Some Critical Properties of the Heisenberg Model*

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A detailed series-extrapolation investigation of some critical properties ($T \to T_c+$) of the Heisenberg model is presented. Systematic use is made of ratio and Padé-approximant techniques, some of the latter being new. Attention is confined to those nearest-neighbor and order-two equivalent-neighbor models which are based on the simple cubic, body-centered cubic, and face-centered cubic lattices. For the face-centered cubic nearest-neighbor classical Heisenberg model, the following estimates are obtained for familiar critical exponents: $\alpha=0$, $-\frac{1}{8}\leqslant\alpha_s\leqslant-\frac{1}{16}$, $\gamma=1.375\pm0.002$, $0.6875\leqslant\nu\leqslant0.7125$, $0\leqslant\eta\leqslant0.07$. Estimates for γ are also obtained for the other nearest-neighbor and equivalent-neighbor classical Heisenberg models, and it is conjectured that $\gamma=1\frac{3}{8}$ may be the exact result in all the cases considered. For the face-centered cubic order-two equivalent-neighbor spin-$\frac{1}{2}$ Heisenberg ferromagnet, it is estimated that $\gamma=1.3744\pm0.0008$. A similar but less precise result is found for the corresponding simple cubic model, and the spin-$\frac{1}{2}$ nearest-neighbor susceptibility series are briefly examined. It is suggested that consideration should be given to the possibility that for ferromagnetic Heisenberg interactions γ has the same value $1\frac{3}{8}$ irrespective of spin and the particular three-dimensional nearest-neighbor or finite-order equivalent-neighbor model considered. Other quantities estimated include various Curie points and singularity amplitudes and the critical values of certain thermodynamic functions. Some attention is given to the simple classical Heisenberg antiferromagnet.

1. INTRODUCTION

Much of the theoretical study of critical phenomena[1] is based on the statistical mechanics of the Ising and Heisenberg models which correspond to special cases of the Hamiltonian

$$\mathcal{H}=-\sum_{(ij)} 2(J_{ij}{}^xS_i{}^xS_j{}^x+J_{ij}{}^yS_i{}^yS_j{}^y+J_{ij}{}^zS_i{}^zS_j{}^z)-mH\sum_{i=1}^{N}S_i{}^z. \quad (1.1)$$

This equation relates to a lattice of N sites in a magnetic field H directed parallel to the z axis. The components $S_i{}^x$, $S_i{}^y$, and $S_i{}^z$ are those of a spin operator $\mathbf{S}_i$ associated with the ith site, m is the magnetic moment per spin, and the first summation is taken over all pairs of sites (ij) in the lattice. However, in the present paper attention is confined to problems in which the interactions are of finite range. When only one of the three quantities $J_{ij}{}^x$, $J_{ij}{}^y$, $J_{ij}{}^z$ is nonzero we have pure Ising coupling, while if all three of these quantities are equal (and nonzero) we have spatially isotropic Heisenberg coupling.

Apart from one-dimensional systems (for which critical behavior is not found for $T\neq0$), exact solutions exist only for certain zero-field properties of various two-dimensional spin-$\frac{1}{2}$ nearest-neighbor Ising lattices.[2–4] The exact critical exponents[5,6] thus obtained are in contradiction with all current approximate theories,[2–4] but are in excellent agreement with numerical estimates based upon extrapolation of the leading terms of the appropriate exact series expansions.[2,3] It is expected therefore that series extrapolation is also the most reliable method when no exact solution is known. Accordingly we adopt this approach in the present paper.

For the Ising model many details of critical behavior are well established.[2–4,7] The results which have most bearing on the present investigations may be summarized as follows: Excluding long-range interactions, the critical exponents appear to depend only on the dimensionality d of the lattice and not on its detailed structure. Furthermore, there is evidence to suggest that they are independent of spin magnitude, and that they have identical values for nearest-neighbor and higher- (finite-) order equivalent-neighbor models. It seems also that in general the critical exponents are simple fractions. Finally, their accepted values are consistent with the majority of the scaling laws, which imply in particular that the exponents are symmetrical about the transition.

For the Heisenberg model, the situation is not so clear. Series-extrapolation investigations have been restricted to high-temperature critical behavior. For general spin, the first six coefficients of the high-temperature expansions of the zero-field susceptibility and specific heat have been known for some time.[8] Conclusions based on these terms are somewhat tentative, and the desirability of longer series was acknowledged.[9,10] In fact, the general spin expansions have very

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[1] For recent reviews see Refs. 2–4.
[2] M. E. Fisher, Rept. Progr. Phys. 30, 615 (1967).
[3] C. Domb, Phil. Mag. Suppl. 9, 149 (1960).
[4] L. P. Kadanoff *et al.*, Rev. Mod. Phys. 39, 395 (1967).
[5] We refer here and elsewhere to results obtained in the thermodynamic limit $N\to\infty$, which is necessary to obtain mathematical singularities. When this limit is taken, we mean by a d-dimensional lattice a lattice which extends to infinity in all its d dimensions.
[6] We conform to the notation and definitions of Ref. 2.
[7] D. S. Gaunt, Proc. Phys. Soc. (London) 92, 150 (1967).
[8] G. S. Rushbrooke and P. J. Wood, Mol. Phys. 1, 257 (1958).
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[10] J. Gammel, W. Marshall, and L. Morgan, Proc. Roy. Soc. (London) A275, 257 (1963).

recently been extended,[11] and in addition in the extreme quantum limit of spin $\frac{1}{2}$ (Refs. 12, 13) and the classical or correspondence limit of infinite spin[14–19] still more terms have been calculated.

In this paper, we consider some properties of the Heisenberg model in the light of this new information. Since the Heisenberg model cannot be ferro- or antiferromagnetic in one and two dimensions,[20] we confine attention to the three-dimensional model and in particular to the simple cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc) lattices. Thus we leave aside discussion of the interesting possibility of some novel kind of phase transition in two dimensions.[21] We investigate not only nearest-neighbor models but also equivalent-neighbor models of order two,[22] and more particularly with an obvious notation the sc (1,2), bcc (1,2), and fcc (1,2) models.

It is convenient to redefine some of the quantities appearing in (1.1) in such a way that the general spin Heisenberg Hamiltonian may be written

$$\mathcal{H}=-\sum_{(ij)}(2J_{ij}/S^2)\mathbf{S}_i\cdot\mathbf{S}_j-(mH/S)\sum_{i=1}^{N}S_i^z. \quad (1.2)$$

In the limit of infinite spin this becomes

$$\mathcal{H}=-\sum_{(ij)}2J_{ij}\mathbf{s}_i\cdot\mathbf{s}_j-mH\sum_{i=1}^{N}s_i^z, \quad (1.3)$$

where $\mathbf{s}_i$ is a classical unit vector. When all the interaction parameters J_{ij} are equal we omit the subscripts.

For convenience, most of the series analyzed in this paper are collected in Tables I, II, and III. For the classical Heisenberg model, the zero-field susceptibility χ_0 and specific heat C_0 have the expansions

$$\chi_0=(Nm^2/3kT)\sum_{r\geqslant 0}a_rK^r,$$
$$C_0=Nk\sum_{r\geqslant 2}b_rK^r, \quad (1.4)$$

where $K=2\beta J$ and the coefficients are presented in Tables I and II. The results of Table I, which are for the nearest-neighbor model, are taken from the work of Joyce and Bowers.[14–16] (The coefficients a_r have been calculated independently by Wood and Rushbrooke,[17] and by Stanley.[18,19]) The coefficients a_r of Table II are for the equivalent-neighbor model of order two and are obtained using the configurational data of Domb and Dalton[22] and the coefficients in terms of general

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TABLE I. Coefficients in the high-temperature expansions of the zero-field susceptibilities and specific heats of some nearest-neighbor classical Heisenberg models.

	Susceptibility		
n	a_n (sc)	a_n (bcc)	a_n (fcc)
0	1.000 000	1.000 000	1.000 000
1	2.000 000	2.666 667	4.000 000
2	3.333 333	6.222 222	14.666 667
3	5.422 222	14.340 741	51.733 333
4	8.518 519	31.861 728	178.459 259
5	13.267 019	70.311 581	606.745 397
6	20.335 991	152.811 632	2042.100 411
7	30.998 964	330.743 405	6821.952 840
8	46.867 340	709.993 599	22 659.360 929
9	70.606 787	1519.806 958	···
	Specific heat		
n	b_n (sc)	b_n (bcc)	b_n (fcc)
2	1.000 000	1.333 333	2.000 000
3	0	0	5.333 333
4	1.133 333	5.066 667	14.266 667
5	0	0	37.925 926
6	1.858 907	14.758 377	100.912 875
7	0	0	273.272 099
8	2.663 671	46.082 502	754.586 974
9	0	0	2116.136 406
10	4.298 002	153.025 422	···

TABLE II. Coefficients a_n in the high-temperature expansions of the zero-field susceptibilities of some equivalent-neighbor classical Heisenberg models.

n	a_n [bcc (1,2)]	a_n [sc (1,2)]	a_n [fcc (1,2)]
0	1.000 000	1.000 000	1.000 000
1	4.666 667	6.000 000	6.000 000
2	20.222 222	34.000 000	34.000 000
3	84.651 852	187.822 222	187.822 222
4	346.987 654	1021.466 667	1021.466 667
5	1403.179 588	5496.788 713	5497.025 750
6	5620.467 741	29 354.159 389	29 357.865 068
7	22 353.980 873	155 851.472 856	155 890.603 607

TABLE III. Coefficients a_n' in the high-temperature expansions of the zero-field susceptibilities of some equivalent-neighbor spin-$\frac{1}{2}$ Heisenberg models.

n	a_n' [bcc (1,2)]	a_n' [sc (1,2)]	a_n' [fcc (1,2)]
0	1.000	1.000	1.000
1	7.000	9.000	9.000
2	42.000	72.000	72.000
3	234.667	548.000	548.000
4	1262.958	4059.375	4059.375
5	6663.225	29 565.575	29 570.075
6	34 736.110	212 869.123	212 951.740
7	179 510.349	1 519 860.768	1 520 865.135

lattice parameters. The coefficients a_r' of Table III also relate to the equivalent-neighbor Heisenberg model of order two, but are for the case of spin $\frac{1}{2}$. They are defined by the equation

$$\chi_0=(Nm^2/kT)\sum_{r\geqslant 0} a'_r K^r, \tag{1.5}$$

where $K=2\beta J$, and are obtained from the results of Domb and Dalton[22] and Domb and Wood.[12]

The plan of the rest of the paper is as follows: Section 2 is devoted to a discussion of our extrapolation techniques. In Secs. 3–6, a detailed numerical investigation of some critical properties of the nearest-neighbor classical Heisenberg ferromagnet is undertaken. In particular, the susceptibility, specific heat, entropy and energy, and second moment of the correlations, all in zero field, are considered in Secs. 3–6, respectively. In Sec. 7, some results for the simple classical Heisenberg antiferromagnet are presented. Sections 8 and 9 are concerned with the zero-field susceptibility of the equivalent-neighbor Heisenberg ferromagnet, for the cases of spin infinity and spin $\frac{1}{2}$, respectively. A summary and discussion will be found in Sec. 10.

