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Confluent singularities and the correction-to-scaling exponent for the $d = 3$ fcc Ising model*

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The susceptibility of the spin-s nearest-neighbor fcc Ising model is studied at zero magnetic field by twelve-term high-temperature series. We find that the data near criticality are consistent with $\chi = A(s)t^{-5/4}[1 + B(s)t^{\Delta_1}]$, $t = 1 - T_c(s)/T$. The correction-to-scaling exponent has the universal value $\Delta_1 = 0.50 \pm 0.05$ in good agreement with ϵ-expansion estimates. The confluent amplitude $B(s)$ vanishes at $s = 1/2$ to within uncertainties. Values of the critical parameters are tabulated for a variety of spins.

I. INTRODUCTION

It has long been appreciated that the pure power laws which characterize the "ideal" scaling behavior of thermodynamic functions near enough to criticality[1,2] are subject to corrections.[3] In addition to so-called background terms,[4] we distinguish singularities at values of the temperature and field variables *away from* the critical point, $t=(T-T_c)/T_c=0$, $h=0$, from those ("confluent") singularities which occur *at* $t=h=0$ but are masked by the dominant, scaling singularities. As an example of the former we may cite the "antiferromagnetic" singularities which occur *at* $T=-T_c(h=0)$ in loose-packed (two-sublattice) ferromagnetic Ising models.[5,6] Such corrections are unrelated to the critical fluctuations[7] and are generally negligible near criticality. The confluent corrections, on the other hand, are a direct byproduct of the same fluctuations responsible for scaling behavior. They may be large (even divergent) near criticality and are only unimportant relative to the scaling contributions. The focus of this paper is the determination of the critical exponent characterizing these confluent corrections in the three-dimensional ($d=3$) Ising model ($n=1$, i.e., one-spin dimension).

Early, more or less phenomenological efforts[8] found a variety of correction exponents, related by scaling laws to the ordinary critical exponents. Wegner[9] was the first to study corrections to scaling in the renormalization-group context. He showed how confluent corrections arise through the dependence of the thermodynamic functions on the fields associated with irrelevant operators. The leading correction comes from the leading irrelevant operator, i.e., the irrelevant operator associated with the least negative[10] eigenvalue $y=-|y|=-\omega$ of the linearized renormalization-group equations. The corresponding corrections to the (reduced) free energy per lattice site are of the form

$$w(t,h)=\lim_{N\to\infty}\frac{1}{N}\ln Z_N=t^{2-\alpha}\,\mathcal{F}\left(\frac{h}{t^{\Delta}}\right)\left[1+\mathcal{G}\left(\frac{h}{t^{\Delta}}\right)t^{\Delta_1}+\cdots\right], \tag{1}$$

$[t=(T-T_c)/T_c,\ h=mH/k_BT_c]$ near criticality, with[11]

$$\Delta_1=\nu\omega\ . \tag{2}$$

The corresponding expression for the (reduced) zero-field susceptibility is

$$\chi=\left.\frac{\partial^2 w}{\partial h^2}\right|_{h=0}=At^{-\gamma}(1+Bt^{\Delta_1}+\cdots)\ . \tag{3}$$

The exponent ω has been calculated[12–14] in the ϵ expansion[15] ($\epsilon=4-d$) through order ϵ^3, giving for $n=1$,

$$\omega=\epsilon-\tfrac{17}{27}\epsilon^2+1.618\epsilon^3+O(\epsilon^4)\ , \tag{4}$$

which is not well converged at $\epsilon=1$ but is estimated by Padé methods to give[14] $\omega\simeq 0.8$ or [using (2) with[16] $\nu=0.638$] $\Delta_1\simeq 0.5$. Additional calculations of Δ_1 at $d=3$ by recursion-relation methods have very recently been reported by Swift and Grover[16a] and by Golner and Riedel.[16b]

The first observation of the correction exponent Δ_1 was reported by one of us,[17] in 1970 (before its theoretical significance[9] was fully appreciated) in the course of a study of the zero-field susceptibility of the spin-s Ising model on the fcc lattice using twelve-term high-temperature series. This study has remained unpublished until the present. In the interim there have been several related developments. Barouch *et al.*[18] have calculated analytically the leading correction to the zero-field susceptibility of the $d=2$, $s=\frac{1}{2}$ Ising model on the square lattice. They find a result of the form

$$\chi = C_0 t^{-7/4} + C_1 t^{-3/4} + \cdots , \qquad (5)$$

in good agreement with previous numerical results of Sykes *et al.*[19] Equation (5) is consistent with the correction factor in (3) being analytic at $t=0$ and might be interpreted as $\Delta_1 = 1$. Actually, there is good evidence in both two[20] and three[17] dimensions (as we shall show below) suggesting that $s=\frac{1}{2}$ (as opposed to $s>\frac{1}{2}$) is a special case and favoring $B(s)=0$ at $s=\frac{1}{2}$ (only) with $0<\Delta_1<1$ and independent of s. Thus (5) probably does *not* constitute an evaluation of Δ_1 in $d=2$, $n=1$. Very recently (in work quite independent from ours) Camp and Van Dyke[20,21] have analyzed high-temperature series for the susceptibility of the spin-s Ising model on a number of lattices ($d=2$ and $d=3$) including the fcc. Their series are shorter than ours (10 terms in place of our 12); however, they reach conclusions which are fully consistent with ours,[17] using analytical methods which are somewhat different. Finally, we note that Greywall and Ahlers[22] have found it necessary to introduce confluent corrections into the analysis of He data near the λ line. He finds $0.4 \lesssim \Delta_1 \lesssim 0.8$ in crude agreement with our conclusions and the ϵ expansion (4).

