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Magnetic Phase Boundary of the Spin-½ Heisenberg Ferromagnetic Model*

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We compute in this paper the exact coefficients, in a magnetic field, of the first eight powers of $x = J/\kappa T$ for the spin-$\frac{1}{2}$ Heisenberg ferromagnetic model for five lattices. We use this result to obtain the magnetic equation of state in the form $\tanh(H/\kappa T) = Mg(x, M^2)$; again we obtain the exact coefficients for the first eight powers of x. From this equation, we are able to extrapolate and determine the magnetic phase boundary with reasonable accuracy for $M < 0.8$. We have investigated the critical exponents ι, β, and δ. We are unable to determine ι; we find an effective β over a range of M of $\beta = 0.35 \pm 0.05$, and we estimate $\delta = 5.0 \pm 0.2$.

I. INTRODUCTION

In a previous paper,[1] to which we shall refer subsequently as I, the free energy $F(H, T)$ of the nearest-neighbor spin-$\frac{1}{2}$ Heisenberg model was expanded as a double power series in the magnetic field H and inverse temperature $1/T$. More precisely, starting with the Hamiltonian

$$\mathcal{H} = -\tfrac{1}{2}J \sum_{\langle i,j \rangle} \vec{\sigma}^{(i)} \cdot \vec{\sigma}^{(j)} - \mu H \sum_i \sigma_3^{(i)} \quad , \tag{1}$$

the associated free energy, given by

$$F(H, T) = -\kappa T \ln \mathrm{Tr} \exp(-\mathcal{H}/\kappa T) \quad , \tag{2}$$

was expanded as a double power series in the variables $x \equiv J/\kappa T$ and $y \equiv \mu H/\kappa T$. In (1), $\vec{\sigma}^{(i)}$ is the Pauli spin vector at site i of a given crystal lattice, σ_3 is the component of $\vec{\sigma}$ in the direction of the external magnetic field H, μ is the associated magnetic moment, and J is the exchange coupling constant (positive for ferromagnetic interactions); the first summation runs over each pair of neighboring sites on the lattice. In (2), κ is Boltzmann's constant.

Noting that, in the absence of spontaneous magnetization, F is necessarily an even function of H, and writing

$$-F/NkT = F_0(x) + \sum_{s=1}^{\infty} [(2s)!]^{-1} y^{2s} F_s(x) \quad , \tag{3}$$

where N is the number of lattice sites (surface effects being ignored), the function $F_0(x)$ was found as a power series in x through x^{10} for the three cubic lattices[2]; face centered cubic (fcc), body centered cubic (bcc), and simple cubic (sc); $F_1(x)$ was found through x^9 for the close-packed fcc lattice, and through x^{10} for the open lattices, bcc and sc; and for all three lattices $F_2(x)$, $F_3(x)$, and $F_4(x)$ were found through x^8.

Analysis of these series, exhibited in detail in I, showed that, for any particular cubic lattice, the series $F_1(x) \cdots F_4(x)$ all diverged at $x = x_c$, corresponding, for positive J, to a ferromagnetic Curie point. The nature of this divergence was examined in detail, the susceptibility critical index γ being found from the series $F_1(x)$ and the existence of a constant high-temperature gap parameter 2Δ being deduced from the sets $F_s(x)$, $s = 1, \ldots, 4$. Explicitly, we found[3] $x_c(\mathrm{fcc}) = 0.249_2$, $x_c(\mathrm{bcc}) = 0.397_3$, $x_c(\mathrm{sc}) = 0.596_2$, $\gamma = 1.43 \pm 0.01$ (all lattices), and $2\Delta = 3.63 \pm 0.03$ (all lattices). We had hoped that we could determine, from the double power series, the degree of the critical isotherm δ and the order of the magnetic phase boundary β (for notation, see I, or below); but we did not succeed in this explicitly and had to appeal to the high-temperature scaling laws to infer $4.46 \leq \delta \leq 5.00$ and $0.36 \leq \beta \leq 0.41$. Nor did we determine the magnetic phase boundary, or saturation magnetization at subcritical temperatures. Essentially, this was because we had not found $F_s(x)$ for sufficiently many values of s, and so were not able to discuss $F(H, T)$ as a function of H.

In the present paper we shall show that, although there remain difficulties in an explicit calculation of β or δ, we can in fact determine the magnetic phase boundary $M(T)$ in the limit $H \to 0$, for this spin-$\frac{1}{2}$ Heisenberg model by a suitable modifica-

tion, and extension, of our previous work. Two things have led us to this new approach. First, it has been shown[4] that for an Ising lattice gas a double power series expansion of the free energy in terms of ρ (the density) and a high-temperature variable can be used to find the boundary of the two-phase region (which, in this case, was known already from low-temperature series work[5,6]), and, second, we have realized that by using $t \equiv \tanh y$ instead of y as the second expansion variable, the coefficient in (3) of a given power of x becomes a finite polynomial in t^2, and can be found in its entirety. This latter fact is stated explicitly, though not fully proven, in the early work of Opechowski.[7] While not absolutely essential to the derivation of a phase boundary,[8] it has provided a major motivation for the present work.

II. COMPUTATION OF COEFFICIENTS

Since our present approach is only a modification of the previous one, and again uses the finite-cluster method, we shall adopt the same notation (which was fully defined in I). Basically, we have to find the partition functions of finite clusters, the latter being specified as $[m, l, \tau]$ where m is the number of sites (spins), l is the number of nearest-neighbor bonds, and τ distinguishes between different topological types. Our fundamental equation, (12) of I,

$$Z_{[\tau]}(H,T)=\sum_{n=0}^{\infty}\frac{x^n}{2^n n!}\left\{\sum_{k=0}^{[m/2]}\mathrm{Tr}(\Gamma_k^n)\times\sum_{p=k}^{m-k}\exp[(m-2p)y]\right\}, \tag{4}$$

where $[\tau]$ is now short for $[m, l, \tau]$, gives

$$\ln Z_{[\tau]}(H,T)=m\ln(2\cosh y)+\ln\left[1+\sum_{n=1}^{\infty}\frac{x^n}{2^n n!}\times\sum_{j=0}^{[m/2]}\beta_{[\tau]}(n,j)t^{2j}\right], \tag{5}$$

where

$$\sum_{j=0}^{[m/2]}\beta_{[\tau]}(n,j)t^{2j}=\frac{1}{2^m}\sum_{k=0}^{[m/2]}\mathrm{Tr}(\Gamma_k^n)(1-t^2)^k\times\sum_{s=0}^{[m/2]-k}\binom{m-2k+1}{2s+1}t^{2s}. \tag{6}$$

Writing

$$\mu_{[\tau]n}\equiv\sum_{j=0}^{[m/2]}\beta_{[\tau]}(n,j)t^{2j}, \tag{7}$$

Eq. (5) can be written

$$\ln Z_{[\tau]}(H,T)=m\ln(2\cosh y)+\sum_{n=1}^{\infty}\frac{x^n}{2^n n!}k_{[\tau]n}, \tag{8}$$

where

$$k_{[\tau]n}\equiv\sum_{j=0}^{X}\alpha_{[\tau]}(n,j)t^{2j} \tag{9}$$

and the k's are related to the μ's as are cumulants to moments. The α's, like the β's, are simply numerical coefficients. Opechowski's theorem, of which we outline a proof below, is that

$$X\leq n. \tag{10}$$

In as far as the finite-cluster formalism holds for H^2 expansions, it holds also for t^2 expansions (these expansions being related by linear equations with constant coefficients), so that (9) can be written

$$k_{[\tau]n}=\sum_{\tau'\subset\tau}n_{\tau'}^{\tau}\varphi_{[\tau']n}+\varphi_{[\tau]n}, \tag{11}$$

where, regarding clusters as connected linear graphs, $\tau'\subset\tau$ implies that τ' is a connected subgraph of τ (containing at least one bond), $\tau'\neq\tau$, and $n_{\tau'}^{\tau}$ is equal to the number of times τ' (as a free graph) can be located on τ (as a labeled graph).[9] And we know (see I) that, for any τ, $\varphi_{[\tau]n}$ vanishes when $n<l$, where l is the number of lines in τ.

By direct calculation for the pair cluster $m=2$, $l=1$, we find $\mu_1=t^2$, i.e., $k_1=t^2$. Thus, for any cluster τ

$$k_{[\tau]1}=\mu_{[\tau]1}=lt^2. \tag{12}$$

Since k_n involves μ_1^n, we expect $k_{[\tau]n}$ to include a term in t^{2n}. The essence of (10) is that there are no higher powers of t^2 in $k_{[\tau]n}$.

To prove (10), we note that, for given n, the clusters $[\tau]$ fall into two classes: clusters $[\tau_1]$ for which $[\frac{1}{2}m]\leq n$, and clusters $[\tau_2]$ for which $[\frac{1}{2}m]>n$. For the clusters $[\tau_1]$, Eq. (7) shows that there is nothing further to prove; the μ's have the desired property and thence, by the moment-cumulant transformation, so also do the k's. Moreover, this property, if true of the k's, is true also of the φ's; Eq. (11) shows that $\varphi_{[\tau]}$ is a linear combination of k's for clusters having no more sites than has $[\tau]$. We now turn to the clusters $[\tau_2]$, and note that for each of these $l>n$, since for any cluster of m sites, l runs from $m-1$ (trees) to $\frac{1}{2}m(m-1)$ (stars). Thus for the clusters $[\tau_2]$, Eq. (11) reads

$$k_{[\tau_2]n}=\sum_{\tau'\subset\tau_2}n_{\tau'}^{\tau_2}\varphi_{[\tau']n}, \tag{13}$$

and we can proceed inductively. For simplicity of exposition, suppose $n=2$. Then the clusters $[\tau_1]$ are all connected graphs with five or fewer sites. Consider next clusters with six sites: l runs from 5 to 15. Start with $l=5$ (a tree); each connected subcluster has fewer than six sites, so

(13) establishes the theorem for $m=6$, $l=5$. Proceed to $l=6$; each subcluster either has fewer than 6 sites or else is a tree, $m=6$, $l=5$; so (13) now establishes the theorem for $m=6$, $l=6$, and so on. For fixed m, we run through the possible values of l in ascending sequence, and for each new graph the right-hand side of (13) involves only subgraphs for which the theorem has already been proved.