2. EXTRAPOLATION PROCEDURES

We are concerned with series of the general form

$$f(z)=\sum_{r=0}^{\infty}\alpha_r z^r, \tag{2.1}$$

where only the first n coefficients are known. We expect $f(z)$ to have singularities at various points z_i of the complex z plane. Certain of these will have physical significance. Thus, the singularity z_c closest to the origin on the positive real axis corresponds to the Curie point of the ferromagnetic problem ($J>0$). Similarly, the singularity z_N closest to the origin on the negative real axis corresponds to the Néel point of the antiferromagnetic problem ($J<0$).

In general, we assume

$$f(z)\sim A_i(1-z/z_i)^{-\lambda_i}+B_i \quad \text{as} \quad z\to z_i- , \tag{2.2}$$

and aim to determine z_i, λ_i, A_i, and B_i (Ref. 23) for the physically significant singularities. In analyzing for singularities of the form (2.2), we use Padé-approximant (PA)[2,24] and ratio[2,3,25] methods. Rather than discussing our various extrapolation procedures as they arise, we prefer to undertake a detailed discussion of them here so as to make Secs. 3–9 more or less independent of each other. We are particularly concerned to emphasize a systematic approach. Several new PA methods are introduced.

[23] Where no ambiguity arises we sometimes omit the subscripts i, c, and N.
[24] G. A. Baker, Phys. Rev. **124**, 768 (1961).
[25] C. Domb and M. F. Sykes, J. Math. Phys. **2**, 63 (1961).

The $[D,N]$ PA to $g(z)$ is the ratio $P_N(z)/Q_D(z)$ of two polynomials of degrees D and N, whose coefficients are chosen so that the coefficients of the expansion of $[D,N]$ in powers of z coincide with those of $g(z)$ through order $D+N$.[26] Thus when using PA's it is natural to attempt first to convert any singularity of interest to a simple pole. If (2.2) holds and provided that $f(z)$ either diverges or vanishes as $z\to z_i-$,[27]

$$D\ln f(z)\sim\lambda(z_i-z)^{-1} \quad \text{as} \quad z\to z_i- , \tag{2.3}$$

where $D=d/dz$. Thus, the logarithmic derivative of $f(z)$ has a simple pole at $z=z_i$ with residue $-\lambda$. The roots and residues of PA's to $D\ln f(z)$ may therefore be used as estimates for z_i and $-\lambda$.

In this paper, we use the more general function

$$[D^p\ln f(z)]^{1/p}\sim[(p-1)!\lambda]^{1/p}(z_i-z)^{-1} \quad \text{as} \quad z\to z_i- \;(p=1,2,\cdots). \tag{2.4}$$

The roots of PA's to (2.4) provide estimates for z_i, while estimates for λ may be determined from the corresponding residues. Three points should be mentioned here: (a) With short series we are restricted to small p since each differentiation "loses" a term. (b) We are satisfied only if results for different values of p are consistent. However, we do not expect convergence to be equally fast in all cases. Indeed, we hope that it will be especially rapid for some particular p. Even if this is not so, comparison of results for various p should allow more accurate estimation of any trends. (c) There will in general be correction terms to (2.2) whose presence will slow convergence. A simple assumption is

$$f(z)\sim Az_i^{\lambda}(z_i-z)^{-\lambda}[1+a(z_i-z)+\cdots], \tag{2.5}$$

whence

$$D\ln f(z)\sim\lambda(z_i-z)^{-1}[1-(a/\lambda)(z_i-z)+\cdots], \tag{2.6}$$

whereas[10]

$$[D^2 f(z)]^{1/2}\sim(\lambda)^{1/2}(z_i-z)^{-1}\times[1+\text{terms of higher order than first}]. \tag{2.7}$$

We see that (2.5) provides an example where the PA's should converge better for $p=2$ than for $p=1$. Thus, (2.7) should be more satisfactorily represented than (2.6) by low-order PA's, and furthermore errors in λ resulting from those in z_i are of higher order for (2.7) than for (2.6).

We next introduce the function

$$[D^{p-1}(f(z))^{1/\lambda}]^{1/p}\sim[A^{1/\lambda}(p-1)!z_i]^{1/p}(z_i-z)^{-1} \quad \text{as} \quad z\to z_i- \;(p=1,2,\cdots), \tag{2.8}$$

which, assuming λ to be known, provides another way of

[26] For further details see Refs. 2 and 24.
[27] If $f(z)$ approaches a nonzero constant as $z\to z_i-$, it is generally interesting to use the first derivative which diverges—see Ref. 2.

converting the dominant part of (2.2) to a simple pole. PA's to (2.8) yield estimates for z_i and A.

Finally, we introduce the function

$$(z_i - z)[D^p \ln f(z)]^{1/p} \sim [(p-1)!\lambda]^{1/p} \quad \text{as} \quad z \to z_i- \quad (p=1,2,\cdots), \qquad (2.9)$$

which may be constructed if z_i is known. PA's to (2.9) evaluated at $z=z_i$ give estimates for λ.

Methods[28] (2.8) and (2.9) use as data λ and z_i, respectively; it is therefore reasonable to expect that they will yield more rapid convergence than method (2.4). Now, exact values of λ or z_i are seldom known; however, methods (2.8) and (2.9) can still be employed with advantage when good estimates for these quantities are available. With the obvious modifications (a)–(c) following (2.4) apply equally well to (2.8) and (2.9). As far as we are aware the general methods (2.4), (2.8), and (2.9) have not been used elsewhere. Previously attention has been restricted to $p=1$, although in one study[10] PA's to $[D^2 \ln f(z)]^{1/2}$ have been employed.

Our general procedure in PA analyses is as follows: Given the first $n+1$ terms of a series, we form all possible PA's with $D+N=1,\cdots,n$ (except perhaps those with D or N zero). The results are displayed in a triangular array with D labeling the rows and N the columns. If the results of the last few orders are substantially the same, we suspect that this Padé table has converged. Calculations are usually undertaken for $p=1$, 2 (and perhaps 3). We regard the roots and residues of PA's to $[D^p \ln f(z)]^{1/p}$ as of *primary importance*. Inspection of these usually suggests ranges of values for z_i and λ for any singularity of interest. Methods (2.8) and (2.9) are then applied at points throughout these ranges. The results are examined for consistency, a procedure which may lead to improved estimates.

Method (2.8) is of particular importance when a certain value of λ is strongly indicated. Using this value in (2.8) should yield good estimates for z_i and A. Using this estimate for z_i in (2.9), a value for λ close to that adopted should then be obtained. In a similar way, when a good estimate for z_i is available we use first method (2.9) and subsequently method (2.8).

We now turn to the ratio method, which rests on the observation that if (2.2) holds for the dominant singularity z_c (say) of (2.1), then with $g=\lambda-1$

$$\alpha_n \sim A\left|\binom{-(1+g)}{n}\right|(z_c)^{-n} \quad \text{as } n\to\infty\,, \qquad (2.10)$$

and therefore

$$r_n = \alpha_n/\alpha_{n-1} \sim (z_c^{-1})(1+g/n) \quad \text{as} \quad n\to\infty\,. \qquad (2.11)$$

To obtain estimates for z_c^{-1}, g, and A given the first few coefficients α_n, it is convenient to employ a suitable procedure based upon the following results[2,3,25]:

$$l_n = nr_n - (n-1)r_{n-1} \qquad \to z_c^{-1} \text{ as } n\to\infty\,; \qquad (2.12)$$

$$g_n = n(z_c' r_n - 1) \qquad \to g \quad \text{as } n\to\infty\,, \quad \text{if } z_c'=z_c; \qquad (2.13)$$

$$\beta_n = nr_n/(n+g') \qquad \to z_c^{-1} \text{ as } n\to\infty\,, \quad \text{for all } g'; \qquad (2.14)$$

$$A_n = \alpha_n (z_c')^n \Big/ \left|\binom{-(1+g')}{n}\right| \to A \quad \text{as } n\to\infty\,, \quad \text{if } z_c'=z_c \text{ and } g'=g. \qquad (2.15)$$

Although z_c and g are rarely known exactly, we may still use (2.13) and (2.15) with advantage provided good estimates for these quantities are available. The β_n, however, converge to z_c for all g', but it is generally true that convergence will be most rapid for g' near g.

We normally follow a procedure similar to that described above in relation to PA studies. Thus we search for consistency between the various methods (2.12)–(2.15), where necessary taking values of g' and z_c' throughout the ranges of previous estimates. In estimating a limit as $n\to\infty$, it is generally useful to construct a Neville table, which is a triangular array in which n labels the rows and $r=0, 1, 2, \cdots$, the columns. Entries e_n^r are generated by the formula

$$e_n^r = [ne_n^{r-1} - (n-r)e_{n-1}^{r-1}]/r \qquad (r=1, 2, \cdots, n\geqslant r)\,, \qquad (2.16)$$

where e_n^0 is the sequence to be extrapolated, and e_n^1 is merely the linear extrapolants. [Exceptionally, for method (2.14) we start with $r=1$, i.e., we take e_n^1 to be the data β_n. This generally yields improved convergence.] While the entries in the later columns of a Neville table tend to magnify any small irregularities in the data, they are of considerable value when the corresponding $1/n$ plot shows a marked steady curvature. Another procedure useful in these circumstances is to replace n in (2.11)–(2.15) by $n+\epsilon$, where varying the small constant ϵ gives a range of sequences and influences curvature. In general results for different values of the "n shift" ϵ must be carefully compared.