In this paper we report a detailed study[17] of the susceptibility of the spin-s nearest-neighbor Ising model on the fcc lattice, based on twelve-term high-temperature series. Although we have such series for a variety of other lattices and thermodynamic functions,[23] we choose the fcc susceptibility because (a) $d=3$ series are better converged than corresponding $d=2$ series of the same length, (b) the analysis of loose-packed lattices is complicated by the presence of antiferromagnetic singularities on the circle of convergence,[5] and (c) susceptibility series are, among available series, typically the smoothest and best converged. We conclude that for $d=3$, $n=1$ the correction index has the universal value

$$\Delta_1 = 0.50 \pm 0.05 , \qquad (6)$$

in agreement with (4) and previous estimates.[17,20] In addition, we give values for the critical temperature $k_B T_c(s)$ and the critical amplitudes [see (3)] $A(s)$ and $B(s)$ for spins $s=\frac{1}{2}, 1, \ldots, 5\frac{1}{2}$, and ∞. The correction amplitude $B(s)$ is an increasing function of spin, with $B(\frac{1}{2})=0$ to within uncertainties.

II. CALCULATIONS

A. Series derivation

The Hamiltonian of the spin-s nearest-neighbor Ising model is (in reduced units)

$$-\beta\mathcal{H}_N = \frac{K}{s^2} \sum_{\langle 12 \rangle} S^z(1) S^z(2) + \frac{h}{S} \sum_1 S^z(1) , \qquad (7)$$

where N is the number of lattice sites, $\langle 12 \rangle$ stands for a nearest-neighbor pair of sites, and the dimensionless coupling K is related to the exchange interaction J by $K = \beta J = J/k_B T$. Each operator S^z takes on the $(2s+1)$ values $S^z = -s, -s+1, \ldots, s-1, s$, so the variable S^z/s always lies in the interval -1 to $+1$. All thermodynamic functions may be derived from the (reduced) free energy per lattice site,

$$w(K, h) = \lim_{N\to\infty} \frac{1}{N} \ln \operatorname{Tr} e^{-\beta\mathcal{H}_N} . \qquad (8)$$

The noninteracting free energy is easily evaluated,

$$w(K=0, h) = \ln(2s+1) + \sum_{k=1}^{\infty} \frac{B_{2k}}{2k(2k)!} \times \left((2s+1)^{2k} - 1\right) \left(\frac{h}{s}\right)^{2k} = \sum_{k=0}^{\infty} \frac{M^0_{2k}(s) h^{2k}}{(2k)!} \qquad (9)$$

(B_{2k} are the Bernoulli numbers[24]), which gives $h=0$ values of the unrenormalized semi-invariants,[25–27] for example,

$$M^0_2(s) = (s+1)/3s. \qquad (10)$$

Established computer codes[26,28] now allow us to generate 12 terms ($k=1, \ldots, 12$) in the high-temperature series for the zero-field correlations and (reduced) susceptibility

$$\chi = \frac{\partial^2 w}{\partial h^2}\bigg|_{h=0} = \frac{1}{s^2} \sum_2 \langle S^z(1) S^z(2) \rangle = M^0_2(s) \left(1 + \sum_{k=1}^{\infty} a_k(s) v^k\right) , \qquad (11)$$

where $v = K M^0_2(s)$. High-temperature series for the spin-s fcc Ising model were first calculated by Domb and Sykes.[29] They obtained the coefficients through $k=6$ as finite polynominals in the variable $X = s(s+1)$. The polynomials[21] $k=7, 8$ and[20] $k=9, 10$ have been added recently by Camp and Van Dyke. Numerical values[30] of the coefficients $a_{11}(s)$ and[31] $a_{12}(s)$ are listed in Table I for a variety of spins. The coefficients $a_{11}(\frac{1}{2})$ and $a_{12}(\frac{1}{2})$ were previously available from Ref. 31.

B. Series analysis

Analysis of the series (11) was initially carried out by standard ratio-Neville and log-derivative-Padé techniques.[32,33] It becomes apparent in any standard analysis that the $s=\frac{1}{2}$ series behaves differently from (better than!) those with $s>\frac{1}{2}$. This is well illustrated in Fig. 1 and Table II, which compare $s=\frac{1}{2}$ and $s=\infty$ (typical of $s>\frac{1}{2}$) behavior under ratio analysis. If it were *exactly* true that $\chi(v) = A(1 - v/v_c)^{-\gamma} = At^{-\gamma}$, then[1] the coefficients a_k could be deduced from the binomial expansion

TABLE I. Coefficients $a_{11}(s)$ and $a_{12}(s)$ for the nearest-neighbor fcc Ising susceptibility, as defined by (11). Lower-order coefficients are available in Refs. 20, 21, and 29. The coefficients are determined numerically and suffer from roundoff error, despite the use of double precision arithmetic, so the tenth figure and beyond may be unreliable.

s	$10^{-11}a_{11}(s)$	$10^{-12}a_{12}(s)$[a]
0.5	1.581 830 429 21	1.581 351 984 73
1.0	2.318 982 137 38	2.418 844 615 73
1.5	2.586 064 135 21	2.731 228 837 28
2.0	2.710 401 911 61	2.878 097 285 01[b]
2.5	2.778 056 387 30	2.958 380 297 10
3.0	2.818 876 226 51	3.006 942 763 34
3.5	2.845 377 705 11	3.038 520 086 10
4.0	2.863 549 825 13	3.060 194 905 28
4.5	2.876 549 374 95	3.075 711 154 74
5.0	2.886 168 087 57	3.087 197 937 22
5.5	2.893 484 161 45	3.095 938 230 81
∞	2.931 975 653 96	3.141 970 324 02

