This is in sharp contrast to the sc and bcc ferromagnets where no such state exists. It would be interesting to investigate the behavior of this bound state for an arbitrary wave vector.

It is interesting to compare the present calculation of the two-magnon optical spectrum with a similar calculation in a Heisenberg antiferromagnet.[14] In that case, the *attractive* interactions caused a resonant peak to develop just below the top of the band. The position of this peak was rather insensitive to the crystal structure and determined by a square-root divergence in the density of states at the zone boundary. This divergence occured as a result of the form of the antiferromagnetic spin waves rather than the structure of the lattice. By contrast, in the present case, we find that the *repulsive* force may lead to a bound state, but the geometry of the lattice is a very important aspect.

ACKNOWLEDGMENT

The author would like to thank T. Moriya for an interesting conversation.

APPENDIX

The Green's function $I_{fcc}(\epsilon)$ is calculated near to the zone boundary. The imaginary part is obtained from (5.2) and the real part from the Kramers-Kronig relation (5.3) using the computations of Frikkee[9] for $\mathrm{Im} I_{fcc}(\epsilon)$ for $-0.96 < \epsilon < 3$ and the asymptotic form (5.2) for $-1 < \epsilon < -0.96$. We estimate that, due to the difficulties of the numerical integration, the real part is correct to about 5%. See Table I.

[1]M. Wortis, Phys. Rev. 132, 85 (1963).
[2]N. D. Mermin and H. Wagner, Phys. Rev. Letters 17, 1133 (1966).
[3]See, for example, P. A. Fleury and R. Loudon, Phys. Rev. 166, 514 (1968).
[4]T. Moriya, J. Phys. Soc. Japan 29, 117 (1970).
[5]R. J. Elliott and R. Loudon, Phys. Letters 3, 189 (1963).
[6]R. Silberglitt and A. B. Harris, Phys. Rev. 174, 640 (1968).
[7]T. Wolfram and J. Callaway, Phys. Rev. 130, 2207 (1963).
[8]F. J. Dyson, Phys. Rev. 102, 1217 (1956); 102, 1230 (1956).
[9]E. Frikkee, J. Phys. C 2, 345 (1969).
[10]D. T. Teaney, in *Critical Phenomena*, edited by M. S. Green and J. V. Sengers, Natl. Bur. Std. (U. S.) Misc. Publ. No. 273 (U. S. GPO, Washington, D. C., 1966), p. 50.
[11]G. S. Rushbrooke and P. J. Wood, Mol. Phys. 1, 257 (1958).
[12]T. R. McGuire, B. E. Argyle, M. W. Shafer, and J. S. Smart, J. Appl. Phys. 34, 1345 (1963).
[13]N. Menyuk, K. Dwight, and T. B. Reed, Phys. Rev. B 3, 1689 (1971).
[14]R. J. Elliott and M. F. Thorpe, J. Phys. C 2, 1630 (1969).

PHYSICAL REVIEW B VOLUME 4, NUMBER 5 1 SEPTEMBER 1971

Spin-$\frac{1}{2}$ Heisenberg Ferromagnet on Cubic Lattices: Analysis of Critical Properties by a Transformation Method*

M. Howard Lee and H. Eugene Stanley
Physics Department and Center for Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 5 November 1969; revised manuscript received 19 April 1971)

The high-temperature series expansions for the spin-$\frac{1}{2}$ Heisenberg ferromagnetic model on cubic lattices are analyzed by a transformation method. Evidence is presented suggesting that the susceptibility critical exponent (γ) and the gap parameter (2Δ) are both smaller than the original estimates obtained by Padé approximant techniques. Specifically, we find that $\gamma = 1.36 \pm 0.04$ and $2\Delta = 3.50 \pm 0.20$. The error limits are to be taken as a reasonable confidence level rather than as a strict bound.

I. INTRODUCTION

Critical properties of all realistic three-dimensional models of magnetism are determined by the method of exact series expansions. It is generally accepted that critical values of the Ising model are, on the whole, reliably established.[1] Critical values of other models, such as the spin-$\frac{1}{2}$ *XY* model[2] and the spin-$\frac{1}{2}$ Heisenberg model,[3] have been determined only recently and with an uncertainty generally greater than in the Ising counterparts. In these extreme quantum models, the noncommutativity of spin operators complicates the evaluation of expansion coefficients enormously; moreover, there is an irregularity in the resulting series, apparently related to the noncommutativity in some way not yet understood, making the job of analysis difficult (and consequently the estimated values not entirely reliable).

For the spin-$\frac{1}{2}$ Heisenberg ferromagnet on regular cubic lattices, which is our main concern, there are now known a sufficient number of high-temperature expansion coefficients for several functions, from which one can make estimates of relevant critical values. However, the generally irregular nature of the coefficients (i.e., the magnitudes of these coefficients change in an irregular fashion) has taxed the capacity of the existing techniques of analysis. Although some critical values (notably the critical points, susceptibility exponent, gap parameter) have been estimated, they are in all probability not immune from some small but significant changes as either higher-order expansion coefficients become known or techniques of analysis become more refined.

Estimates for the critical point and exponent are usually made from a high-temperature series expansion by ratio and Padé approximant methods. Although the two methods are not directly related and employ different standards of reliability, estimates made by them are often comparable and consistent. When the two methods yield inconsistent values as they are in some cases known to do, it becomes difficult to decide which values are more reliable. If a series behaves very irregularly, the ratio method is essentially useless. In such a situation one has only the Padé approximant method to rely on. Since any result of series extrapolations (from a finite number of terms) is not rigorous, it is desirable to analyze a series by as many different methods as available to guard against some possible systematic errors.

The series for the $S=\frac{1}{2}$ Heisenberg ferromagnet are of the irregular kind and have been analyzed largely by the Padé approximant method. We provide here an analysis of these series by a transformation method. While this method is not new, we believe that it has not been hitherto applied with advantage to high-temperature series expansions. A series whose coefficients of expansion change in an irregular fashion indicates the presence of more than one singularity. The transformation method seeks to isolate the physical singularity, so that the series represents essentially an expansion of the physical singularity.

II. HEISENBERG MODEL

The Heisenberg model is defined by the Hamiltonian

$$\mathcal{H} = -2J\sum_{ij} \mathbf{S}_i \cdot \mathbf{S}_j - \mu H \sum_i S_i^z , \qquad (1)$$

where S_i is the spin operator at site i of a given cubic lattice, S_i^z is the z component of S_i which is the same as the direction of the external magnetic field H, μ is the magnetic moment, and J is the exchange coupling constant ($J>0$ for ferromagnetic coupling). The first sum in (1) is over pairs of nearest-neighbor sites only.

The Heisenberg model, which is a natural generalization of the Ising model, may be realized in many realistic magnetic systems. Recently, much effort has been expended in obtaining critical properties of this model by the method of exact series expansions as in the three-dimensional Ising model.[1] For the case of $S=\frac{1}{2}$ on the fcc, bcc, and simple cubic (sc) lattices, Baker *et al.*[3] have considerably extended the evaluation of the expansion coefficients for the susceptibility, specific heat, and some higher field derivatives of the free energy, all of which should diverge as the critical point is approached. The susceptibility series, usually the best behaved and hence used to determine the critical point, are markedly less regular than the susceptibility series of the Ising model. The other series are even less regular. A thorough analysis of these series is given by Baker *et al.* using the Padé approximant techniques almost exclusively.

Among these estimated critical values, the susceptibility exponent (γ) and the gap parameter (2Δ) are of special interest to us. The susceptibility exponent is estimated[3] to be $\gamma = 1.43 \pm 0.01$ for all three cubic lattices, and the gap parameter, less reliably, $2\Delta = 3.63 \pm 0.03$ for the fcc lattice (evidence for the other lattices is not satisfactory).

If this estimated value for the susceptibility exponent, $\gamma \approx 1.43$, by Baker *et al.* is correct (as indeed their extensive evidence tends to support it), it raises certain difficult questions. First, the susceptibility exponent for the $S=\infty$ Heisenberg model on the same cubic lattice is estimated to be $\gamma \simeq 1.38$.[4] As the series for $S=\infty$ are on the whole regular, this value can be accepted with reasonable confidence. Then the small difference between the values of γ for $S=\frac{1}{2}$ and $S=\infty$, if it really exists, would suggest that γ might be, at least, weakly spin dependent. However, this sort of spin dependence is inconsistent with the basic assumptions of scaling laws.[5] Second, quite independently, Bowers and Woolf[6] have advanced, based on somewhat indirect but reasonable evidence, that $\gamma \simeq 1.38$ for all cubic lattices *and* for all spin values.

In order to resolve this apparent discrepancy, it seemed to us that a reexamination of the series for $S=\frac{1}{2}$ by some other methods of analysis, other than the Padé approximant method, might be in order. Baker *et al.* have made abundantly clear that their estimates are necessarily subject to the basic procedural assumption of Padé analysis being tenable. There are two well-known important shortcomings inherent in the Padé approximant method. First, Padé analysis seeks convergence and mutual consistency rather than trend. This kind of criterion has an obvious built-in danger. Second, the Padé approximant method unfortunately places too heavy an emphasis on initial coefficients of a series. Clearly the asymptotic behavior of a series should not significantly depend on initial coefficients.

It is for these reasons that any analysis of a finite-termed series by the Padé approximant method ought to be complemented, if possible, by the ratio method. The ratio method uses only ratios of successive coefficients and incorporates a final extrapolation.[7] It works best when the physical singularity unambiguously determines the radius of convergence. That is, when the physical singularity is the only singularity or when it is by far the nearest singularity (to the origin of the $K=J/kT$ plane). In such cases, extrapolations by the ratio method can be exceedingly accurate and reliable. If nonphysical singularities exist near the circle of convergence, as in the case of $S=\frac{1}{2}$, the analysis of a series by the ratio method becomes nontrivial.

III. TRANSFORMATION METHOD

A thermodynamic function $f(K)$, such as the susceptibility, is generally assumed to obey, near its critical point, a power law

$$f(K)\sim (K_c - K)^{-q}, \quad K\to K_c^- \tag{2}$$

where q is the critical exponent. The function $f(K)$ being analytic can be given a power series expansion about the origin in the form of $f(K)=\sum_{n=0}^{N} a_n K^n$, convergent up to the circle of convergence determined by K_c. If K_c is the only singularity or the nearest singularity of $f(K)$, the values of K_c and q may be determined if a sufficient number of the expansion coefficients a_n are known (usually about 10 for three-dimensional lattices).