For loose-packed lattices the ratios r_n exhibit marked odd/even oscillations, whose effects may be minimized by using alternate pairs of points when, for example, Eqs. (2.12) and (2.16) are replaced by

$$l_n = \tfrac{1}{2}[nr_n - (n-2)r_{n-2}] \to z_c^{-1} \quad \text{as} \quad n\to\infty\,, \qquad (2.17)$$

$$e_n^r = [ne_n^{r-1} - (n-2r)e_{n-2}^{r-1}]/(2r) \qquad (r=1, 2, \cdots, n\geqslant 2r)\,. \qquad (2.18)$$

Sometimes, given the first few terms of a series expansion of some property, estimates are required of its value throughout some physical region of the independent variable. Such estimates may be obtained by

[28] We shall often refer to an extrapolation procedure by means of the associated equation.

either constructing and evaluating a "mimic function"[29] or evaluating PA's to the series, or forming partial sums of the series and estimating their limit.[30]

TABLE IV. Curie roots and corresponding critical exponents from PA's to $D \ln\chi$ for some nearest-neighbor classical Heisenberg models.

fcc lattice							
			$10^4\times$(Curie root)				
D/N	1	2	3	4	5	6	
1	3086	3118	3132	3137	3139	3142	
2	3137	3144	3140	3142	3159		
3	3144	3141	3141	3136			
4	3140	3141	3141				
5	3142	3136					
6	···						
			$10^3\times$(Critical exponent)				
D/N	1	2	3	4	5	6	
1	1270	1310	1334	1344	1350	1356	
2	1346	1364	1351	1358	1481		
3	1364	1355	1354	1345			
4	1351	1354	1355				
5	1359	1346					
6	···						
bcc lattice							
			$10^4\times$(Curie root)				
D/N	1	2	3	4	5	6	7
1	4369	5202	4550	5115	4637	5055	4693
2	4713	4824	4844	4850	4855	4858	
3	4834	4850	4852	···	4859		
4	4847	4852	4849	4862			
5	4851	4842	4864				
6	4857	4859					
7	4859						
			$10^3\times$(Critical exponent)				
D/N	1	2	3	4	5	6	7
1	1018	1718	1006	1805	1003	1835	1013
2	1225	1314	1336	1345	1354	1359	
3	1325	1345	1349	···	1363		
4	1342	1349	1344	1369			
5	1347	1337	1376				
6	1357	1362					
7	1361						
sc lattice							
			$10^4\times$(Curie root)				
D/N	1	2	3	4	5	6	7
1	6250	7347	6451	7337	6610	7194	6692
2	6811	6838	6882	6927	6927	6919	
3	6839	6774	···	6927	6927		
4	6883	···	6841	6919			
5	6933	6929	6920				
6	6929	6935					
7	6919						
			$10^3\times$(Critical exponent)				
D/N	1	2	3	4	5	6	7
1	1042	1692	1006	1914	1023	1851	1037
2	1296	1312	1347	1392	1391	1380	
3	1312	1291	···	1391	1392		
4	1348	···	1303	1380			
5	1400	1395	1382				
6	1395	1402					
7	1380						

TABLE V. Curie roots and corresponding critical exponents from PA's to $(D^2 \ln\chi)^{1/2}$ for the fcc classical Heisenberg model.

		$10^5\times$(Curie root)			
D/N	1	2	3	4	5
1	31 341	31 467	31 442	31 442	31 468
2	31 512	31 446	31 442	31 442	
3	31 447	31 442	31 445		
4	31 441	31 446			
5	31 441				
		$10^4\times$(Critical exponent)			
D/N	1	2	3	4	5
1	13 505	13 833	13 746	13 744	13 884
2	14 008	13 763	13 744	13 746	
3	13 768	13 747	13 761		
4	13 743	13 765			
5	13 743				

Numerical estimates obtained in this paper are given either in the form $l_1 \leqslant q \leqslant l_2$, where l_1 and l_2 are nonrigorous bounds apparently supported by the extrapolation procedures, or in the form $q \pm \epsilon$, where ϵ is an indication of the apparent accuracy of these procedures.

3. ZERO-FIELD SUSCEPTIBILITY OF THE NEAREST-NEIGHBOR CLASSICAL HEISENBERG FERROMAGNET

We are now in a position to consider the critical behavior of the initial susceptibility of the nearest-neighbor classical Heisenberg ferromagnet. The relevant series expansions have already been given in Table I.

We first determine the "Curie roots"[31] and the corresponding residues of PA's to $D \ln\chi$ for the three cubic lattices. Unfortunately, in no case do these results (Table IV) lead to very precise estimates of either the Curie point K_c or the critical exponent γ. (It is, however, perhaps worth mentioning that if we were prepared to assume γ to be lattice-independent, then we should conclude its value to be approximately 1.37.)

Following the general procedure described in Sec. 2, we next perform similar calculations with $(D^2 \ln\chi)^{1/2}$. The results of Table V, which are for the fcc lattice, show very rapid convergence. All PA's of the last three orders bar one yield (after rounding[32]) values in the ranges

$$K_c = 0.31444 \pm 0.00003, \quad \gamma = 1.375 \pm 0.002 \text{ (fcc)}. \tag{3.1}$$

Since there are no discernible trends in these later approximants, we feel confident in adopting (3.1) as initial Padé estimates.

Now experience with the Ising model indicates that the critical exponents may well be simple fractions; therefore the estimate (3.1) strongly suggests that here $\gamma = 1\frac{3}{8}$ may be the exact result. We therefore form PA's

[29] M. F. Sykes, J. L. Martin, and D. L. Hunter, Proc. Phys. Soc. (London) **91**, 671 (1967); also D. S. Gaunt and C. Domb, J. Phys. **C1**, 1038 (1968).

[30] One method of estimating this limit is given in C. Domb and M. F. Sykes, Proc. Roy. Soc. (London) **A235**, 247 (1956).

[31] The Curie root is in general the smallest positive real root of the Padé denominator. Any nonphysical real roots between the origin and the Curie root usually have very small residues and may therefore be easily identified.

[32] In the following, we omit this qualification, which is, however, usually necessary.

TABLE VI. Curie roots (in units of 10^{-5}) of PA's to $(D\chi^{8/11})^{1/2}$ for the fcc classical Heisenberg model.

D/N	1	2	3	4	5	6
1	31 472	31 437	31 447	31 445	31 444	31 447
2	31 435	31 445	31 445	31 443	31 445	
3	31 445	31 445	31 445	31 445		
4	31 445	31 445	31 445			
5	31 442	31 445				
6	31 445					

to $(D\chi^{8/11})^{1/2}$ [method (2.8), $p=2$] for the fcc lattice. The Curie roots of the Padé denominators (Table VI) show very rapid convergence, which supports the conjecture $\gamma=1\frac{3}{8}$. All PA's of the last four orders (bar the [5,1]) have roots in the range

$$K_c=0.31445\pm0.00002 \text{ (fcc)}, \tag{3.2}$$

which is our final Padé estimate for the Curie point of the fcc lattice and is in excellent agreement with the initial estimate (3.1). From the residues of these PA's, the following estimate for the amplitude of the ferromagnetic singularity of the fcc lattice may be obtained:

$$A=0.8385\pm0.0009 \text{ (fcc)}. \tag{3.3}$$

As a check on consistency, we evaluate PA's to $(K_c-K)(D^2\ln\chi)^{1/2}$ at $K=K_c=0.31445$ [method (2.9), $p=2$]. The results (Table VII) show, as expected, very rapid convergence, nearly the entire Padé table yielding γ between 1.374 and 1.376, which is very satisfactory.

When we apply methods (2.4), (2.8), and (2.9) with $p=1$ and $p=3$ to the fcc lattice, we obtain results entirely consistent with those found for $p=2$. However, since these investigations do not permit estimates as precise as those presented above, we do not propose to discuss them in any detail. The marked improvement in convergence obtained in PA calculations by going from $p=1$ to $p=2$ suggests that, for the fcc lattice, the ferromagnetic singularity in the susceptibility *may* be of the form discussed at (c) above.

Unfortunately for the loose-packed lattices, convergence is not much improved by taking $p>1$. However, a comparison of the results of PA calculations with $D\ln\chi$ (Table IV) and $(D^2\ln\chi)^{1/2}$ yields the initial estimates

$$K_c=0.4864\pm0.0012,\quad \gamma\approx1.37 \text{ (bcc)},$$
$$K_c=0.6919\pm0.0015,\quad \gamma\approx1.38 \text{ (sc)}. \tag{3.4}$$

TABLE VII. Estimates (in units of 10^{-4}) for the critical exponent γ of the fcc classical Heisenberg model from PA's to $(K_c-K)\times(D^2\ln\chi)^{1/2}$ evaluated at $K=K_c=0.31445$.

D/N	1	2	3	4	5
1	13 796	13 760	13 759	13 738	13 760
2	13 761	13 759	13 760	13 759	
3	13 759	13 760	13 759		
4	13 847	13 759			
5	13 760				

TABLE VIII. Curie roots (in units of 10^{-4}) of PA's to $\chi^{8/11}$ and $(D\chi^{8/11})^{1/2}$ for the bcc classical Heisenberg model.

				$\chi^{8/11}$				
D/N	1	2	3	4	5	6	7	8
1	5077	4813	4922	4840	4889	4850	4877	4855
2	5187	4890	4875	4870	4867	4866	4865	
3	4898	4870	4869	4850	4865	4860		
4	4880	4869	4871	4864	4864			
5	4872	4862	4865	4864				
6	4868	4865	4864					
7	4866	4862						
8	4865							
				$(D\chi^{8/11})^{1/2}$				
D/N	1	2	3	4	5	6	7	
1	4691	5023	4730	4974	4767	4944	4793	
2	4867	4865	4862	4861	4862	4862		
3	4865	4868	4861	4861	4862			
4	4862	4861	4862	4862				
5	4861	4861	4862					
6	4862	4862						
7	4862							

For the Ising model, γ is almost certainly lattice-independent in any given dimension; therefore, in the light of the estimates (3.4), it seems logical to use PA methods (2.8) and (2.9) to investigate how *consistent* the susceptibility series of the loose-packed lattices are with $\gamma=1\frac{3}{8}$.

In Tables VIII and IX will be found the Curie roots of PA's to $(D^{p-1}\chi^{8/11})^{1/p}$ for $p=1$ and $p=2$. These Padé tables, whose mutual consistency is noteworthy, lead (with the assumption $\gamma=1\frac{3}{8}$) to the final Padé estimates

$$K_c=0.4863\pm0.0003 \text{ (bcc)},$$
$$K_c=0.6918\pm0.0005 \text{ (sc)}. \tag{3.5}$$

These estimates are centrally within the ranges of (3.4), which is encouraging and may perhaps be regarded as indirect evidence for $\gamma=1\frac{3}{8}$. From the residues of these

TABLE IX. Curie roots (in units of 10^{-4}) of PA to $\chi^{8/11}$ and $(D\chi^{8/11})^{1/2}$ for the sc classical Heisenberg model.