[a]Reference 31.
[b]This coefficient is given incorrectly in Ref. 30.

$$M_2^0 a_k = A v_c^{-k}\binom{\gamma+k-1}{k} , \qquad (12)$$

and the ratio of successive coefficients would be

$$\rho_k \equiv a_k/a_{k-1} = (1/v_c)\left[1+(\gamma-1)/k\right] . \qquad (13)$$

The actual structure of $\chi(v)$ is, of course, more complicated; however, (13) remains asymptotically true for large k, provided[34] that (a) $\chi(v) \sim At^{-\gamma}$ near v_c, (b) there are no singularities in the disk $|v| < v_c$, and (c) there are no singularities on the circle of convergence $|v| = v_c$ stronger than (a). The form of corrections terms to (13) depends on the behavior of $\chi(v)$ on the circle of convergence. If $\chi(v) = A(v)t^{-\gamma} + B(v)$, with $A(v)$ and $B(v)$ analytic in the neighborhood of v_c and throughout the *closed* disk[35] $|v| \leq v_c$, then there is a theorem due to Darboux, which guarantees that the correction terms go as integral powers of k^{-1},

$$\rho_k = \frac{1}{v_c}\left(1+\frac{\gamma-1}{k} + b_2 k^{-2} + b_3 k^{-3} + \cdots\right) , \qquad (14)$$

and the coefficients $b_2, b_3, \ldots$ can be deduced from the expansion of $A(v)$ about v_c. On the other hand, if there are additional singularities on the circle of convergence, then the correction terms will in general contain nonintegral powers of k^{-1}. In particular, a single confluent singularity of form (3) gives

$$M_2^0 a_k = A v_c^{-k}\binom{\gamma+k-1}{k}\left[1+BR_k(\gamma,\Delta_1)\right] , \qquad (15)$$

where

$$R_k(\gamma,\Delta_1) = \left(\frac{\gamma-\Delta_1}{\gamma}\right)\left(\frac{\gamma-\Delta_1+1}{\gamma+1}\right)\cdots\left(\frac{\gamma-\Delta_1+k-1}{\gamma+k-1}\right) \xrightarrow[k \text{ large}]{} \frac{\Gamma(\gamma)}{k^{\Delta_1}\Gamma(\gamma-\Delta_1)} \qquad (16)$$

and the ratios go as

$$\rho_k = (1/v_c)\{1+(1/k)[\gamma-1-\Delta_1 BR_k(\gamma,\Delta_1)] + O(k^{-2}) + O(k^{-2-\Delta_1})\} , \qquad (17)$$

so the leading correction to (13) varies with $k^{-1-\Delta_1}$, which dominates k^{-2}, provided $0<\Delta_1<1$. Corrections like (14) are naturally incorporated by a Neville extrapolation, which effectively fits ρ_k to a polynomial in k^{-1} (see $s=\frac{1}{2}$ in Table II). On the other hand, the presence of singular corrections as in (17) makes polynomial approximations poor and leads to slow monotonic trends in the Neville tables (see $s=\infty$ in Table II). It is common, for example, to form successive estimates γ_k of the exponent γ from the local slope of the ratio plots ρ_k vs k^{-1}. When singular corrections are present, it is clear from (17) that for large k,

$$\gamma_k \sim \gamma - \Delta_1 BR_k(\gamma,\Delta_1) \sim \gamma - \frac{\Delta_1 B\Gamma(\gamma)}{k^{\Delta_1}\Gamma(\gamma-\Delta_1)} , \qquad (18)$$

which converges to γ from below ($B>0$) more slowly than any integral power of k^{-1}. This effect

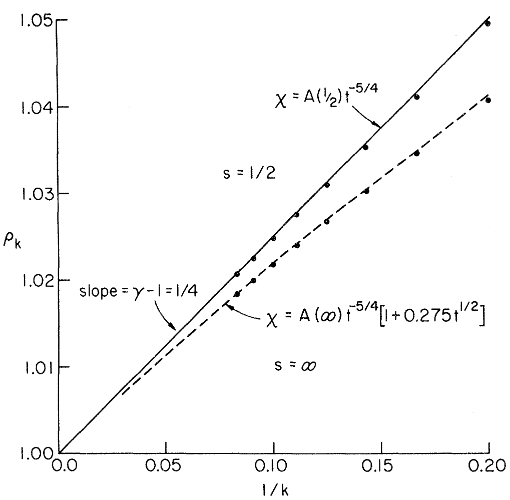

FIG. 1. Normalized ratio plots for the $s=\frac{1}{2}$ and $s=\infty$ fcc Ising susceptibility. Critical temperatures are taken from Table VI. Dots show the data points. The solid line follows the asymptotic expression $v_c\rho_k = 1+(\gamma-1)/k$, which is exact when $\chi = At^{-\gamma}$. The dashed line shows the ratios derived from the $s=\infty$ mimic function (19), which has the same asymptotic behavior but contains a confluent correction. Note how closely the dotted line fits the $s=\infty$ data and how slowly it approaches its asymptote.

