High-temperature-series study of the spin-1/2 Heisenberg ferromagnet

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We have extended existing high-temperature-series expansions for the spin-1/2 Heisenberg ferromagnet, for both the zero-field free energy and susceptibility. Series are obtained to order 13 for the simple cubic and body-centered cubic lattices and to order 12 for the face-centered cubic lattice, an addition of three terms in each case. The series are analyzed by a battery of methods and more precise estimates of the critical temperatures and exponents obtained. We also obtain estimates of the specific heat and susceptibility of the standard two- and three-dimensional lattices as functions of temperature, in the high-temperature region. [S0163-1829(96)03418-2]

I. INTRODUCTION

In this paper, we consider the thermodynamic properties of the spin-1/2 quantum Heisenberg ferromagnet, described by the Hamiltonian

$$H=-2J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j-g\mu_B H\sum_i S_i^z. \tag{1}$$

The model is defined on any regular lattice and the exchange interaction is restricted to nearest neighbors. This is a generic model for studies of magnetism in solids and, although the simplest such model, has resisted exact solution except in one dimension.

We derive high-temperature-series expansions for the above Hamiltonian, for the zero-field free energy and susceptibility, in powers of the variable $K=J/kT$. Series are obtained through order K^{12} for the triangular (tri) and face-centered cubic (fcc) lattices, and through order K^{13} for the square (sq), simple cubic (sc), and body-centered cubic (bcc) lattices. Our work extends by three terms the earlier classic work on this subject by Baker and Rushbrooke and their co-workers.[1,2] It is, of course, well known that the Mermin-Wagner theorem[3] precludes any state of conventional long-range order at finite temperatures in two dimensions. In three dimensions it is generally believed that a conventional phase transition occurs at finite temperature, although a rigorous proof of such exists only for the classical spin-∞ case,[4] and for the antiferromagnet with $S\geqslant 1$.[5]

Previous work[1,2] for the $S=\frac{1}{2}$ model has obtained values of the critical exponent $\gamma=1.43\pm0.01$. For $S=\infty$ the renormalization-group estimate of γ is[6] $\gamma=1.386\pm0.004$, with the addition of a confluent singularity with correction exponent $\Delta_1=0.55$. For this classical model McKenzie, Domb, and Hunter[7] derived 12th-order series for the sc and fcc lattices and 11th-order series for the bcc lattice. Their analysis appeared to be completely consistent with the field theory predictions. However, more recent analyses give the slightly larger value $\gamma=1.40$ for both the fcc lattice[8] and the sc lattice,[9] the latter based on a 14th-order series.[10]

It is believed, from general universality principles, that critical exponents should be independent of the spin quantum number S, and hence that the $S=\frac{1}{2}$ and $S=\infty$ models should have identical exponents. One of the motivations for the present work was to see if extended series for the $S=\frac{1}{2}$ model would give an estimate of γ closer to the classical series and field theory results, thus resolving an apparent discrepancy.

II. DERIVATION OF THE SERIES

We follow essentially the same steps as in the work of Baker *et al.*[1] Rushbrooke, Baker, and Wood based on a finite-cluster method. For completeness, the main steps are summarized below.

The logarithm of the partition function corresponding to the Hamiltonian H on an infinite lattice L can be written as a sum over all connected clusters embeddable in L:

$$\frac{1}{N}\ln Z=\sum_G C_G^{(L)}\Phi_G(K,H), \tag{2}$$

where the sum is over the set of clusters $\{G\}$, $C_G^{(L)}$ is the usual ''weak lattice constant'' of G in L, and $\Phi_G(K,H)$ is referred to as the ''reduced partition function'' for G. The coupling constant $K=J/kT$, as usual.

The reduced partition function can be obtained in the following way. Denote by A_G the logarithm of the partition function of cluster G (some examples are given in Appendix A). Then

$$\Phi_G=A_G-\sum_{k=1}^{G-1}T_{Gk}\Phi_k, \tag{3}$$

where T_{Gk} is the number of ways in which the (smaller) cluster k can be embedded in cluster G. In this way, the Φ's for all clusters are obtained recursively.

Standard methods exist for generating the clusters and computing the lattice constants. For example, for the fcc series to order K^{12} the list contains 19 859 distinct clusters. For the loose-packed sc and bcc lattices to order K^{13} a total of 6236 clusters needs to be considered. For each cluster in the list, it is necessary to identify all subclusters and their embedding factors T_{Gk}. Again, standard methods exist for doing this.