				$\chi^{8/11}$				
D/N	1	2	3	4	5	6	7	8
1	7174	6855	6971	6868	6941	6897	6930	6906
2	7018	6940	6916	6911	6913	6916	6916	
3	6943	6884	6910	6912	6935	6916		
4	6919	6910	6915	6917	6915			
5	6912	6913	6917	6916				
6	6913	6907	6915					
7	6915	6916						
8	6916							
				$(D\chi^{8/11})^{1/2}$				
D/N	1	2	3	4	5	6	7	
1	6706	7079	6728	7075	6801	7016	6835	
2	6911	6896	6900	6920	6921	6917		
3	6896	6899	6894	6921	6920			
4	6900	6895	6908	6917				
5	6921	6921	6918					
6	6921	6921						
7	6917							

TABLE X. Estimates (in units of 10^{-3}) for the critical exponent γ of the bcc classical Heisenberg model from PA's to $(K_c-K)D\ln\chi$ and $(K_c-K)(D^2\ln\chi)^{1/2}$ evaluated at $K=K_c=0.4863$.

D/N	1	2	3	4	5	6	7
			$(K_c-K)D\ln\chi$				
1	1290	1348	1358	1364	1367	1369	1371
2	1353	1363	1368	1376	1372	1374	
3	1360	1370	1386	1373	1373		
4	1365	1379	1373	1373			
5	1368	1372	1373				
6	1370	1375					
7	1371						
			$(K_c-K)(D^2\ln\chi)^{1/2}$				
D/N	1	2	3	4	5	6	
1	1377	1366	1384	1378	1381	1379	
2	1366	1373	1380	1380	1380		
3	1383	1380	1380	1380			
4	1379	1380	1380				
5	1381	1380					
6	1379						

TABLE XI. Estimates (in units of 10^{-3}) for the critical exponent γ of the sc classical Heisenberg model from PA's to $(K_c-K)D\ln\chi$ and $(K_c-K)(D^2\ln\chi)^{1/2}$ evaluated at $K=K_c=0.6918$.

D/N	1	2	3	4	5	6	7
			$(K_c-K)D\ln\chi$				
1	1336	1361	1375	1382	1380	1379	1378
2	1363	1426	1388	1381	1324	1378	
3	1376	1388	1366	1379	1379		
4	1384	1382	1379	1379			
5	1380	1372	1379				
6	1378	1378					
7	1378						
			$(K_c-K)(D^2\ln\chi)^{1/2}$				
D/N	1	2	3	4	5	6	
1	1390	1391	1408	1371	1371	1377	
2	1391	1389	1397	1371	1371		
3	1408	1397	1393	1376			
4	1373	1369	1377				
5	1369	1372					
6	1378						

same PA's we estimate

$$A=0.868\pm0.012 \text{ (bcc)},\quad A=0.970\pm0.010 \text{ (sc)}. \tag{3.6}$$

Naturally, we now use the estimates (3.5) in conjunction with the PA method (2.9). The results for the extreme values of (3.5) differ from those for the central values by only about $\pm1\%$. Furthermore, we are reasonably confident that the central values are, in fact, correct to four figures. Consequently, we present in Tables X and XI only the results for these values. These are very satisfactory, the last two orders of PA's yielding, with few exceptions,

$$p=1:\quad \gamma=1.370\text{–}1.375 \text{ (bcc)},\quad 1.379\text{–}1.378 \text{ (sc)},$$
$$p=2:\quad \gamma=1.381\text{–}1.379 \text{ (bcc)},\quad 1.369\text{–}1.378 \text{ (sc)},$$

which are all within $\pm\frac{1}{2}\%$ of $1\frac{3}{8}$.

We feel that the above PA calculations for the loose-packed lattices certainly demonstrate that the susceptibility series of these lattices are consistent with the conjecture $\gamma=1\frac{3}{8}$. They therefore provide evidence for the lattice independence of this critical exponent.

As regards ratio analyses, the method given by (2.12) and (2.17) leads to rather inexact estimates for the Curie points which, however, do include those given previously. To provide better estimates we turn to method (2.14).

Since $\beta_n\rightarrow K_c^{-1}$ as $n\rightarrow\infty$ irrespective of the value of g', we may take $g'=\frac{3}{8}$ and subsequently use the results to estimate g from method (2.13). The sequences β_n (Table XII) show rather rapid convergence and yield the estimates 3.180 ± 0.001 (fcc), 2.0563 ± 0.0008 (bcc), and 1.4455 ± 0.0005 (sc) for K_c^{-1}. These give

$$K_c=0.31447\pm0.00010 \text{ (fcc)},\quad K_c=0.4863\pm0.0002 \text{ (bcc)},\quad K_c=0.6918\pm0.0003 \text{ (sc)}, \tag{3.7}$$

which are in excellent agreement with the PA estimates (3.2) and (3.5). In fact, for the loose-packed lattices the ratio estimates (3.7) are firmer than the PA estimates (3.5) and therefore supersede them.

Next, we investigate $g=\gamma-1$ using the ratio method (2.13) with the estimate (3.7) for the Curie points. The results of Table XIII correspond to our adopted values of K_c, namely, 0.31445 (fcc), 0.4863 (bcc), and 0.6918 (sc). For the fcc lattice, the last five linear intercepts lie between 0.372 and 0.373 and are thus within 0.8% of $\frac{3}{8}$. For the loose-packed lattices, it is useful to smooth the oscillations by forming averages of successive pairs of linear intercepts. In the case of the bcc lattice, the

TABLE XII. $10^4\times\beta_n$ and extrapolants for the susceptibilities of some nearest-neighbor classical Heisenberg models ($g'=\frac{3}{8}$).

	fcc			bcc			sc		
n/r	1	2	3	1	2	3	1	2	3
1	29 091			19 394			14 545		
2	30 877			19 649			14 035		
3	31 354			20 487			14 459		
4	31 539	31 725		20 313			14 364		
5	31 627	31 759	31 782	20 528	20 538		14 488	14 495	
6	31 677	31 776	31 794	20 455	20 526		14 427	14 458	
7	31 708	31 786	31 798	20 543	20 555	20 557	14 468	14 454	14 447
8	31 728	31 789	31 794	20 505	20 556	20 566	14 442	14 457	14 457
9	···	···	···	20 550	20 558	20 559	14 463	14 456	14 456

TABLE XIII. $10^4 \times g_n$ and extrapolants for the susceptibilities of some nearest-neighbor classical Heisenberg models.

	fcc, $K_c'=0.31\,445$		bcc, $K_c'=0.4863$		sc, $K_c'=0.6918$	
n/r	0	1	0	1	0	1
1	2578		2968		3836	
2	3060	3541	2694		3060	
3	3274	3704	3625	3953	3760	3722
4	3389	3733	3219	3743	3474	3888
5	3455	3719	3659	3710	3872	4039
6	3500	3724	3415	3809	3625	3926
7	3533	3730	3679	3731	3818	3683
8	3556	3722	3515	3816	3675	3826
9	···	···	3689	3724	3800	3735

last four such averages are between 0.3760 and 0.3775, that is, within 0.7% of $\frac{3}{8}$. Convergence is slower for the sc lattice, but g close to 0.375 is certainly indicated.

Taking $g=\frac{3}{8}$ and our adopted values of K_c, we finally use method (2.15) to estimate the amplitudes of the ferromagnetic singularities. From Table XIV, we estimate

$$A=0.839\pm0.003 \text{ (fcc)},$$
$$A=0.866\pm0.003 \text{ (bcc)}, \qquad (3.8)$$
$$A=0.971\pm0.003 \text{ (sc)},$$

in good agreement with the results (3.3) and (3.6) of PA calculations.

In Table XXIX are collected our final estimates for K_c, γ, and A. In general, each entry in this table is either the appropriate Padé or ratio estimate, depending on which is the more accurate. [The estimates 1.375 $\pm$0.010 for the critical exponents γ of the bcc and sc lattices are obtained using the estimates (3.7) for K_c in conjunction with both the ratio method (2.13) and the PA method (2.9).]

4. ZERO-FIELD SPECIFIC HEAT OF THE NEAREST-NEIGHBOR CLASSICAL HEISENBERG FERROMAGNET

In this section, the critical behavior of the zero-field specific heat of the classical Heisenberg ferromagnet is investigated. Attention is confined to the fcc lattice, since the series (Table I) for the loose-packed lattices have $b_{2n+1}=0$ (Ref. 33) and are therefore too short for accurate extrapolation.

TABLE XIV. $10^4 \times A_n$ and extrapolants for the susceptibilities of some nearest-neighbor classical Heisenberg models ($g'=\frac{3}{8}$).

	fcc, $K_c'=0.31\,445$			bcc, $K_c'=0.4863$			sc, $K_c'=0.6918$	
n/r	0	1	2	0	1	2	0	1
0	10 000			10 000			10 000	
1	9148	9148		9431			10 063	
2	8882	8616		9012	9012		9770	9770
3	8757	8506		8979	8753		9773	9628
4	8684	8468	8414	8870	8727		9711	9653
5	8637	8446	8414	8855	8669		9733	9674
6	8603	8433	8408	8808	8685		9714	9720
7	8577	8425	8405	8800	8663	8658	9723	9698
8	8558	8419	8399	8775	8676	8667	9715	9715
9	···	···	···	8770	8663	8664	9720	9707

It is important to determine whether or not the specific-heat series indicates a singularity at the Curie point as previously determined from the susceptibility. On the basis of PA and ratio calculations (the details of which we omit to save space) we feel justified in concluding that, as expected, the specific heat does have its dominant singularity at the same value of K as the susceptibility. We therefore use the precise estimate $K_c=0.31445\pm0.0002$ obtained from the susceptibility in analyzing the critical behavior of the specific heat.

Following standard procedure, we assume that $C_0 \sim C(K_c-K)^{-(1+g)}+D$ as $K\to K_c-$ and use the ratio method (2.13) to obtain an estimate for the index $1+g$. The results (Table XV) suggest that $1+g$ is negative, which means that the specific heat does not diverge as $T\to T_c+$, but approaches some (nonzero) constant D. Therefore, according to our definition,[6] the critical exponent for the high-temperature behavior of the specific heat is zero, i.e.,

TABLE XV. $10^4 \times (1+g_n)$ and extrapolants for the specific heat of the fcc classical Heisenberg model ($K_c'=0.31\,445$).

n/r	0	1
3	5156	
4	3646	
5	1796	
6	0201	
7	−0393	−3957
8	−0537	−1544
9	−0635	−1423

$$\alpha=0. \qquad (4.1)$$

When the critical exponent λ of some property is zero, it is frequently useful to consider the exponent λ_s of the singular part of that property.[2] In the present circumstances $\alpha_s=1+g$, and we feel able to conclude on the basis of Table XV and other such sequences that

$$\tfrac{1}{16}\leqslant -\alpha_s\leqslant \tfrac{1}{8}. \qquad (4.2)$$

Although the results (4.1) and (4.2) have been obtained specifically for the fcc lattice, it seems very probable on general grounds that they will hold for all three-dimensional nearest-neighbor classical Heisenberg models.