TABLE II. Sample Neville tables for $s=\frac{1}{2}$ and $s=\infty$. Shown in the first column are the biased ratio estimates from (13),

$$(v_c^{-1})_k^{\mathrm{Nev}} = (k_B T_c(s)/JM_2^0(s))_k^{\mathrm{Nev}} = k\rho_k(s)/(k+\gamma-1)$$

and

$$(\gamma)_k^{\mathrm{Nev}} = 1 + k(v_c(s)\rho_k(s)-1),$$

using $\gamma=\frac{5}{4}$, $v_c^{-1}(\frac{1}{2})=9.7953$, and $v_c^{-1}(\infty)=10.5236$. Subsequent columns give the linear, quadratic, and cubic extrapolants. The rule of thumb in interpreting Neville tables is to read the bottom of the column which is most nearly constant. Note that for $s=\frac{1}{2}$ the left-hand columns are already well converged, while $s=\infty$ contains slow monotonic trends out to the cubic extrapolants.

	k	$(v_c^{-1})_k^{\mathrm{Nev}}$				$(\gamma)_k^{\mathrm{Nev}}$			
	6	9.7905	9.7921	9.8017	9.8248	1.2469	1.2453	1.2482	1.2578
	7	9.7912	9.7956	9.8045	9.8083	1.2470	1.2473	1.2522	1.2576
	8	9.7918	9.7957	9.7960	9.7820	1.2471	1.2475	1.2479	1.2407
$s=\frac{1}{2}$	9	9.7922	9.7953	9.7940	9.7898	1.2471	1.2472	1.2462	1.2427
	10	9.7925	9.7952	9.7948	9.7966	1.2471	1.2471	1.2466	1.2476
	11	9.7927	9.7953	9.7956	9.7977	1.2471	1.2471	1.2473	1.2493
	12	9.7930	9.7952	9.7951	9.7936	1.2471	1.2471	1.2468	1.2452
	6	10.4520	10.5647	10.5336	10.5319	1.2075	1.2297	1.2328	1.2351
	7	10.4667	10.5545	10.5291	10.5231	1.2108	1.2305	1.2325	1.2322
	8	10.4768	10.5479	10.5280	10.5263	1.2133	1.2312	1.2332	1.2345
$s=\infty$	9	10.4842	10.5433	10.5269	10.5248	1.2154	1.2317	1.2336	1.2342
	10	10.4898	10.5398	10.5262	10.5245	1.2170	1.2321	1.2338	1.2343
	11	10.4941	10.5373	10.5258	10.5246	1.2185	1.2325	1.2341	1.2348
	12	10.4975	10.5353	10.5254	10.5245	1.2196	1.2328	1.2343	1.2350

is visible in the $s=\infty$ ratios of Fig. 1.

The $s>\frac{1}{2}$ data are, then qualitatively consistent with the hypothesis of a confluent singularity of the form (3). To test this hypothesis and to make quantitative estimates of the parameters of (3), we developed a very simple generalization of the ratio method.[36] The ratio method in its simplest form uses three successive coefficients a_k to construct estimates of v_c^{-1}, γ, and A on the basis of (12). In the method of "four fits"[37,38] we accept as universal the value[16,31] $\gamma=\frac{5}{4}$ (see, however, Sec. III A) and use four successive coefficients a_{k-1}, a_k, a_{k+1}, and a_{k+2} to solve (15) for estimates $(v_c^{-1})_k$, A_k, B_k, and $(\Delta_1)_k$ of the critical parameters. It is easy to show that this procedure is convergent as $k\to\infty$, provided that (a) there are no singularities within the disk $|v|<v_c$ and (b) there are no singularities on the circle of convergence stronger than (3). The rapidity of the convergence is expected to be good, if singularities in addition to (3) are weak and far outside the circle of convergence. Table III shows some typical examples. Note that the estimates of v_c^{-1}, in particular, are extremely rapidly convergent as k increases (cf. $s=\infty$ in Table II). Even the confluent amplitude and index, B_k and $(\Delta_1)_k$, are quite stably determined for $s>\frac{1}{2}$, although small long-term trends are still apparent, due presumably to competing singularities in $\chi(v)$. We interpret the good con-

TABLE III. Successive four-fit estimates of the parameters of (3) for spins $s=\frac{1}{2}$, 1, and ∞. $v_c^{-1}(s)=k_B T_c(s)/JM_2^0(s)$ with $M_2^0(s)=(s+1)/3s$. $A(s)$ and $B(s)$ are the dominant and confluent amplitudes and Δ_1 is the correction-to-scaling index.

	k	v_c^{-1}	A/M_2^0	B	Δ_1
	1	9.7977	0.9754	0.0252	1.0275
	2	9.7912	0.9790	−0.0025	2.0061
	3	9.7905	0.9793	0.0000	8.6183
	4	9.7904	0.9793	0.0000	6.9290
$s=\frac{1}{2}$	5	9.7900	0.9795	0.0000	−11.6670
	6	9.7963	1.0204	−0.0368	−0.0819
	7	9.7938	0.9748	0.0216	0.7752
	8	9.7945	0.9704	0.0156	0.3567
	9	9.7959	0.9970	−0.0153	−0.1553
	10	9.7949	0.9630	0.0218	0.1924
	1	10.3163	0.7333	0.3638	0.3254
	2	10.2220	0.8840	0.1868	0.8330
	3	10.2186	0.8882	0.2065	0.8972
	4	10.2279	0.8704	0.1488	0.6233
$s=1$	5	10.2285	0.8683	0.1471	0.5992
	6	10.2288	0.8674	0.1461	0.5874
	7	10.2292	0.8654	0.1438	0.5624
	8	10.2293	0.8647	0.1428	0.5530
	9	10.2296	0.8631	0.1407	0.5319
	10	10.2298	0.8616	0.1388	0.5127
	1	10.6667	0.4737	1.1111	0.2375
	2	10.5115	0.8005	0.2963	0.6553
	3	10.5195	0.7876	0.3014	0.5949
	4	10.5216	0.7826	0.3025	0.5701
$s=\infty$	5	10.5204	0.7861	0.3034	0.5902
	6	10.5210	0.7840	0.3017	0.5767
	7	10.5212	0.7833	0.3009	0.5717
	8	10.5214	0.7824	0.2996	0.5655
	9	10.5216	0.7812	0.2976	0.5562
	10	10.5218	0.7799	0.2953	0.5468