If nonphysical singularities K_i with strengths q_i exist near the circle of convergence, the power series expansion may be useful if and only if $N\to\infty$, where N is the total number of exactly determined expansion coefficients. For a finite N (~ 10), the existence of these singularities is manifested through an irregular variation in the values of a_n. In extreme cases, the behavior of a_n may seem randomly changing in both sign and magnitude. In others the behavior, while irregular, may still be comparatively smooth, indicating that the strengths (q_i) of nonphysical singularities are weak compared with the critical strength of the physical singularity (i.e., $|q_i|\ll q$). But if they are not sufficiently weak (i.e., $|q_i|\lesssim q$), their influence may very well persist asymptotically. For these cases, obtaining one or two additional higher-order coefficients (always a laborious task) is not expected to be of much direct benefit. This sort of irregular behavior makes it difficult to determine K_c and q unambiguously.

Suppose by some means the locations of all the principal singularities of $f(K)$ are known and $q>|q_i|$. Consider a conformal transformation, say, $K^* = G(K)$. If, by the transformation, nonphysical singularities K_i are mapped onto K_i^* in such a way that now K_i^* are farther removed from the transformed circle of convergence (determined by K_c^*). Then since the transformed series, say, $f(K^*)=\sum_{n=0}^{N} \times b_n K^{*n}$, is dominated by the nearest and strongest singularity, K_c^*, it should be possible to apply the ratio method for the analysis of the series. It will be seen that the transformation can also improve the analysis by the Padé approximant method.

What kind of transformation can one apply? For a completely convergent series, almost any conformal transformation may suffice. But for functions, which are or can be given in terms of only a finite number of expansion coefficients, it is essential to find the "right" transformation. The desired transformation must be one which gives

$$f(K^*)\sim (K_c^* - K^*)^{-q}, \quad K^*\to K_c^{*-} . \tag{3}$$

It must also determine the nth transformed coefficient b_n solely by the n exactly known coefficients a_n. That is, $b_n = f(a_n, a_{n-1}, a_{n-2}, \ldots a_1, a_0)$. Thus transformations such as $K^* = G(0)+G(K)$, where $G(0)$ is a nonzero constant, are to be excluded.

As is well known, the critical point and exponent can be obtained by approximating the series expansion in the form of N zeros and D poles (the $[N, D]$ Padé approximants). The critical point is usually given by one of real positive poles which appear most consistently among the $[N, D]$ Padé elements and which converge to some apparent value. The critical exponent is given by the residue at that pole. Among the Padé elements the more important or reliable elements are the main diagonal ones (i.e., $N=D$) and the next diagonal ones (i.e., $N=D\pm 1$).

If a transformation leaves the diagonal elements of the Padé approximants to $f(K)$ invariant, there is little advantage to be gained by the transformation in so far as Padé analysis is concerned. Among Padé approximants, the most commonly used are Padé approximants to the logarithmic derivative of $f(K)$, which converts the singularities into simple poles. It can be shown that under a bilinear transformation the invariant elements are the less important $[N, D=N+2]$. Thus this type of transformation may indeed hasten the convergence of the main diagonal elements for the logarithmic derivative of a function.

The transformation method has been used before. The ideas and applications of this method are found in Danielian and Stevens,[8] Baker, Gammel, and Willis,[9] Gaunt and Fisher,[10] Baker,[11] and Guttmann,[12] among others. References to more recent work may be found in Lee and Stanley.[13] The most notable results seem to be due to Gaunt and Fisher, who have analyzed the activity and virial series by this method for phase transitions in a hard-sphere lattice gas model.

IV. EXTRAPOLATION PROCEDURES

We shall briefly describe two principal extrapolation procedures used in this paper in connection with the transformation method.

A. Ratio Method

The ratio method rests on the observation that if $f(K)$ obeys a power law near the critical point K_c, ratios of successive coefficients $\rho_n = a_n/a_{n-1}$ are given by

$$\lim_{n\to\infty} \rho_n = K_c^{-1}\left[1 + (q-1)\frac{1}{n} + O\left(\frac{1}{n^2}\right)\right] \quad . \tag{4}$$

Then, K_c^{-1} represents the asymptotic limit ($n\to\infty$) and $(q-1)$ the limiting slope of ρ_n. Estimates for these parameters can be made by extrapolations provided that the true nature of asymptotic behavior is indicated in the incomplete series.[1] The trend of successive ratios may be obtained by constructing a ratio plot or a Neville table. If ratios are smooth or regular, estimates for K_c and q can be made with a minimum uncertainty.

For the transformed series, ratios of successive coefficients $r_n = b_n/b_{n-1}$ are given by

$$\lim_{n\to\infty} r_n = K_c^{*-1}\left[1 + (q-1)\frac{1}{n} + O\left(\frac{1}{n^2}\right)\right] . \tag{5}$$

Given the value for K_c^*, we can then get the value for K_c by the inverse transformation equation $K = G^{-1}(K^*)$.

B. Padé Approximant Method

The $[N, D]$ Padé approximant[11] to $f(K)$ is an approximation by a rational function in the form of the ratio of two polynomials of degrees N and D. Their coefficients are chosen such that the coefficients of the expansion of the rational function, in powers of K, coincide with those of $f(K)$ through order $N+D$. Advantages of Padé approximants to the logarithmic derivatives of $f(K)$ are apparent since the singularities are only simple poles, which are easier to approximate.

The general procedure of Padé analysis, given the first n terms of a series, is to obtain all possible Padé approximants with $N+D = 1, 2, \ldots, n-1$. If the results of the last few orders are subtantially unchanged, the Padé table is regarded as having converged. This procedure may be further varied to check self-consistency.

V. ZERO-FIELD SUSCEPTIBILITY

The zero-field initial susceptibility is defined in the usual way:

$$\chi = kT \frac{\partial^2}{\partial H^2} \ln Z \big|_{H=0} , \tag{6}$$

where

$$Z = \mathrm{tr}\, e^{-\mathcal{H}/kT} . \tag{7}$$

The reduced susceptibility, $\tilde{\chi} = \chi kT/N\mu^2$, can be given a power series expansion in the form

$$\tilde{\chi}(K) = 1 + \sum_{n=1} a_n K^n , \tag{8}$$

where $K = J/kT$. The exact values of the expansion coefficients a_n for 3 cubic lattices (fcc, bcc, and sc) have been analyzed up to $n = 6$ by Domb and Sykes,[14] Gammel *et al.*,[15] and Baker.[16] Subsequently, Baker *et al.*[3] have calculated a_7, a_8, a_9 for the fcc lattice and a_7, a_8, a_9, a_{10} for the bcc and sc lattices. These values are reproduced in Table I.

The critical points are normally determined from the susceptibility since the series for the susceptibility are found most regular (hence easiest to pin down K_c accurately). Earlier estimates[14,15] based on 6 terms are $K_c = 0.246$, 0.392, and 0.588 for the fcc, bcc, and sc lattices, respectively, and $\gamma \simeq \frac{4}{3}$ for all 3 lattices. Estimates given by Baker *et al.*[3] using the extended series are $K_c = 0.2492$, 0.3973, and 0.5962 for the fcc, bcc, and sc lattices, respectively, and $\gamma = 1.43 \pm 0.01$ for all 3 cubic lattices.[17] These estimates are obtained using Padé analysis of the susceptibility series, by attaining a high degree of mutual self-consistency between the quoted values of K_c and $\gamma = 1.43$.

An examination of the susceptibility series reveals that unlike other susceptibility series (e.g., the Ising,[1] XY,[2] or $S=\infty$ Heisenberg susceptibility[4]) these series are markedly irregular. The irregu-

TABLE I. Exact coefficients of the susceptibility series expansions for the $S=\frac{1}{2}$ Heisenberg model on the fcc, bcc, and sc lattices. After Baker *et al.* (Ref. 3).

n	a_n(fcc)	a_n(bcc)	a_n(sc)
0	1	1	1
1	6	4	3
2	30	12	6
3	138	34.666666	11
4	611.25	95.833333	20.625
5	2658.55	262.7	39.025
6	11432.5125	708.0416666	68.7770833
7	48726.72619	1893.289683	119.4297619
8	206142.3674	5012.108631	216.1622768
9	866895.5063	13235.51327	387.1938327
10		34737.96523	658.3415398

TABLE II. Singularities of the susceptibility series on the fcc lattice given by Padé approximants to the logarithmic derivative of the series.

D/N	2	3	4	5	6
2			0.2411	0.2526 0.5362	0.2505 −0.9387
3		0.2482 $0.1300 \pm 0.3757i$	0.2495 $0.2119 \pm 0.3605i$	0.2491 $0.1899 \pm 0.3389i$	
4	0.2483 $0.1335 \pm 0.3756i$	$0.2443 \pm 0.0149i$ $0.1506 \pm 0.4271i$	0.2492 $0.1894 \pm 0.3477i$ −1.152		
5	0.2498 $0.2205 \pm 0.3912i$ −2.228 0.8657	0.2493 $0.1906 \pm 0.3546i$ −0.6903 2.232			
6	0.2491 $0.1959 \pm 0.3272i$ −1.480				

larity is evidently due to the presence of nonphysical singularities. It will be seen that some of the nonphysical singularities lie close to the circle of convergence (in the case of the sc lattice, the physical singularity actually is *not* the nearest singularity). Although it is not clear whether there is any physical significance behind these extra singularities, it is assumed that their removal will make the series behave more regularly. The interference by the nonphysical singularities may otherwise make the results of Padé analysis less than totally reliable, since this method of analysis at any rate is significantly influenced by these early coefficients which are interfered most and are meaningless in so far as the asymptotic behavior of the series is concerned.

Padé analysis can, nevertheless, be used to determine the *approximate* locations of physical and nonphysical singularities in the K plane. The results are given in Tables II, III, and IV for the fcc, bcc, and sc lattices, respectively. In these tables are shown singularities which are given consistently by Padé approximant analysis (these shall be called the principal singularities).