Finally, we need to consider how one calculates the cluster partition functions $A_G=\ln Z_G$. This can be done in various ways[2] but, for the $S=\frac{1}{2}$ system, the most efficient approach

uses group theoretical techniques, based on the theory of the symmetric group. The Hamiltonian for cluster G can be written in terms of Pauli matrices as

$$H_G = -\tfrac{1}{2} J \sum_{\langle ij \rangle} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j - \tfrac{1}{2} g \mu_B H \sum_i \sigma_i^z$$
$$= -\tfrac{1}{2} JP - \tfrac{1}{2} g \mu_B H M, \quad (4)$$

where $P \equiv \Sigma_{\langle ij \rangle} \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j$ and $M = \Sigma_i \sigma_i^z$. The first sum is over all bonds (edges) of cluster G while the second is over all sites (vertices). Because the two terms in H_G commute, we can write

$$Z_G = \mathrm{Tr}\{e^{-\beta H_G}\}$$
$$= \mathrm{Tr}\{e^{\beta JP/2} e^{\beta g \mu_B H M/2}\}$$
$$= \sum_{r=0}^{\infty} \frac{K^r}{2^r r!} \mathrm{Tr}\{P^r e^{\beta \mu_B H M/2}\}. \quad (5)$$

The operator P can be written as $P = \Sigma_{\langle ij \rangle}(2P_{ij} - 1)$ where P_{ij} is the permutation which interchanges spins at sites i and j. Hence, if the basis states are chosen to belong to the irreducible representations of the symmetric group of order n_G, where n_G is the number of sites in the cluster, P and P^r will be automatically block diagonalized. In this way, Z_G becomes

$$Z_G = \sum_{r=0}^{\infty} \frac{K^r}{2^r r!} \left\{ \sum_{k=0}^{[n_{G/2}]} \mathrm{Tr}(T_k^r) \sum_{m=k}^{n_G - k} e^{(n_G - 2m)y} \right\} \quad (6)$$

with $y = \frac{1}{2} \beta g \mu_B H$. Here Γ_k is the matrix representation of P in the irreducible representation k. Some further details about the generation of these basis states and the dimensionalities of the irreducible subspaces are given in Appendix B. Despite this simplification, the largest matrix is of dimension 1001, and calculation of the powers of these matrices is by far the most time consuming part of the computation.

Since we only require Z_G to order H^2, for the calculation of the initial susceptibility, we expand

$$\sum_{m=k}^{n_G - k} e^{(n_G - 2m)y} = u_k + \tfrac{1}{2} v_k (\beta g \mu_B H)^2 + \cdots$$

with

$$u_k = n_G + 1 - 2k,$$

$$v_k = \tfrac{1}{3}(n_G - 2k)(n_G - 2k + 1)(n_G - 2k + 2)$$

and obtain

$$Z_G = Z_{G0} + \tfrac{1}{2} (\beta h \mu_B H)^2 Z_{G2} + \cdots \quad (7)$$

with

$$Z_{G0} = \sum_{r=0}^{\infty} \frac{\mu_{r0}}{2^r r!} K^r, \quad Z_{G2} = \sum_{r=0}^{\infty} \frac{\mu_{r2}}{2^r r!} K^r \quad (8)$$

and

$$\mu_{r0} = \sum_{k=0}^{[n_{G/2}]} u_k \mathrm{Tr}(\Gamma_k^r), \quad \mu_{r2} = \sum_{k=0}^{[n_{G/2}]} v_k \mathrm{Tr}(\Gamma_k^r). \quad (9)$$

Finally

$$A_G = \ln Z_G = \ln Z_{G0} + \tfrac{1}{2} (\beta g \mu_B H)^2 Z_{G2} / Z_{G0} + \cdots \quad (10)$$

gives the logarithm of the partition function for cluster G.

Combining these various steps finally yields series for the zero-field free energy per site,

$$-\beta f(K) = \ln 2 + \sum_{n=1}^{\infty} \frac{e_n}{2^n n!} K^n, \quad (11)$$

and for the dimensionless zero-field susceptibility,

$$\overline{\chi} \equiv \frac{kT\chi}{(g\mu_B)^2} = 1 + \sum_{n=1}^{\infty} \frac{\alpha_n}{2^n n!} K^n. \quad (12)$$

In Table I we give the integer coefficients e_n and α_n for the five lattices sq, tri, sc, bcc, and fcc. We add three new coefficients to the previous series[1] of each of the three-dimensional lattices. Baker *et al.* quote the value 750 651 187 968 for e_{10} for the fcc lattice, which is slightly in error, due to two incorrect lattice constants. Our value is 750 412 309 248. We are unaware of previous tabulations for the two-dimensional lattices.

From (11) we can derive the specific heat series

$$C/k = \sum_{n=2}^{\infty} \frac{e_n}{2^n (n-2)!} K^n. \quad (13)$$

III. EVALUATION OF THERMODYNAMIC FUNCTIONS AT HIGH TEMPERATURES

As no exact results for thermodynamic functions are known, it seems worthwhile to use the expansion to estimate values of the specific heat and susceptibility numerically as functions of temperature. This is done by forming Padé approximants to the function $f(K)$,

$$f(k) \equiv \frac{P_N(K)}{Q_M(K)},$$

and evaluating these approximants for any K. For high temperatures, $K \ll 1$, all approximants give essentially the same result. As K increases the spread of estimates from different approximants increases, giving rise to increasing error bars. The procedure fails close to the radius of convergence of the series, which may or may not correspond to a physical phase transition.