TABLE IV. Observed series ratios compared with those derived from best mimic functions for $s=\frac{1}{2}$ and $s=\infty$. Ratios are defined by (13). The mimic functions are given in the text at (19) and thereafter.

	$s=\frac{1}{2}$ ratios		$s=\infty$ ratios	
	actual	mimic	actual	mimic
1	12.0	12.2441	12.0	12.0196
2	11.0	11.0197	11.4	11.4664
3	10.6061	10.6116	11.1789	11.2011
4	10.4029	10.4075	11.0413	11.0525
5	10.2797	10.2851	10.9510	10.9578
6	10.1984	10.2034	10.8875	10.8921
7	10.1409	10.1451	10.8405	10.8439
8	10.0978	10.1014	10.8042	10.8070
9	10.0642	10.0674	10.7754	10.7778
10	10.0373	10.0412	10.7520	10.7541
11	10.0153	10.0179	10.7326	10.7345
12	9.9970	9.9994	10.7162	10.7180

vergence as confirmation of the *Ansatz* (3). In reading the results quoted in Sec. III B (Table V), we have extrapolated linearly against k^{-1} and have taken the last ($k=10$) such extrapolant with an assigned uncertainty equal to one-half of the net extrapolation.[39] This procedure is admittedly *ad hoc*, but the magnitudes of the extrapolations are rather small, anyway.

To illustrate how well the form (3) fits the series data, we compare in Table IV the actual $s=\infty$ ratios $\rho_k(s)$ with those derived by expanding the best $s=\infty$ mimic function

$$\chi(v)=0.256t^{-5/4}(1+0.275t^{1/2}) ,\quad t=(1-10.5236v) . \tag{19}$$

The corresponding normalized ratios are shown as the dashed line in Fig. 1. The fit which (19) provides for the $s=\infty$ ratios is fully as good as the fit which $\chi(v)=0.972t^{-5/4}$, $t=(1-9.7953v)$, provides for the $s=\frac{1}{2}$ ratios.

While not entirely free of ambiguities, a straightforward Padé analysis lends some support to the ratio methods discussed above. One may consider, for example, Padé approximants to (i) $(d/dv)\ln(dC/dv)$ and (ii) $[(v_c-v)(d/dv)\ln(dC/dv)]_{v=v_c}$, where $C(v)\equiv(v_c-v)^{5/4}\chi(v)$. According to hypothesis, $dC/dv\sim(v_c-v)^{-(1-\Delta_1)}$. Method (i) not only yields an estimate of Δ_1 but in addition tests the confluence of the correction term. In Table V we show estimates of Δ_1 and v_c^*, the position of the correction singularity, in the cases $s=1$ and $s=\infty$. In forming $C(v)$ we have used the values of v_c from the "four-fit" ratio method; these values (shown in Table VI) are not greatly different from those determined in a "naive" ratio analysis. The estimates of Δ_1 are somewhat greater than the proposed $\Delta_1=\frac{1}{2}$ and the location of the singularity of the correction term appears to differ by 2–3% from the "four-fit" values used to form $C(v)$. A preliminary check of the $s=\infty$ model on the *bcc* lattice indicates similar behavior. One does not fare so well in attempting to apply method (ii), which forces the correction to be exactly confluent. For example, in the $s=\infty$ case the low-order diagonal and near-diagonal approximants indicate $\Delta_1\simeq0.54$, but approximants beyond [3/4] are plagued by real zero-pole pairs lying very close to v_c producing defective estimates for Δ_1. The $s=1$ case is similar in this regard. These extrapolants may be providing an indication that the structure of the singularity is in fact quite complicated. A more systematic Padé analysis has been carried out by Camp and Van Dyke[20] in the accompanying paper.

III. RESULTS AND CONCLUSIONS

A. Universality

Earlier work on the spin-s Ising model[21,33] using eight-ten-term series noted a small spin dependence of the susceptibility exponent, with $\gamma(s=\frac{1}{2})=1.25$, $\gamma(s=\infty)=1.23$, and $\gamma(s)$ for other spins at intermediate values. This trend is clearly present, when the twelve-term data are analyzed by conventional methods, as seen, for example, in Table II. Such a continuous spin dependence, if real, would be in violation of the principle of universality[40] and inconsistent with the renormalization group approach. Our analysis shows that *the twelve-term high-temperature susceptibility series are consistent with the universal value* $\gamma=\frac{5}{4}$ *for all* s, *provided that a confluent correction of the form* (3) *is assumed.* Since such corrections are, indeed, predicted by the renormalization group analysis,[9] the inference in favor of universality would seem strong.