A. Susceptibility for fcc Lattice

The principal singularities of the susceptibility on the fcc lattice appear to be (i) a positive real pole at $K = K_1 \cong 0.25$, which is the physical singularity, (ii) a pair of complex poles at $K = K_2(\overline{K}_2) \cong 0.19 \pm i0.35$,

TABLE III. Singularities of the susceptibility series on the bcc lattice given by Padé approximants to the logarithmic derivative of the series.

D/N	2	3	4	5	6
2			0.3980 −0.5871	0.4020 −0.4621	0.3966 −0.3194
3		0.3922 −0.4212	0.4119 −0.5167	0.3995 −0.6744	0.3891 −0.3638
4	0.3926 −0.4021	0.3960 −0.4747 $-0.0937 \pm 0.3682i$	0.3953 −0.4694 $-0.0674 \pm 0.3314i$	0.3971 −0.4347 $-0.0575 \pm 0.4279i$	
5	0.5109 −0.5055 $0.0011 \pm 1.110i$	0.3953 −0.4692 $-0.0669 \pm 0.3319i$	0.3958 −0.4766 $-0.0796 \pm 0.3700i$		
6	0.4003 −0.5329 $-0.0806 \pm 0.8320i$	0.3970 −0.4239 $-0.0359 \pm 0.4368i$			
7	0.4074 −0.5564 $-0.0056 \pm 0.7954i$				[7, 2] 0.3931 −0.3878

TABLE IV. Singularities of the susceptibility series on the sc lattice given by Padé approximants to the logarithmic derivative of the series.

D/N	2	3	4	5	6
2		$0.3206 \pm 0.0952i$	0.7904 −0.4572	0.3552	0.2728
3	1.991 $0.3230 \pm 0.1734i$	0.5180 $0.0148 \pm 0.2551i$	0.6272 $-0.1757 \pm 0.4239i$	0.5658 $-0.1601 \pm 0.5749i$	0.6365 $-0.0153 \pm 0.5782i$
4	0.5700 −1.612 $-0.0582 \pm 0.3692i$	0.5944 −0.6318 $-0.0671 \pm 0.4984i$	0.5964 −0.6815 $-0.0780 \pm 0.5003i$	0.5950 −0.7261 $-0.0786 \pm 0.5069i$	
5	0.6163 −0.9250 $-0.1243 \pm 0.4763i$ 1.323	0.5965 −0.6784 $-0.0780 \pm 0.4997i$ 10.25	0.5956 $-0.0749 \pm 0.5055i$		
6	0.5828 −0.8020 $-0.1050 \pm 0.5226i$	0.5948 −0.7139 $-0.0798 \pm 0.5066i$			
7	0.6052 −0.7655 $-0.0717 \pm 0.5266i$				

(iii) a negative real pole at $K = K_3 \cong -1$, and (iv) a second positive real pole at $K = K_4 \cong 2$. The physical singularity $K_1 \equiv K_c \cong 0.25$, shown most consistently in the Padé table (Table II), determines the radius of convergence of the power series, being the nearest real positive singularity. The complex poles, K_2 and $\overline{K}_2$, also shown consistently, lie somewhat beyond the circle of convergence.[18] The negative real pole, shown to range from − 0.7 to − 2.2, probably centers on $K \cong -1$ if it exists at all.[19] Based solely on this Padé table, the existence of a second positive real pole is indeed to be doubted. But we shall show more substantial evidence for its existence.

If these singularities do exist, it would imply that the susceptibility has the form

$$\overline{\chi}(K) \sim (K_c - K)^{-\gamma}(K_2 - K)^{-q_2}(\overline{K}_2 - K)^{-\overline{q}_2} \times (K_3 - K)^{-q_3}(K_4 - K)^{-q_4}. \quad (9)$$

If $\gamma \gg |q_i|$, $i = 2, 3$, and 4, the series expansion about $K = 0$ is expected to be dominated by the physical singularity. That is, the values for the expansion coefficients a_n are largely determined by the expansion of $(K_c - K)^{-\gamma}$. Other singularities contribute to the expansion coefficients a_n in the form of small interference, diminishing as $n \to \infty$. An examination of the susceptibility series shows that although the ratios of the coefficients look relatively smooth, there is slight curvature, suggesting that the condition $\gamma \gg |q_i|$, $i = 2, 3$, or 4, is probably not satisfied. Since $K_2(\overline{K}_2)$ and K_3 lie in a proximity to the circle of convergence, we may expect the interference to come mainly from these singularities. The interference is thus determined not only by the closeness of nonphysical singularities to the circle of convergence but also by the relative strengths of these singularities.

Relative strengths of the singularities can be qualitatively observed through an increase or a decrease in interference by transforming the singularities. Consider the following bilinear transformation:

$$K^* = K/(1 + tK), \quad (10)$$

where t is a real number. Depending upon the value

TABLE V. Principal singularities of the susceptibility and their transformation according to the bilinear transformation.

		(a) fcc		
	$t=0$	$t=\frac{1}{2}$	$t=1$	$t=2$
K_c	0.25	0.22	0.20	0.17
$K_2(\overline{K}_2)$	$0.19 \pm 0.35i$	$0.18 \pm 0.23i$	$0.23 \pm 0.23i$	$0.21 \pm 0.15i$
K_3	~ -1	~ -2	$\sim (\pm)\infty$	~ 1
K_4	~ -2	~ 1	~ 0.7	~ 0.4
		(b) bcc		
	$t=0$	$t=\frac{1}{2}$	$t=1$	$t=2$
K_c	0.40	0.33	0.28	0.22
$K_2(\overline{K}_2)$	$-0.07 \pm 0.43i$	$0.88 \pm 0.38i$	$0.16 \pm 0.39i$	$0.22 \pm 0.21i$
K_3	−0.45	−0.58	0.83	−4.5
		(c) sc		
	$t=0$	$t=1$	$t=2$	$t=3$
K_c	0.60	0.38	0.27	0.21
$K_2(\overline{K}_2)$	$-0.08 \pm 0.50i$	$0.16 \pm 0.45i$	$0.25 \pm 0.29i$	$0.24 \pm 0.18i$
K_3	−0.70	−2.33	1.75	0.64
K_4	~ 25	0.70	0.49	0.25

TABLE VI. Coefficients of the transformed susceptibility series for the fcc lattice.

n	$b_n(\frac{1}{2})$	$b_n(1)$	$b_n(2)$
1	6	6	6
2	33	36	42
3	169.5	204	282
4	841.5	1121.25	1847.25
5	4103.425	6057.55	11916.55
6	19789.075	32373.7625	76100.0125
7	94657.04494	171681.0512	482493.8762
8	449768.7559	904869.2132	3042285.584
9	2125342.763	4745041.979	19096820.32

for t, the nonphysical singularities can be mapped in different relations to the physical singularity. In Table V are given the values of singularities for $t=0$, $\frac{1}{2}$, 1, and 2. If the interference comes mainly from the negative real pole K_3, then as may be observed from Table V(a), the bilinear transformation with $t=\frac{1}{2}$ and 1 should reduce the interference the most. If the interference comes from the negative real pole *and* complex poles, the bilinear transformation with $t=1$ and probably 2 would best serve to reduce the interference.

The series expansion for the susceptibility in powers of K^* is obtained from (8) by applying the bilinear transformation (10):

$$\tilde{\chi}(K^*;t)=1+\sum_{n=1} b_n(t)K^{*n}\,, \tag{11}$$

where

$$b_n(t)=f(a_n, a_{n-1}, \ldots, a_1; t). \tag{12}$$

The values for the expansion coefficients $b_n(t)$ are given in Table VI for $t=\frac{1}{2}$, 1, and 2. Ratios of successive coefficients of the transformed series show that for $t=\frac{1}{2}$ there is nearly as much interference as for $t=0$, but for $t=1$ the series is very regular, and for $t=2$ the series just begins to be regular. This would indicate that while the negative real pole

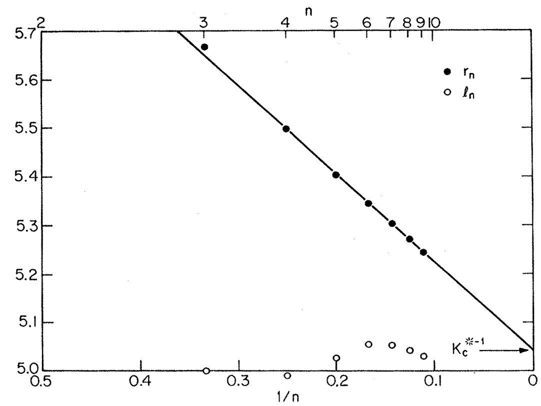

FIG. 1. Ratios of coefficients and linear extrapolants of the transformed susceptibility series $\tilde{\chi}(K^*;\ 1)$ for the fcc lattice.

gives the most interference, the complex poles provide a not negligible amount of interference (i.e., $|q_3|>|q_2|$).