In Fig. 1 we show the specific heat C/k versus kT/qJ for the sq and sc lattices. For small K (high T) the approximants are well converged and estimates are accurate to high precision (10^{-4}–10^{-6}). The error bars for lower T are confidence limits, based on the spread of a range of approximants. The specific heat for the sq lattice appears to be exhibiting a broad peak, as expected, at $kT/J \cong 0.6$, although the series do not converge well in the vicinity of the peak. For the sc lattice the specific heat begins to rise sharply in the vicinity of $kT/J \cong 1.7$, consistent with the expected cusp at T_c. This is discussed further in the following section.

In Fig. 2 we show the susceptibility versus kT/qJ. Again the series allow accurate estimates of χ to be obtained for $kT/J \geq 0.8$ for the sq lattice. Below $kT/J \cong 1$ the susceptibil-

TABLE I. High-temperature expansion coefficients e_n and α_n for various lattices.

	n	e_n	α_n		n	e_n	α_n
sq	1	0	4		8	−7 804 944	2 231 209 728
	2	6	16		9	723 961 728	71 938 507 776
	3	−12	64		10	2 596 523 904	2 446 325 534 208
	4	−84	416		11	−856 142 090 496	92 886 269 386 752
	5	1 200	4 544		12	6 383 648 984 832	3 995 799 894 239 232
	6	3 120	23 488		13	1 356 696 930 401 280	180 512 165 153 832 960
	7	−249 312	−207 616	bcc	1	0	8
	8	920 928	4 205 056		2	12	96
	9	86 274 816	198 295 552		3	−24	1 664
	10	−1 232 035 584	−2 574 439 424		4	168	36 800
	11	−40 970 012 160	−112 886 362 112		5	1 440	1 008 768
	12	1 391 730 516 480	3 567 419 838 464		6	24 480	32 626 560
	13	20 983 074 318 336	94 446 596 145 152		7	−297 024	1 221 399 040
tri	1	0	6		8	28 017 216	51 734 584 320
	2	9	48		9	−533 681 664	2 459 086 364 672
	3	18	408		10	41 156 316 672	129 082 499 311 616
	4	−306	3 600		11	−503 287 538 688	7 432 690 738 003 968
	5	−3 240	42 336		12	53 001 415 916 544	464 885 622 793 134 080
	6	49 176	781 728		13	−1 839 416 689 004 544	31 456 185 663 820 136 448
	7	1 466 640	13 646 016	fcc	1	0	12
	8	−13 626 000	90 893 568		2	18	240
	9	−1 172 668 032	−1 798 204 416		3	108	6 624
	10	75 256 704	70 794 720 768		4	180	234 720
	11	1 392 243 773 184	7 538 546 211 840		5	−5 040	10 208 832
	12	18 426 692 664 576	63 813 109 782 528		6	162 000	526 810 176
sc	1	0	6		7	14 565 600	31 434 585 600
	2	9	48		8	563 253 408	2 127 785 025 024
	3	−18	528		9	17 544 639 744	161 064 469 168 128
	4	−162	7 920		10	750 412 309 248	13 483 480 670 745 600
	5	2 520	149 856		11	56 646 776 913 408	1 237 073 710 591 635 456
	6	33 192	3 169 248		12	4 973 976 625 190 400	123 437 675 536 945 410 048
	7	−1 019 088	77 046 528				

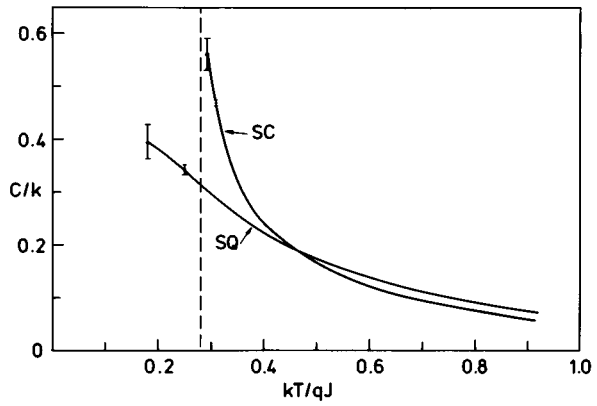

FIG. 1. Specific heat versus temperature for the square (sq) and simple cubic (sc) lattices. The dashed vertical line is the estimated critical temperature for the sc lattice.