In summary, then, Eq. (9) reads

$$k_{[\tau]n}=\sum_{j=0}^{n}\alpha_{[\tau]}(n,j)t^{2j} \quad . \tag{14}$$

Hence, by the moment-cumulant transformation, (7) reads

$$\mu_{[\tau]n}=\sum_{j=0}^{\min(n,[m/2])}\beta_{[\tau]}(n,j)t^{2j} \quad . \tag{15}$$

The computation proceeds by first using Eq. (6) to find the numbers $\beta_{[\tau]}(n,j)$. We then transform to the numbers $\alpha_{[\tau]}(n,j)$ and then, by (11), to numbers $\varphi_{[\tau]}(n,j)$, where

$$\varphi_{[\tau]n}=\sum_{j=0}^{n}\varphi_{[\tau]}(n,j)t^{2j} \quad . \tag{16}$$

Finally, we have to form the scalar products

$$f(n,l)\equiv\textstyle\sum_{\tau}N_{[\tau]}^{(\text{lattice})}\varphi_{[\tau]}(n,j)/N \quad , \tag{17}$$

where $N_{[\tau]}^{(\text{lattice})}$ denotes the number of times the graph $[\tau]$ can be located on (i.e., weakly embedded in) the particular physical lattice under consideration. Ignoring boundary effects, $N_{[\tau]}^{(\text{lattice})}$ is proportional to N, the number of lattice sites, so that $F(H,T)$ is properly an extensive thermodynamic quantity.

For reasons discussed in I (p. 805), the calculation, which was performed on the KDF9 machine at Newcastle, was confined to clusters (graphs) with $l\leq 8$. There are 358 such graphs, all of which occur on the fcc lattice. They are depicted in Ref. 10, where the matrix elements $n_{\tau'}^{\tau}$ and the lattice counts $N_{[\tau]}^{(\text{lattice})}$ also are listed. The necessary coefficients $\mathrm{Tr}\Gamma_n^k$ had, of course, been found in our previous calculation. With the restriction $l\leq 8$, we are working accurately through terms in x^8, and so confine n in (5) to $n\leq 8$.

In place of (3), we have thus obtained (for the three cubic lattices, fcc, bcc, and sc, and the two planar lattices, pt, and ps) the free-energy expansions

$$-F(H,T)/NkT=\ln(2\cosh y)+\mathfrak{F}_0(x)+\sum_{j\geq 1}\mathfrak{F}_j(x)t^{2j} \quad , \tag{18}$$

where

$$\mathfrak{F}_j(x)=\sum_{n=1}^{\infty}\frac{x^n}{2^n n!}f(n,j) \quad , \tag{19}$$

and we know the coefficients $f(n,j)$ for $n\leq 8$ and $j\leq 8$. The series $\mathfrak{F}_0(x)$ is, of course, simply the series $F_0(x)$ of (3), and will not be discussed further here. Nor shall we present explicitly the coefficients $f(n,j)$, $1\leq j\leq 8$; for it is more useful to give, instead, expressions derived from them (see Sec. III). But it is appropriate to comment here on the structure of these coefficients and the checks to which the calculations have been submitted.

To take the checking procedures first, the most searching of these is to confirm that $\varphi_{[\tau]n}=0$ when $n<l$, in all cases. A second check derives from Eq. (6) when $t^2=1$. For this gives

$$\sum_{j=0}^{[m/2]}\beta_{[\tau]}(n,j)=\frac{\mathrm{Tr}(\Gamma_0^n)}{2^m}\sum_{s=0}^{[m/2]}\binom{m+1}{2s+1}$$

$$=\mathrm{Tr}(\Gamma_0^n)=l^n \quad .$$

(see Baker, Rushbrooke, and Gilbert,[11] and references therein). Consequently,

$$\ln\left[1+\sum_{n=1}^{\infty}\frac{x^n}{2^n n!}\sum_{j=0}^{[m/2]}\beta_{[\tau]}(n,j)\right]=\tfrac{1}{2}lx \quad ,$$

Hence, from (5), (8), and (9),

$$\alpha_{[\tau]}(1,1)=l \tag{20}$$

and

$$\sum_{j=0}^{n}\alpha_{[\tau]}(n,j)=0, \quad n>1. \tag{21}$$

We have checked (20) and (21) explicitly on all the α's, $[\tau]=1,2,\ldots,358$. Third, by rearrangement of our previous expansion (3),[1,2] directly transforming from y to t_s, one of us[12] has already published what amounts to the coefficients $f(n,j)$ for $j\leq 4$. The present, entirely independent, calculations agree exactly with those results.[13] Indeed, these calculations are equivalent to having taken the series in (3) as far as $s=8$, instead of stopping at $s=4$, though a direct continuation of the previous approach, up to $s=8$, would have been impracticable on account of round-off error or machine overflow. An advantage of the present method is that, as outlined above, it proceeds throughout in integer arithmetic (and the numbers are never excessively large). In particular, the $f(n,j)$ are integers.

As for the structure of the $f(n,j)$ coefficients, Eq. (10) (the Opechowski theorem) implies

$$f(n,j)=0, \quad \text{when} \quad n<j \quad .$$

Put otherwise, the series $\mathfrak{F}_j(x)$ in (18) starts with a term in x^j.

III. MAGNETIC EQUATION OF STATE

Our primary objective of obtaining the mag-

netic equation of state, namely, the interrelationship between magnetization M, field H, and temperature T, is now easily achieved. Since

$$M = -\left(\frac{\partial F}{\partial H}\right)_T ,$$

Eq. (18) gives immediately

$$M = tb_0(x) + t^3 b_1(x) + \cdots + t^{17} b_8(x) + \cdots , \qquad (22)$$

where

$$b_0(x) = 1 + 2\sum_{n=1}^{\infty} \frac{x^n}{2^n n!} f(n, 1) , \qquad (23)$$

$$b_j(x) = 2\sum_{n=1}^{\infty} \frac{x^n}{2^n n!} [(j+1)f(n, j+1) - jf(n, j)], \quad j \geq 1 , \qquad (24)$$

and we have chosen to measure M in units of $N\mu$, so that its maximum, saturation, value is unity.

The series $b_0(x)$ is precisely the series $F_1(x)$ of (3), namely, the high-temperature expansion of the zero-field susceptibility. It was discussed in detail in I and, as stated in the Introduction, is known through x^{10} for open lattices and through x^9 for close-packed lattices. Except in so far as we shall subsequently employ the best available estimates of the Curie temperatures, which were derived in I from these longer series, only the terms of $b_0(x)$ through x^8 are used in the present work.

The series $b_j(x)$, $j = 1 \cdots 8$, are also known through terms in x^8; and, since $f(n, j) = 0$ when $n < j$, Eq. (24) shows that $b_j(x)$, like $\mathfrak{F}_j(x)$, starts with a term in x^j. This implies that if we were to group together like powers of x on the right-hand side of (22), then the coefficient of x^n would be a finite (odd) polynomial in t of degree $2n+1$, so that the field-dependent coefficients of successive powers of x through x^8 are known exactly. But this regrouping of the terms is not pertinent to our present approach.

The series $\mathfrak{F}_0(x)$ of (18), i.e., $F_0(x)$ of (3), does not enter into the magnetic equation of state. Essentially, as discussed in I, its second derivative is the series for the zero-field specific heat.

Although Eq. (22) is one form of the desired magnetic equation of state, it is more profitable to revert this series and obtain t as a double power series in x and M. This is because our principal aim is to find the magnetic phase boundary, i.e., the spontaneous magnetization in limitingly small field at temperatures below the Curie point T_c and (22) cannot be used as it stands for this purpose, both because $t \to 0$ implies $M \to 0$, and because $b_0(x)$ diverges for $T \leq T_c$. To this end we have used Lagrange's reversion formula,[14] thereby obtaining the expansion

$$t = Mc_0(x) + M^3 c_1(x) + \cdots + M^{17} c_8(x) + \cdots \qquad (25)$$

where

$$c_0(x) = [b_0(x)]^{-1} \qquad (26)$$

and $c_j(x)$ is given by the coefficient of ξ^j in

$$\frac{1}{2j+1} \sum_{k=0}^{\infty} \binom{2j+k}{k} (-1)^k [c_0(x)]^{2j+k+1} \times [\xi b_1(x) + \xi^2 b_2(x) + \cdots]^k . \qquad (27)$$

The operations entailed by (27) are easily computerized, and can be so organized that the calculation proceeds in integer arithmetic without the risk of round-off error.

The expression (27) shows that the series $c_j(x)$, just as $b_j(x)$ and $\mathfrak{F}_j(x)$, starts with a term in x^j. Thus the terms displayed in (25) include all terms in powers of x through x^8. Grouping together like powers of x on the right-hand side of (25), therefore yields,

$$t = Mg(x, M^2) , \qquad (28)$$

where

$$g(x, M^2) = 1 + \sum_{n \geq 1} \frac{x^n}{2^n n!} p_n(M^2) ; \qquad (29)$$

$p_n(M^2)$ is a polynomial in M^2 of degree n. These polynomials epitomize our high-temperature expansion knowledge of the Heisenberg spin-$\frac{1}{2}$ model, apart from the series $F_0(x)$ and either one or two extra known coefficients in the series $F_1(x)$. We present these polynomials in the Appendixes to this paper.

IV. PHASE BOUNDARY

Equation (28) shows that $H \to 0$, i.e., $t \to 0$, corresponds to one or the other of two possibilities, either $M = 0$ or

$$g(x, M^2) = 0 . \qquad (30)$$

For a ferromagnetic substance, $M = 0$ is the stable solution for $T > T_c$ and an unstable solution for $T < T_c$. An implicit equation for the spontaneous magnetization as a function of temperature, for $T \leq T_c$, is provided by Eq. (30). It is the solution of this equation, as a curve in the T, M plane, which we call the magnetic phase boundary.

If this curve exists, then Eq. (25) shows that it cuts the temperature axis ($M = 0$) at that temperature at which $c_0(x)$ vanishes. But, from (26) and (23), $c_0(x)$ is simply the zero-field inverse susceptibility. Thus, on this theory, the magnetic phase boundary necessarily cuts the temperature axis at the Curie point as determined by the vanishing of the inverse susceptibility.

Inspection of the polynomials $p_n(M^2)$ reveals that, in all cases, $p_n(1) = 0$. In view of (29) and (30), this means that if the line $M = 1$ cuts the magnetic phase boundary, it must do so as $x \to \infty$, i.e., at

$T=0$. Indeed, Eqs. (22)–(24) show that $t=1$ implies $M=1$ [because the numbers $f(n, j)$ are zero when $n<j$]. And $t=1$ implies either $H\to\infty$ or $T=0$. That this property transfers from Eq. (22) to the reverted equation (28), is a satisfactory check on the reversion arithmetic.