Since the series for $t=1$ appears to have the least interference from the nonphysical singularities, we shall rely for the asymptotic properties on the analysis of this series. In Fig. 1, ratios of coefficients $r_n(1)=b_n(1)/b_{n-1}(1)$ together with linear extrapolants $l_n(1)=nr_n-(n-1)r_{n-1}$ are displayed in a conventional ratio plot. The values for r_n and l_n are given in Table VII (fcc). The trend of ratios $r_n(1)$, with increasing n, appears to be fairly well settled along the asymptotic line we have provided. Our reading of the intercept at $n=\infty$ is $K_c^{*-1}=5.042\pm0.010$ ($K_c^*=0.1983\pm0.004$).[20,21] Using this value of the intercept and the slope of the asymptote, we obtain from (5), $\gamma=1.36\pm0.04$. The inverse transformation $K=G^{-1}(K^*)$ gives $K_c=0.2475\pm0.0010$.[20]

Although the series for $t=2$ is not as regular as the series for $t=1$, essentially the same estimates are given by the coefficients $b_n(2)$. From a ratio plot of $b_n(2)$, we obtain $K_c^{*-1}(2)=6.043\pm0.20$ ($K_c^*=0.1655\pm0.0006$), $\gamma=1.36\pm0.06$, and by the inverse

TABLE VII. Ratios of coefficients and linear extrapolants for the three cubic lattices based on the coefficients of the transformed series $b_n(t)$.

n	r_n(1; fcc)	$l_n(1)$	r_n(1; bcc)	$l_n(1)$	r_n(2; sc)	$l_n(2)$
1	6		4		3	
2	6	6	4	4	4	5
3	$5\frac{2}{3}$	5	3.916667	3.75	3.916667	3.75
4	5.496324	4.985293	3.827128	3.558511	3.885638	3.792553
5	5.402497	5.027192	3.777762	3.580301	3.876934	3.842115
6	5.344366	5.053708	3.742182	3.564281	3.869958	3.835081
7	5.303092	5.055452	3.714659	3.549521	3.857719	3.784285
8	5.270641	5.043484	3.691922	3.532766	3.841578	3.728587
9	5.243898	5.029954	3.673678	3.527721	3.825157	3.693791
10			3.659109	3.527993	3.810973	3.683317

TABLE VIII. Singularities of $\tilde{\chi}(K^*; 1)$ on the fcc lattice given by Padé approximants to $d/dK^* \ln\tilde{\chi}(K^*; 1)$.

D/N	2	3	4	5	6
2	0.2017	0.1935	0.1975	0.1976	0.2020 ± 0.0129i
3	0.1972 0.3388 ± 0.3838i	0.1982 0.1717 ± 0.3627i	0.1989 0.1622 ± 0.2528i	0.1993 0.2005 ± 0.2188i	
4	0.1989 0.2051 ± 0.2635i	0.1996 0.2374 ± 0.2292i 0.6283	0.1995 0.2276 ± 0.2291i 0.7097		
5	0.1996 0.2352 ± 0.2291i −10.66 0.6445	0.1995 0.2285 ± 0.2298i −2.229 0.6906			
6	0.1995 0.2278 ± 0.2293i −4.677 0.7048				

transformation, $K_c = 0.2473 \pm 0.0015$. These values compare favorably with the estimates provided by the series for $t = 1$.

The Padé approximant analysis of the transformed series $\tilde{\chi}(K^*; 1)$ is given in Table VIII. The bilinear transformation maps K_3 away from the origin, whereas K_4 toward the origin, while leaving K_c and $K_2(\overline{K}_2)$ relatively unaffected. As may be thus expected, the second positive pole is shown more consistently in Padé analysis of $\tilde{\chi}(K^*; 1)$ than in the Padé analysis of $\tilde{\chi}(K)$, whereas the negative real pole is the opposite. The physical and complex poles are shown more or less the same in both tables. In comparing the Padé tables of $\tilde{\chi}(K)$ and $\tilde{\chi}(K^*; 1)$ it is useful to note that what remains invariant under the bilinear transformation are the [2, 4] and [3, 5] Padé approximants (out of the 12 approximants shown). Particularly, the [3, 5] Padé approximant may be regarded as a link between the two Padé tables. Based on Table VIII, a reasonable estimate for the critical point is $K_c^* = 0.199 \pm 0.001$ or $K_c = 0.248 \pm 0.002$. This value is consistent with the estimate given by ratio analysis.

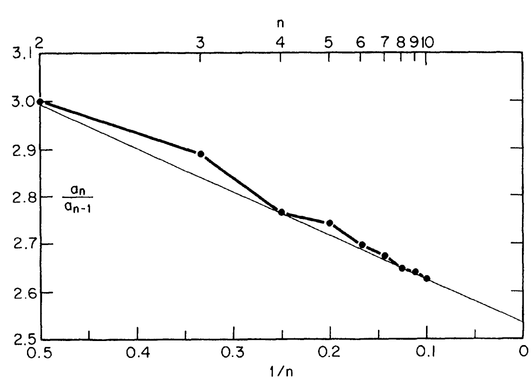

FIG. 2. Ratios of coefficients of the susceptibility series $\tilde{\chi}(K)$ for the bcc lattice. Successive ratios are linked to emphasize the effect of the interference by nonphysical singularities. Ratios are expected to converge onto the asymptotic line (solid line), obtained by removing the interference (redrawn from Fig. 3).

B. Susceptibility for bcc Lattice

The principal singularities of the susceptibility on the bcc lattice appear to be (i) a positive real pole at $K = K_c \cong 0.40$, which is the physical singularity, (ii) a pair of complex poles at $K = K_2(\overline{K}_2) \cong -0.07 \pm i0.43$, and (iii) a negative real pole at $K = K_3 \cong -0.45$. All these singularities are fairly consistently shown in the Padé table (see Table III). Since the complex poles and the negative real pole lie quite close to the circle of convergence, they are expected to interfere significantly with the series expansion of $(K_c - K)^{-\gamma}$ as one can clearly see in Fig. 2.

As in the case of the fcc lattice, we shall apply to the series the bilinear transformation (10) with $t = \frac{1}{2}$, 1 , and 2. In Table V(b) we give the values of the corresponding singularities. If only the negative real pole K_3 were to interfere the most, the transformation with $t = 2$ would be preferred. If on the other hand the negative real pole and the complex poles were to interfere roughly equally, the transformation with $t = \frac{1}{2}$ and 1 would undoubtedly serve the best. In Table IX the values of the expansion coefficients $b_n(t)$ are given. Ratios of coefficients show that for $t = 1$ the sequence of ratios is very regular; for $t = \frac{1}{2}$ the sequence is fairly regular but not as regular as for $t = 1$; and for $t = 2$ the sequence is not regular although considerably more so than for $t = 0$. This relative behavior suggests that the interference

TABLE IX. Coefficients of the transformed susceptibility series for the bcc lattice.

n	$b_n(\frac{1}{2})$	$b_n(1)$	$b_n(2)$
1	4	4	4
2	14	16	20
3	$47\frac{2}{3}$	$62\frac{2}{3}$	$98\frac{2}{3}$
4	$157\frac{1}{3}$	239.833 333	479.833
5	512.616 66	906.033 333	2 309.366
6	1 651.583 33	3 390.541 667	11 029.708
7	5 276.935 51	12 594.706 35	52 365.122
8	16 738.882 9	46 498.678 08	247 400.330
9	52 826.220 3	170 821.160 1	1 164 072.361
10	166 032.464 6	625 053.278 7	5 458 269.914

comes from the negative real pole and the complex poles more or less equally.

Since the series for $t=1$ appears to be most regular (i.e., least interfered by the nonphysical singularities in the series expansion), we shall rely for the asymptotic properties on the analysis of this series. In Fig. 3, ratios of coefficients $r_n(1)$ and linear extrapolants $l_n(1)$ are displayed in a ratio plot. The values for $r_n(1)$ and $l_n(1)$ for the bcc lattice are given in Table VII (bcc). A comparison with Fig. 2 shows a dramatic change in the behavior of the expansion coefficients.

The trend of $r_n(1)$ appears to be rather well settled along the asymptotic line we have provided in Fig. 3. Based on the intercept and the slope of the asymptote we estimate: $K_c^{*-1}=3.534\pm 0.010$ ($K_c^*=0.2829\pm 0.0015$)[22] and $\gamma=1.36\pm 0.04$. The inverse transformation gives $K_c=0.3946\pm 0.0015$.[20]

Although the series for $t=\frac{1}{2}$ and 2 are not as regular as the series for $t=1$, essentially the same estimates are given by them. From a ratio plot of $b_n(\frac{1}{2})$, we obtain $K_c^{*-1}(\frac{1}{2})=3.031\pm 0.020$, $\gamma=1.36\pm 0.06$, and $K_c=0.3951\pm 0.0035$. From a ratio plot of $b_n(2)$, we obtain $K_c^{*-1}(2)=4.532\pm 0.025$, $\gamma=1.36\pm 0.06$, and $K_c=0.3949\pm 0.0040$. Both series provide estimates for K_c and γ which are comparable with the estimates given by the series for $t=1$.

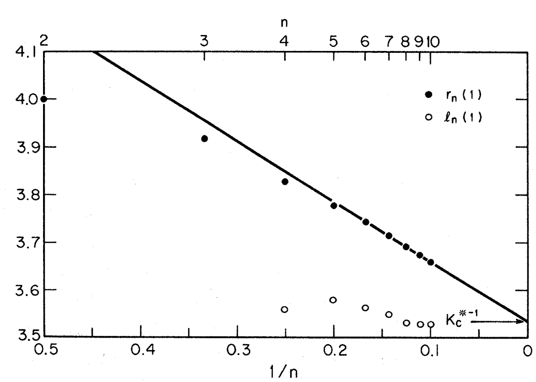

FIG. 3. Ratios of coefficients and linear extrapolants of the transformed susceptibility series $\tilde{\chi}(K^*;1)$ for the bcc lattice.

Padé approximant analysis of $\tilde{\chi}(K^*;1)$ is given in Table X. Based on the Padé table (Table X), a reasonable estimate for the critical point is $K_c^*=0.283\pm 0.002$ or $K_c=0.395\pm 0.003$, which is consistent with the estimate given by ratio analysis. There is slight evidence of a second positive real pole at $K^*\cong 0.7$ or $K\cong 2.3$ (not shown in our Table X).

C. Susceptibility for sc Lattice

Compared with the singularities of the susceptibility on the fcc and bcc lattices, the principal singularities for the sc lattice are given far less consistently by Padé approximants (see Table IV). This implies that not as much information is contained in this susceptibility series (with 10 coefficients) as in the series for the other lattices (with 9 and 10 coefficients, respectively, for the fcc and bcc lattices). Based on the coordination numbers, we might argue that the susceptibility series for the sc would need at least 3 or 4 more coefficients to contain a comparable degree of information.

The principal singularities for the susceptibility on the sc lattice appear to be (i) a positive real singularity at $K=K_c\cong 0.60$, (ii) a pair of complex poles at $K=K_2(\overline{K_2})\cong -0.08\pm i0.50$, and (iii) a negative real pole at $K=K_3\cong -0.70$. There is slight evidence of a second positive real pole (not shown in Table IV) at $K=K_4\cong 25$. Unlike in the two previous cases, the physical singularity is *not* the nearest singularity, and the radius of convergence of the power series is instead given by the complex poles. Thus the series expansion is expected to be quite irregular (see Fig. 4).