5. ZERO-FIELD ENTROPY AND ENERGY OF THE NEAREST-NEIGHBOR CLASSICAL HEISENBERG FERROMAGNET

Recalling that we write the zero-field specific heat in the form

$$C_0=Nk\sum_{r\geqslant 2} b_r K^r \quad (K=2J/kT), \qquad (5.1)$$

[33] The coefficient b_l of K^l in the specific-heat series involves all graphs of l lines and vertices all of even degree, which can be formed from the nearest-neighbor links of the lattice when multiple bonding is allowed. For the loose-packed lattices, there are no such graphs for l odd and therefore in this case $b_{2n+1}=0$.

it is easy to show that

$$\frac{S(\infty)-S(T)}{Nk}=\frac{1}{Nk}\int_T^\infty \frac{C_0}{T}dT=\sum_{r\geqslant 2} b_r K^r/r \qquad (5.2)$$

and

$$\frac{E(\infty)-E(T)}{NkT}=\frac{1}{NkT}\int_T^\infty C_0 dT=\sum_{r\geqslant 2} b_r K^r/(r-1), \qquad (5.3)$$

where S and E are the entropy and energy, respectively, and where the expansions apply for $H=0$ and $T\geqslant T_c$.

By evaluation of the available terms of the expansions and approximation of the remainders (see Sec. 2), the quantities (5.2) and (5.3) may be estimated over the entire high-temperature region. These quantities are independent of the interaction energy J. Because of this their critical values, for which we obtain the estimates

	fcc	bcc	sc
$[S(\infty)-S(T_c)]/Nk$	0.314 ± 0.002	0.338 ± 0.006	0.415 ± 0.014
$[E(\infty)-E(T_c)]/NkT_c$	0.468 ± 0.004	0.533 ± 0.004	$0.69\ \pm 0.02$,

(5.4)

are particularly useful for comparison with experiment.

6. ZERO-FIELD SPIN PAIR CORRELATION FUNCTION OF THE NEAREST-NEIGHBOR CLASSICAL HEISENBERG MODEL

In this section, we are concerned with the reduced longitudinal spin pair correlation function $\Gamma(\mathbf{r},T,H)$. For general spin, a suitable definition is

$$\Gamma(\mathbf{r},T,H)=\langle(S_0^z-\langle S^z\rangle)(S_\mathbf{r}^z-\langle S^z\rangle)\rangle/\tfrac{1}{3}S(S+1). \qquad (6.1)$$

For a detailed discussion of the relevant general theory we refer to the work of Fisher,[2,34–36] Burford,[37] and Fisher and Burford.[38] Assuming there is only a single correlation length κ^{-1} which diverges at the critical point, it is usual to write the scaling relation

$$\Gamma\simeq G(\kappa r)/r^{d-2+\eta} \quad (r\to\infty,\, T\to T_c,\, H=0), \qquad (6.2)$$

for the long-range behavior of the correlations. The high-temperature behavior of κ is given by

$$\kappa\sim F(1-T_c/T)^\nu \quad \text{as} \quad T\to T_c+. \qquad (6.3)$$

It is now convenient to introduce the correlation moments

$$\mu_t=\sum_\mathbf{r} r^t\Gamma(\mathbf{r}), \qquad (6.4)$$

and to write for their zero-field high-temperature critical behavior

$$\mu_t\sim A_t(1-T_c/T)^{-\gamma_t} \quad \text{as} \quad T\to T_c+. \qquad (6.5)$$

Using (6.2)–(6.5), it can be shown[2,35–38] that

$$\gamma_t=(t+2-\eta)\nu, \qquad (6.6)$$

which, in the case of the reduced susceptibility ($t=0$), yields

$$\gamma=\gamma_0=(2-\eta)\nu. \qquad (6.7)$$

The numerical investigations of this section are as follows: First, using the series expansions of Fisher and Burford[2,35,37] as verified by Jasnow and Wortis,[39] we estimate γ_2 for the nearest-neighbor classical Heisenberg model. Second, we interpret this result in terms of exponents ν and η by accepting (6.6) for $t=0$ and $t=2$ and using

$$\nu=\tfrac{1}{2}(\gamma_2-\gamma_0), \qquad (6.8)$$

$$\eta=2-\gamma_0\nu^{-1}, \qquad (6.9)$$

with $\gamma=\gamma_0=1\tfrac{3}{8}$. We undertake this analysis since the current estimates of Fisher and Burford[2,35,37] are, of necessity, based on values for K_c and γ obtained from shorter susceptibility expansions.

For the three cubic lattices, the results of evaluating PA's to $(K_c-K)D\ln\mu_2$ at $K=K_c$ are presented in Table XVI. (Throughout this section we use the accurate estimates for the Curie points obtained from the susceptibility series.) The series for the fcc lattice is much the smoothest, and consequently we confine attention to it. (The other series provide no evidence that γ_2 is lattice-dependent.)

While the PA results give us confidence in the assertion

$$\gamma_2\geqslant 2.75 \text{ (fcc)}, \qquad (6.10)$$

TABLE XVI. Estimates (in units of 10^{-3}) for the critical exponent γ_2 of some nearest-neighbor classical Heisenberg models from PA's to $(K_c-K)D\ln\mu_2$ evaluated at $K=K_c$.

	fcc, $K_c=0.31\,445$			bcc, $K_c=0.4863$			sc, $K_c=0.6918$		
D/N	1	2	3	1	2	3	1	2	3
1	2748	2752	2754	2586	2715	2737	2694	2749	2776
2	2752	2756		2724	2754		2752	2918	
3	2754			2744			2778		

[34] M. E. Fisher, Natl. Bur. Std. (U. S.) Misc. Publ. **273**, 21 (1966).
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[38] M. E. Fisher and R. J. Burford, Phys. Rev. **156**, 583 (1967).
[39] D. Jasnow and M. Wortis (to be published). We have not used the two new terms given here.

TABLE XVII. $10^3 \times g_n$ and extrapolants for the second correlation moment of the fcc classical Heisenberg model.

n/r	0	1	2	3	4
2	3031				
3	2351	0990			
4	2135	1487	1984		
5	2031	1617	1812	1697	
6	1971	1671	1778	1745	1769

it is difficult to obtain from them an estimated upper bound. We therefore employ the ratio method (2.13). Since the $1/n$ plot has a considerable curvature, later columns of the Neville table (Table XVII) are useful, and we estimate

$$2.74 \leqslant \gamma_2 \leqslant 2.80 \text{ (fcc)}. \quad (6.11)$$

Further evidence may be obtained by assuming (see Sec. 2) r_n to be of the form $K_c^{-1}[1+g/(n+\epsilon)]$ [compare (2.11)]. In general, results for different ϵ must be critically compared. However, when an accurate estimate for K_c^{-1} is available from some other source, it is important to ensure that the convergence of the sequence $l_n(\epsilon)=(n+\epsilon)r_n-(n-1+\epsilon)r_{n-1}$ [compare (2.12)] to this limit is smooth. Here $\epsilon=-\frac{1}{2}$ is satisfactory in this respect; therefore we use this value in forming the sequence $g_n(\epsilon)=(n+\epsilon)(K_c r_n-1)$ [compare (2.13)]. The following successive estimates for γ_2-1 result: 2.273, 1.959, 1.868, 1.828, 1.807. This sequence certainly supports the (nonrigorous) upper bound of (6.11).

Combining (6.10) and (6.11), we obtain our final estimate

$$2.75 \leqslant \gamma_2 \leqslant 2.80 \text{ (fcc)},$$

which, using (6.8) and (6.9), gives

$$0.6875 \leqslant \nu \leqslant 0.7125 \text{ (fcc)}, \quad (6.12)$$

$$0 \leqslant \eta \leqslant 0.07 \text{ (fcc)}. \quad (6.13)$$

7. SIMPLE CLASSICAL HEISENBERG ANTIFERROMAGNET

Simple antiferromagnetic ordering is possible on loose-packed lattices. It is well known[2,38] that for the classical Heisenberg model, the mathematical problem of a simple antiferromagnet in a finite or zero staggered field[2] is precisely equivalent to that of the corresponding ferromagnet in the appropriate uniform field. Thus, Secs. 3–6 may be simply reinterpreted in terms of antiferromagnetism. Some particularly important consequences of this symmetry are the following: The Curie and Néel points are related by the equality $(2J/kT_c)=(2|J|/kT_N)$. The critical values of the entropy, energy, etc., at the Curie and Néel points are the same. All the critical exponents for the ferromagnet and antiferromagnet are identical. (N.B. For the antiferromagnet these exponents are defined, where necessary, with reference to a staggered field.)

For comparison with experiment, it is important to obtain results for antiferromagnets in uniform fields. To investigate the initial physical susceptibility of the simple classical Heisenberg antiferromagnet we use the series of Table I, taking $K=2\beta J$ to be negative, and restricting attention to the loose-packed bcc and sc lattices.

Starting with the reduced susceptibility ξ defined by

$$\xi=(3kT/Nm^2)\chi, \quad (7.1)$$

we follow a procedure similar to that of Fisher and Sykes[40,41] for the spin-$\frac{1}{2}$ Ising model and attempt to remove the dominant ferromagnetic singularity by computing

$$\phi=(1-K/K_c)^{\gamma}\xi, \quad (7.2)$$

where here $\gamma=1\frac{3}{8}$. Using our estimates $K_c=0.4863$ (bcc) and $K_c=0.6918$ (sc), we find

$$\phi(K)=1-0.160806K-0.227534K^2 +0.121741K^3-0.267445K^4+0.224921K^5 -0.485872K^6+0.527412K^7-1.093833K^8 +1.333827K^9-\cdots \text{ (bcc)} \quad (7.3)$$

and

$$\phi(K)=1+0.0124320K-0.103108K^2 +0.0366111K^3-0.0431506K^4+0.0603836K^5 -0.0393274K^6+0.0527043K^7-0.0421989K^8 +0.0636318K^9-\cdots \text{ (sc)}.$$

Apart from initial effects, the coefficients of both the series (7.3) alternate regularly in sign as must be the case asymptotically if the antiferromagnetic singularity dominates. Unfortunately, however, the magnitudes of the coefficients are not sufficiently regular to allow accurate assessment of the behavior of the physical susceptibility in the region of the Néel point. If we dismiss the possibility that our value for γ is incorrect, there remain two likely causes of this: (a) the use in (7.2) of an insufficiently accurate estimate of K_c; (b) the effect of singularities other than that at the Néel point.