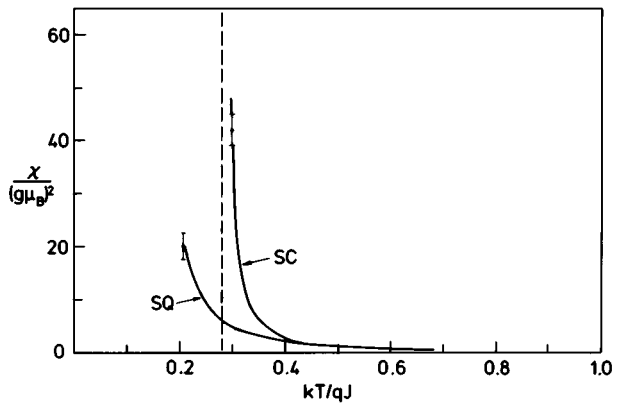

FIG. 2. Susceptibility versus temperature for the square (sq) and simple cubic (sc) lattices. The dashed vertical line is the estimated critical temperature for the sc lattice.

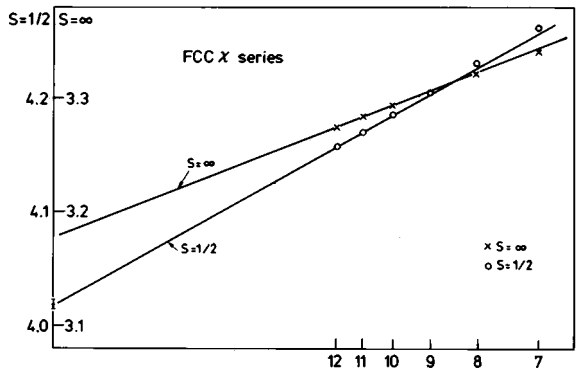

FIG. 3. Ratio plot for the susceptibility series for the fcc lattice, for both $S=1/2$ and $S=\infty$.

ity begins to rise sharply but the series become too irregular to estimate the location of the peak or its height accurately. For the sc lattice, as T approaches the transition temperature, the susceptibility exhibits the expected divergence. This is taken up in the following section.

The behavior of the specific heat and susceptibility for the other lattices is broadly similar to the above, and we do not display these. While the series results are only accurate for moderate and high temperatures, they could be combined with other techniques, such as low-temperature approximations or finite-lattice results, to provide accurate estimates of thermodynamic properties over the entire range of temperatures.

IV. CRITICAL POINT ESTIMATES

As mentioned above, the three-dimensional systems will have a second-order phase transition at a critical temperature T_c, which depends on the lattice. It is believed that the singularities of thermodynamic functions follow a conventional power law, with universal exponents γ, α, etc.

Methods of extracting critical temperatures and exponents from power series have been reviewed recently by Guttmann.[10] We have tried many of the methods, and summarize our findings below. It is useful, in this context, to consider also the corresponding series for the classical spin-∞ cases.

A. fcc lattice

We start with the susceptibility series for the fcc lattice. As usual series for this lattice appear to be the most regular. A standard ratio plot is shown in Fig. 3, for both $S=\frac{1}{2}$ and $S=\infty$. The $S=\frac{1}{2}$ series points show considerable residual curvature indicating the presence of strong corrections to the asymptotic scaling form. Two-point estimates of K_c and γ from the last four ratios give

$$K_c: \quad 0.249\,41, \quad 0.248\,99, \quad 0.248\,92,$$

$$\gamma: \quad 1.440, \quad 1.4219, \quad 1.4190.$$

With a degree of caution one might estimate $K_c \cong 0.2488$ and $\gamma = 1.41$. The classical series points are quite linear on this scale. Neville-Aitken extrapolation, which allows for higher powers of $1/n$, does not lead to improved estimates.

TABLE II. Estimates of critical temperature $K_c = J/kT_c$ and exponent γ from poles and residues of Padé approximants to $(d/dK)\ln X$ for the fcc lattice.

D/N	3	4	5	6	7
3		0.249 48	0.249 14	0.248 78	0.249 09
		1.442	1.427	1.410	1.426
4		0.249 21		0.248 97	0.249 18
		1.430		1.419	1.431
5	0.249 26	0.248 94	0.249 03	0.249 07	
	1.432	1.418	1.422	1.424	
6	0.248 55	0.249 03	0.249 10		
	1.397	1.422	1.426		
7	0.248 93	0.249 07			
	1.417	1.424			

If the function has an appreciable confluent term, so that

$$\chi(K) = C_0\left(1-\frac{K}{K_c}\right)^{-\gamma}\left[1+b\left(1-\frac{K}{K_c}\right)^{\Delta_1}\right]+\cdots, \quad (14)$$

then a modified analysis technique is required. We have used a modified Neville-Aitken method[10] with $\Delta=0.5$, as well as five- and four-point fits as proposed by Ferer and co-workers.[8,11] The modified Neville-Aitken extrapolants are inferior to the direct method, and no consistent solution is obtained from the N-point fits. These results suggest that a confluent correction, if present, has a sufficiently small amplitude as to be unobservable.