As in the previous two cases, we shall apply the bilinear transformation (10) to the series. In Table V(c) we give the values of the singularities for $t=0$, 1, 2, and 3, and in Table XI the values of the corresponding expansion coefficients. Referring to Table V(c), if the interference comes from the complex poles and the negative real pole approximately equally, the optimum choice for t seems to be $t=2$.

TABLE X. Singularities of $\tilde{\chi}(K^*; 1)$ on the bcc lattice given by Padé approximants to $d/dK^* \ln\tilde{\chi}(K^*; 1)$.

D/N	2	3	4	5	6
2		0.2813 −0.4125	0.2665 ± 0.0061i	0.2791	0.2846
3	0.2816 −0.9397	0.2795	0.2789	0.2738	0.2841 0.1916 ± 0.4930i
4	0.2819 −0.6724	0.2789	0.2795 −2.303	0.2831 0.2144 ± 0.2260i −0.3678	
5	0.2985 ± 0.0156i −1.042	0.2833 0.1454 ± 0.2659i −0.8840	0.2842 0.1471 ± 0.3890i −0.7229		
6	0.2811 0.1446 ± 0.1277i −0.9992	0.2840 0.1831 ± 0.3607i −0.5723			
7	0.2843 0.1069 ± 0.4265i −0.8703				[7, 2] 0.2844 −0.2533

Ratio plots of these coefficients show that only the sequence of ratios of $b_n(2)$ can be considered as regular. The others show signs of becoming regular. Since even the series for $t = 2$ is not sufficiently regular, we need additional coefficients to establish the trend of ratios more firmly. Thus our estimates here must necessarily be more tentative than those given for the other lattices.

In Table VII (sc) the values of $r_n(2)$ and $l_n(2)$ are given. Ratio analysis of $b_n(2)$ gives the following estimates: $K_c^{*-1} = 3.678 \pm 0.020$ (or $K_c^* = 0.2791 \pm 0.0015$) and $\gamma = 1.36 \pm 0.06$. Using the inverse transformation we obtain $K_c = 0.5959 \pm 0.0050$. The other series provide comparable estimates.

Padé approximant analysis of $\tilde{\chi}(K^*; 2)$ is given in Table XII. As may be observed, the physical singularity is given much more consistently here than in the Padé table (Table IV) of the original series. Except for the [2, 4] and [3, 5] Padé approximants, there is considerable improvement in the consistency of the physical singularity. This is not unexpected since by the transformation the physical singularity has become the nearest singularity. Based on the Padé table (Table XII), a reasonable estimate for the critical point is $K_c^* = 0.272 \pm 0.003$ or $K_c = 0.596 \pm 0.015$. The second positive real pole is also rather consistently shown at $K_4^* \cong 0.49$, corresponding to $K_4 \cong 25$, which is shown only inconsistently in the Padé table of $\tilde{\chi}(K)$.

In summary, the critical values given by ratio analysis of the transformed susceptibility series are $K_c = 0.2475 \pm 0.0015$, 0.3946 ± 0.0015, and 0.5959 ± 0.0050 for the fcc, bcc, and sc lattices, respectively, and $\gamma = 1.36 \pm 0.04$ for the 3 cubic lattices. Padé analysis of the transformed series has provided the estimates $K_c = 0.248 \pm 0.002$, 0.394 ± 0.003, and 0.596 ± 0.015 for the three respective lattices. Our reasons for having given less weight to the estimates by Padé analysis are based on our belief that since the interference by the nonphysical singularities are still present in the early coefficients of the transformed series, the results of Padé analysis cannot be taken as accurate as those of ratio analysis.

The estimates of the critical values obtained by Baker *et al.* using the Padé analysis of the original susceptibility series are $K_c = 0.2492$, 0.3973, and 0.5962 (with an error quoted to be about 10^{-3} for all three) for the fcc, bcc, and sc lattices, respectively, and $\gamma = 1.43 \pm 0.01$ for the three cubic lattices. Although these values for the critical points do considerably dis-

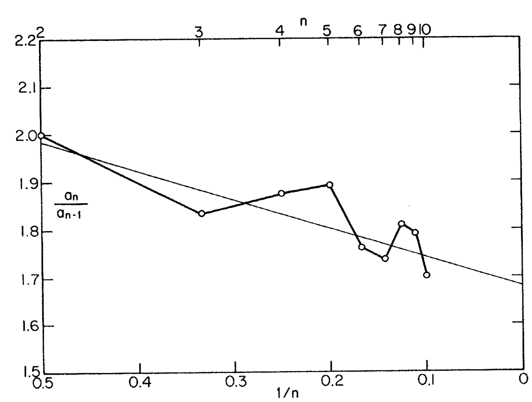

FIG. 4. Ratios of coefficients of the susceptibility series $\tilde{\chi}(K)$ for the sc lattice. Successive ratios are linked to emphasize the effect of the interference by nonphysical singularities. Ratios are expected to converge onto the asymptotic line drawn as $n \to \infty$, obtained by removing the interference.

TABLE XI. Coefficients of the transformed susceptibility series on the sc lattice.

n	$b_n(1)$	$b_n(2)$	$b_n(3)$
1	3	3	3
2	9	12	15
3	26	47	74
4	74.625	182.625	362.625
5	214.525	708.025	1771.525
6	613.152 083	2 740.027 083	8639.402 083
7	1733.967 262	10 570.254 76	42 063.292 26
8	4 860.239 36	40 606.453 94	204385.556 0
9	13 557.792 05	155 326.056 9	990790.088 4
10	37 725.590 5	591 943.398 4	4 791 209.715

agree with our estimates by ratio analysis, we contend that the comparison is not proper. This is because the presence of the nonphysical singularities will, as stated before, necessarily make the Padé values (given in four-place accuracy) suspect. If, on the other hand, the estimates of Baker *et al.* are accepted at three-place accuracy, as we have done for our Padé values, their estimates are in agreement with our estimates by Padé analysis of the transformed series. The disagreement between their value of the critical exponent $\gamma \cong 1.43$ and our value $\gamma \cong 1.36$ can also be resolved if we similarly accept their value at one order lower accuracy (i.e., $\gamma \cong 1.4$).

Our result $\gamma \cong 1.36$, if correct, can at once resolve the two issues earlier discussed. Namely, it restores the argument of an essential spin independence of the critical exponents (as is assumed by scaling laws) which had been left in some doubt by the previous higher value of the critical exponent γ. Also, it lends support to Bowers and Woolf[6] who have suggested that $\gamma \cong 1.38$ irrespective of the nearest-neighbor or finite-order equivalent model.

VI. HIGHER FIELD DERIVATIVES OF FREE ENERGY

Essam and Fisher[23] first suggested the idea of studying the $H=0$ critical behavior of higher field derivatives of the free energy. It is defined as

$$F_p(K) = \lim_{H\to 0} -kT \frac{\partial^{2p}}{\partial H^{2p}} \ln Z, \quad p = 2, 3, 4, \ldots$$

$$= \lim_{H\to 0} \frac{\partial^{2p-2}}{\partial H^{2p-2}} \chi. \tag{13}$$

Obviously, higher field derivatives of the free energy represent a family of many-spin correlation functions. Since F_p are obtained from the susceptibility, whose critical behavior is of a power law, it seems reasonable to make the following two assumptions: (i) The dominant critical behavior of F_p is of the power-law form

$$F_p(K) \sim (K_c - K)^{-\gamma_p}, \quad K \to K_c^- \tag{14}$$

where the exponents satisfy $\gamma_p > \gamma_{p-1} > \cdots > \gamma_2 > \gamma_1 \equiv \gamma$. The inequalities for the exponents derive from the fact that since F_p are obtained by taking derivatives of the susceptibility, the strength of the singularity can only increase with p. (ii) The principal singularities of F_p are those of the susceptibility. This assumption need not, indeed, may not, be strictly correct, as there may be *additional* nonphysical singularities associated with higher spin correlations. However, if the strength of the physical singularity is much greater than the strengths of these extra nonphysical singularities, the interference by these singularities should vanish rapidly with order. Both assumptions can be tested by obtaining power series expansions of F_p as in the case of the susceptibility. The interest in F_p comes from that accord-

TABLE XII. Singularities of the $\tilde{\chi}(K^*; 2)$ on the sc lattice given by Padé approximants to $d/dK^* \ln\tilde{\chi}(K^*; 2)$.

D/N	2	3	4	5	6
2		0.2609	0.2612	0.2541	0.2998 ± 0.0076i
3	0.2610	0.2612	0.2614	0.2666 0.1998 ± 0.1880i	0.2699 0.2686 ± 0.2217i
4	0.2664 0.1668 ± 0.2784i 0.7248	0.2705 0.2415 ± 0.2705i 0.5656	0.2717 0.2558 ± 0.2869i 0.4995	0.2719 0.2552 ± 0.2895i 0.4903	
5	0.2703 0.2394 ± 0.2686i 0.5749	0.2720 0.2534 ± 0.2920i 0.4767	0.2719 0.2549 ± 0.2896i 0.4888		
6	0.2716 0.2563 ± 0.2844i 0.5089	0.2719 0.2549 ± 0.2896i 0.4890			
7	0.2718 0.2560 ± 0.2891i 0.4940				[7, 2] 0.2739 0.5756

TABLE XIII. Exact coefficients of the series expansions for pth higher field derivative of the free energy for the three cubic lattices. After Baker *et al.* (Ref. 3).

n	$a_n^{(2)}$	$a_n^{(3)}$	$a_n^{(4)}$
		fcc	
1	24	51	87.53
2	327	1290	3506.12
3	3345	22405.5	91295.29
4	28653	305205	1788855.13
5	217479.7	3500313.93	28551488.46
6	1512289.6	35291185.89	389818850.65
7	9841725.23	321858058.80	4704418456.45
8	60808494.14	2708643241.72	51360029876.09
		bcc	
1	16	34	58.35
2	138	552	1509.18
3	888.67	6099.67	25162.20
4	4765.33	52503.33	313676.07
5	22629.8	379025.45	3170734.86
6	98445.57	2399790.29	27325927.82
7	401005.34	13726858.00	207675673.84
8	1551082.47	72402512.75	1425491650.98
		sc	
1	12	25.5	43.77
2	73.5	298.5	821.29
3	324.5	2317.25	9729.06
4	1176	13785	84932.58
5	3761.35	68094.21	595047.50
6	11002.25	293181.50	3527771.24
7	30058.27	1135642.09	18340359.35
8	77850.24	4044279.24	85750103.00

ing to scaling theories the gap parameter $2\Delta_p \equiv \gamma_p - \gamma_{p-1}$ is constant for all p. For the Ising model in three dimensions, it has been estimated that $\Delta = 1.56 \pm 0.03$.[24]

The series expansions for the *reduced* higher field derivatives of the free energy are given in the form

$$\tilde{F}_p(K) = 1 + \sum_{n=1} a_n^{(p)} K^n. \qquad (15)$$

Baker *et al.*[3] have obtained the exact values of the coefficients $a_n^{(p)}$ for $p = 2$, 3, and 4, up to $n = 8$, on the fcc, bcc, and sc lattices. These values are reproduced in Table XIII. The sequences of coefficients in these series are generally smooth indicating that the expansion coefficients are dominated by the expansion of $(K_c - K)^{-\gamma_p}$. However, owing to curvature in these sequences, it is difficult to obtain reliable estimates for the critical parameters directly from ratios of coefficients.