We are left with the problem of plotting the phase boundary between the points (0, 1) and (T_c, 0) in the T, M plane. Equation (30) is an implicit equation to this curve, if it exists. For any value of M in the range (0, 1) we can evaluate the coefficients $p_n(M^2)$ in Eq. (29), thus obtaining (exactly) the terms through x^8 in the expansion of $g(x, M^2)$ as a power series in x. When a function $f(z)$, is given by a power series in z of which we know only a finite number of terms, experience has shown that it is profitable to construct Padé approximants (PA) to this series.[15] The zeros of the numerators of these PA's may be expected to approximate to those of the function itself, while those of the denominators reflect points at which the function is singular. These zeros may be anywhere in the complex z plane, but physical interest normally centers on roots lying on the positive real axis. With this is mind, it is natural to start by forming PA's to these series for $g(x, M^2)$ and finding the zeros of their numerators.

Our most thorough studies have been confined to the fcc lattice, in the belief that, for series of a given length, convergence will be most rapid for close-packed lattices. We shall present these in some detail, and refer only briefly to those for the bcc and sc lattices.

TABLE I. Roots (multiplied by 10^4) of numerators of PA's to $g(x, M^2)$, fcc latice.

M	[3, 3]	[3, 4]	[4, 3]	[4, 4]	[3, 5]	[5, 3]
1	∞	∞	∞	∞	∞	∞
0.95	4354	5202	5333	c. c.	5283	6044
0.9	3806	4039	4094	4568	3687	4197
0.85	3408	3480	3513	3658	c. c.	3548
0.8	3135	3153	3183	3274	c. c.	3200
0.75	2944	2929	2966	3043	3113	2977
0.7	2803	2745	2812	2888	2921	2820
0.65	2697	c. c.	2692	2778	2796	2703
0.6	2614	c. c.	2589	2697	2707	2612
0.55	2548	c. c.	2456	2636	2641	2539
0.5	2493	2635	c. c.	2590	2592	2478
0.45	2445	2573	c. c.	2555	2555	2367
0.4	2396	2538	c. c.	2529	2529	c. c.
0.35	2315	2522	2588	2511	2511	2531
0.3	c. c.	2543	c. c.	2494	2499	2511
0.25	c. c.	c. c.	c. c.	2422	2488	2507
0.2	c. c.	c. c.	c. c.	2264	2471	2512
0.15	2297	c. c.	c. c.	2390	2448	2526
0.1	2339	c. c.	c. c.	2420	2432	c. c.
0.05	2346	2440	c. c.	2432	2432	c. c.
0	2347	2405	c. c.	2436	2438	c. c.

Table I shows, for values of M ranging from 0 to 0.95, the relevant zeros of the numerators of the most significant PA's to $g(x, M^2)$ for the fcc lattice. We take the relevant zero to be the smallest positive real root, and it is these that are listed, except that occasionally it is necessary to ignore a smaller root which coincides closely with a root of the denominator. For example, for the [3, 3] approximant when $M=0.4$, the root listed is at $x=0.23959$. There is, in fact, also a root of the numerator at $x=0.10656$, but there is a root of the denominator at $x=0.10654$. The symbol c. c. implies a complex pair rather than a real root; though here again some discretion must be exercised. As an example, we may cite the [5, 3] approximant when $M=0$. The numerator has a positive real root at $x=1.7162$, but clearly, the relevant root is the complex pair $0.2558\pm0.0059i$.

Inspection of Table I reveals rather poor convergence, between the different PA's. In this connection it may be significant that about half the PA's give evidence of a second positve real root (of the numerator) somewhat larger than that listed. This is particularly true of the [4, 4] and [3, 5] approximants, for which this second root is in the range 0.29 to 0.31 for $M\leq 0.4$, and then increases more rapidly, being about 0.5 when $M=0.75$. This makes one wonder whether $g(x, M^2)$ vanishes in a simple manner at the phase boundary, or has, perhaps, a branch point there. In fact, we know that when $M=0$, it does have such a branch point, for when $M=0$, Eq. (30) is simply the equation $\chi(x)^{-1}=0$, where $\chi(x)$ is the zero-field susceptibility which, near the Curie point, behaves like $(x_c-x)^{-\gamma}$ with $\gamma=1.43$.

For this reason we have felt it profitable to consider not the vanishing of $g(x, M^2)$, but the singularities in its logarithmic derivative $\partial \ln g(x, M^2)/\partial x$. Taking the logarithmic derivative necessarily converts a branch point into a simple pole, to which PA's should do good justice. Indeed, this way, we are now doing for general M precisely what we did in I when locating the Curie point from the temperature dependence of the zero-field susceptibility. Table II lists the smallest positive real roots of the denominators of the most significant PA's to $\partial \ln g(x, M^2)/\partial x$, and we give the entries to one more significant figure than those listed in Table I, since it is clear that convergence, between results from different approximants, has been appreciably improved. Moreover, denominators of PA's to $\partial \ln g(x, M^2)/\partial x$ show no evidence of a positive real root other than the one listed.

Table II repays careful examination. First, we observe that the entries in the bottom row, $M=0$, are necessarily the corresponding entries from Table VII of I (in which we were looking for the

TABLE II. Roots (multiplied by 10^5) of denominators of PA's to $\partial \ln g(x, M^2)/\partial x$, fcc lattice. Last column is mean (to four figures) of previous columns.

M	[3, 2]	[3, 3]	[4, 2]	[3, 4]	[4, 3]	[5, 2]	Av
1	∞	∞	∞	∞	∞	∞	
0.95	45701	94844	c.c.	c.c.	c.c.	46674	
0.9	43477	55699	c.c.	52138	52976	42218	
0.85	39023	41207	42089	37959	39919	37200	3957
0.8	35176	34994	35001	33514	35201	33676	3459
0.75	32357	31682	31805	31148	29695	31309	3133
0.7	30328	29684	29850	29594	29579	29658	2978
0.65	28850	28374	28515	28473	28455	28461	2852
0.6	27759	27459	27553	27627	27565	27565	2759
0.55	26944	26790	26836	26973	26872	26876	2688
0.5	26332	26286	26296	26462	26322	26329	2634
0.45	25870	25900	25918	26064	25862	25867	2591
0.4	25518	25601	25488	25757	25394	25397	2553
0.35	25249	25371	25257	25526	c.c.	24523	
0.3	25042	25201	25061	25361	26187	c.c.	
0.25	24883	25087	24900	25252	25454	c.c.	
0.2	24764	25034	24753	25168	25213	24556	
0.15	24687	25018	24516	25067	25070	24885	
0.1	24666	24948	25449	24988	24991	24970	
0.05	24701	24857	24879	24955	25021	24984	
0	24732	24824	24829	24948	c.c.	24983	2488

Curie point). The more extensive work of that paper, using a longer series and a variety of alternative procedures for locating x_c, led us to conclude that $x_c = 0.2492$. Of the approximants in Table II [3, 4] comes closest to realizing this value. Second, we note that the [3, 3] and [3, 4] approximants give values of x which increase monotonically with M. Third, we note that for M in the range 0.45 to 0.65 there is good convergence not just between these two approximants, but over the wider set. In the final column we list, for $0.4 \leq M \leq 0.85$ (which includes the range of particularly good convergence), the straight average (to four figures only) of the values given by the six successive approximants. The value 2488 against $M = 0$ comes, likewise, from averaging the entries in the bottom row of Table II, counting the [3, 4] entry twice (to compensate for the missing value from the [4, 3] approximant).

In Table III we give, to three figures only, the values of T/T_c as calculated for given M from the [3, 3], [3, 4], and final columns of Table II. In Fig. 1 we show this (normalized) phase boundary, the full curve being drawn through the points of the last column of Table III over the range $0.45 \leq M \leq 0.85$ (as nearly as is consistent with having a smooth curve). In Fig. 1 we show also the low-temperature limiting $T^{3/2}$ law resulting from spin-wave theory. There is no adjustable parameter in this spin-wave curve, whose equation[16] is

$$M = 1 - 0.02932(\kappa T/J)^{3/2} = 1 - 0.2357(T/T_c)^{3/2} ,$$

on using the value 0.2492 for x_c. Our phase boundary appears to join satisfactorily with this spin-wave curve, which it must approach from below.[17]

Over the range $0.7 \geq M \geq 0.45$ we present the phase boundary with some confidence. Though estimates of accuracy are necessarily subjective, we suspect the full curve gives T/T_c to within about 1%. Moreover, over this range, our curve seems virtually identical with that given by second-order Green's-function theory.[18] On the other hand, for $M \leq 0.4$ we are, of course, more interested in $1 - T/T_c$ than in T/T_c, and, as is clear from Table III, we certainly do not know this with comparable accuracy.

We shall now refer very briefly to the corresponding results for the bcc and sc lattices. For the bcc lattice we can follow the same procedure as led to Table III above. We shall, however, now quote only numbers for comparison with the last column of Table III (namely, straight averages over the six most relevant PA's), and we have used $x_c = 0.3973$ (from our previous work on the longer susceptibility series). For $M = 0.65$, 0.6, 0.55, 0.5, and 0.45, we now find $T/T_c = 0.872$, 0.900, 0.924, 0.943, and 0.957, quite extraordinarily close to the fcc values listed in Table III. This is not, perhaps, as surprising as it may at first seem, for the spin-wave curve for the bcc lattice, namely,

TABLE III. Phase boundary, fcc lattice, as calculated from columns 3, 5, and 8 of Table II.