TABLE XVIII. The [5,4] PA to $\phi(K)$ for the bcc and sc classical Heisenberg models.

$$[D,N]=P_N(K)/Q_D(K)=\sum_{r=0}^{N} p_r K^r \Big/ \sum_{s=0}^{D} q_s K^s$$

	Numerator bcc	Numerator sc		Denominator bcc	Denominator sc
p_0	+1.000 000	+1.000 000	q_0	+1.000 000	+1.000 000
p_1	+0.385 757	−5.292 029	q_1	+0.546 563	−5.304 461
p_2	−2.684 874	−0.493 719	q_2	−2.369 449	−0.324 665
p_3	−0.444 539	+4.145 953	q_3	−0.822 940	+3.566 443
p_4	+1.129 456	−2.231 199	q_4	+0.658 898	−2.071 660
			q_5	+0.128 422	+0.116 098

[40] M. F. Sykes and M. E. Fisher, Physica **28**, 919 (1962).
[41] M. E. Fisher and M. F. Sykes, Physica **28**, 939 (1962).

TABLE XIX. Estimated values of the quantity $(6|J|/Nm^2)\chi$ at various points of the high-temperature ranges of the bcc and sc simple classical Heisenberg antiferromagnets.

bcc				sc			
$-1/K$	$(6\|J\|/Nm^2)\chi$	$-1/K$	$(6\|J\|/Nm^2)\chi$	$-1/K$	$(6\|J\|/Nm^2)\chi$	$-1/K$	$(6\|J\|/Nm^2)\chi$
3.500	0.15465	2.100	0.18135	3.500	0.17526	1.550	0.23883
3.250	0.16005	2.095	0.18135	3.250	0.18269	1.500	0.23902
3.000	0.16559	2.090	0.18135	3.000	0.19064	1.490	0.23900
2.750	0.17114	2.085	0.18134	2.750	0.19912	1.480	0.23896
2.500	0.17636	2.080	0.18132	2.500	0.20808	1.470	0.23889
2.350	0.17902	2.075	0.18131	2.250	0.21737	1.465	0.23884
2.300	0.17976	2.070	0.18129	2.000	0.22661	1.460	0.23879
2.250	0.18040	2.065	0.18127	1.750	0.23483	1.455	0.23873
2.200	0.18090	2.060	0.18124	1.650	0.23731	1.450	0.23867
2.150	0.18124	2.05634	0.18122	1.600	0.23822	1.4455	0.23860

To investigate (a) we repeat our analysis at various points throughout the ranges (3.7), but unfortunately the magnitudes of the coefficients of $\phi(K)$ remain irregular. Regarding (b), analyses of the series (7.3) show that, apart from the antiferromagnetic singularity, they have a well-defined singularity for small positive K. It may well be therefore that our difficulty is principally caused by the "interference" of residual singularities at $K=+K_c$. [No attempt to account for such correction terms is made in (7.2).]

If we write

$$\phi \sim A_N'(1-K/K_N')^{1-\epsilon}+B_N' \quad \text{as} \quad K\to K_N+, \quad (7.4)$$

then PA calculations certainly give $K_N \approx -K_c$ (the equality holds rigorously) and ϵ small. (The bcc lattice provides some evidence, admittedly rather inconclusive, that $\epsilon \geqslant 0$. This suggests that the susceptibility gradient may be infinite at the Néel point as is the case for the spin-$\frac{1}{2}$ Ising model.[40,41])

To estimate ϕ and therefore χ in the high-temperature region we may either extrapolate partial sums of the series (7.3) or evaluate PA's to them (see Sec. 2). Using the method of partial sums, we estimate B_N' in (7.4) to be 0.954 (bcc) and 0.884 (sc). PA's (see Table XVIII for details of the [5,4] PA's which should be among the most reliable) lead to the estimates 0.967 (bcc) and 0.895 (sc) for B_N'. We conclude that

$$\begin{aligned}\phi(K_N)&=B_N'\approx 0.960 \text{ (bcc)},\\ \phi(K_N)&=B_N'\approx 0.889 \text{ (sc)}.\end{aligned} \quad (7.5)$$

The assignment of uncertainties is difficult but the results (7.5) should be accurate to within a few percent.

Corresponding to (7.4), we can write

$$\xi \sim A_N(1-K/K_N)^{1-\epsilon}+B_N \quad \text{as} \quad K\to K_N+. \quad (7.6)$$

Then using (7.2), we find that our estimates (7.5) are equivalent to

$$\begin{aligned}\xi(K_N)&=B_N\approx 0.370 \text{ (bcc)},\\ \xi(K_N)&=B_N\approx 0.343 \text{ (sc)}.\end{aligned} \quad (7.7)$$

In Table XIX are listed estimated values of the quantity

$$(6|J|/Nm^2)\chi=-K(1-K/K_c)^{-11/8}\phi(K), \quad (7.8)$$

at various points of the range $K_N \leqslant K \leqslant 0$. These are obtained using the [5,4] PA's of Table XVIII. The general behavior seems similar to that found for the spin-$\frac{1}{2}$ Ising model.[40,41] In particular, a flat maximum just above the Néel point is suggested. However, it should be emphasized that the results are rather unreliable in the critical region, where numerical uncertainties are relatively large.

8. ZERO-FIELD SUSCEPTIBILITY OF THE EQUIVALENT-NEIGHBOR CLASSICAL HEISENBERG FERROMAGNET

The first seven coefficients of the high-temperature series expansions of the zero-field susceptibilities of the bcc (1,2), sc (1,2), and fcc (1,2) classical Heisenberg models have already been presented in Table II. In this section, we estimate Curie temperatures K_c and critical exponents γ using these series. Our primary concern is to establish whether, starting with the nearest-neighbor model, the inclusion of equal-strength second-neighbor interactions leaves the value of γ unchanged, as seems to be the case for the spin-$\frac{1}{2}$ Ising model.[2,22]

From the roots of PA's to $(D^p \ln\chi)^{1/p}$ with $p=1$, 2, and 3 and from Neville tables for the ratios, we obtain the preliminary estimates

$$K_c=0.2640 \text{ [bcc (1,2)]}, \quad 0.1965 \text{ [sc (1,2)]}, \quad 0.1963 \text{ [fcc (1,2)]}. \quad (8.1)$$

To find more accurate estimates for these Curie points we first verify that g is near 0.375 and then employ the ratio method (2.14) taking $g'=\frac{3}{8}$. From these results (Table XX) and from other similar sequences we feel able to conclude that $K_c^{-1}=3.7911 \pm 0.0012$ [bcc (1,2)], 5.087 ± 0.004 [sc (1,2)], 5.090 ± 0.005 [fcc (1,2)]. On inversion these give the final estimates

$$\begin{aligned}K_c&=0.26378\pm 0.00009 \text{ [bcc (1,2)]},\\ K_c&=0.19658\pm 0.00015 \text{ [sc (1,2)]},\\ K_c&=0.19646\pm 0.00020 \text{ [fcc (1,2)]},\end{aligned} \quad (8.2)$$

which are close to the initial estimates (8.1).

TABLE XX. β_n's and extrapolants for the susceptibilities of some equivalent-neighbor classical Heisenberg models ($g'=\frac{3}{8}$).

bcc (1,2) $10^4\beta_n$

n/r	1	2	3	4	5
1	33 939				
2	36 491				
3	37 210				
4	37 477	37 743			
5	37 618	37 829	37 886		
6	37 699	37 862	37 895	37 899	
7	37 750	37 878	37 899	37 902	37 903

sc (1,2) $10^3\beta_n$

n/r	1	2	3	4	5
1	4364				
2	4772				
3	4910				
4	4972	5034			
5	5006	5056	5071		
6	5026	5067	5077	5081	
7	5039	5073	5081	5083	5084

fcc (1,2) $10^3\beta_n$

n/r	1	2	3	4	5
1	4364				
2	4772				
3	4910				
4	4972	5034			
5	5006	5057	5072		
6	5027	5068	5078	5082	
7	5040	5074	5082	5085	5086

Taking values for K_c throughout the ranges (8.2), we investigate the value of γ using PA method (2.9) with $p=1$ and $p=2$ and ratio method (2.13). Results for typical values of K_c are presented in Tables XXI–XXIII, which are for the bcc (1,2), sc (1,2), and fcc (1,2) models, respectively. For the bcc (1,2), the Padé table for $p=1$ is largely increasing, while that for $p=2$ is largely decreasing. Comparison suggests the estimate 1.372 ± 0.005 for their common limit. This result is supported by the Neville table, which is again substantially increasing, and appears to have a limiting value in the range 1.375 ± 0.004. For the sc (1,2) and fcc (1,2) convergence is not quite so rapid, but it appears reasonable to conclude that in both cases the limit lies in the range 1.37 to 1.38. It is not easy to give final estimates for γ, since the uncertainties must reflect those in K_c. However, a detailed study makes us confident that

$$\gamma=1.375\pm0.005. \tag{8.3}$$

[If, as seems unlikely, there are any differences between the values of this critical exponent for the bcc (1,2),

TABLE XXI. Estimates (in units of 10^{-3}) for the critical exponent γ of the bcc (1,2) classical Heisenberg model, using $K_c=0.26380$.

From evaluating PA's to $(K_c-K)D\ln\chi$ at $K=K_c$

D/N	1	2	3	4	5
1	1358	1350	1367	1365	1366
2	1350	1354	1365	1366	
3	1372	1366	1366		
4	1365	1366			
5	1366				

From evaluating PA's to $(K_c-K)(D^2\ln\chi)^{1/2}$ at $K=K_c$

D/N	1	2	3	4
1	1367	1359	1377	1377
2	1363	1378	1377	
3	1377	1377		
4	1377			

From g_n's and extrapolants

n/r	0	1	2	3	4
3	1313				
4	1325	1363			
5	1334	1368	1377		
6	1340	1370	1374	1370	
7	1344	1371	1373	1372	1374

TABLE XXII. Estimates (in units of 10^{-3}) for the critical exponent γ of the sc (1,2) classical Heisenberg model, using $K_c=0.19666$.

From evaluating PA's to $(K_c-K)D\ln\chi$ at $K=K_c$

D/N	1	2	3	4	5
1	1334	1329	1341	1346	1352
2	1329	1332	1350	1373	
3	1341	1350	1361		
4	1347	1372			
5	1353				

From evaluating PA's to $(K_c-K)(D^2\ln\chi)^{1/2}$ at $K=K_c$

D/N	1	2	3	4
1	1359	1371	1372	1377
2	1371	1372	1369	
3	1372	1370		
4	1377			

From g_n's and extrapolants

n/r	0	1	2	3	4
3	1259				
4	1278	1335			
5	1291	1345	1359		
6	1301	1351	1363	1367	
7	1309	1355	1366	1371	1375

TABLE XXIII. Estimates (in units of 10^{-3}) for the critical exponent γ of the fcc (1,2) classical Heisenberg model, using $K_c=0.19658$.