We have used a number of Padé approximant methods. Direct Padé analysis of the logarithmic derivative series gives estimates of K_c and γ as shown in Table II. The estimates are quite regular and suggest $K_c \cong 0.2491$ and $\gamma \cong 1.425$ with some uncertainty. It is noticeable that higher-order approximants indicate a trend to lower K_c and γ and hence one should be cautious in assigning confidence limits. It also needs to be borne in mind that the presence of any additive term to the leading singularity is not well handled by simple D log Padé approximants.

A somewhat more sophisticated approach is to allow for a correction term as in (14). Adler and co-workers[12,9] have proposed two such methods based on Padé approximants. Here we use their method $M2$ in which the series is first transformed to a variable y,

$$y = 1-\left(1-\frac{K}{K_c}\right)^{\Delta_1},$$

and the Padé approximants to

$$G(y) = \Delta_1(y-1)\,\frac{d}{dy}\ln\chi(y)$$

are evaluated at $y=1$. These provide estimates of γ for given estimates of K_c and Δ_1. The optimum estimates are taken to be where different approximants best coincide. In the present case this occurs for $K_c \cong 0.2490$ and Fig. 4 shows estimates of γ versus Δ, for this value of K_c. We note that the convergent region covers a rather broad range of Δ_1 values, which includes $\Delta_1=1.0$, corresponding to an analytic correction, but not the field theory prediction $\Delta_1=0.55$. The correspond-

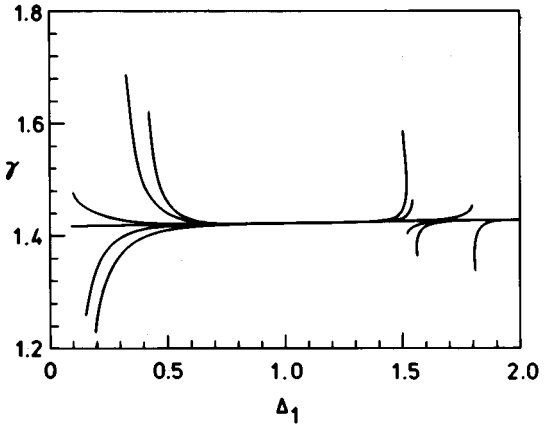

FIG. 4. Padé approximant estimates of γ versus Δ_1 for $K_c=0.2490$, for the fcc lattice susceptibility, based on method M2 of Adler *et al.* (Refs. 9 and 12).

ing γ estimate is approx. $\gamma\cong 1.42$. Changing the K_c estimate worsens the convergence and in no case favors a smaller Δ_1 value.

Finally, we have explored an alternative approach, based on first-order differential approximants, in which the series coefficients are fitted to

$$KP_N(K)\chi' + Q_M(K)\chi = R_L(K),$$

which defines a differential approximant $[L/M;N]$. Singular points of χ are represented by zeros of $P_N(K)$ and estimates of the exponent are given by

$$\gamma = Q_M(K_c)/K_c P_N'(K_c).$$

In Table III we show estimates of K_c and γ from higher-order approximants. As can be seen, these numbers are quite widely scattered, and it is not clear with the present series how one should choose final estimates.

In summary, none of the methods of analysis are particularly successful. From the trend of the ratio plot and the results given by Padé and differential approximants one might state, rather conservatively,

$$K_c = 0.2490 \pm 0.0004, \quad \gamma = 1.41 \pm 0.02,$$

TABLE III. Estimates of critical temperature $K_c = J/kT_c$ and exponent γ from $[L/M;N]$ differential approximants to X for the fcc lattice. Defective approximants are not shown.

L	M	N	K_c	γ	L	M	N	K_c	γ
1	5	5	0.249 07	−1.429	5	3	2	0.249 76	−1.490
2	4	5	0.249 66	−1.466	7	1	2	0.247 49	−1.309
2	5	4	0.249 47	−1.453					
3	4	4	0.249 67	−1.481	1	4	4	0.248 36	−1.372
4	3	4	0.248 29	−1.216	2	3	4	0.248 90	−1.414
4	4	3	0.249 51	−1.449	2	4	3	0.248 55	−1.386
6	3	2	0.249 13	−1.397	3	3	3	0.248 71	−1.398
8	1	2	0.247 33	−1.274	4	2	3	0.246 99	−1.278
					4	3	2	0.248 51	−1.384
1	4	5	0.250 40	−1.529					
1	5	4	0.250 09	−1.504					

