Calculation of the Scaling Function for the Heisenberg Model*

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We present a method for calculating the "Griffiths" scaling function $h(\epsilon/M^{1/\beta})$ directly from high-temperature series expansions. The scaling function is calculated for the first time for the $S=\frac{1}{2}$ and ∞ Heisenberg models, and comparison with experimental data on $CrBr_3$, EuO, Ni, and disordered Pd_3Fe is favorable. We observe an apparent lattice independence of the scaling functions calculated, consistent with the "universality hypothesis."

The static-scaling hypothesis[1] makes predictions concerning (i) relations among critical-point exponents (such as $\alpha+2\beta+\gamma=2$), and (ii) the mathematical form of the equation of state in the critical region. At present there exists a great deal of *experimental* evidence to support predictions (i) and (ii)[2]; however, *theoretical* calculations on model systems almost exclusively concern critical-point exponents and hence pertain only to prediction (i).

One notable exception is the recent calculation of the scaling-function equation of state for the Ising model.[3] The calculation of Ref. 3 depends crucially upon the knowledge of *low*-temperature as well as *high*-temperature series expansions; unfortunately, low-temperature expansions are not available for many interaction Hamiltonians, and in such cases the calculation of Ref. 3 cannot be generalized. In particular, since a large fraction of the experimental evidence supporting (ii) concerns magnetic systems,[2] it would be desirable to obtain a theoretical prediction of the scaling function for the Heisenberg model of magnetism.

The purpose of the present work is to present a method of calculating scaling functions that depends only upon the existence of high-temperature series expansions and hence is applicable to Ising, planar, Heisenberg, ... systems. Moreover, we feel that this method is significantly simpler to apply than the method utilized in Ref. 3. To illustrate this method we calculate the scaling function for the $S=\frac{1}{2}$ and ∞ Heisenberg models, and compare the theoretical predictions with experimental data on the insulating ferromagnetic $CrBr_3$. We discuss the possible dependence of the scaling function upon spin quantum number S, in the light of the universality hypothesis.[4] Also we calculate the Ising-model scaling function for various lattices and compare our work with that of Ref. 3.

The static-scaling hypothesis may be formulated[1,5] by the statement that the singular part of a thermodynamic potential (or, equivalently, the magnetic field) is a generalized homogeneous function; that is, for all positive λ,

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

where H, ϵ, and M denote, respectively, magnetic field, reduced temperature $(T-T_c)/T_c$, and magnetization; the exponents β and δ are defined by $M\sim|\epsilon|^{\beta}$, when $H=0$, and $H\sim M^{\delta}$, when $\epsilon=0$. The main assumption is that (1) is true in the critical region, i.e., for sufficiently small ϵ and M.

The "Griffiths"[1] scaling function $h(x)$ may be obtained from (1) by setting $\lambda=(1/M)^{\delta+1}$, where

$$H\left(\frac{\epsilon}{M^{1/\beta}},1\right)=\frac{H(\epsilon,M)}{M^{\delta}}\equiv h\left(\frac{\epsilon}{M^{1/\beta}}\right)\ . \qquad (2)$$

However, the function $h(x)$ defined in Eq. (2) would not be characteristic of the critical region since both arguments of $H(\epsilon/M^{1/\beta},1)$ in (2) are not small near the critical point. To obviate this difficulty, we return to (1) and set $\lambda=(c/M)^{\delta+1}$, where c is an arbitrary fixed small number. Therefore (2) is replaced by

$$H\left(\frac{\epsilon c^{1/\beta}}{M^{1/\beta}},c\right)=\frac{c^{\delta}H(\epsilon,M)}{M^{\delta}}=c^{\delta}h\left(\frac{\epsilon}{M^{1/\beta}}\right)\ , \qquad (2')$$

so that the function $h(x)$ becomes

$$h(x)=H(xc^{1/\beta},c)/c^{\delta}\ . \qquad (3)$$

Hence *if* we knew the function $H(\epsilon,M)$, then $h(x)$ could be obtained by fixing $M=c$ and allowing for ϵ the corresponding values $xc^{1/\beta}$. In fact, the most we know about $H(\epsilon,M)$, either for the Ising model or for the Heisenberg model, is a finite number of terms in a series expansion.