M	T/T_c [3, 3]	[3, 4]	Av
0.95	0.262		
0.9	0.446	0.479	
0.85	0.602	0.657	0.629
0.8	0.709	0.744	0.719
0.75	0.784	0.801	0.794
0.7	0.836	0.843	0.835
0.65	0.875	0.876	0.872
0.6	0.904	0.903	0.902
0.55	0.927	0.925	0.925
0.5	0.944	0.943	0.945
0.45	0.959	0.957	0.960
0.4	0.970	0.969	0.975
0.35	0.978	0.977	
0.3	0.985	0.984	
0.25	0.990	0.988	
0.2	0.992	0.991	
0.15	0.992	0.995	
0.1	0.995	0.998	
0.05	0.999	1.000	
0	1.0	1.0	1.0

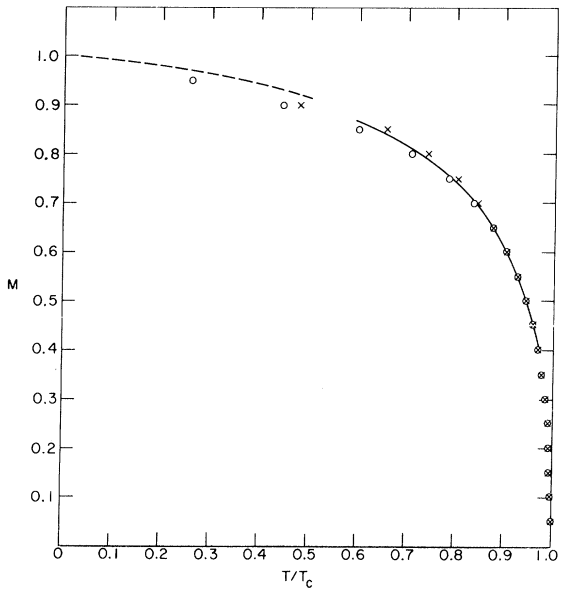

FIG. 1. Magnetic phase boundary, fcc lattice. ⊙ from [3, 3] PA of Table III, × from [3, 4] PA of Table III. Full curve from last column of Table III. Broken curve, $T^{3/2}$ law from spin-wave theory.

$$M = 1 - 0.0587(\kappa T/J)^{3/2} ,$$

becomes, on taking $x_c = 0.3973$,

$$M = 1 - 0.2344(T/T_c)^{3/2} ,$$

in which the coefficient differs by less than 1% from that for the fcc lattice.

For the sc lattice our Padé tables are appreciably less well converged. The [3, 2] Padé of Table III behaves rather oddly. Ignoring this and then averaging over the five remaining approximants, using $x_c = 0.5962$, we find for $M = 0.75$ and 0.65, the values $T/T_c = 0.74$ and 0.82 (and we should have obtained these answers, to two figures only, by averaging simply the [3, 4] and [4, 3] approximants). In the range $0.55 \geq M \geq 0.30$, the [4, 2] and [5, 2] approximants fail to exist, so that we shall quote only the mean of the [3, 4] and [4, 3] approximants to give $T/T_c = 0.88$ when $M = 0.55$. These values are 5 or 6% lower than the corresponding values for the fcc lattice; which is roughly in accordance with the results of second-order Green's-function theory.[19]

Finally, we ought to examine what happens when we apply the same analysis to the series data for a two-dimensional lattice, and we shall look at the results for the plane triangular lattice. We know from the work of Mermin and Wagner[20] that for any two-dimensional lattice there can not in fact be a magnetic phase boundary, for as $H \to 0$, $M \to 0$ if $T \neq 0$. Nevertheless, as we have seen, there is a sense in which our procedure yields $M = 1$ at $T = 0$, and, in so far as when $M = 0$ we are examining the divergence of the zero-field susceptibility, the possibility of a pseudo-critical-point (T_c^*, at which the susceptibility diverges but there is no onset of magnetization) cannot be rigorously excluded (see, for example, Stanley and Kaplan[21] and de Jongh *et al.*[22]). Thus, it is possible that we shall find a pseudo-phase-boundary, simply because, in dealing with finite series, we may have to pass continuously from the pseudo-critical-point ($M = 0$, $T = T_c^*$) to the saturation point $M = 1$, $T = 0$.

Tables IV and V give for the triangular lattice the quantities equivalent to those displayed for the fcc lattice in Tables I and II (except that in both cases the x values have been multiplied by 10^4, whereas those in Table II were multiplied by 10^5). Although Table IV is not well converged, there might seem to be some evidence of a pseudo-phase-boundary. It should, however, be observed regarding the three approximants which use all the known coefficients, that the numerators of the [3, 5] and [5, 3] approximants necessarily have a real root (which, as we see, is in most cases positive), whereas with the [4, 4] approximant, where there is no such necessity, there are consistently only complex roots (which, in fact, do not lie near the real axis). Turning now to Table V, we observe first that the evidence for a pseudo-critical-point (at $M = 0$) is, in fact, very weak; the only approximants we have, [3, 2], [3, 3], and [3, 4], give no evidence of convergence. Second, what should perhaps be the best approximants, [3, 4] and [4, 3],

TABLE IV. Roots (multiplied by 10^4) of numerators of PA's to $g(x, M^2)$, pt lattice.

M	[3, 3]	[3, 4]	[4, 3]	[4, 4]	[3, 5]	[5, 3]
0.95	11590	17970	21193	c. c.	17557	c. c.
0.9	10880	13979	16163	c. c.	11865	31821
0.85	10175	11770	13022	c. c.	9055	17262
0.8	9550	10449	11222	c. c.	8416	13456
0.75	9024	9599	10148	c. c.	8406	11781
0.7	8589	9017	9477	c. c.	8145	10844
0.65	8231	8596	9044	c. c.	7776	10231
0.6	7940	8276	8756	c. c.	7309	9783
0.55	7708	8023	8555	c. c.	6445	9436
0.5	7531	7810	8407	c. c.	c. c.	9163
0.45	7406	7620	8291	c. c.	c. c.	8948
0.4	7327	7434	8198	c. c.	c. c.	8779
0.35	7282	7229	8121	c. c.	c. c.	8649
0.3	7263	6967	8059	c. c.	c. c.	8548
0.25	7258	6547	8009	c. c.	c. c.	8472
0.2	7261	c. c.	7971	c. c.	c. c.	8415
0.15	7266	c. c.	7942	c. c.	c. c.	8375
0.1	7272	c. c.	7922	c. c.	c. c.	8347
0.05	7275	c. c.	7910	c. c.	c. c.	8331
0	7276	c. c.	7906	c. c.	c. c.	8326

are, overall, the most oddly behaved. Indeed, if we believed in a pseudo-phase-boundary and wished to plot it, it is only in the neighborhood of $M=0.55$ that we could do so with any conviction. But most marked is the contrast between Table V and Table II. It is clear that there is a qualitative difference as regards satisfactory convergence between the results for two- and three-dimensional lattices; and we are content to leave the matter there.

V. CRITICAL EXPONENTS

We turn now to an examination of the extent to which, from our magnetic equation of state, we can determine the critical exponents β and δ. Here β denotes the degree of the magnetic phase boundary, defined by

$$M_0(T)\sim B(1-T/T_c)^{\beta} \quad \text{as} \quad T\to T_c^- \tag{31}$$

[we now use $M_0(T)$ to denote the spontaneous magnetization at the temperature T], and δ denotes the degree of the critical isotherm, defined by

$$H\sim DM^{\delta}, \quad T=T_c, \quad M\to 0^+ \quad . \tag{32}$$

Equation (31) refers, of course, to the limit $H\to 0$. It is convenient to introduce a third exponent, ι, defined by the hypothesis that

$$M=M_0(T)+M_1(T)H^{\iota}+\cdots \tag{33}$$

in the neighborhood of the phase boundary $T\leq T_c$. The value of ι is closely related to the existence or nonexistence of an initial susceptibility $\chi(0)$ at temperatures below the Curie point for

$$\chi(0)=\lim_{H\to 0}\left(\frac{\partial M}{\partial H}\right)_T$$

and if $\iota=1$ then $\chi(0)=M_1(T)$, but if $\iota<1$ then $\chi(0)$ diverges. Now for the Ising model it is virtually certain, from the work of Essam and Fisher,[23] that the initial susceptibility exists (and deverges as $T\to T_c$), and thus that $\iota=1$. But for the Heisenberg model, this is by no means the case; indeed spin-wave theory gives[24] $\iota=\frac{1}{2}$. To anticipate our results, we have not found it possible unambiguously to determine ι from the series expansions with which we are here concerned. But the investigation of the problem is of intrinsic interest, and also has a bearing on the determination of β; we shall therefore take it first, and then go on to discuss β and δ, respectively.

A. Exponent ι

We start by replacing Eq. (33) by the essentially equivalent equation

$$M=M_0(x)+M_1(x)t^{\iota}+\cdots \quad , \tag{34}$$

where, as throughout, $x=J/\kappa T$ and $t=\tanh(\mu H/\kappa T)$. If $\iota=1$, $M_1(x)$ is now the "reduced" susceptibility $\chi(0)\kappa T/\mu$. Assuming that for sufficiently small t only the terms displayed in (34) matter, this equation yields

$$\left(\frac{\partial \ln t}{\partial x}\right)_M=\frac{1}{\iota}\left[\frac{-M_0'(x)}{M-M_0(x)}+\frac{M_1'(x)}{M_1(x)}\right] \quad , \tag{35}$$

and for $x>x_c$, i.e., $T<T_c$, it is only the first term on the right-hand side of (35) that we expect to be singular (as a function of x). The singularity in this term occurs when $M_0(x)$ attains the value M. Denoting by x_p the value of x for which $M_0(x_p)=M$, and writing

$$M_0(x)=M_0(x_p)+(x-x_p)M_0'(x_p)+\cdots \quad , \tag{36}$$

we find, effectively,

$$\left(\frac{\partial \ln t}{\partial x}\right)_M\sim\frac{1}{\iota}\frac{1}{x-x_p} \quad . \tag{37}$$

But,

$$\left(\frac{\partial \ln t}{\partial x}\right)_M=\frac{\partial \ln g(x, M^2)}{\partial x} \quad ,$$

so that x_p is simply the value of x on the magnetic phase boundary which we have determined, for given M, in Sec. III above, and which is listed for the fcc lattice in Table II. Thus, the residues of the PA's at the poles listed in Table II should converge (if our series are long enough) to $1/\iota$.

This argument is valid provided $x>x_c$, i.e., $M\neq 0$. When $M=0$, however, by (25), $g(x, 0)=c_0(x)$, where $c_0(x)$ is the zero-field inverse susceptibility; consequently, the residue of $\partial \ln g(x, 0)/\partial x$ is necessarily γ, the susceptibility exponent.[25] Thus, if

TABLE V. Roots (multiplied by 10^4) of denominators of PA's to $\partial \ln g(x, M^2)/\partial x$, pt lattice.