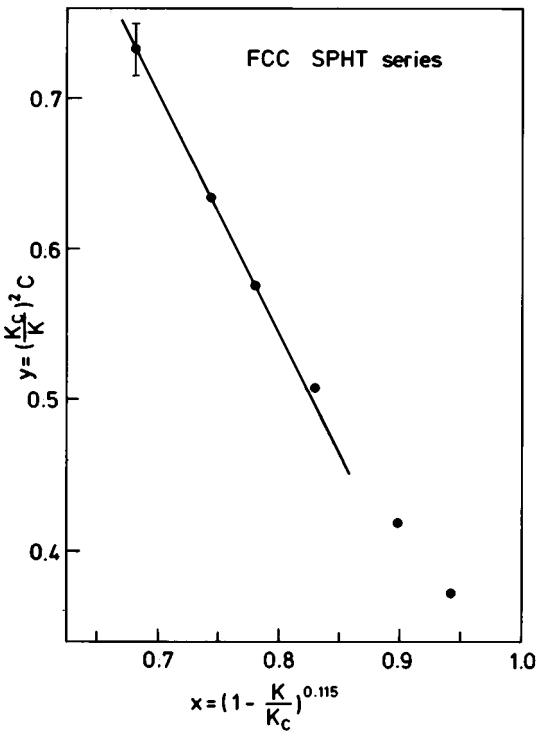

FIG. 5. Specific heat for fcc lattice fitted to asymptotic form.

with no indication of the confluent term predicted by field theory.

The amplitude of the dominant singularity can be obtained from Padé approximants to $(K_c-K)\chi^{1/\gamma}$ or alternatively from Padé approximants to $\chi(1-K/K_c)^{\lambda}$. These methods give, from the fcc lattice, the estimate

$$C_0 \cong 1.131 \pm 0.005.$$

The specific heat is expected to behave in the vicinity of the critical point as

$$C = \left(\frac{K}{K_c}\right)^2 \left[A - B\left(1 - \frac{K}{K_c}\right)^{\alpha}\right] \tag{15}$$

where A and B are constant amplitudes. The series itself is too irregular to allow direct estimates of the exponent α. The field theory prediction is $\alpha=0.115$, which yields a cusp of height A at $K=K_c$. We have assumed this value of α and have attempted to estimate the amplitudes A and B by fitting the values of C obtained in the previous section to Eq. (15). Figure 5 shows a plot of $(K_c/K)^2 C$ versus $(1-K/K_c)^{0.115}$, with a line of best fit which covers the interval $0.8<K/K_c<0.96$. The estimates are $A=1.82$ and $B=1.59$, somewhat larger values than given by Baker *et al.*[1]

B. sc lattice

We consider the analysis of the susceptibility series for the simple cubic lattice. The ratios show complex oscillatory behavior and no sensible extrapolation seems possible. Table IV shows estimates of K_c and γ from poles of Padé approximants to the logarithmic derivative series. These are reasonably consistent and indicate

TABLE IV. Estimates of critical temperature $K_c = J/kT_c$ and exponents γ for the sc lattice from poles and residues of Padé approximants to $(d/dK)\ln X$.

D/N	4	5	6	7	8
4		0.5950	0.5949	0.5973	0.5962
		1.411	1.408	1.453	1.430
5	0.5956	0.5949	0.5950	0.5965	
	1.420	1.408	1.411	1.438	
6	0.5950	0.5955	0.5957		
	1.410	1.418	1.421		
7	0.5948	0.5957			
	1.407	1.421			
8	0.5968				
	1.443				

$$K_c \cong 0.5960 \pm 0.0005, \quad \gamma \cong 1.42.$$

Consistent singularities are also observed at $K \cong -0.7$, presumably corresponding to the antiferromagnetic critical point, and at $K \cong -0.08 \pm 0.51i$. It is the presence of these singularities that results in the complex oscillatory behavior of the series. Differential approximants give estimates consistent with the above.

We have also estimated the leading amplitude of the susceptibility and the specific heat amplitudes. These are given in Table VI below, and discussed in the following section.

C. bcc lattice

We have repeated the above steps for the bcc susceptibility series. The ratios are again oscillatory but much less erratic than for the sc lattice. D log Padé approximants show a consistent physical singularity at $K \cong 0.3968$ together with a strong antiferromagnetic singularity at $K \cong -0.415$. Estimates of K_c and γ are shown in Table V. Our overall estimates are

$$K_c \cong 0.3968 \pm 0.0002, \quad \gamma \cong 1.415.$$

Again, differential approximants give very similar results. Amplitudes for χ and C have been estimated and are given in Table VI.

TABLE V. Estimates of critical temperature $K_c = J/kT_c$ and exponent γ for the bcc lattice from poles and residues Padé approximants to $(d/dK)\ln X$. The asterisk denotes a defective approximant.