From evaluating PA's to $(K_c-K)D\ln\chi$ at $K=K_c$

D/N	1	2	3	4	5
1	1331	1325	1339	1344	1351
2	1325	1329	1346	1307	
3	1339	1346	1363		
4	1344	1309			
5	1352				

From evaluating PA's to $(K_c-K)(D^2\ln\chi)^{1/2}$ at $K=K_c$

D/N	1	2	3	4
1	1354	1370	1369	1380
2	1370	1369	1370	
3	1369	1370		
4	1382			

From g_n's and extrapolants

n/r	0	1	2	3	4
3	1258				
4	1276	1332			
5	1290	1342	1357		
6	1299	1348	1360	1364	
7	1307	1353	1365	1372	1378

sc (1,2), and fcc (1,2) models, they are not detected by our methods.]

In the light of our estimate (8.3) and our general approach of looking for simple fractions which do justice to our conclusions, it appears probable that $\gamma=1\frac{3}{8}$ is the exact result in the three cases considered. This suggests that γ has the same value for the nearest-neighbor model and the equivalent-neighbor model of order two.

9. ZERO-FIELD SUSCEPTIBILITY OF THE EQUIVALENT-NEIGHBOR SPIN-$\frac{1}{2}$ HEISENBERG MODEL

We analyze here the susceptibility series of Table III, which are for the bcc (1,2), sc (1,2), and fcc (1,2) spin-$\frac{1}{2}$ Heisenberg models. We might well expect the critical exponent γ of the Heisenberg model to be independent of spin, as seems to be the case for the Ising model.[2,9] If so, then bearing in mind the results of Domb and Dalton[22] and Sec. 8 of this paper, we should perhaps expect to find $\gamma=1\frac{3}{8}$ for all three-dimensional nearest-neighbor and higher finite-order equivalent-neighbor Heisenberg models, irrespective of spin. Unfortunately, however, according to Baker *et al.* (Ref. 13), $\gamma=1.43\pm0.01$ for the three cubic lattices with nearest-neighbor spin-$\frac{1}{2}$ Heisenberg interactions. Faced with this contradiction, the best approach here is obviously to let the series of Table III stand on their own, and to undertake a direct analysis similar to that of Sec. 3.

We start with a discussion of the Curie roots and corresponding residues of PA's to $D\ln\chi$ for the fcc (1,2)

TABLE XXIV. Curie roots and corresponding critical exponents from PA's to $D\ln\chi$ for the fcc (1,2) spin-$\frac{1}{2}$ Heisenberg model.

		$10^5\times$(Curie root)			
D/N	1	2	3	4	5
1	14 685	14 750	14 743	14 745	14 754
2	14 762	14 744	14 745	14 743	
3	14 745	14 745	14 744		
4	14 745	14 745			
5	14 742				
		$10^4\times$(Critical exponent)			
D/N	1	2	3	4	5
1	13 586	13 766	13 742	13 752	13 801
2	13 816	13 745	13 749	13 740	
3	13 748	13 750	13 744		
4	13 750	13 748			
5	13 737				

TABLE XXV. Curie roots (in units of 10^{-6}) of PA's to $\chi^{8/11}$ for the fcc (1,2) spin-$\frac{1}{2}$ Heisenberg model.

D/N	1	2	3	4	5	6
1	147 651	147 430	147 455	147 450	147 451	147 464
2	147 420	147 453	147 451	147 451	147 450	
3	147 455	147 451	147 451	147 451		
4	147 453	147 451	147 451			
5	147 451	147 452				
6	147 451					

TABLE XXVI. Estimates (in units of 10^{-5}) for the critical exponent γ of the fcc (1,2) spin-$\frac{1}{2}$ Heisenberg model from PA's to $(K_c-K)D\ln\chi$ evaluated at $K=K_c=0.147451$.

D/N	1	2	3	4	5
1	137 615	137 490	137 498	137 500	137 503
2	137 496	137 500	137 500	137 498	
3	137 500	137 501	137 500		
4	137 500	137 500			
5	137 503				

TABLE XXVII. Curie roots and corresponding critical exponents from PA's to $D\ln\chi$ for the sc (1,2) spin-$\frac{1}{2}$ Heisenberg model.

		$10^5\times$(Curie root)			
D/N	1	2	3	4	5
1	14 685	14 750	14 760	14 756	14 761
2	14 762	14 762	14 757	14 758	
3	14 762	14 762	14 759		
4	14 758	14 759			
5	14 759				
		$10^4\times$(Critical exponent)			
D/N	1	2	3	4	5
1	13 586	13 766	13 805	13 787	13 811
2	13 816	13 815	13 793	13 798	
3	13 815	13 816	13 799		
4	13 797	13 799			
5	13 799				

model. The convergence of these results (Table XXIV) is remarkably rapid, there being only one approximant of the last three orders which does not yield values in the ranges

$$K_c=0.14744\pm0.00002\ [\text{fcc}\ (1,2)], \qquad (9.1)$$

which is an initial estimate, and

$$\gamma=1.3744\pm0.0008\ [\text{fcc}\ (1,2)], \qquad (9.2)$$

which is a final estimate. If we insist on a simple fraction for γ, the estimate (9.2) strongly suggests $\gamma=1\frac{3}{8}$. Consequently, we obtain our final estimate for the Curie point

$$K_c=0.147451\pm0.000003\ [\text{fcc}\ (1,2)] \qquad (9.3)$$

from PA's to $\chi^{8/11}$ (Table XXV). Using the central value of (9.3) in PA method (2.9) with $p=1$, the results of Table XXVI are obtained. All approximants of the last four orders yield $\gamma=1.3750\pm0.0001$ and all of the last three $\gamma=1.37500\pm0.00003$, which is extremely satisfactory. The exceptionally rapid convergence of Tables XXV and XXVI and their mutual consistency give us additional confidence in the conjecture $\gamma=1\frac{3}{8}$.

Table XXVII contains results of PA calculations with $D\ln\chi$ for the sc (1,2) model. Fluctuations, both among PA's of a given order and from one order to another, are more marked than for fcc (1,2); furthermore, there is some indication that the Padé tables are decreasing. With these points in mind, we obtain

$$K_c=0.14750\pm0.00012\ [\text{sc}\ (1,2)] \qquad (9.4)$$

TABLE XXVIII. Curie roots (in units of 10^{-5}) of PA's to $\chi^{8/11}$ for the sc (1,2) spin-$\frac{1}{2}$ Heisenberg model.

D/N	1	2	3	4	5	6
1	14 765	14 743	14 746	14 749	14 750	14 751
2	14 742	14 745	14 732	14 751	14 743	
3	14 745	14 761	14 750	14 754		
4	14 745	14 750	14 753			
5	14 751	14 759				
6	14 736					

as an initial estimate and

$$\gamma=1.377\pm0.005\ [\text{sc }(1,2)] \qquad (9.5)$$

as a final estimate. The estimate (9.5) suggests that the exact result for sc (1,2) is also $\gamma=1\frac{3}{8}$. Consequently, we determine the Curie roots of PA's to $\chi^{8/11}$ for sc (1,2). These are displayed in Table XXVIII, which leads to our final estimate

$$K_c=0.14753\pm0.00008\ [\text{sc }(1,2)]. \qquad (9.6)$$

Naturally we evaluate PA's to $(K_c-K)D\ln\chi$ at $K=K_c$ using various values throughout the range (9.6). These calculations, of which we omit the details, are entirely consistent with our previous conclusions.

We do not give here any analysis of the susceptibility series of fcc (1,2) and sc (1,2) using either PA methods with $p>1$ or ratio techniques. These are omitted since, while they serve to confirm the above conclusions, they do not provide more accurate estimates of either γ or K_c.

Unfortunately, we do not obtain very rapid convergence when we apply any of our methods to the susceptibility series of bcc (1,2). This is not altogether surprising since the effective coordination number is only 14. We are therefore not dealing with much "closer packing" than is the circumstance for fcc (1), where fast convergence is certainly not in evidence.[13] Although the bcc (1,2) series does not permit precise estimates for critical parameters, it is not inconsistent with $\gamma=1\frac{3}{8}$.

10. SUMMARY AND DISCUSSION

Against the background sketched in Sec. 1, and using the extrapolation techniques of Sec. 2, we have estimated various critical parameters of the Heisenberg model. For convenience, many of our results are collected in Table XXIX. Of particular importance in the theory of critical phenomena are the values of the various critical exponents; consequently much of this section is devoted to a consideration of our results for such quantities.

In Secs. 3–6, the three-dimensional nearest-neighbor classical (i.e., infinite-spin) Heisenberg ferromagnet was studied. In Sec. 3, the critical behavior of the high-temperature initial susceptibility was investigated with particular regard to the value of the appropriate critical exponent γ. Evidence was presented which supports the conjecture that $\gamma=1\frac{3}{8}$ exactly for each of the three cubic lattices. (The evidence was especially convincing for the fcc lattice.) Estimates for the Curie points K_c and the amplitudes A_c of the ferromagnet singularity were also obtained for these three lattices. In Sec. 4, the zero-field high-temperature specific heat of the fcc lattice was investigated. For the critical exponents, the estimates $\alpha=0$ and $-\frac{1}{8}\leqslant\alpha_s\leqslant-\frac{1}{16}$ were found. The critical values of the entropy and energy of the three cubic lattices

TABLE XXIX. Some high-temperature critical parameters of the Heisenberg model.

a) Nearest-neighbor models

Spin	Property	Parameter	Estimated value sc (1)	Estimated value bcc (1)	Estimated value fcc (1)	Remarks
∞	Initial ferromagnetic susceptibility χ_0	K_c	0.6918 $\pm$0.0003	0.4863 $\pm$0.0002	0.31445 $\pm$0.00002	
		γ	1.375 $\pm$0.010	1.375 $\pm$0.010	1.375 $\pm$0.002	
		A_c	0.971 $\pm$0.003	0.866 $\pm$0.003	0.8385 $\pm$0.0009	
∞	Zero-field specific heat, C_0	α_s			$-\frac{1}{8}\leqslant\alpha_s\leqslant-\frac{1}{16}$	$\alpha=0$ for fcc (1)
∞	Critical entropy and energy	$(S_\infty-S_c)/Nk$	0.415 $\pm$0.014	0.338 $\pm$0.006	0.314 $\pm$0.002	
		$(E_\infty-E_c)/NkT_c$	0.69 $\pm$0.02	0.533 $\pm$0.004	0.468 $\pm$0.004	
∞	Zero-field spin pair correlation function, Γ	γ_2			$2.75\leqslant\gamma_2\leqslant2.80$	ν and η are obtained from γ and γ_2 using $\nu=\frac{1}{2}(\gamma_2-\gamma)$ and $\eta=2-\gamma\nu^{-1}$.
		ν			$0.6875\leqslant\nu\leqslant0.7125$	
		η			$0\leqslant\eta\leqslant0.07$	
∞	Initial antiferromagnetic susceptibility χ_0	ϵ	≈0	≈0	...	
		B_N	≈0.343	≈0.370	...	

b) Equivalent-neighbor models of order-2

Spin	Property	Parameter	Estimated value bcc (1,2)	Estimated value sc (1,2)	Estimated value fcc (1,2)	Remarks
∞	Initial ferromagnetic susceptibility, χ_0	K_c	0.26378$\pm$0.00009	0.19658$\pm$0.00015	0.19646 $\pm$0.00020	
		γ	⟵	1.375 $\pm$0.005	⟶	
$\frac{1}{2}$	Initial ferromagnetic susceptibility, χ_0	K_c		0.14753$\pm$0.00008	0.147451$\pm$0.000003	
		γ		1.377 $\pm$0.005	1.3744 $\pm$0.0008	

were estimated in Sec. 5. In Sec. 6, we obtained the estimate $2.75 \leqslant \gamma_2 \leqslant 2.80$ for the high-temperature critical exponent of the second moment of the zero-field longitudinal spin pair correlation function of the fcc lattice. Assuming there to be only a single correlation length which diverges at the critical point, we used our results for γ and γ_2 to obtain the estimates $0.6875 \leqslant \nu \leqslant 0.7125$ and $0 \leqslant \eta \leqslant 0.07$ for the correlation critical exponents introduced in (6.2) and (6.3).