M	[3, 2]	[3, 3]	[4, 2]	[3, 4]	[4, 3]	[5, 2]
0.95	24522	c. c.	c. c.	13924	c. c.	11711
0.9	27457	c. c.	c. c.	47495	c. c.	12045
0.85	23848	c. c.	c. c.	c. c.	33966	11834
0.8	18754	15928	16493	6270	19061	11403
0.75	14907	9714	11868	10275	10218	10914
0.7	12325	8298	10379	14040	10371	10371
0.65	10570	7955	9599	19051	9745	9756
0.6	9336	8060	9163	27615	9122	9123
0.55	8448	8445	8445	46643	8448	8535
0.5	7815	9071	8377	113138	7524	8022
0.45	7387	9947	8182	4×10^7	c. c.	7588
0.4	7140	11069	7981	c. c.	c. c.	7256
0.35	7068	12345	7740	819930	c. c.	7112
0.3	7169	13514	7385	81096	c. c.	7306
0.25	7447	14198	6668	37357	c. c.	7941
0.2	7885	14174	c. c.	25499	c. c.	9117
0.15	8422	13601	c. c.	21494	c. c.	11655
0.1	8949	12871	c. c.	20321	c. c.	121564
0.05	9334	12321	c. c.	20191	c. c.	c. c.
0	9475	12123	c. c.	20243	c. c.	c. c.

TABLE VI. Estimates of $1/\iota^*(M)$. For numbers in parentheses see text.

M	fcc (6)	bcc (6)	sc (5)
0.95	2.05 (3)		
0.9	1.90 (5)	2.30 (5)	
0.85	1.58 (5)	1.77 (5)	2.45 (4)
0.8	1.45	1.46	1.84 (4)
0.75	1.35 (5)	1.43	1.88
0.7	1.30	1.30	1.79
0.65	1.28	1.31	1.82
0.6	1.29	1.31	1.65 (3)
0.55	1.29	1.32	1.61 (3)
0.5	1.29	1.32	1.57 (3)
0.45	1.30	1.35	1.54 (3)
0.4	1.29	1.40 (5)	1.51 (3)
0.35	1.32	1.40 (5)	1.47 (3)
0.3	1.34 (4)	1.41	1.43
0.25	1.39 (4)	1.33 (5)	1.53
0.2	1.37 (5)	1.37	1.40
0.15	1.38	1.40	1.40
0.1	1.41 (5)	1.45	1.41
0.05	1.42	1.44 (5)	1.41
0	1.41 (5)	1.47 (5)	1.41

we were dealing with infinite series, we would expect the residues of $\partial \ln g(x, M^2)/\partial x$, at the poles which determine the magnetic phase boundary, to have value $1/\iota$ (presumably constant along the phase boundary) for $M \neq 0$ and to jump to γ when $M = 0$.

Unfortunately, we are not dealing with infinite series but with finite series, $\partial \ln g(x, M^2)/\partial x$ being known through terms in x^7 only. It is by forming PA's to these finite series that we have located the singularity at $x = x_p(M)$; and the residue, which we will denote by $1/\iota^*(M)$, is incapable of showing the discontinuous behavior at $M = 0$ which we expect. It is tied to the value γ at $M = 0$, and must move continuously away from this value. Of course, the nonuniformity of behavior which we would expect the infinite series to reveal should not affect the phase boundary itself, for x_p must decrease continuously to x_c as $M \to 0$. Thus, we are satisfied that we have adequately located the phase boundary, even though the residues $1/\iota^*(M)$ cannot adequately converge to $1/\iota$. The best we can hope of these is that, as M increases from 0 to 1, $1/\iota^*(M)$ will decrease from γ to 1 if $\iota = 1$, or will increase from γ to 2 if $\iota = \frac{1}{2}$.

In a parallel study of the spin-$\frac{1}{2}$ Ising model, Gaunt and Baker[26] have found that as M increases from 0 to 1, $1/\iota^*(M)$ does in fact decrease monotonically from γ (1.25 for the bcc lattice and 1.75 for the ps lattice) to a value very close to unity. This is satisfactory, since, as we have said already, we expect $\iota = 1$ for the Ising model. In the present, Heisenberg, case the position is less satisfactory. Table VI lists, for the three cubic lattices, the mean values of the residues given by the different PA's for each value of M. For the fcc and bcc lattices we have listed the mean of the residues of the [3, 2], [3, 3], [4, 2], [3, 4], [4, 3], and [5, 2] PA's if these all exist, but for the sc lattice we have omitted the [3, 2] approximant which, as we have said above, is badly out of step in this case. Where not all the PA's exist (due to the absence of real poles), we have taken the mean of those which do exist (and indicate the number of approximants over which we have averaged by the figure in parentheses to the right of the mean). In a very few cases we have omitted an approximant which is particularly out of line with the others; the most significant instance being the omission of the [5, 2] approximant for the bcc lattice when $M = 0$. That this is irregular is clearly seen in Table VIII of paper I.

That the bottom line of Table VI does not yield precisely $\gamma = 1.43$ is simply because in finding γ in I we were using rather longer series and a more thorough analysis. Looking now at what happens as we move away from $M = 0$, we notice that $1/\iota^*(M)$ is apparently "strongly" tied to the value γ, in that if plotted against M it would approach this value horizontally. This "strong" tying is also clearly exhibited by the Ising-model results of Gaunt and Baker.[26] But as we move still further away from $M = 0$, to the middle range of M, we find that for the fcc and bcc lattices $1/\iota^*(M)$ decreases, whereas for the sc lattice it increases. Finally, for relatively large M, $1/\iota^*(M)$ increases, in all cases, to a value of the order of 2, though (except for the fcc lattice) there are too few approximants left to carry the table right up to $M = 0.95$.

It is impossible to draw a firm conclusion from these figures. If one believes in $\iota = \frac{1}{2}$ on other grounds, then one might see some support for this here. All we can confidently say is that, evidently, the Heisenberg model behaves rather differently in respect to $\iota^*(M)$ than does the Ising model, and we doubt if this is entirely due to our using relatively shorter series.

B. Exponent β

We next look at the problem of determining β, defined by Eq. (31). Perhaps the most obvious approach, having found the phase boundary, is to follow the common procedure of experimentalists and plot $\ln M_0$ against $\ln \Delta T$, where[27] $\Delta T \equiv (T_c - T)/T_c$. We expect this plot to exhibit linearity as $\Delta T \to 0$, with a gradient given by β. Unfortunately, it is immediately apparent, from both Tables II and III, that for small M our knowledge of the phase boundary is not sufficiently precise for this approach to be practicable. In the region of rel-

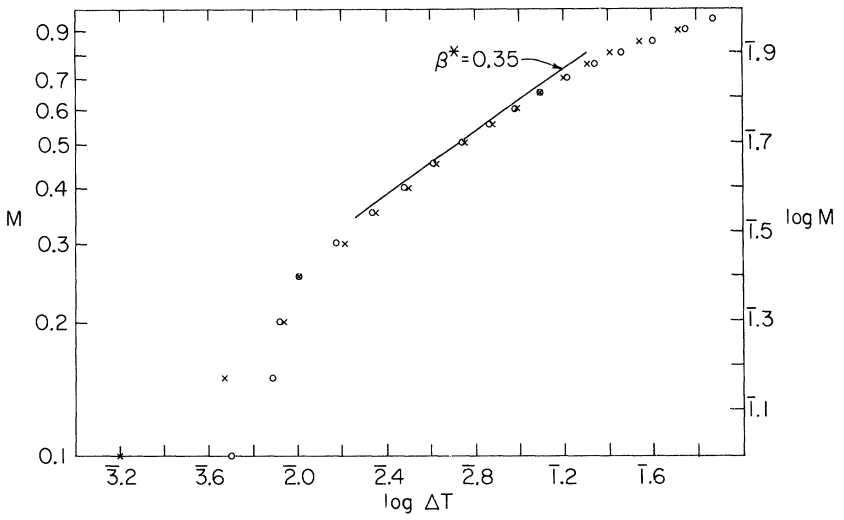

FIG. 2. $\text{Log}_{10}M$ against $\log_{10}\Delta T$, fcc lattice. Symbols same as for Fig. 1; basic data, Table II.

atively small M, say $0.3 \geq M \geq 0.05$, there is neither adequate agreement between different approximants nor sufficiently smooth behavior of any one approximant for convincing conclusions to be drawn. We can, however, say more than this. If we were to pin our faith to one particular approximant, say the [3, 3] approximant, and follow this right down to very small M, we should inevitably[28] eventually obtain the classical exponent $\beta = 0.5$. We have verified this for the [3, 3] approximant taking $M = 0.001$ and $M = 0.002$ (though it necessitates finding x_p to eight significant figures), and indeed find $\beta = 0.5$ (to one significant figure). The reason is that x_p has been located as the zero of a finite polynomial (the denominator of the appropriate PA) whose coefficients are themselves rational functions of M^2. If we follow this zero as a function of M, we shall necessarily find $\beta = 0.5$. For both reasons, therefore, we must confine attention to that range of M, above 0.3, for which the phase boundary is known with some precision.

If we define an "effective" β by

$$\beta^*(M) = \frac{\partial \ln M(T)}{\partial \ln \Delta T}, \tag{38}$$

then the best we can hope is to determine $\beta^*(M)$ over the range of M for which we know the phase boundary with some confidence, say $0.4 \leq M \leq 0.7$. For larger M, in as far as the phase boundary approaches the spin-wave limit, $\beta^*(M)$ must tend to zero as M tends to saturation.[29] Figure 2 shows plots of $\log M$ against $\log \Delta T$ as given by the [3, 3] and [3, 4] approximants of Table II, and we observe that over the range $0.4 \leq M \leq 0.7$ an effective gradient is fairly well defined. For larger M, β^* appreciably decreases (though Table II is not well converged for large M). For $M \leq 0.3$ the approximants are too irregular for the gradients to have any meaning.[30]

Confining further attention to the region $0.4 \leq M \leq 0.7$, in Table VII we list the gradients of lines joining successive points of Fig. 2, together with those similarly calculated from the last (average) column of Table II. We include this last column because it gives some indication of the behavior of approximants other than [3, 3] and [3, 4]; but clearly, its gradient 0.26 over the range $0.4 \leq M \leq 0.45$ is appreciably too low (as is to be expected from the last entry in the right-hand column of Table III). Ignoring this figure, we can conclude[31] that for $0.4 \leq M \leq 0.7$

$$\beta^* = 0.35 \pm 0.05 \quad . \tag{39}$$

An alternative approach to finding β^* is given by use of the cyclic rule

$$\left(\frac{\partial \ln t}{\partial \ln M}\right)_x = -\left(\frac{\partial \ln t}{\partial x}\right)_M \left(\frac{\partial x}{\partial \ln M}\right)_t \tag{40}$$

at points near the phase boundary $t = 0$. From (38) and (37) we see that, as a function of x, the right-hand side of (40) behaves like

$$-\frac{1}{\iota^*\beta^*} \quad \frac{(x_p - x_c)x_p}{x_c} \quad \frac{1}{x - x_p} \quad .$$

TABLE VII. Estimates of $\beta^*(M)$ from columns 3, 5, and 8 of Table II; fcc lattice.

