japan 28, 259 (1970).

[10]N. Menyuk, K. Dwight, and T. B. Reed, Phys. Rev. B 3, 1689 (1971).

[11]J. S. Kouvel and J. B. Comly, in *Critical Phenomena in Alloys, Magnets, and Superconductors*, edited by R. E. Mills, E. Ascher, and R. I. Jaffee (McGraw-Hill, New York, 1971).

[12]M. Vicentini-Missoni, R. I. Joseph, M. S. Green, and J. M. H. Levelt Sengers, Phys. Rev. B 1, 2312 (1970).

[13]P. Schofield, Phys. Rev. Letters 22, 606 (1969).

[14]B. D. Josephson, J. Phys. C 2, 1113 (1969).

[15]C. Domb and D. S. Gaunt, J. Phys. Suppl. 32, C1 (1971).

[16]M. S. Green, M. J. Cooper, and J. M. H. Levelt Sengers, Phys. Rev. Letters 26, 492 (1971); see also M. J. Cooper (unpublished).

[17]D. D. Betts, A. J. Guttmann, and G. S. Joyce, J. Phys. C 4, 1994 (1971).

[18]T. Schneider, G. Srinivasan, and E. Stoll (unpublished).

[19]D. S. Gaunt and C. Domb, J. Phys. C 3, 1442 (1970).

[20]S. Milošević and H. E. Stanley, following paper (henceforth referred to as II), Phys. Rev. B 6, 1002 (1972).

[21]H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena*, (Oxford U. P., London, 1971).

[22]A. Hankey and H. E. Stanley, Phys. Rev. B 6 (to be published); see also T. S. Chang, A. Hankey, and H. E. Stanley, Bull. Am. Phys. Soc. 17, 277 (1972).

[23]J. Aczel, *Lectures on Functional Equations* (Academic, New York, 1966); our attention to this book was drawn by M. J. Cooper [Phys. Rev. 168, 183 (1968)].

[24]G. A. Baker, Jr., in *Advances in Theoretical Physics*, edited by K. A. Brueckner (Academic, New York, 1965), Vol. 1, p. 1.

[25]J. Zinn-Justin, Phys. Rept. 1, 55 (1971), and references contained therein.

[26]D. S. Gaunt and G. A. Baker, Phys. Rev. B 1, 1184 (1970). In Sec. II, we generally use the same notation as Ref. 26, but we call $q\equiv 1/\iota$.

[27]The possibility $q\neq 1$ corresponds to $\chi=\infty$ on the phase boundary. It may seem unreasonable to estimate more than two decimal places of q, but we noticed that a remarkable consistency in PA's to $f(v)$ (to the fifth decimal place) can be obtained if one uses some particular prediction of Table I, rather than some over-all average (in which case the consistency is only to the second decimal place). Moreover, if one tries the choice $q=1$, which is believed (Ref. 26) to be the true one, the mentioned consistency becomes still further weakened (see Table II).

[28]In deriving expression (2.11b) we have used results of J. W. Essam and D. L. Hunter, J. Phys. C 2, 392 (1968), concerning the amplitudes for higher-order derivatives of magnetization with respect to field.

[29]M. F. Sykes, J. W. Essam, and D. S. Gaunt, J. Math. Phys. 6, 283 (1965). Only the first of the "four expressions" is *strictly* derived from low-temperature expansions, the next three being expansions about $x=0$, i.e., the critical isotherm. The point is that expansions such as $M=1-2\sum_s sL_s(u)\mu^s$ are valid for *arbitrary* μ (temperature), not just for low temperature (small μ),

where $u \equiv e^{-4J/kT}$ and $\mu \equiv e^{-2mH/kT}$. They are, of course, actually expansions about $\mu = 0$ ($H = \infty$), and hence the name "high-field expansions" might be more appropriate. We wish to thank Dr. Gaunt for having emphasized this point to us.

[30]M. E. Fisher, J. Math. Phys. 4, 278 (1963); Rept. Progr. Phys. 30, 615 (1967), particularly Table II.

[31]D. S. Gaunt, Proc. Phys. Soc. (London) 92, 150 (1967).

[32]G. A. Baker, Jr., J. Eve, and G. S. Rushbrooke, Phys. Rev. B 2, 706 (1970). The polynomials $P_n(M)$ were derived from Ref. 35.

[33]T. Asano, Phys. Rev. Letters 24, 1409 (1970).