In Sec. 7 the simple classical Heisenberg antiferromagnet was examined. A mathematical equivalence with the problem of the ferromagnet was noted and exploited. Assuming the physical susceptibility of the simple antiferromagnet to be of the form $(Nm^2/3kT) \times [A_N(1-K/K_N)^{1-\epsilon}+B_N]$ just above the Néel point, numerical investigations for the bcc and sc lattices showed ϵ to be small. Estimates for B_N were made.

In Sec. 8, an investigation of the initial susceptibility of the bcc (1,2), sc (1,2), and fcc (1,2) equivalent-neighbor classical Heisenberg models was undertaken. Evidence was obtained which indicated that, in each of these cases, $\gamma = 1\frac{3}{8}$ is probably the exact result. The Curie points were estimated.

In Sec. 9, the Curie points and critical exponents γ of the sc (1,2) and fcc (1,2) spin-$\frac{1}{2}$ Heisenberg models were estimated. The evidence, which was particularly convincing for fcc (1,2), suggested that for both these models the exact value of γ is again very probably $1\frac{3}{8}$.

In discussing our results, we turn first to the nearest-neighbor classical Heisenberg ferromagnet and to various of the existing equalities[2,4,42] and inequalities[2,4,43] which connect the critical exponents. Using these it is possible with our present information to indulge in considerable speculation, but we are content to present some of the apparently more important points. (Although strictly the following remarks are for spin infinity and the fcc lattice with only nearest-neighbor interactions, arguments advanced later suggest that they may be of wider relevance.)

Actually we have already used relations of the type mentioned, for in deriving our values for ν and η in Sec. 6 we employed the formula $\gamma_t = (t+2-\eta)\nu$ for $t=0$ and $t=2$. Our estimates satisfy the Josephson inequality $d\nu \geqslant 2-\alpha$,[43] and also include values satisfying the stronger inequality $d\nu \geqslant 2-\alpha_s$ and the scaling law $d\nu = 2-\alpha_s$.[2] Now, the scaling laws imply that the critical exponents are symmetrical about the transition, and such symmetry is apparently not a general property of the Heisenberg model. In this connection, Fisher[2] has discussed some difficulties arising when γ' is undefined. Although difficulties of the above type occur for the nearest-neighbor spherical model,[44] the scaling relations $\alpha_s+2\beta+\gamma=2$, $\gamma=\beta(\delta-1)$, and $2\Delta=\gamma+2-\alpha_s$ involving the high-temperature critical exponents α_s, γ, and Δ are still satisfied with $\alpha_s = -1$. It seems, therefore, that the results

$$\tfrac{11}{32} \leqslant \beta \leqslant \tfrac{3}{8}, \tag{10.1}$$

$$4\tfrac{2}{3} \leqslant \delta \leqslant 5, \tag{10.2}$$

$$3\tfrac{7}{16} \leqslant 2\Delta \leqslant 3\tfrac{1}{2}, \tag{10.3}$$

obtained by using our values in these equations, may have some relevance. The result (10.1) suggests that β is greater than $\frac{1}{3}$, which is a value sometimes considered.[42] For a numerical investigation of the gap exponent 2Δ in the case of the spin-$\frac{1}{2}$ Heisenberg model see Baker *et al.*[13]

Turning to the simple classical Heisenberg antiferromagnet, it seems logical in the spirit of the work of Fisher,[2] to investigate the possibility of an algebraic connection between ϵ and α or α_s. It is therefore interesting that the numerical work of Secs. 4 and 7 allows, among others, the possibilities $\epsilon=\alpha=0$ and $-\frac{1}{8} \leqslant \epsilon = \alpha_s \leqslant -\frac{1}{16}$. (There is, however, some rather inconclusive evidence that for the bcc lattice $\epsilon \geqslant 0$.)

We have found it to be probable that, for classical Heisenberg interactions, the equivalent-neighbor bcc (1,2), sc (1,2), and fcc (1,2) models have the same common value of γ, namely, $1\frac{3}{8}$, as do the nearest-neighbor sc, bcc, and fcc models. This result is not unexpected since similar behavior appears to be the case for the spin-$\frac{1}{2}$ Ising model.[2,22] We are naturally led to expect that $\gamma = 1\frac{3}{8}$ may well be the exact result for all equivalent-neighbor classical Heisenberg models of finite order (including nearest-neighbor ones).

The evidence for $\gamma = 1\frac{3}{8}$ in the case of certain spin-$\frac{1}{2}$ equivalent-neighbor Heisenberg models of order two is rather good. This requires further consideration since Baker *et al.*[13] give $\gamma = 1.43 \pm 0.01$ for the three cubic lattices with nearest-neighbor spin-$\frac{1}{2}$ Heisenberg interactions. In the light of the previous paragraph, we feel reluctant to accept that for the spin-$\frac{1}{2}$ Heisenberg model the value of γ is not the same for nearest-neighbor models and equivalent-neighbor models of order two.

Now, for the spin-$\frac{1}{2}$ Heisenberg model the nearest-neighbor susceptibility series[13] do not yield convergence comparable to that found in Sec. 9 of this paper for the equivalent-neighbor series. Consequently, as regards γ, we feel that the value 1.43 given in the former case is, despite the relatively long series available there, less firmly established than the value 1.375 in the latter case. In fact, a study of the results of Baker *et al.*[13] and a detailed ratio analysis shows that, while the estimate $\gamma = 1.43$ is perhaps the most reasonable, the possibility that $\gamma = 1\frac{3}{8}$ cannot be ignored for nearest-neighbor models.

We therefore suggest that $\gamma = 1\frac{3}{8}$ for all equivalent-neighbor spin-$\frac{1}{2}$ Heisenberg models of finite order (including nearest-neighbor ones) must be seriously considered. Furthermore, if $\gamma = 1\frac{3}{8}$ for the extreme quantum limit of spin $\frac{1}{2}$, as well as the classical limit of infinite

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spin, it seems rather unlikely that a different value will apply for intermediate spin. The early work of Gammel *et al.*[10] for general spin provides some evidence (see particularly their Table 5) to support this idea. This leads to the possibility that for ferromagnetic Heisenberg interactions, the critical exponent γ has the same value irrespective of spin and the particular three-dimensional nearest-neighbor or finite-order equivalent-neighbor model considered.[45] Additional terms of the spin-$\frac{1}{2}$ equivalent-neighbor series would provide a useful means of testing this suggestion more thoroughly. The calculation of the required lattice constants[3] can be handled by electronic computer and it is hoped to extend the equivalent-neighbor series as far as the nearest-neighbor ones.

[45] This naturally suggests the similar behavior of other critical exponents. In the absence of detailed numerical evidence the assumption of such behavior might prove useful.

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Magnetic Symmetry and Antiferromagnetic Resonance in CoO

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The irreducible corepresentations of the Shubnikov (magnetic) space group of ordered CoO (C_c2/c) have been deduced, and the magnon symmetries at various points in the Brillouin zone have been investigated. The antiferromagnetic resonance frequencies in CoO have been determined experimentally to be at 216.0, 221.0, and 248.0 cm^{-1} (each $\pm 0.2\%$). These results are compared with the neutron-scattering results and postulated magnon dispersion relations of Sakurai, Buyers, Cowley, and Dolling. It is suggested that the exchange constants J_1 and J_2 are about one order of magnitude smaller than previously assumed.

1. INTRODUCTION

At high temperatures CoO assumes the NaCl structure. Below its Néel temperature antiferromagnetic CoO suffers a small tetragonal distortion and both a single-spin-axis structure and a multi-spin-axis structure have been proposed for the orientations of the spins. Antiferromagnetic resonance frequencies for CoO were calculated by Tachiki[1] and some experimental work has been done by Milward.[2] Neutron-scattering measurements have recently been performed both above and below the Néel temperature by Sakurai *et al.*[3]

2. COREPRESENTATIONS OF ANTIFERROMAGNETIC CoO STRUCTURE

In its paramagnetic state CoO assumes the NaCl structure so that the Co^{2+} ions form a fcc lattice. (See Fig. 1.) There have been two alternative suggestions concerning the arrangement of the spins in CoO at low temperatures. Below the Néel temperatures CoO is no longer exactly cubic but acquires a small tetragonal distortion. According to Shull *et al.*[4] and Roth[5] the spins are aligned in ferromagnetic sheets parallel to (111) planes with alternate signs in successive sheets. The actual spin direction was claimed to be in the [11$\bar{7}$] direction and therefore at an angle of 11° 30′ to the z axis.[5] It is clear that such an orientation of the spins is not compatible with the retention of tetragonal symmetry, and an alternative multi-spin-axis structure for

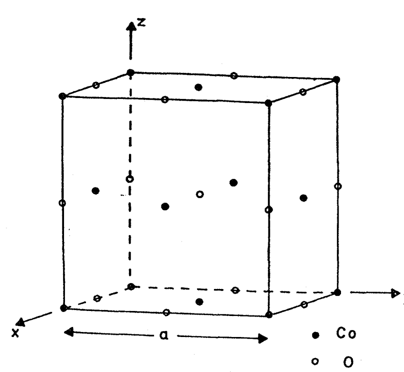

FIG. 1. The structure of paramagnetic CoO (NaCl structure).

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