Range	[3, 3]	[3, 4]	Av
0.35–0.4	0.39	0.41	
0.4–0.45	0.38	0.38	0.26
0.45–0.5	0.36	0.37	0.32
0.5–0.55	0.34	0.35	0.32
0.55–0.6	0.33	0.34	0.32
0.6–0.65	0.30	0.33	0.30
0.65–0.7	0.28	0.31	0.29

If then, for a given value of M, we form PA's to the left-hand side of (40) as a function of x [which, from (28) and (29) is known as a power series in x through the term in x^8], and locate x_p from the vanishing of a denominator, then if r denotes the residue of the approximant at this pole, we shall have

$$\iota^*\beta^* = -[(x_p - x_c)x_p]/(x_c r). \tag{41}$$

In combining Eq. (41) with our previous estimates of $1/\iota^*(M)$ to find $\beta^*(M)$, we shall keep to the central range of M, for which both sets of appropriate Padé tables show the best apparent convergence. Taking the mean of the [3, 4], [4, 3], [4, 4], [3, 5], and [5, 3] approximants to the right-hand side of (41), using $x_c = 0.2492$, we find for $\iota^*\beta^*$, for the fcc lattice, at $M = 0.5$, 0.55, and 0.6 the values 0.289, 0.263, and 0.247. Combining these with the corresponding values of $1/\iota^*(M)$ from Table VI, yields $\beta^*(0.5) = 0.37$, $\beta^*(0.55) = 0.34$, and $\beta^*(0.6) = 0.32$; estimates consistent with Eq. (39).

We shall comment only very briefly on corresponding results for the bcc and sc lattices, since for these lattices the estimates of $\iota^*\beta^*$ are appreciably less well converged, and have not been taken below $M = 0.6$. If, for $M = 0.6$, we follow the procedure of the last paragraph for the bcc lattice (but omit the [4, 4] approximant to $\iota^*\beta^*$ which is markedly out of line with the other four) we again find $\beta^*(0.6) = 0.32$. Although the close agreement is doubtless accidental, we certainly expect Eq. (39) to hold also for the bcc lattice since, as we have noted, there is near coincidence between the bcc and fcc phase boundaries. On the other hand, for the sc lattice we can hardly say better than that at $M = 0.6$, $\iota^*\beta^*$ lies in the range 0.20 to 0.25; taking $1/\iota^* = 1.65$ from Table VI, this gives β^* in the range 0.33 to 0.41. In view of the uncertainty, both here and for other values of M, it seems wisest not to attempt to draw conclusions regarding β^* for the sc lattice; we simply do not know the phase boundary with sufficient accuracy.

It will have been noticed that in using Eq. (41) we have located $x_p(M)$ from poles of PA's to $\partial \ln t/\partial \ln M$, regarded as a function of x, rather than from poles of PA's to $\partial \ln t/\partial x$, as in Sec. IV. Fortunately, over the range of M with which we are here concerned, this makes no significant difference. Indeed, in their parallel study of the Ising model,[26] Gaunt and Baker have used $\partial \ln t/\partial \ln M$ as the basic function for determining the phase boundary. They preferred it to $\partial \ln t/\partial x$ because its approximants showed better convergence for large M. This is not the case for the Heisenberg model, for which we find that approximants to $\partial \ln t/\partial x$ are better converged than those to $\partial \ln t/\partial \ln M$ both for large M and for small M. But over the middle range of M, roughly $0.55 \leq M \leq 0.75$, for both the fcc and bcc lattices, the two methods agree to within the 1% accuracy that we have quoted. For the sc lattice the agreement is less good. This all correlates rather strongly with the value of $1/\iota^*$ (see Table VI and Table III in Ref. 26). We can locate the phase boundary satisfactorily from $\partial \ln t/\partial \ln M$ when $1/\iota^*$ is close to unity.

C. Exponent δ

Finally, we look at the problem of determining the exponent δ, defined by Eq. (32). Since t is proportional to H when H is small, it is convenient to define $\delta^*(M)$ by

$$\delta^*(M) = \frac{\partial \ln t}{\partial \ln M} \quad \text{at } x = x_c \tag{42}$$

and natural to expect that $\delta = \lim \delta^*(M)$ as $M \to 0$. If we were dealing with infinite series rather than with polynomial approximations to them, and could sum the series, then this expectation would doubtless be justified. But in fact, from Eqs. (28) and (29),

$$\ln t = \ln M + \sum_{n \geq 1} \frac{x^n}{2^n n!}\, q_n(M^2) \ , \tag{43}$$

where the q_n's are related to the p_n's of (29) as are cumulants to moments, and $q_n(M^2)$ is a polynomial in M^2 of degree n. Consequently,

$$\frac{\partial \ln t}{\partial \ln M} = 1 + \sum_{n \geq 1} \frac{x^n}{2^n n!}\, d_n(M^2) \ , \tag{44}$$

where

$$d_n(M^2) = 2M^2 q_n'(M^2) \ . \tag{45}$$

Now we know (44) through terms in x^8 (and thereafter extend the series by the method of PA's). From (45), as $M \to 0$, $d_n(M^2) \to 0$; therefore,

$$\delta^*(M) \to 1 \quad \text{as} \quad M \to 0 \ ,$$

inevitably, when the work is based on a finite rather than on an infinite series. It is little comfort that the true situation is doubtless one of nonuniformity of convergence.

In these circumstances the best we can hope is that the finite series effect will be unimportant for larger values of M, and that $\delta^*(M)$ found for these larger values of M already shows a dependence on M which is typical of its true (infinite series) behavior. To investigate this, we now, for given M, form PA's to the right-hand side of (44) and evaluate these approximants at $x = x_c$. We shall concentrate on the fcc lattice, taking $x_c = 0.2492$.

TABLE VIII. Estimates of $\delta^*(M)$, and $t(M)$ on critical isotherm; fcc lattice.

M	δ^*	t
0.975	10.53 ± 0.01	0.752 ± 0.001
0.95	9.41 ± 0.01	0.580 ± 0.001
0.9	8.01 ± 0.01	0.365 ± 0.002
0.85	7.19 ± 0.05	0.237 ± 0.002
0.8	6.63 ± 0.1	0.157 ± 0.002
0.75	6.22 ± 0.2	0.104 ± 0.004
0.7	5.90 ± 0.2	0.068 ± 0.004
0.65	5.64 ± 0.4	0.044 ± 0.004
0.6	5.42 ± 0.05	0.028 ± 0.008
0.55	5.17 ± 0.15	
0.5	4.8 ± 0.2	
0.2	1.93 ± 0.5	
0.15	1.50 ± 0.2	
0.1	1.15 ± 0.2	
0.05	1.04 ± 0.1	

Table VIII shows what happens. For $M \geq 0.85$ the Padé table [to the right-hand side of (44) evaluated at x_c] shows very good convergence. It does not matter whether we take δ^* from the mean of the [4, 4], [3, 5], and [5, 3] approximants or include also the earlier approximants [3, 3], [3, 4], and [4, 3]. Thereafter, we are led to lean more heavily on the later approximants (and take the mean of the [4, 4], [3, 5], and [5, 3] results, omitting one only if it is badly out of line), though we have paid some attention to all six approximants in listing the inevitably subjective "uncertainties." With odd exceptions (e.g., at $M = 0.65$), things are fairly satisfactory down to $M = 0.5$; thereafter, there is a region of considerable uncertainty until we reach $M = 0.2$, when we are clearly approaching the limiting value of unity.

Although for large M, $\delta^*(M)$ is well defined, its dependence on M is not linear. This leads us to consider plotting δ^* not against M but against the corresponding value of t, for which purpose we must form Padé tables to the right-hand side of (28), regarded as a function of x to be evaluated at $x = x_c$. Again, these Padé tables are well converged for large M, and the third column of Table VIII lists the values of t, for given M, on the critical isotherm. There is no point, however, in taking this column below $M = 0.6$ since the uncertainty in t, though still numerically small, is becoming commensurate with t itself. We now find that a plot of $\delta^*(M)$ against $t(M)$ is remarkably linear over the range $0.975 \geq M \geq 0.8$, an extrapolation to $t = 0$ yielding $\delta^* = 5.6$. For $M < 0.8$ the points start falling below this line.

We do not, however, regard 5.6 as the best estimate we can make of δ; rather we regard it as an upper bound. There are two reasons for this. First, when a similar analysis is applied to Ising model series (by Gaunt and Baker), $\delta^*(M)$ is again a linear function of $t(M)$ for large M, but the extrapolant (5.4 for bcc and 5.7 for sc lattices) is larger than can be maintained on other grounds.[32] Second, we can be guided by mean field theory. From its basic equation

$$\mu H/\kappa T_c = -M + \tfrac{1}{2}(T/T_c)\ln[(1+M)/(1-M)] , \quad (46)$$

we easily derive the isothermal

$$M = 3^{1/3}(\mu H/\kappa T_c)^{1/3} - \tfrac{3}{5}(\mu H/\kappa T_c) ,$$

which has the form

$$M = aH^{1/\delta} - bH$$

(since $\delta = 3$ on the mean field approximation). Hence,

$$\delta^* = \delta + cH^{1-1/\delta}$$

or equivalently (to this approximation)

$$\delta^* = \delta + dt^{1-1/\delta} ,$$

where $t = \tanh(\mu H/\kappa T_c)$. This suggests that we should plot δ^* not against t but against $t^{1-1/\delta}$. Without pretending that the argument is a strong one,[33] we are led to plot δ^* against $t^{0.8}$, since we expect δ to be fairly close to 5. The result of so doing is shown in Fig. 3. Here the upper points show δ^* plotted against t, while the lower points (more accurately, points further to the right) show δ^* plotted against $t^{0.8}$, in each case for $0.9 \geq M \geq 0.65$. At its lower end the second curve does seem appreciably more linear, and extrapolates to a value about 5.1. We must, however, draw attention to the uncertainties[34] in the data of Table VIII, which (for this second plot) we have indicated by hatched rectangles in Fig. 3. In view of these uncertainties, we incline to conclude[35] that $\delta = 5 \pm 0.2$.