In order to test the present procedure of obtaining $h(x)$ we will first consider the Ising model. Gaunt and Baker[6] provided the following expansion of $H(\epsilon,M)$:

$$H(\epsilon,M)\cong(\epsilon+1)\tanh^{-1}\left[M\sum_{n=0}^{L}\psi_n(M)\,v^n\right]$$
$$\equiv(\epsilon+1)\tanh^{-1}[M\tau(M,v)]\ , \qquad (4)$$

where $\psi_n(M)$ are polynomials in M^2 of degree n, $v\equiv\tanh[K_c/(\epsilon+1)]$, $K_c\equiv J/kT_c$, and J is the exchange parameter in the Hamiltonian. The polynomials $\psi_n(M)$ were calculated[6] through order $L = 8, 12$, and 12 for the fcc, bcc, and sc lattices, respectively. Following (3) we should get a closed-form expression for the right-hand side of (4) when $M = c$, where c is a very small positive constant.[7] Formally, this problem is similar to one encountered[6] in the process of determination of the phase boundary from (4), and here we will adopt the similar attitude, namely, we will assume that the function $\tau(M = c, v)$ in (4) vanishes at the phase boundary with the power-law form

$$\tau(c, v) = \sum_{n=0}^{L} \psi_n(c) v^n = (v_0 - v)^q f(v) , \quad (5)$$

where v_0, q, and $f(v)$ are to be estimated by the method of Padé approximants (PA's). Thus one first must find v_0 and q by considering PA's to $(d/dv) \times [\ln \tau(c, v)]$, and afterwards $f(v)$ can be determined by studying the product $(v_0 - v)^{-q} \tau(c, v)$. Gaunt and Baker[6] noticed that the series (5) was not sufficiently lengthy for reliable estimates for v_0 and q to be obtained unless $c \gtrsim 0.6$. Since the smaller the value of c, the wider the range of x in (3) may be, we will choose $c = 0.6$ for our further analysis.

In the case of the bcc lattice we found $v_0 = 0.1658$ and $q = 1.076$; PA's to $f(v)$ were consistent up to five decimal places, and we rather arbitrarily chose the [4, 4] PA, with the result

$$\tau(0.6v) = \left(1 - \frac{v}{0.1658}\right)^{1.076} \left(\frac{1 - 4.566v + 5.406v^2 + 5.842v^3 + 0.3907v^4}{1 - 5.936v + 17.603v^2 - 37.098v^3 + 25.812v^4}\right). \quad (6)$$

Inserting (6) into (4), using the resulting form for $H(\epsilon, 0.6)$ in (3), and choosing[6] $\beta = \frac{5}{16}$, $\delta = 5$, we finally obtain

$$h(x) = [(0.195x + 1)/0.07776] \tanh^{-1}[0.6\tau(0.6, \tilde{v})] , \quad (7)$$

where $\tau(0.6, \tilde{v})$ is given by (6) and $\tilde{v} \equiv \tanh[0.15743/(0.195x + 1)]$.

Comparing $h(x)$ in (7) with Ref. 3, we find good agreement[8] in the range $-x_0 \le x \lesssim 1.1$; $-x_0$ is the lowest possible value of x and is determined by $x_0 = \mathcal{B}^{-1/\beta}$, where $\mathcal{B}$ is the amplitude defined by $M(\epsilon, H = 0) = \mathcal{B}(-\epsilon)^\beta$. The largest discrepancy is not larger than 3%, and it occurs at those values of x where different PA's of Ref. 3 agree to within 10%. More striking is the fact that in Ref. 3 four *separate expressions* were needed for $h(x)$ in the interval $-x_0 \le x \lesssim 1.1$, while in the present approach *a single expression*, Eq. (7), suffices. In fact, the upper limit of $\simeq 1.1$ for x is determined only by the smallness of the number of terms in the original series (5). For $x \gtrsim 1.1$ we may use the "fifth expression" of Gaunt and Domb (derived also from high-temperature expansions), and it satisfactorily matches our expression $h(x)$ (valid for $x \lesssim 1.1$).