Padé approximant analysis of these relatively short series is not expected to be meaningful (there are in effect only 7 terms available for getting Padé approximants). While the results of our Padé analysis are too scattered to be conclusive, the whole picture of the singularities seems not inconsistent with our second assumption. Baker *et al.* have noted that these series are not well suited for Padé analysis because $\tilde{F}_p$ seem to vanish for some small negative real K. These zeros are then reflected as poles close to the origin in the logarithmic derivatives of the function (to which we make Padé approximants).

If the principal singularities of $\tilde{F}_p$ are those of $\tilde{\chi}$, then the interference by nonphysical singularities ($K_2, \overline{K}_2, K_3$, and K_4) can be essentially removed by the same transformation used for $\tilde{\chi}$ in Sec. V. Consider the bilinear transformation (10) for $\tilde{F}_p(K)$. In terms K^*, we have

$$\tilde{F}_p(K^*; t) = 1 + \sum_{n=1} b_n^{(p)}(t) K^{*n}. \qquad (16)$$

The optimum choice of t for the fcc, bcc, and sc lattices are then expected to be $t = 1$, 1, and 2, respectively, if our assumption (ii) is reasonably correct. The values of $b_n^{(p)}(t)$ for $p = 2$, 3, and 4 on the three cubic lattices are given in Table XIV.

A. fcc Lattice

Ratios of coefficients $b_n^{(p)}(1)$ for $\tilde{F}_p(K^*; 1)$, to-

TABLE XIV. Coefficients of the expansion for pth higher field derivative of the transformed free energy for the three cubic lattices.

n	$b_n^{(2)}$	$b_n^{(3)}$	$b_n^{(4)}$
		(1; fcc)	
1	24	51	87.53
2	351	1341	3 593.65
3	4 023	25 036.5	98395.06
4	39 693	376 342.5	2 073 346.90
5	353 493.7	4 860 777.93	36 268 792.76
6	2 921 327.1	56 075 361.51	551 395 415.4
7	22 802 879.33	592 557 856.5	7 508 771 544
8	170 145 854.8	5 836 437 316	93 541 008 792
		(1; bcc)	
1	16	34	58.35
2	154	586	1 567.53
3	1 180.67	7 237.67	28238.90
4	7 861.33	72 492.33	393 748.54
5	47 591.13	627 878.78	4 582 507.37
6	268 840.57	4 883 741.54	46 575 588.99
7	1 440 606.41	34 955 889.17	425 852 331.3
8	7 403 950.43	234 121 613.3	3 575 559 263.2
		(2; Sc)	
1	12	25.5	43.76
2	97.5	349.5	908.82
3	666.5	3 613.25	13 189.29
4	4 101	31474.5	153 512.58
5	23 501.35	243 948.21	1 534 987.20
6	127 879.75	1 735 599.62	13 720 978.15
7	668 686.22	11 560 156.79	112 461 140.5
8	3 387 120.66	73 050 677.65	859 934 931.6

gether with those of the susceptibility $\tilde{\chi}(K^*;1)$, are plotted in a conventional ratio plot (see Fig. 5). We observe that the sequences of $\tilde{F}_2$, $\tilde{F}_3$, and $\tilde{F}_4$ all approach the same intercept, provided by $\tilde{\chi}(K^*;1)$. We further observe that gaps between two nearest branches of the sequences are nearly constant. A reasonable estimate of the intercept at $n=\infty$ for each of $\tilde{F}_p$ is $K_c^{*-1}=5.04\pm0.20$, which is consistent with the earlier estimate given by the susceptibility series $\tilde{\chi}(K^*;1)$: $K_c^{*-1}=5.042\pm0.010$. Hence, we shall assume the estimate provided by the susceptibility series as the more nearly correct value of the critical point and use it in the analysis of the exponents for the higher field derivatives.

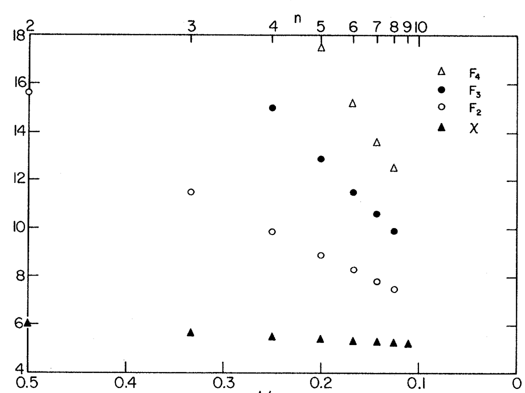

FIG. 5. Ratios of coefficients of $\tilde{\chi}(K^*;1)$ and $\tilde{F}_p(K^*;1)$ for the fcc lattice. Observe that all the asymptotes approach the same intercept and the gap between two nearest asymptotes at a given n becomes nearly constant as $n\to\infty$.

For the values of the exponents γ_p, we could directly make estimates of the limiting slopes from ratio plots as in the susceptibility exponent γ.

TABLE XV. Analysis of γ_2 for the fcc lattice based on $K_c^{*-1}(1)=5.042$. In constructing all Neville tables, more digits must be retained than are here displayed.

n	$r_n^{(2)}$ (1; fcc)	$s_n^{(2)}$	$g_n^{(2)}$	$l_n^{(2)}$	$q_n^{(2)}$
1	24	18.958	4.7600		
2	14.625	19.166	4.8013	4.8426	
3	11.461538	19.26	4.819	4.87	4.86
4	9.866518	19.30	4.827	4.85	4.85
5	8.905694	19.32	4.831	4.85	4.84
6	8.264156	19.33	4.834	4.85	4.85
7	7.805658	19.35	4.837	4.85	4.86
8	7.461595	19.36	4.839	4.85	4.86

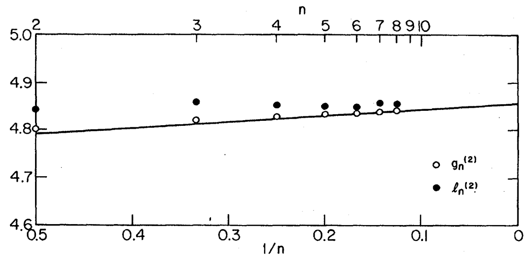

FIG. 6. Limiting exponents and linear extrapolants for γ_2 on the fcc lattice. The intercept of g_n at $n=\infty$ represents the value for γ_2. $K_c^{*-1}=5.042$.

However, by taking advantage of the accurately known K_c^{*-1}, a somewhat more convincing analysis can be obtained by the following procedure. The nth limiting slope $s_n^{(p)}$ is given by the relation

$$s_n^{(p)}=n(r_n^{(p)}-K_c^{*-1}), \tag{17}$$

where $r_n^{(p)}=b_n^{(p)}/b_{n-1}^{(p)}$. Here, s_n can be accurately calculated up to the known number of the expansion coefficients. The nth limiting exponent $g_n^{(p)}$ may be analogously defined by

$$g_n^{(p)}=1+s_n^{(p)}/K_c^{*-1}, \tag{18}$$

where $g_\infty^{(p)}\equiv\gamma_p$. When $s_n^{(p)}$ or $g_n^{(p)}$ are plotted sequentially in a $1/n$ ratio plot, and if these values fall on a straight line, reliable estimates for $s_\infty^{(p)}$ or $g_\infty^{(p)}$ can be made.

In Table XV, we have given successive values of r_n, s_n, and g_n for $p=2$. In addition, values of the linear extrapolants $l_n=[ng_n-(n-1)g_{n-1}]$ and the quadratic extrapolants $q_n=\frac{1}{2}[nl_n-(n-2)l_{n-1}]$ are given, forming a partial Neville table. For a limited number of terms available ($n=8$), these extrapolants are not expected to provide accurate estimates but only to indicate the nature of the trend of a sequence. In Fig. 6, the limiting exponents g_n and the linear extrapolants l_n are displayed in a ratio plot. As may be observed, the last few g_n fall on a straight line (asymptote) we have provided. The values of the linear extrapolants, which appear to converge onto the asymptote slowly and in a mildly oscillatory fashion, tend to support the trend established by g_n. A reasonable estimate for g_∞ is $\gamma_2(\text{fcc})=4.86\pm0.02$.

In Table XVI, we have given values of extrapolants for $p=3$. In Fig. 7, the nth limiting exponents g_n and the linear extrapolants l_n are displayed in a ratio plot. As may be observed, the last few g_n fall on a straight line. The values of the linear extrapolants appear to advance towards the intercept of the asymptote. A reasonable estimate for g_∞ is $\gamma_3(\text{fcc})=8.34\pm0.03$.

In Table XVII, we have given the values of r_n, s_n, and g_n for $p=4$ and a complete Neville table based on g_n. In Fig. 8, the limiting exponents g_n are displayed in a ratio plot and in Fig. 9 the values of the linear and quadratic extrapolants are given. As in the cases of $p=2$ and 3 these extrapolants advance towards the intercept of the asymptote, which is given by g_∞: $\gamma_4(\text{fcc})=11.79\pm0.05$.