We would add only that if the above argument has any validity, then the finite series effect, which causes δ^* eventually to approach unity, sets in for our series at about $M = 0.6$.

VI. SUMMARY AND CONCLUSION

We have shown that it is possible to locate the magnetic phase boundary for the Heisenberg spin-$\frac{1}{2}$ model with acceptable accuracy from an expansion of the magnetic free energy in powers of $J/\kappa T$ and $\tanh(\mu H/\kappa T)$, i.e., of essentially high-temperature variables. The phase boundary is not accurately determined for a magnetization greater than about 80% of the saturation value, but by then we are entering the realm of spin-wave theory. For the fcc lattice our phase boundary agrees closely with that given by Cooke and Gersch, using second-order Green's-function

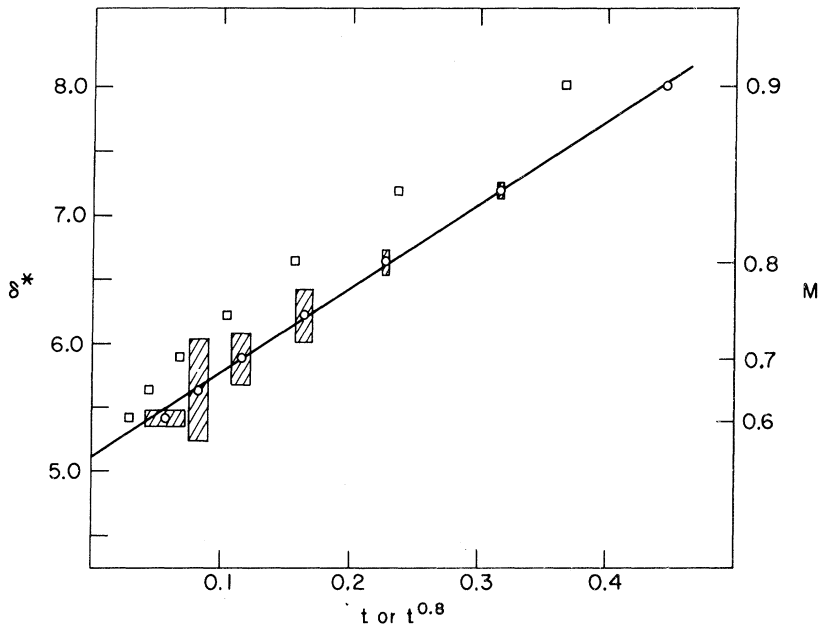

FIG. 3. ⊡ $\delta^*(M)$ against t, ⊙ $\delta^*(M)$ against $t^{0.8}$, fcc lattice.

theory. Likewise for the sc lattice, although we know the phase boundary less accurately, our results agree within their precision, with the second-order Green's-function treatment. For the bcc lattice we find a magnetic phase boundary barely distinguishable from that for the fcc lattice, which is in keeping with the similarity of their limitingly low-temperature forms provided by spin-wave theory.

On this latter point, it is interesting to observe that the experimental results for the magnetic phase boundary of the bcc Heisenberg ferromagnetic $Cu(NH_4)_2Br_4\ 2H_2O$ reported by Wielinga[36] lie very much closer to the Cooke and Gersch fcc phase boundary than to the corresponding phase boundary for the sc lattice, notwithstanding that, as regards lattice coordination number, the bcc is closer to the sc than to the fcc lattice.

In contrast to this, we have found that there are intrinsic difficulties in determining the critical exponents β and δ, relating, respectively, to the phase boundary and the critical isotherm. Although by using rather longer series we could have located the phase boundaries with greater precision, this is probably not the case as regards these critical exponents, whose exact determination escapes us as much in principle as in practice. Longer series might well clarify the question of ι and the existence or nonexistence of an initial susceptibility at subcritical temperatures; but without radically new methods, or a rigorous proof of the scaling laws, it seems unlikely that much more can be said about the magnitudes of β and δ.

In this paper we have not tried to estimate β itself; only to say something about an effective β over the range for which we know the phase boundary with some confidence, namely, $0.4 \leq M \leq 0.7$, for which we have given $\beta^* = 0.35 \pm 0.05$. In I, invoking the scaling laws, we concluded $0.36 \leq \beta \leq 0.41$, though the tempting assumptions $\gamma = \frac{10}{7}$ and $2\Delta = \frac{25}{7}$ led to $\beta = \frac{5}{14} = 0.357$; a value which we still rather favor. If this is so, it is clear that the true value of β may well remain effective up to, say, $M = 0.6$ or $T/T_c = 0.9$. In any case, it should be noted that in determing the value $\beta = 0.38 \pm 0.04$ for Cu $(NH_4)_2$ Br_4 $2H_2O$, Wielinga leaned heavily on the saturation magnetization measurements in the region of $M = 0.6$ and $T/T_c = 0.9$.

Regarding δ, we believe we can say with confidence that $\delta < 5.6$. In I we concluded $4.46 \leq \delta \leq 5.00$, while the fractional values for γ and 2Δ led to $\delta = 5$. We have allowed ourselves here to say 5.0 ± 0.2, and believe there is some positive evidence for this. Longer series could improve our confidence, but some uncertainty over the validity of the extrapolation procedure used must inevitably remain.

ACKNOWLEDGMENTS

Finally, we would express our thanks to Dr. K. Pirnie for programming assistance; and to Dr. D. S. Gaunt and Dr. P. J. Wood for helpful discussions in the course of this work.

APPENDIX A: FACE-CENTERED-CUBIC LATTICE

$$p_1(M^2) = -12 + 12M^2 ,$$

$$p_2(M^2) = 48 - 360M^2 + 312M^4 ,$$

$$p_3(M^2) = 288 + 6\,384M^2 - 18\,624M^4 + 11\,952M^6 ,$$

$$p_4(M^2) = 288 - 69\,408M^2 + 681\,120M^4 - 1\,222\,272M^6 + 610\,272M^8 ,$$

$$p_5(M^2) = -13\,632 - 172\,608M^2 - 16\,961\,280M^4 + 73\,509\,120M^6 - 95\,359\,680M^8 + 38\,998\,080M^{10} ,$$

$$p_6(M^2) = 1\,017\,792 + 8\,860\,992M^2 + 252\,075\,072M^4 - 3\,144\,229\,056M^6 + 8\,518\,176\,000M^8 - 8\,625\,755\,520M^{10} + 2\,989\,854\,720M^{12} ,$$

$$p_7(M^2) = 77\,429\,760 + 65\,179\,392M^2 - 186\,057\,984M^4 + 97\,083\,899\,136M^6 - 547\,553\,147\,904M^8 + 1\,072\,326\,447\,360M^{10} - 889\,210\,586\,880M^{12} + 267\,396\,837\,120M^{14} ,$$

$$p_8(M^2) = 3\,306\,207\,744 - 13\,523\,091\,456M^2 - 41\,071\,441\,920M^4 - 1\,914\,333\,448\,704M^6 + 26\,782\,383\,496\,704M^8 - 95\,894\,560\,355\,328M^{10} + 146\,698\,249\,098\,240M^{12} - 102\,955\,962\,332\,160M^{14} + 27\,335\,511\,866\,880M^{16} .$$

APPENDIX B: BODY-CENTERED-CUBIC LATTICE

$$p_1(M^2) = -8 + 8M^2 ,$$

$$p_2(M^2) = 32 - 176M^2 + 144M^4 ,$$

$$p_3(M^2) = -128 + 2\,912M^2 - 6\,720M^4 + 3\,936M^6 ,$$

$$p_4(M^2) = 2\,112 - 49\,472M^2 + 229\,184M^4 - 327\,936M^6 + 146\,112M^8 ,$$

$$p_5(M^2) = -30\,848 + 961\,408M^2 - 7\,272\,960M^4 + 18\,680\,320M^6 - 19\,209\,600M^8 + 6\,871\,680M^{10}$$

$$p_6(M^2) = 829\,568 - 24\,130\,688M^2 + 242\,365\,824M^4 - 944\,997\,504M^6 + 1\,648\,880\,640M^8 - 1\,314\,305\,280M^{10} + 391\,357\,440M^{12} ,$$

$$p_7(M^2) = -14\,608\,896 + 719\,391\,744M^2 - 8\,992\,936\,960M^4 + 47\,457\,141\,760M^6 - 121\,337\,169\,408M^8 + 158\,991\,006\,720M^{10} - 103\,015\,019\,520M^{12} + 26\,192\,194\,560M^{14} ,$$

$$p_8(M^2) = 571\,524\,096 - 26\,098\,339\,840M^2 + 380\,321\,157\,120M^4 - 2\,507\,078\,153\,216M^6 + 8\,543\,360\,842\,752M^8 - 16\,035\,492\,759\,552M^{10} + 16\,735\,590\,574\,080M^{12} - 9\,106\,773\,903\,360M^{14} + 2\,015\,599\,057\,920M^{16} .$$

APPENDIX C: SIMPLE-CUBIC LATTICE

$$p_1(M^2) = -6 + 6M^2 ,$$

$$p_2(M^2) = 24 - 108M^2 + 84M^4 ,$$

$$p_3(M^2) = -96 + 1\,560M^2 - 3\,264M^4 + 1\,800M^6 ,$$

$$p_4(M^2) = 144 - 21\,456M^2 + 93\,744M^4 - 124\,704M^6 + 52\,272M^8 ,$$

$$p_5(M^2) = 2\,784 + 283\,296M^2 - 2\,423\,040M^4 + 5\,929\,920M^6 - 5\,715\,360M^8 + 1\,922\,400M^{10} ,$$

$$p_6(M^2) = 184\,224 - 4\,290\,528M^2 + 61\,205\,472M^4 - 244\,855\,008M^6 + 408\,312\,000M^8 - 306\,308\,160M^{10} + 85\,752\,000M^{12} ,$$

$$p_7(M^2) = -6\,059\,136 + 94\,389\,504M^2 - 1\,619\,869\,440M^4 + 9\,624\,972\,672M^6 - 24\,564\,677\,760M^8 + 30\,799\,077\,120M^{10} - 18\,831\,052\,800M^{12} + 4\,503\,219\,840M^{14} ,$$

$$p_8(M^2) = 24\,005\,376 - 2\,698\,927\,104M^2 + 47\,855\,764\,992M^4 - 380\,555\,467\,008M^6 + 1\,371\,468\,809\,472M^8 - 2\,542\,146\,098\,688M^{10} + 2\,541\,133\,969\,920M^{12} - 1\,307\,420\,835\,840M^{14} + 272\,338\,778\,880M^{16} .$$