We also calculated expressions for $h(x)$ analogous to (7) for the fcc and sc lattices. We find that the normalized functions $h(x)/h(0)$, when plotted against x/x_0, differ for all three lattices by at most 2%, thereby supporting (but of course not proving) the idea of universality of the scaling functions.[3,4,9]

Next we apply the present approach to the case of the nearest-neighbor $S = \frac{1}{2}$ Heisenberg model, for which Baker *et al.*[10] have calculated expansions analogous to (4),

$$H(\epsilon, M) \simeq (\epsilon + 1) \tanh^{-1} \left[M \sum_{n=0}^{L} \frac{z^n}{2^n n!} P_n(M) \right]$$

$$\equiv (\epsilon + 1) \tanh^{-1} [M g(z, M)] , \quad (8)$$

where $z \equiv K_c/(\epsilon + 1)$ and $P_n(M)$ is a polynomial in M^2 of degree n. In analogy with (5), we assume that the function $g(z, M)$ for fixed $M = c$ vanishes at the phase boundary,

$$g(z, c) = 1 + \sum_{n=1}^{L} \frac{z^n}{2^n n!} P_n(c) \sim (z_0 - z)^q \phi(z) . \quad (9)$$

The PA analysis is not reliable for $c < 0.4$, so we shall choose $c = 0.4$. Again the PA's to $\phi(z)$ are extremely consistent (providing $0.4 < c < 0.85$) and we present here the expression for $g(z, c)$, for the fcc lattice, using the [3, 3] P. A.,

$$g(z, 0.4) = \left(1 - \frac{z}{0.25526}\right)^{1.29} \times \left(\frac{1 + 3.789z + 1.671z^2 + 3.612z^3}{1 + 3.775z + 4.622z^2 + 14.397z^3}\right). \quad (10)$$

Combining (10), (8), and (3), we obtain

$$h(x) = \frac{(0.4)^{1/\beta} x + 1}{(0.4)^\delta} \tanh^{-1}[0.4 g(\tilde{z}, 0.4)] , \quad (11)$$

where

$$\tilde{z} = 0.2492/[(0.4)^{1/\beta} x + 1] . \quad (12)$$

We deliberately have not written the explicit values for $(0.4)^{1/\beta}$ and $(0.4)^\delta$ (as we had in the Ising-model case) since there is now an alternative to choose either $\beta = 0.35$, $\delta = 5$ as in Ref. 10 or to take $\beta = 0.385$, $\delta = 4.71$, which follows from combining the more accurate[11] estimates $\gamma = 1.43$ and $2\Delta = 3.63$ with the scaling relations $\Delta = \gamma + \beta$ and $\beta\delta = \gamma + \beta$.[12]

For large x, Eq. (11) will break down for the reasons discussed above. Hence we calculate $h(x)$ for large x using the method of Ref. 3,[13] with the

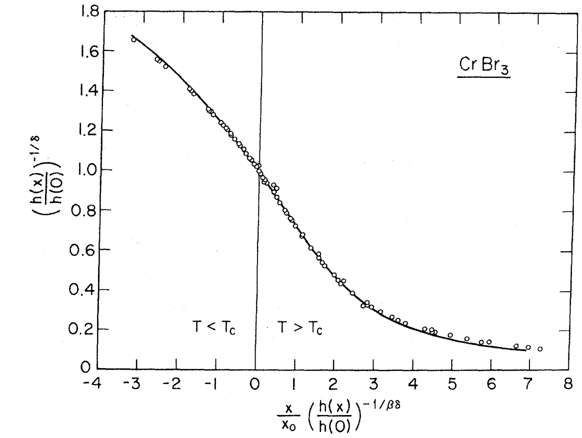

FIG. 1. Scaling function for the $S=\frac{1}{2}$ Heisenberg model, compared with essentially the entire range of the Ho-Litster data (Ref. 2) on $CrBr_3$. The slight discrepancy for large values of the abscissa is due to the difference between the value $\gamma = 1.43$ used in the calculation (Ref. 11) and $\gamma = 1.215$ measured (Ref. 2) for $CrBr_3$. This is essentially a plot of "scaled magnetization" $M/H^{1/\beta}$ vs "scaled temperature" $\epsilon/H^{1/\beta\delta}$, with the results presented in terms of the Griffiths function $h(x)$.