Based on these results for γ_p, [25] we obtain for the gap parameter $2\Delta_2=3.50\pm0.10$, $2\Delta_3=3.48\pm0.15$, and $2\Delta_4=3.46\pm0.25$. We may conclude that $2\Delta=3.50\pm0.20$.

B. bcc and sc Lattices

Ratios of coefficients $b_n(1)$ for $\tilde{F}_p(K^*;1)$ on the bcc lattice are displayed in a ratio plot (see Fig. 10). As in the case of the fcc lattice, the sequences of $\tilde{F}_p$ are all seen to approach the same intercept provided by $\tilde{\chi}(K^*;1)$ and gaps are nearly constant. We observe essentially the same pattern for the series of $\tilde{F}_p(K^*;2)$ on the sc lattice (see Fig. 11).

The exponents γ_p are analyzed using the procedure outlined in the preceding part for the closed-packed lattice. Our analysis shows that the results for open lattices are on the whole less satisfactory than for the closed-packed lattice. (This is not surprising since there are only 8 terms in the series—the

TABLE XVI. Analysis of γ_3 for the fcc lattice based on $K_c^{*-1}(1)=5.042$.

n	$r_n^{(3)}$ (1; fcc)	$s_n^{(3)}$	$g_n^{(3)}$	$l_n^{(3)}$	$q_n^{(3)}$
1	51	45.958	10.115		
2	26.294118	42.504	9.430	8.75	
3	18.670022	40.884	9.109	8.46	8.33
4	15.031754	39.96	8.925	8.37	8.28
5	12.915836	39.37	8.807	8.34	8.29
6	11.536294	38.96	8.728	8.33	8.30
7	10.567170	38.68	8.671	8.33	8.32
8	9.849565	38.46	8.628	8.33	8.34

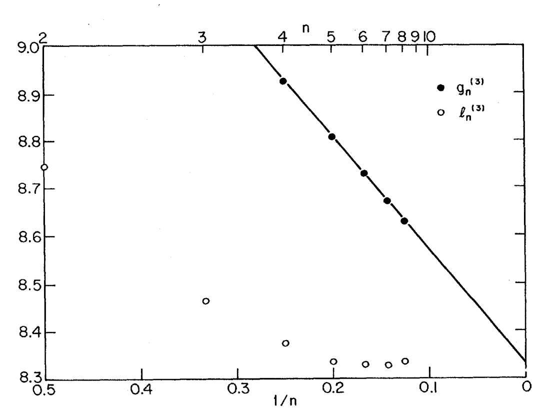

FIG. 7. Limiting exponents and linear extrapolants for γ_3 on the fcc lattice. $K_c^{*-1}=5.042$.

TABLE XVII. Analysis of γ_4 for the fcc lattice based on $K_c^{*-1}(1) = 5.042$ by constructing a Neville table.

n	$r_n^{(4)}$ (1; fcc)	s_n	g_n	l_n	q_n
1	87.529412	82.487	17.360		
2	41.056452	72.03	15.286	13.21	
3	27.380279	67.01	14.291	12.30	11.85
4	21.071657	64.12	13.717	11.99	11.68
5	17.492872	62.25	13.347	11.87	11.68
6	15.203026	60.97	13.092	11.81	11.70
7	13.617762	60.03	12.906	11.79	11.75
8	12.457565	59.33	12.766	11.79	11.77

same number for the fcc lattice.) Various extrapolants for open lattices, especially for the sc lattice, do not show clear signs of convergence and our estimates become necessarily more subjective. In Tables XVIII–XX, we have given values of extrapolants for γ_p on the bcc lattice. Based on these values, our estimates are $\gamma_2 = 4.8 \pm 0.1$, $\gamma_3 = 8.1 \pm 0.3$, and $\gamma_4 = 11.7 \pm 0.5$. In Tables XXI–XXIII, we have given values of extrapolants for the sc lattice. Based on these values, our estimates are $\gamma_2 = 4.8 \pm 0.5$, $\gamma_3 = 8.2 \pm 1.0$, and $\gamma_4 = 11.5 \pm 1.5$.

The sequences for $\tilde{\chi}(K^*; t)$ and $\tilde{F}(K^*; t)$ approaching the same critical point with a nearly equal gap suggest that our assumption about the principal singularities must be basically tenable. Our results on the fcc lattice obtained by the transformation method seem to constitute a fairly reasonable evidence for $2\Delta_p = 2\Delta \cong 3.50$. The results for open lattices are generally not well convergent enough to lend further support for the lattice independence of the critical exponents γ_p.

Baker *et al.*[3] have analyzed the series of $\tilde{F}_p(K)$ by constructing the Neville table (and not by the Padé approximant techniques for the reasons stated earlier). Among these series, the best estimate for K_c seems to come from the series of $\tilde{F}_4(K)$ on the fcc lattice. The values of successive extrapolants for this series, given in *their* Table XXIV, show that while there are signs of convergence in the sequences of extrapolants (linear, quadratic, etc.), the presence of curvature leads us to question whether their seventh and final entry ($K = 4.022$) is as close to the asymptotic value as they seem to have indicated. For the series of $\tilde{F}_2(K)$ and $\tilde{F}_3(K)$ on the fcc lattice, the values of extrapolants cease to progress montonically. Thus, the results of Neville tables are on the whole inconclusive. The sequences for open lattices are much less regular and their estimates are at best only tentative (i.e., $K_c \cong 0.4$ for the bcc lattice and $K_c \cong 0.6$ for the sc lattice).

Since the series of $\tilde{F}_p(K)$ do not yield the critical point unambiguously, it is difficult to expect that this approach can yield reliable estimates for the exponents γ_p. An examination of the Neville tables (Tables XXV–XXVII of Ref. 3) reveals that while the estimates given by Baker *et al.* may be the best that can be made based on the extrapolants of the Neville tables, *none* of the values for the exponents are shown to converge satisfactorily. Indeed, to show convergence, which is expected to be slow owing to the presence of nonphysical singularities,

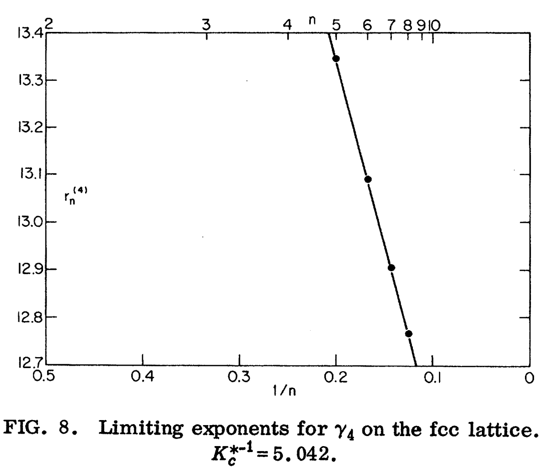

FIG. 8. Limiting exponents for γ_4 on the fcc lattice. $K_c^{*-1} = 5.042$.

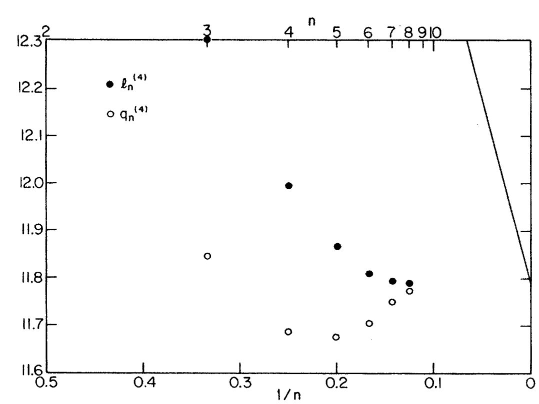

FIG. 9. Linear extrapolants and quadratic extrapolants for γ_4 on the fcc lattice. The solid line represents the asymptote for the limiting exponents redrawn from Fig. 8. $K_c^{*-1} = 5.042$.

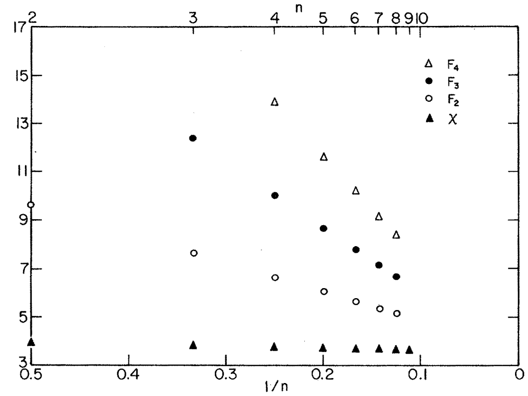

FIG. 10. Ratios of coefficients of $\tilde{X}(K^*;\ 1)$ and $\tilde{F}_p(K^*;1)$ for the bcc lattice.

TABLE XIX. Analysis of γ_3 for the bcc lattice based on $K_c^{*-1}(1)=3.534$.

n	$r_n^{(3)}$ (1; bcc)	s_n	g_n	l_n	q_n
1	34	30.47	9.62		
2	17.235 29	27.40	8.75	7.89	
3	12.350 97	26.45	8.48	7.95	8.0
4	10.015 981	25.93	8.34	7.89	7.8
5	8.661 313	25.64	8.25	7.92	8.0
6	7.778 160	25.46	8.21	7.96	8.0
7	7.157 604	25.37	8.18	8.01	8.1
8	6.697 630	25.31	8.16	8.05	8.2

one would probably need more than eight coefficients. Thus, it seems to us that it is not too unreasonable to regard the estimates given by Baker *et al.*, $\gamma_2\cong 5.06$, $\gamma_3\cong 8.69$, $\gamma_4\cong 12.32$, and $2\Delta\cong 3.63$ (our values are $\gamma_2\cong 4.86$, $\gamma_3\cong 8.34$, $\gamma_4\cong 11.79$, and $2\Delta\cong 3.50$) for the fcc lattice, as only tentative.