[34]T. Asano, J. Phys. Soc. Japan 29, 350 (1970).

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

[36]There is even the third possibility, $\beta = 0.39$ and $\delta = 4.49$, which follows from the values $\gamma = 1.36$ and $2\Delta = 3.50$, obtained in the very recent analysis of M. H. Lee and H. E. Stanley, Phys. Rev. B 4, 1613 (1971). However, if we accept this choice for β and δ we would have, for the sake of consistency, to perform a similar reanalysis of the series obtained in Ref. 32, but this would be beyond the scope of the present work.

[37]The values of β and δ are roughly within the confidence limits of the only numerical evaluation of these critical exponents (Ref. 32), $\beta = 0.35 \pm 0.05$ and $\delta = 5.0 \pm 0.2$.

[38]See, e.g., the discussion in Ref. 31.

[39]Since the choice $\gamma = 1.40$ and $2\Delta = 3.50$ implies a weaker estimation of the amplitudes A_{2r-1} we considered two possible sets $A_1 = 1.127$, $A_3 = -4.7$, and $A_5 = 178$, the average values, and $A_1 = 1.130$, $A_3 = -5.2$, and $A = 180$, the extreme of the Padé predictions. The first set results in the following expression:

$$h_2(x) = x^{\gamma}(0.8873 + 0.4856x^{-2\beta} + 0.0728x^{-4\beta} + \cdots),$$

which matches with Eq. (3.7a) at $x = 3.5$ with accuracy less than 1%. The second set ($A_1 = 1.130$, $A_3 = -5.2$, $A_5 = 180$) yields the expression

$$h_2(x) = x^{\gamma}(0.8850 + 0.5315x^{-2\beta} + 0.2373x^{-4\beta} + \cdots),$$

which overlaps with the Eq. (3.7a) at $x = 1$ with the same accuracy, i.e., less than 1%. We expect the second $h_2(x)$ expression to be more reliable as it meets with the small-x formula (3.7a) in the same region where the corresponding formulas for $\gamma = 1.43$ and $2\Delta = 3.63$ overlap (cf. Sec. III C).

[40]R. F. Wielinga, in *Progress in Low Temperature Physics*, edited by C. J. Gorter (North-Holland, Amsterdam, 1970), Vol. VI, pp. 333–373. See, e.g., the recent comparison of the data for EuO and EuS with the $S = \infty$ Heisenberg model in J. Als-Nielsen, O. W. Dietrich, W. Kunnmann, and L. Passell, Phys. Rev. Letters 27, 741 (1971).

[41]R. L. Stephenson and P. J. Wood, Phys. Rev. 173, 475 (1968).

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

[43]Recently, M. Ferer, M. A. Moore, and M. Wortis (Ref. 45) observed that the coefficients in the high-temperature series expansions of higher-order derivatives of magnetization with respect to field as calculated in Ref. 41 are in error. This might be a reason for the slight inconsistency in Table VI.

[44]See, e.g., G. S. Joyce and R. G. Bowers, Proc. Phys. Soc. (London) 88, 1053 (1966); H. E. Stanley, Phys. Rev. 158, 546 (1967). Recently R. G. Bowers and M. E. Woolf [*ibid.* 177, 917 (1969)] have argued that $\gamma = 1.375 \pm 0.002$, but see Ref. 45 and G. Paul and H. E. Stanley [Phys. Rev. B 5, 3715 (1972)] for arguments suggesting that there may be pitfalls in the Bowers-Woolf approach.

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

[46]H. E. Stanley and D. D. Betts, Phys. Rev. B 6, (to be published).

[47]From Table VII it follows that in the case $\beta = 0.38$ and $\gamma = 1.38$ the amplitude B of the phase boundary [$M = B(-\epsilon)^{\beta}$; $B = x_0^{-\beta}$] is equal to 1.22. During our study of possible choices for the parameter a in Eq. (4.6) we noticed that almost all choices for a imply $B \cong 1.20 \pm 0.04$ and therefore we cannot agree with the statement of Als-Nielsen *et al.* (Ref. 40) that the theoretical prediction for the $S = \infty$ Heisenberg model is $B = 1.12$.

[48]We have studied the higher-order derivatives of magnetization with respect to field (as was done for $S = \frac{1}{2}$ in Sec. III B) and found that the Stephenson and Wood estimates ($\gamma = 1.38$, $\beta = 0.38$, $K_c = 0.1573$) gave the most reliable results.

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