It would be more satisfying to have concluded for

TABLE V. Padé-approximant estimates of the position and power of the correction singularity for the $s=1$ and $s=\infty$ fcc Ising model by method (i) described in the text. In forming $C(v)$ we have used $v_c^{-1}(1)=10.2316$ and $v_c^{-1}(\infty)=10.5236$.

L/M	v_c^*	Δ_1	v_c^*	Δ_1
2/2	12.1990	0.79	10.6177	0.54
2/3	10.9553	0.70	10.6408	0.56
3/2	10.8711	0.68	10.9124	0.63
3/3	10.7840	0.66	10.6997	0.57
3/4	10.6131	0.61	10.7191	0.57
4/3	a	a	10.7134	0.57
4/4	10.6157	0.61	10.7164	0.58
4/5	10.6132	0.61	10.7206	0.58
5/4	10.5273	0.56	10.7143	0.57
5/5	a	a	10.6535	0.54

[a]The real pole splits into a complex pair in these entries.

TABLE VI. Critical temperatures, amplitudes, and exponents of the susceptibility of the nearest-neighbor spin-s Ising model on the fcc lattice. The model is defined by Eqs. (7)–(11). Parametrization of the critical behavior is given by (3). Unless otherwise noted, numbers are obtained from four-fit analysis with $\gamma = \frac{5}{4}$. Assignment of uncertainties is outlined at the end of Sec. II B. Entries for the confluent exponent Δ_1 are defined in Sec. III B.

s	$M_2^0(s)$	$v_c^{-1}(s)$	$k_B T_c(s)/J$	$A(s)$	$B(s)$	Δ_1
0.5	1	9.7953 ± 0.0005[a]	9.7953 ± 0.0005[a]	0.972 ± 0.002[b]	0.00 ± 0.02[b]	...[c]
1.0	$\frac{2}{3}$	10.2316 ± 0.0009	6.8211 ± 0.0006	0.565 ± 0.005	0.122 ± 0.009	0.51(0.34)
1.5	$\frac{5}{9}$	10.3647 ± 0.0010	5.7582 ± 0.0006	0.452 ± 0.004	0.178 ± 0.012	0.54(0.40)
2.0	$\frac{1}{2}$	10.4233 ± 0.0014	5.2117 ± 0.0007	0.400 ± 0.003	0.214 ± 0.012	0.55(0.44)
2.5	$\frac{7}{15}$	10.4546 ± 0.0010	4.8788 ± 0.0004	0.368 ± 0.003	0.229 ± 0.012	0.55(0.44)
3.0	$\frac{4}{9}$	10.4731 ± 0.0010	4.6547 ± 0.0004	0.348 ± 0.003	0.241 ± 0.011	0.55(0.44)
3.5	$\frac{3}{7}$	10.4851 ± 0.0010	4.4936 ± 0.0004	0.334 ± 0.003	0.248 ± 0.011	0.55(0.45)
4.0	$\frac{5}{12}$	10.4932 ± 0.0010	4.3722 ± 0.0004	0.324 ± 0.003	0.254 ± 0.011	0.55(0.45)
4.5	$\frac{11}{27}$	10.4990 ± 0.0010	4.2774 ± 0.0004	0.316 ± 0.002	0.258 ± 0.011	0.55(0.45)
5.0	$\frac{2}{5}$	10.5033 ± 0.0010	4.2013 ± 0.0004	0.310 ± 0.002	0.261 ± 0.011	0.55(0.45)
5.5	$\frac{13}{33}$	10.5066 ± 0.0009	4.1390 ± 0.0004	0.305 ± 0.002	0.263 ± 0.011	0.55(0.46)
∞	$\frac{1}{3}$	10.5236 ± 0.0009	3.5079 ± 0.0003	0.256 ± 0.002	0.275 ± 0.010	0.55(0.46)

[a]This value from direct ratio analysis compares with 9.794 ± 0.001 from Ref. 16 and 9.7950 ± 0.0005 from Ref. 31.

[b]This value from direct ratio analysis compres with 0.9750 ± 0.0003 from Ref. 28 [based on a slightly different $T_c(\frac{1}{2})$] and 0.963 ± 0.002 from Ref. 31.

[c]There is no evidence of a confluent singularity in the data of Table III for $s = \frac{1}{2}$, a conclusion in agreement with Ref. 31.

fixed $s > \frac{1}{2}$ that (3) makes 1.25 a *better* susceptibility exponent than 1.23. Unfortunately, we have been unable to do this. The four-fit analysis described in Sec. II B assumed $\gamma = \frac{5}{4}$, in accordance with well-established $s = \frac{1}{2}$ results.[16,31] If we assume instead $\gamma = 1.23$, following the apparent ratio estimates for $s = \infty$, the convergence of the $s = \infty$ four-fit estimates

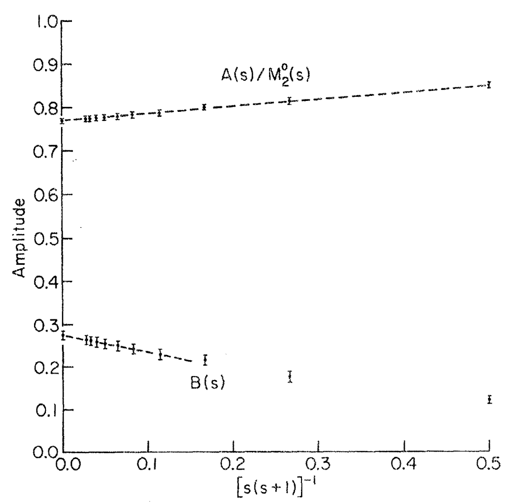

FIG. 2. Leading and confluent amplitudes for the spin-s fcc Ising susceptibility, as defined by Eq. (3). $M_2^0(s) = (s+1)/3s$. Data are taken from Table VI. $s = \frac{1}{2}$ is not shown. Dashed straight lines emphasize the linearity of the data for large s.