VII. CONCLUSIONS

We have shown that the irregularly behaving susceptibility and other series for the $S=\frac{1}{2}$ Heisenberg ferromagnet can be given ratio analysis by the application of a transformation method. This method of analysis has given us estimates for the critical values (K_c and γ_p), which are at variance with the earlier estimates based on Padé analysis, but which seem to be more consistent with other known results. We have argued that the discrepancy between the two results can be resolved if the estimates by Padé analysis are taken at one order lower accuracy (due to the presence of nonphysical singularities). The correctness of our contention, no doubt, can be further tested when additional higher-order coefficients of these series are known.

Based on our study of this and other related models of magnetism, it appears that the irregular behavior of a series due to the presence of *complex poles* has its origin in noncommutation of certain quantum-mechanical spin operators. When a series expansion is interfered by such nonphysical singularities, the effects of the interference must be isolated before the asymptotic behavior of the series can be deduced.

The transformation of various susceptibility series indicates that the assumption of a power-law behavior for the susceptibility is amply justified. On the other hand, our singular lack of success with the transformation of the specific-heat series suggests that the specific heat may obey a more complicated form than the generally accepted simple power law.

As has been pointed out, the ideas of using a transformation method are not new. To our knowledge, this method has not been previously applied to the degree we have used for the $S=\frac{1}{2}$ Heisenberg model. Danielian and Stevens[8] have considered the transformation method for the Heisenberg susceptibility series, but the limited number of then available coefficients (about 6 terms) probably made it

TABLE XVIII. Analysis of γ_2 for the bcc lattice based on $K_c^{*-1}(1)=3.534$.

n	$r_n^{(2)}$ (1; bcc)	s_n	g_n	l_n	q_n
1	16	12.47	4.53		
2	9.625	12.18	4.45	4.37	
3	7.666 667	12.40	4.51	4.63	4.8
4	6.658 385	12.50	4.54	4.62	4.6
5	6.053 825	12.60	4.56	4.68	4.8
6	5.648 963	12.69	4.59	4.72	4.8
7	5.358 590	12.77	4.61	4.75	4.8
8	5.139 468	12.84	4.63	4.76	4.8

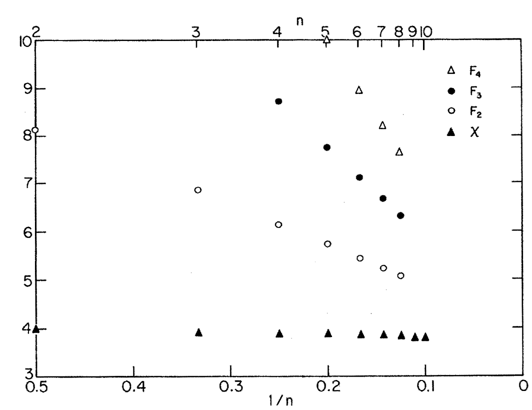

FIG. 11. Ratios of coefficients of $\tilde{X}(K^*;\ 2)$ and $\tilde{F}_p(K^*;\ 2)$ for the sc lattice.

TABLE XX. Analysis of γ_4 for the bcc lattice based on $K_c^{*-1}(1) = 3.534$ by constructing a Neville table.

n	$r_n^{(4)}$ (1; bcc)	s_n	g_n	l_n	q_n
1	58.352 941	54.82	16.51		
2	26.862 903	46.66	14.20	11.89	
3	18.014 910	43.44	13.29	11.47	11.3
4	13.943 479	41.64	12.78	11.25	11.0
5	11.638 157	40.52	12.47	11.20	11.1
6	10.163 778	39.78	12.26	11.21	11.2
7	9.143 252	39.26	12.11	11.23	11.3
8	8.396 242	38.90	12.01	11.28	11.4

TABLE XXI. Analysis of γ_2 for the sc lattice based on $K_c^{*-1}(2) = 3.678$.

n	$r_n^{(2)}$ (2; sc)	s_n	g_n	l_n	q_n
1	12	8.32	3.26		
2	8.125	8.89	3.42	3.57	
3	6.835 897	9.47	3.58	3.89	4.0
4	6.153 038	9.90	3.69	4.04	4.2
5	5.730 639	10.26	3.79	4.19	4.4
6	5.441 379	10.58	3.88	4.30	4.5
7	5.229 024	10.86	3.95	4.40	4.6
8	5.065 336	11.10	4.02	4.47	4.7

TABLE XXII. Analysis of γ_3 for the sc lattice based on $K_c^{*-1}(2) = 3.678$.

n	$r_n^{(3)}$ (2; sc)	s_n	g_n	l_n	q_n
1	25.5	21.82	6.93		
2	13.705 882	20.06	6.45	5.97	
3	10.338 340	19.98	6.43	6.39	6.6
4	8.710 856	20.13	6.47	6.60	6.8
5	7.750 662	20.36	6.54	6.79	7.1
6	7.114 623	20.62	6.61	6.95	7.3
7	6.660 613	20.88	6.68	7.10	7.5
8	6.319 177	21.13	6.74	7.22	7.6

TABLE XXIII. Analysis of γ_4 for the sc lattice based on $K_c^{*-1}(2) = 3.678$ by constructing a Neville table.

n	$r_n^{(4)}$ (2; sc)	s_n	g_n	l_n	q_n
1	43.764 706	40.09	11.90		
2	20.766 129	34.18	10.29	8.68	
3	14.512 492	32.50	9.84	8.93	9.0
4	11.639 181	31.84	9.66	9.12	9.3
5	9.999 097	31.61	9.59	9.33	9.7
6	8.938 823	31.57	9.58	9.53	9.9
7	8.196 292	31.63	9.60	9.70	10.1
8	7.646 507	31.75	9.63	9.87	10.3

impossible for them to carry out a systematic study.

ACKNOWLEDGMENTS

We are grateful to many of our colleagues for having assisted us in completing this work. Thanks are due to D. D. Betts (Alberta), W. Derbyshire (Colorado State), R. V. Ditzian (Toronto), C. J. Elliott (Alberta), R. W. Gibberd (Texas), D. L. Hunter (Brookhaven), and G. Paul (MIT).

---

*Research supported in part by Advanced Research Projects Agency, in part by the NSF, and in part by the Research Corporation.

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

[2]D. D. Betts, C. J. Elliott, and M. H. Lee, Can. J. Phys. 48, 1566 (1970); M. H. Lee, J. Math. Phys. 12, 61 (1971).

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

[4]H. E. Stanley, Phys. Rev. 158, 546 (1967); R. L. Stephenson and P. J. Wood, *ibid.* 173, 475 (1968); G. S. Joyce and R. G. Bowers, Proc. Phys. Soc. (London) 88, 1053 (1966).

[5]L. P. Kadanoff *et al.*, Rev. Mod. Phys. 39, 395 (1967), and references contained therein.

[6]R. G. Bowers and M. E. Woolf, Phys. Rev. 117, 917 (1969).

[7]The ratio method repairs some of the shortcomings of the Padé approximant method. It seeks, for example, trends and it relies increasingly on final coefficients. Further, its application is elementary, whereas the more sophisticated Padé method invariably requires the usage of high-speed computers.

[8]A. Danielian and K. W. H. Stevens, Proc. Phys. Soc. (London) B70, 326 (1957).

[9]G. A. Baker, Jr., J. L. Gammel, and J. G. Willis, J. Math. Anal. Appl. 2, 405 (1961).

[10]D. S. Gaunt and M. E. Fisher, J. Chem. Phys. 43, 2840 (1965).

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

[12]A. J. Guttmann, Ph.D. thesis, 1969 (unpublished); see also A. J. Guttmann and C. J. Thompson, Phys. Letters 28A, 679 (1969).

[13]M. H. Lee and H. E. Stanley, J. Phys. (Paris) 32S, 352 (1971).

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

[15]J. Gammel, W. Marshall, and L. Morgan, Proc. Phys. Soc. (London) A275, 257 (1963).

[16]G. A. Baker, Jr., Phys. Rev. 136, A1376 (1964).

[17]Based solely on Tables VII–IX of Ref. 3, we would consider $K_c = 0.249 \pm 0.001$, 0.396 ± 0.001, and 0.595 ± 0.003 as reasonable estimates for the critical points of the fcc, bcc, and sc lattices, respectively. The more refined estimates of the critical points by Baker *et al.* (Ref. 3) are obtained through mutual self-consistency between the quoted critical points and $\gamma = 1.43$ (see Tables XII, XIII for fcc; XV, XVII for bcc; and XX, XXII for sc). The attained consistency is quite remarkable.

[18]The reality condition requires that complex singularities must occur in pairs of complex conjugates. The existence of nonphysical singularities is not well understood although it is clear that noncommutativity of spin operators *and* the lattice structure must enter into it in some complicated way.

[19]If the negative real pole exists, it runs counter to the common belief that antiferromagnetic ordering cannot be produced in an fcc lattice with nearest-neighbor interactions only.

[20]The error limit is to be taken as a reasonable confidence level rather than a strict bound. In any case, we are not claiming accuracy any better than is indicated by our choice of error limits.

[21]There is in these ratios a mild oscillation about the asymptote, diminishing with n, the presence of which unfortunately prevents further analysis of the intercept by constructing a Neville table. The Neville table, whose extrapolants (linear, quadratic, etc.) are formed by obtaining the slope of successive pairs of ratios, cannot provide a useful estimate when extrapolants do not progress monotonically. When there is an oscillation, however small, it becomes further exaggerated with each sequence of extrapolants. The existence of this small oscillation in our case is evidently due to the complex poles. Our transformation has reduced, but not entirely removed, the interference of these nonphysical singularities.

[22]There is in these ratios a mild oscillation about the asymptote, diminishing with increasing n. Thus, as in the fcc lattice, the Neville table does not provide a convergent estimate of the intercept.

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

[24]C. Domb and D. L. Hunter, Proc. Roy. Soc. (London) 86, 1147 (1965); J. W. Essam and D. L. Hunter, J. Phys. C 1, 312 (1968).

[25]Actually the error limits should be somewhat larger, since the critical point is uncertain to about 0.2% (i.e., $\gamma_2 = 4.86 \pm 0.10$, $\gamma_3 = 8.34 \pm 0.15$, $\gamma_4 = 11.79 \pm 0.25$).