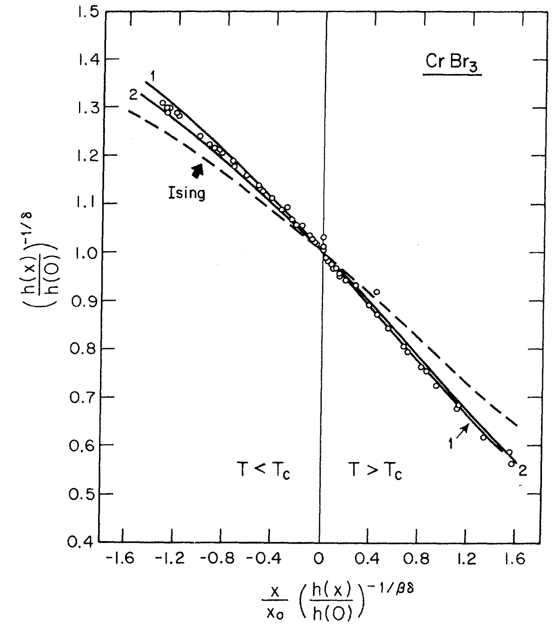

FIG. 2. Central portion of Fig. 1 is shown enlarged here. Curve 1 was calculated with $\beta = 0.385$, $\delta = 4.71$ (as in Fig. 1), while curve 2 was calculated with $\beta = 0.35$, $\delta = 5$. Also shown is the scaling function for the Ising model.

result (for $\gamma = 1.43$, $2\Delta = 3.63$, $\beta = 0.385$, and $\delta = 4.71$)

$$h(x) = x^{\gamma}\ \frac{0.9328 + 0.2805\, x^{-2\beta}}{1 - 0.2472\, x^{-2\beta}} \quad . \tag{13}$$

This expression meets with (11) in the vicinity of $x = 1.25$ with an accuracy better than 0.5%.

Figure 1 compares our $S=\frac{1}{2}$ Heisenberg-model calculation of $h(x)$ with experimental data on the insulating ferromagnet $CrBr_3$[2]. Figure 2 is an enlargement of the central portion of Fig. 1, and

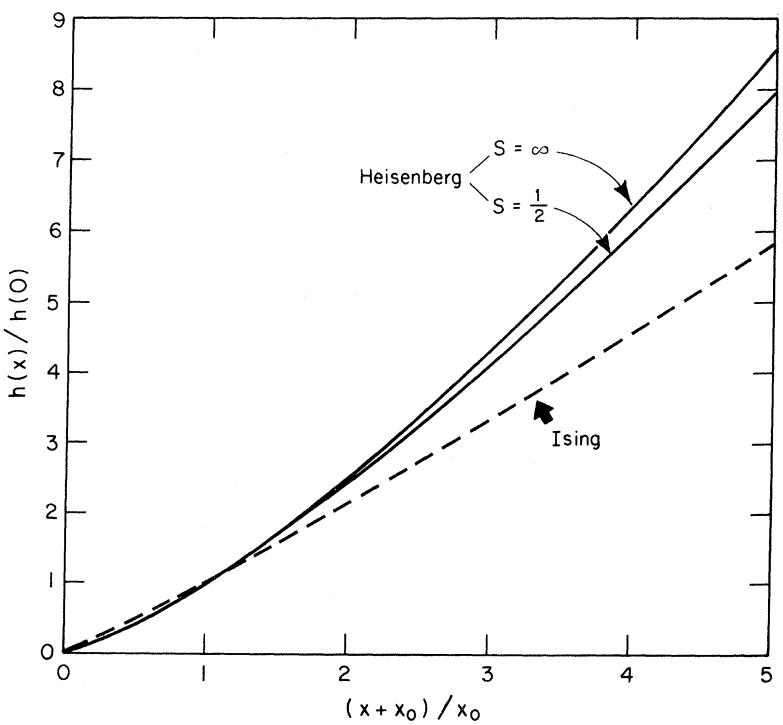

FIG. 3. Comparison of calculations for the fcc lattice for the Ising model and the $S=\frac{1}{2}$ and $S=\infty$ Heisenberg models.

contains additional comparison with the Ising model.