does not become noticeably worse than that shown in Table III.[41] We have also tried leaving γ free and using five successive a_k's to extract "five-fit" estimates for $(v_c)_k$, A_k, B_k, $(\Delta_1)_k$, *and* $(\gamma)_k$ via (15). The introduction of a fifth parameter leads to results with noticeably more scatter than is evident in Table III, and no firm conclusion can be drawn.[42] It is reassuring, however, to find (see Sec. III B) that, under the assumption $\gamma = \frac{5}{4}$ for all s, the correction exponent Δ_1 *does* turn out universal.

B. Parameters of the critical susceptibility

Table VI shows our four-fit evaluations[43] of the parameters (3) of the critical susceptibility of the nearest-neighbor fcc Ising model (7) for a variety of spins, as based on twelve-term high-temperature series. Numbers are derived from data such as Table III. Extrapolation and uncertainties are discussed at the end of Sec. II B. The column giving the correction exponent Δ_1 lists both the last ($k = 10$) estimate $(\Delta_1)_k$ and the corresponding linear extrapolant (bracketted). We conclude conservatively that the correction-to-scaling exponent (2) has the universal value[43]

$$\Delta_1 = 0.50 \pm 0.05 \quad \text{for all } s > \tfrac{1}{2} \tag{20}$$

in agreement with renormalization-group results.[12–14]

The amplitudes $A(s)/M_2^0(s)$ and $B(s)$ are exhibited in Fig. 2. Both show rather linear behavior when plotted versus $[s(s+1)]^{-1}$. The confluent amplitude vanishes at $s=\frac{1}{2}$ to within uncertainties,

$$B(\tfrac{1}{2}) = 0.00 \pm 0.02 . \qquad (21)$$

If it is true that $B(\frac{1}{2})$ vanishes identically, it is certainly an intriguing "accident."

We close on a note of warning: The (fcc) susceptibility series are particularly clean. Similar analysis of other fcc series[23] (e.g., second-moment series) does not yield results of equal clarity.

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[1]M. E. Fisher, Rept. Prog. Phys. 30, 615 (1967).

[2]*Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1972–1974), Vols. 1–4.

[3]D. S. Gaunt, Proc. Phys. Soc. Lond. 92, 150 (1967); D. S. Gaunt and G. A. Baker, Jr., Phys. Rev. B 1, 1184 (1970); M. S. Green, M. J. Cooper, and J. M. H. Levelt Sengers, Phys. Rev. Lett. 26, 492 (1971); M. J. Cooper, J. Phys. (Paris) 32, C1-349 (1971); C. Domb and D. S. Gaunt, *ibid.* 32, C1-344 (1971). These works contain earlier references.

[4]For example, the energy density of magnetic systems has critical behavior $t^{1-\alpha}$ but is, of course, finite at $t=0$ $(T=T_c)$, with a background term which is usually assumed analytic, constant $+a_1 t+\cdots$.

[5]In zero field and on loose-packed lattices the free energy has the symmetry $w(J,T)=w(-J,T)=w(J,-T)$, so in the complex T plane there are symmetric singularities at $T=\pm T_c$. Field-related quantities like the susceptibility lack the symmetry but retain some singular behavior at $T=-T_c$. See M. F. Sykes and M. E. Fisher, Physica (Utr.) 28, 919 (1962).

[6]Other examples are provided by the low-temperature Ising series, such as A. J. Guttmann, C. J. Thompson, and B. W. Ninham, J. Phys. C 3, 1641 (1970); C. Domb and A. J. Guttmann, *ibid.* 3, 1652 (1970).

[7]They may, of course, be related to critical fluctuations belonging to other phase transitions, as in the antiferromagnetic example cited above.

[8]See Ref. 3 and footnote 5 of Ref. 9.

[9]F. J. Wegner, Phys. Rev. B 5, 4529 (1972). See also F. J. Wegner, in *Renormalization Group in Critical Phenomena and Quantum Field Theory: Proceedings of a Conference*, edited by J. D. Gunton and M. S. Green (Temple U.P., Philadelphia, Pa., 1974), pp. 73–82.

[10]We ignore here the special effect of marginal operators. Discussion is given in Ref. 9.

[11]The definition (2) makes $\Delta_1>0$ and departs from Wegner (Ref. 9), who would have $\Delta_j=-\omega\nu$.

[12]The term $O(\epsilon)$ was originally noted in Ref. 9 and first appeared in F. Wegner, Phys. Rev. B 6, 1891 (1972).

[13]The term $O(\epsilon^2)$ was added by A. Aharony, Phys. Rev. B 8, 3349, 4270 (1973).

[14]The full calculation $O(\epsilon^3)$ was carried through by Callan-Symanzik techniques, E. Brezin, J. C. Le Guillou, and J. Zinn-Justin, Phys. Rev. D 8, 2418 (1973); and Phys. Rev. B 8, 5330 (1973).

[15]Technically, what has been calculated is the index of the leading irrelevant operator *near four dimensions*. In identifying this at $\epsilon=1$ with the $d=3$ correction exponent, we make the added assumption that there is no crossing in going from four to three dimensions.