APPENDIX D: PLANE-TRIANGULAR LATTICE

$$p_1(M^2) = -6 + 6M^2,$$

$$p_2(M^2) = 24 - 108M^2 + 84M^4,$$

$$p_3(M^2) = 24 + 1\,296M^2 - 3\,048M^4 + 1\,728M^6,$$

$$p_4(M^2) = -1\,296 - 9\,072M^2 + 69\,840M^4 - 105\,984M^6 + 46\,512M^8,$$

$$p_5(M^2) = -4\,896 - 18\,144M^2 - 1\,123\,200M^4 + 3\,948\,480M^6 - 4\,356\,000M^8 + 1\,553\,760M^{10},$$

$$p_6(M^2) = 359\,904 + 592\,800M^2 + 11\,265\,696M^4 - 108\,004\,320M^6 + 240\,888\,960M^8 - 207\,397\,440M^{10} + 62\,294\,400M^{12},$$

$$p_7(M^2) = 3\,151\,296 + 16\,170\,048M^2 - 35\,578\,368M^4 + 2\,219\,228\,928M^6 - 9\,843\,511\,104M^8 + 15\,972\,264\,000M^{10} - 11\,251\,820\,160M^{12} + 2\,920\,095\,360M^{14},$$

$$p_8(M^2) = -214\,622\,976 + 30\,950\,400M^2 - 911\,121\,408M^4 - 30\,397\,316\,352M^6 + 312\,908\,501\,760M^8 - 902\,373\,502\,464M^{10} + 1\,149\,509\,975\,040M^{12} - 685\,160\,985\,600M^{14} + 156\,608\,121\,600M^{16}.$$

APPENDIX E: PLANE-SQUARE LATTICE

$$p_1(M^2) = -4 + 4M^2,$$

$$p_2(M^2) = 16 - 56M^2 + 40M^4,$$

$$p_3(M^2) = -64 + 688M^2 - 1\,248M^4 + 624M^6,$$

$$p_4(M^2) = 96 - 8\,288M^2 + 30\,176M^4 - 35\,328M^6 + 13\,344M^8,$$

$$p_5(M^2) = 1\,856 + 97\,344M^2 - 675\,840M^4 + 1\,423\,360M^6 - 1\,212\,480M^8 + 365\,760M^{10},$$

$$p_6(M^2) = 64 - 1\,120\,832M^2 + 14\,703\,040M^4 - 50\,582\,592M^6 + 73\,789\,440M^8 - 49\,080\,960M^{10} + 12\,291\,840M^{12},$$

$$p_7(M^2) = -570\,112 + 12\,943\,872M^2 - 315\,780\,864M^4 + 1\,696\,377\,088M^6 - 3\,808\,890\,624M^8 + 4\,220\,160\,000M^{10} - 2\,294\,772\,480M^{12} + 490\,533\,120M^{14},$$

$$p_8(M^2) = 3\,681\,792 - 150\,519\,808M^2 + 6\,734\,360\,576M^4 - 55\,223\,961\,088M^6 + 180\,758\,358\,528M^8 - 298\,530\,462\,720M^{10} + 265\,595\,581\,440M^{12} - 121\,889\,295\,360M^{14} + 22\,702\,256\,640M^{16}.$$

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

[2]The corresponding results for the two-dimensional, plane triangular (pt) and plane square (ps), lattices were published separately: G. A. Baker, Jr., H. E. Gilbert, J. Eve, and G. S. Rushbrooke, Phys. Letters 25A, 207 (1967).

[3]We take this opportunity to correct the equations on p. 811 of I which, as observed by R. F. Wielinga (thesis, Leiden, 1968) should have read

$$\frac{\chi(0)\kappa T}{N\mu^2} \sim \left(\frac{0.422}{0.3973 - x}\right)^{1.43} = \frac{1.09}{(1 - T_c/T)^{1.43}} \quad \text{(bcc)}$$

and

$$\frac{\chi(0)\kappa T}{N\mu^2} \sim \left(\frac{0.679}{0.5962 - x}\right)^{1.43} = \frac{1.20}{(1 - T_c/T)^{1.43}} \quad \text{(sc)}.$$

We are grateful to Dr. Wielinga for bringing this to our attention.

[4]G. A. Baker, Jr., and J. Kahane, J. Math. Phys. 10, 1647 (1969).

[5]J. W. Essam, and M. E. Fisher, J. Chem. Phys. 38, 802 (1963).

[6]M. F. Sykes, J. W. Essam, and D. S. Gaunt, J. Math. Phys. 6, 283 (1965).

[7]W. Opechowski, Physica 4, 181 (1937).

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

[9]In I, n_τ^τ, was denoted $t_{(m,l,\tau)}^{[m,l,\tau]}$.

[10]George A. Baker, Jr., H. E. Gilbert, J. Eve, and G. S. Rushbrooke, BNL Report No. 50053(T-460) (unpublished).

[11]G. A. Baker, Jr., G. S. Rushbrooke, and H. E. Gilbert, Phys. Rev. 135, A1272 (1964).

[12]G. A. Baker, Jr., Phys. Rev. Letters 20, 990 (1968). The numbers tabulated therein are the quantities $2j(-1)^{j+1}f(n,j)/2^n n!$ with $j = m + 1$.

[13]Except only as regards $g_{3,8}$, for each lattice, where discrepancies of the order of 1 in 10^9 reflect round-off error in the $F_4^*(8)$ entries of I, as noted therein.

[14]See E. T. Copson, *Functions of a Complex Variable* (Oxford U. P., Oxford, 1935), p. 125.

[15]For present purposes, PA's are adequately defined in I. We continue to use the notation $[D,N]$ to denote the PA which has as numerator a polynomial of degree N and as denominator a polynomial of degree D. $D+N$ equals the number of terms in the given series which are used in constructing the approximant. For series whose coefficients are known through x^8, we shall hope to find reasonable convergence between conclusions drawn from the [3,3], [3,4], [4,3], [4,4], [3,5], and [5,3] approximants.

[16]F. J. Dyson, Phys. Rev. 102, 1230 (1956).

[17]The extra terms, up to $(T/T_c)^4$, given by Dyson increase $1-M$ by about 7% when $T/T_c=0.3$ and by about 14% when $T/T_c=0.5$.

[18]J. F. Cooke and H. A. Gersch, Phys. Rev. 153, 641 (1967).

[19]See Ref. 18, and Ref. 3, p. 102.

[20]N. D. Mermin and H. Wagner, Phys. Rev. Letters 17, 1133 (1966).

[21]H. E. Stanley and T. A. Kaplan, Phys. Rev. Letters 17, 913 (1966).

[22]L. J. de Jongh, A. C. Botterman, F. R. de Boer, and A. R. Miedema, J. Appl. Phys. 40, 1363 (1969).

[23]J. W. Essam and M. E. Fisher, J. Chem. Phys. 38, 802 (1963).

[24]This result is not confined to first-order spin-wave theory. The best references, for which we are indebted to Professor M. E. Fisher, are V. G. Vaks, A. I. Larkin, and S. A. Pikin, Zh. Eksperim. i Teor. Fiz. 53, 281 (1968); 53, 1089 (1968) [Soviet Phys. JETP 26, 188 (1968); 26, 647 (1968)].

[25]We recall that in I, from somewhat longer series examined in a variety of ways, γ was found to be close to 1.43 for the Heisenberg spin-$\frac{1}{2}$ problem.

[26]D. S. Gaunt and G. A. Baker, Jr., Phys. Rev. B 1, 1184 (1970), Table III.

[27]It is convenient to work in terms of $(T_c-T)/T_c$ rather than T_c-T although, of course, this in no way affects the conclusions. And where no confusion can arise, we shall drop the suffix zero from M_0.

[28]Nonclassical exponents are normally derived as the residues of PA's at poles. For the Ising model $M_0(T)$ is known explicitly as a power series in $\exp(-2J/\kappa T)$, and $\partial \ln M_0/\partial T$ can be examined in the neighborhood of T_c. See G. A. Baker, Jr., Phys. Rev. 124, 768 (1961) or Ref. 23.

[29]This is true also of the Ising model, but not of the "classical" ($s=\infty$) Heisenberg model. See R. E. Watson, M. Blume, and G. H. Vineyard, Phys. Rev. 181, 811 (1969).

[30]The increased gradient in the region near $M=0.2$ is simply due to irregularity in the approximants, and has nothing to do with the ultimate limit of 0.5 discussed above.

[31]In drawing up Table VII we have, for each approximation, used for x_c the value given by the corresponding entry in the bottom line of Table II. Had we instead used always $x_c=0.2492$ there would have been some changes in the numbers in Table VII, but our conclusion would have been unaltered.

[32]D. S. Gaunt, M. E. Fisher, M. F. Sykes, and J. W. Essam, Phys. Rev. Letters 13, 713 (1964); D. S. Gaunt, Proc. Phys. Soc. (London) 92, 150 (1967).

[33]A further argument, leading to the same conclusions, is given in Gaunt and Baker, Ref. 26.

[34]It might be thought that some of these uncertainties would be avoided if we were to start from Eq. (22) and derive directly a series expansion for δ^* of the form $\Sigma_{n\geq 0} c_n(t)\, x^n$ where the coefficients $c_n(t)$ are finite polynomials which are known exactly. Unfortunately, PA's to this series, evaluated at x_c for fixed t, fail to converge at all over the interesting range of t.

[35]The same result, but with weaker limits, comes from analysis of the series for the bcc and sc lattices.

[36]R. F. Wielinga, thesis, Leiden, 1968, Chap. V, Fig. 6 (unpublished).

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Susceptibility and Fluctuation. II. Determination of the Frequency Moments*

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The frequency moment appearing in a relation between susceptibility and fluctuation is expressed in terms of measurable quantities. A discussion is given of a determination of the critical exponent for the staggered magnetic susceptibility of $RbMnF_3$.

I. INTRODUCTION

In a discussion[1] of the relation between the critical exponents of susceptibility and of fluctuation near a critical temperature T_c a frequency moment of a spectral density was introduced. If this moment $\bar{\omega}$ goes to zero at T_c, these two critical exponents are equal. In the present work $\bar{\omega}$ is re-