D/N	4	5	6	7	8
4		0.3971	0.3967	0.3969	0.3969
		1.424	1.415	1.419	1.421
5	0.3958*	0.3968	0.3968	0.3970	
	1.396	1.417	1.418	1.423	
6	0.3969	0.3968	0.3968		
	1.419	1.418	1.417		
7	0.3968	0.3969			
	1.417	1.419			
8	0.3968				
	1.418				

TABLE VI. Estimated critical parameters from the three-dimensional lattices.

	sc	bcc	fcc
$K_c = J/kT_c$	0.5960(5)	0.3968(2)	0.2490(4)
K_c (Ref. 2)	0.595(3)	0.396(2)	0.249(1)
C_0	1.25(2)	1.138(2)	1.131(5)
A	1.21	1.44	1.82
B	0.85	1.13	1.59

V. DISCUSSION AND SUMMARY

We have computed the exact series expansions for the susceptibility and specific heat for the spin-1/2 Heisenberg ferromagnet for the standard two- and three-dimensional lattices. The previous series have been extended by three additional terms.

Assuming an asymptotic form

$$\chi = C_0 \left(1 - \frac{K}{K_c}\right)^{-\gamma} + \cdots,$$

we have analyzed the series to obtain estimates of the critical ''temperature'' $K_c = J/kT_c$, the exponent γ, and the amplitude C_0. These are shown in Table VI. Our estimate of γ, based on all three lattices (fcc, sc, and bcc) and using a variety of techniques, is

$$\gamma = 1.41 \pm 0.02.$$

The renormalization-group result is 1.386 ± 0.004. The most recent series estimates from the classical spin-∞ model are $\gamma = 1.40$. The uncertainties in these estimates are such that these should not be regarded as inconsistent. Nevertheless, it is perhaps annoying that the series estimates, for both $S = 1/2$ and $S = \infty$, seem higher than the field theory result, despite allowances for confluent and analytic correctons. In all likelihood the series are simply too short to yield the correct exponent. Analysis of the three-dimensional (3D) Ising model series shows that estimates of γ continue to change slowly when increasing the number of terms from about 12 to 20.[14] Experience would suggest that the Heisenberg series would not converge any more rapidly.

The additional three terms have allowed us to refine the estimates of critical temperature considerably, and these are shown in Table VI, together with the previous estimates. We have also obtained considerably more precise estimates of the susceptibility amplitude C_0.

These specific heat series are, as usual, considerably less regular and are difficult to analyze for critical properties. Assuming the scaling form

$$C = A - B\left(1 - \frac{K}{K_c}\right)^{\alpha}$$

and the renormalization group estimate of α, we have estimated the amplitudes A and B, given in Table VI. These differ considerably from previous work,[1,2] which used $\alpha = 0.2$. The specific heat for the Heisenberg model is believed to have a cusp at the critical point and thus we estimate the value of specific heat at this point to be $C/Nk = 1.21$, 1.44, and 1.82, respectively, for the sc, bcc, and fcc

TABLE VII. Some low-order clusters with their partition functions A_G and reduced partition functions Φ_G.

	A_G					Φ_G				
r	1	2	3	4	5	1	2	3	4	5
1		3	−6	−6	120		3	−6	−6	120
	2	−4	−4	80	−208	2	−4	−4	80	−208
2		6	−12	−36	480				−24	240
	4	−4	−32	224	544		4	−24	64	960
3		9	0	−162	0			18	−72	−1080
	6	0	−108	0	7 776			−24	−432	5520
4		9	−18	−90	1 080				$0(K^6)$	
	6	0	−48	336	4 176				−96	1920
5		9	−18	−66	840				$0(K^6)$	
	6	−4	−84	256	1 616			12	−112	320
6		12	−6	−216	360					−240
	8	4	−136	−176	11 408				−64	−640
7		12	−24	−48	960				72	−480
	8	0	−64	0	2 048				−128	−2240

lattices. It would be interesting to compare these with experimental values but we are not aware of such results.

The computation of three additional series coefficients reported here was carried out using the same algorithmic procedure as used by Baker *et al.* 28 years ago, and has been possible because of the enormous increase in computing performance during this period. Nevertheless, it still required substantial CPU time and memory. It is difficult to conceive of any radically more efficient approach to this quantum system, unlike classical systems where a variety of methods exist. Therefore we are not optimistic about prospects to further extend these series significantly in the short to medium term.

We have recently received a report from Butera and Comi[15] in which they report an impressive increase in the length of series for the classical spin-∞ Heisenberg model for the sc and bcc lattices, in each case to order K^{19}. Analysis of these series gives $\gamma=1.403(6)$ and 1.396(3) from the sc and bcc lattices. These results are slightly lower than previous series estimates but still higher than the renormalization-group results.

Note added in proof. Since submission of this paper we have refined the algorithm used to derive series coefficients, and have extended the series for the loose-packed lattices by one term, to order x^{14}. The new coefficients are

$e_{14}=-1\ 798\ 371\ 774\ 277\ 632$ (sq),
$-27\ 667\ 884\ 260\ 938\ 752$ (sc),
$246\ 102\ 905\ 022\ 713\ 856$ (bcc)

and

$\alpha_{14}=-5\ 636\ 771\ 173\ 998\ 592$ (sq),
$8\ 443\ 006\ 907\ 441\ 565\ 696$ (sc),
$2\ 284\ 815\ 238\ 218\ 471\ 260\ 160$ (bcc).