[16]M. A. More, D. Jasnow, and M. Wortis, Phys. Rev. Lett. 22, 940 (1969).

[16a]J. Swift and M. K. Grover, Phys. Rev. B (to be published).

[16b]G. R. Golner and E. K. Riedel, Phys. Rev. B (to be published).

[17]M. Wortis, paper presented at Newport Beach Conference on Phase Transitions, January, 1970 (unpublished).

[18]F. Barouch, B. M. McCoy, and T. T. Wu, Phys.Rev. Lett. 31, 1409 (1973); 32, 35 (E) (1974).

[19]M. F. Sykes, D. S. Gaunt, P. D. Roberts, and J. A. Wyles, J. Phys. A 5, 624 (1972).

[20]W. J. Camp and J. P. Van Dyke, following paper, Phys. Rev. B 11, 2579 (1975).

[21]J. P. Van Dyke and W. J. Camp, Phys. Rev. B 9, 3121 (1974).

[22]D. S. Greywall and G. Ahlers, Phys. Rev. Lett. 28, 1251 (1972); Phys. Rev. A 7, 2145 (1973). See also, G. Ahlers, *ibid.* 8, 530 (1973).

[23]D. M. Saul and M. Wortis (unpublished).

[24]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965), p. 810.

[25]F. Englert, Phys. Rev. 129, 567 (1963).,

[26]M. Wortis, D. Jasnow, and M. A. Moore, Phys. Rev. 185, 805 (1969).

[27]M. Wortis, in Ref. 2, Vol. 3.

[28]M. Ferer and M. Wortis, Phys. Rev. B 6, 3426 (1972). Each spin value required about 10 min of computer time on an IBM 360/75.

[29]C. Domb and M. F. Sykes, Phys. Rev. 128, 168 (1962). A typographical error in order $k=4$ is noted and rectified in Ref. 21. Our coefficients are related to the $h_k(s)$ of Domb and Sykes (see also Refs. 20 and 21) by $h_k(s)=a_k(s)\,(\frac{1}{3}X)^k$.

[30]Our coefficients for $s=1$, 2, and ∞ appear in an article by C. Domb in Ref. 2, Vol. 3.

[31]Our program satisfies extensive checks through order $k=11$. Comparison with results of M. F. Sykes, D. S. Gaunt, P. D. Roberts, and J. A. Wyles [J. Phys. A 5, 640 (1972)] suggests that for the fcc lattice (only) our a_{12} contains a small systematic error. The magnitude of the error is so small (10^{-6}) that it is undetectable in

the analysis undertaken herein.

[32]D. S. Gaunt and A. J. Guttmann, in Ref. 2, Vol. 3. D. L. Hunter and G. A. Baker, Jr., Phys. Rev. B 7, 3346 (1973); 1, 3377 (1973).

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

[34]There is good evidence from series that all these provisos are, in fact, true for the high-temperature fcc Ising susceptibility.

[35]M. G. Darboux, J. Math. 3, 377 (1878); and M. Hamy, *ibid.* 4, 203 (1908), as cited by B. W. Ninham, J. Math. Phys. 4, 679 (1963) and C. Domb, Adv. Phys. 19, 339 (1970).

[36]A method very similar to ours was developed in Ref. 20, where the parameters in the asymptotic expression [see (17)]

$$\rho_k = \frac{1}{v_c}\left(1 + \frac{\gamma - 1}{k} + \frac{a}{k^{1+\Delta_1}} + \frac{b}{k^2} + \cdots\right)$$

are fit to successive ratios. It is also pointed out in Ref. 20 that another (more sophisticated) method [due to G. A. Baker, Jr. and D. L. Hunter, Phys. Rev. B 7, 3377 (1973)] gives consistent results.

[37]D. M. Saul, Ph. D. thesis (University of Illinois, 1974) (unpublished), Appendix B.

[38]M. A. Moore, D. M. Saul, and M. Wortis, J. Phys. C 7, 162 (1974); D. M. Saul, M. Wortis, and D. Stauffer, Phys. Rev. B 9, 4964 (1974).

[39]In practice, we form the Neville table and quote the last entry in the linear extrapolant column. For example, for $s=\infty$ this reads $k_B T_c(\infty)/M_2^0(\infty)\, J = 10.5236$, which is larger by 0.0018 than the $k=10$ direct estimate, so we assign ± 0.0009 as uncertainty.

[40]Continuous variation of the critical exponents can occur for special cases where the energy scales like the dimensionality, as in the Baxter model, R. J. Baxter, Phys. Rev. Lett. 26, 832 (1971); however, this exception is not relevant to the Ising model and can be understood within the renormalization-group context, as shown by L. P. Kadanoff and F. J. Wegner, Phys. Rev. B 4, 3989 (1971) and in Ref. 9.

[41]Nor, on the other hand, does it become any better. The $s=\frac{1}{2}$ four-fit analysis with $\gamma = 1.23$ *is* noticeably poor; however, the point is not that 1.23 is a candidate for a universal γ but rather that four-fit analysis cannot rule out $\gamma = 1.23$ *for* $s=\infty$.

[42]There *is* still some trend towards $\gamma_k < \frac{5}{4}$ for $s > \frac{1}{2}$, though perhaps a little less than in the direct ratio analysis.

[43]As mentioned in Sec. I, our results are in substantial agreement with those of Ref. 20. The dependence $T_c(s)$ is empirically parametrized in Eq. (3.9) of Ref. 21.