For the classical Heisenberg model ($S=\infty$), a somewhat modified procedure applied to the series of Stephenson and Wood[14] leads to the result

$$h(x)=\frac{0.8K_c}{M^\delta}\left(1-\frac{z}{0.1577}\right)^{1.33}\times\left(\frac{3-22.169z+23.71z^2+9.512z^3}{1-7.823z+10.745z^2+1.697z^3}\right), \qquad (14)$$

where $z=K_c/(xM^{1/\beta}+1)$ and M is found from the expression $M(xM^{1/\beta}+1)=0.8K_c$ $(K_c=0.1573)$.

To compare $h(x)$ for $S=\infty$ with $h(x)$ for $S=\frac{1}{2}$, we plot in Fig. 3 the dependence upon $(x+x_0)/x_0$ of $h(x)/h(0)$, because this quantity does not require for its calculation the specification of the critical-point exponents.[15] In the region where (11) and (14) are valid, the discrepancy between the $S=\frac{1}{2}$ and $S=\infty$ scaling functions is at worst 10%; whether this discrepancy is genuine or spurious (because of the slow convergence of the series) we cannot answer firmly.

In summary, we have presented a method that affords a simple reliable calculation of the scaling function $h(x)$; this method is applicable to models for which no low-temperature series are available. The scaling functions for the Ising and Heisenberg models were calculated and of the two the Heisenberg calculation was found to agree considerably better with experimental data on $CrBr_3$, EuO, Ni, and disordered Pd_3Fe. Finally, we have noted a striking lattice independence (and possible spin independence) of the scaling function.

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[1]R. B. Griffiths, Phys. Rev. 158, 176 (1967), and references contained therein.

[2]See, e.g., J. T. Ho and J. D. Litster, Phys. Rev. Letters 22, 603 (1969).

[3]D. S. Gaunt and C. Domb, J. Phys. C 3, 1442 (1970). The method of Ref. 3 possesses, inherently, a better accuracy of the values x_0 and $h(0)$ (related to "critical amplitudes"), and the discrepancy between our results and those of Ref. 3 is essentially the same as the discrepancy between determining low-temperature exponents from high-temperature expansions (instead of using low-temperature expansions); cf. Fig. 5 of Ref. 6.

[4]R. B. Griffiths, Phys. Rev. Letters 24, 1489 (1970); L. P. Kadanoff (unpublished).

[5]A. Hankey and H. E. Stanley (unpublished). See also H. E. Stanley, *Introduction to Phase Transitions and Critical Phenomena* (Oxford U.P., London, 1971), Chap. 11.

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

[7]In (3) the product $xc^{1/\beta}$ appears as the argument of H where the variable ϵ was, and therefore it should be small. For example, if $x=4$, $c=0.8$, and $\beta=\frac{5}{16}$, then $xc^{1/\beta}\cong 2$, which is not of the order of ϵ in the critical region.

[8]When we compare with Ref. 3, we actually plot $h(x)/h(0)$ against $(x+x_0)/x_0$.

[9]P. G. Watson, J. Phys. C 2, 2158 (1969); M. Ferer, M. A. Moore, and M. Wortis, Phys. Rev. B 3, 3911 (1971).

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

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

[12]We have calculated an expression for $h(x)$ similar to (11) for a bcc lattice, and numerical comparison with (11) supports the conjecture that $h(x)/h(0)$ is independent of lattice structure.

[13]To do this, it was necessary to calculate the *amplitudes* A_{2r-1} for the behavior of the $(2r-1)$ derivative of M with respect to H. We found, using the series of Ref. 11, the values $A_1=1.072\pm0.002$,

$$A_3=-4.05\begin{cases}+0.09\\-0.06\end{cases} \quad \text{and} \quad A_5=130\begin{cases}+3\\-5\end{cases}.$$

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

[15]An exception to this statement is that the plot for $S=\infty$ depends upon a choice of δ; however, only an imperceptible change was noted on varying δ in the range $4.28\le\delta\le5$.