The analysis of the series is not affected significantly.

TABLE VIII. Dimensionalities of $\Delta^{(k)}$ (upper row) and $D^{(k)}$ (lower row) for $n=2$–14.

$n/k=$	0	1	2	3	4	5	6	7
2	1	2						
	1	1						
3	1	3						
	1	2						
4	1	4	6					
	1	3	2					
5	1	5	10					
	1	4	5					
6	1	6	15	20				
	1	5	9	5				
7	1	7	21	35				
	1	6	14	14				
8	1	8	28	56	70			
	1	7	20	28	14			
9	1	9	36	84	126			
	1	8	27	48	42			
10	1	10	45	120	210	252		
	1	9	35	75	90	42		
11	1	11	55	165	330	462		
	1	10	44	110	165	132		
12	1	12	66	220	495	792	924	
	1	11	54	154	275	297	132	
13	1	13	78	286	715	1287	1716	
	1	12	65	208	429	572	429	
14	1	14	91	364	1001	2002	3003	3432
	1	13	77	273	637	1001	1001	429

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APPENDIX A

We list in Table VII, for illustrative purposes, some low-order clusters together with their partition functions A_G and reduced partition functions Φ_G. In each case, the upper line is for zero field and the lower line is the H^2 term. To avoid fractions the coefficient of K^r is multiplied by $2^r r!$. Note the extensive cancellation which occurs in the reduced partition functions. This can be used to eliminate some high-order clusters from the list.

APPENDIX B

We provide here a summary of procedures involved in generating basis states belonging to irreducible representations of the symmetric group, expanding on details given in Ref. 2 and in standard books on group theory (e.g., Ref. 13).

Consider a cluster with n sites. There are 2^n basis states, conveniently taken to be eigenstates of the z component of total spin $\Sigma\sigma_i^z$ and labeled $(m_1,m_2,\ldots,m_n)$ with $m_1=\pm 1$. This set may be sorted into orthogonal sectors labeled by $k=0,1,2\ldots,[n/2]$, where k is the number of up spins, providing representations $\Delta^{(k)}$ of the symmetric group $S(n)$, of dimensionalities

$$\dim\Delta^{(k)}=\binom{n}{k}.$$

These representations are, in general, reducible and can be decomposed as

$$\Delta^{(k)}=D^{(0)}\oplus D^{(1)}\oplus\cdots\oplus D^{(k)},$$

where the $D^{(k)}$ are irreducible representations (irreps) and

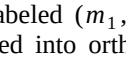
$$\dim D^{(k)}=\dim\Delta^{(k)}-\dim\Delta^{(k-1)}.$$

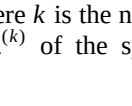
The irreps $D^{(k)}$ correspond to Young tableaux,[13] with two rows with $n-k$ and k squares, respectively.

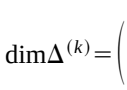
Table VIII lists the dimensionalities of $\Delta^{(k)}$ and $D^{(k)}$ for $n=2$–14. The upper row in each case is the dimension of $\Delta^{(k)}$ and the lower is $\dim D^{(k)}$. The largest irreducible sector dealt with in this work has dimension 1001.

Each tableau of a given form has a number of distinct realizations, equal to the dimensionality of the irrep. For each realization we define a Young operator which, when operating on a given function, yields a basis function belonging to that irrep. Since all irreps are contained within the maximal sector ($[n/2]$ up spins), we need only work within this sector. The procedure is best illustrated by example.

We consider the simple case $n=3$. The tableaux and Young operators are

k = 0  $Y_0 = e + (12) = (13) + (23) + (123) + (132)$

k = 1  $Y_{11} = [e - (13)][e + (12)]$

 $Y_{12} = [e - (12)][e + (13)]$

where (ij) denotes a permutation of i and j, etc.

We consider the three states with one up spin, $|001\rangle$, $|010\rangle$, and $|100\rangle$, where, for convenience, we denote down spins by 0 rather than -1. $k=0$ is the symmetric (identity) representation and the corresponding basis function is

$$1\Psi_0\rangle=\frac{1}{\sqrt{3}}\{|001\rangle+|010\rangle+|100\rangle\}.$$

For $k=1$ we construct

$$Y_{11}|001\rangle=|001\rangle-|100\rangle,$$

$$Y_{12}|001\rangle=|001\rangle-|010\rangle.$$

These are orthogonalized using the standard Gram-Schmidt procedure to form a basis for the $k=1$ irrep. These steps have been computerized to give a program which generates an orthonormal basis for any irrep.

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