Three-dimensional Heisenberg ferromagnet: A series investigation

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We present new twelfth-order high-temperature series for the susceptibility, correlation length, and free energy of the nearest-neighbor classical Heisenberg ferromagnet in zero field on a fcc lattice. Checks corroborating the correctness of the series are discussed. Standard analysis of these series produces results in essential agreement with the renormalization-group calculations and several other series analyses. However, a more reliable confluent singularity analysis suggests slightly larger values, $\gamma = 1.40^{+0.03}_{-0.01}$ and $\nu = 0.72 \pm 0.01$, as well as a confluent correction of just the size to cause the observed standard analysis underestimate.

I. INTRODUCTION

For a number of years, there has been a real discrepancy between the values of the Heisenberg indices.[1-8] Not only have series results disagreed with renormalization-group results, but different applications of the same method have led to different results, so that recent, seemingly reliable studies led to a number of different values, e.g., values of the susceptibility index were in the range $1.38 < \gamma < 1.42$. This situation is summarized in Table I.

In an attempt to better understand the differences between the various series results, we have derived new twelfth-order series for the classical Heisenberg model; our analysis of these new longer series has been influenced by the lessons learned in eliminating the Ising discrepancies.[9-11] The Heisenberg discrepancy may seem superficially similar to the Ising situation where the consensus of recent series work, based largely on new very long series, suggests that the earlier series analysis overestimated the indices (e.g., $\gamma \sim 1.25$) with the new estimates being indistinguishable from renormalization-group predictions (e.g., $\gamma \sim 1.24$). These modifications do not rely solely on the very long series. Recent reanalysis of correct twelfth order, $S = \frac{1}{2}$ Ising series indicates the traditional $\gamma = \frac{5}{4}$ is too high.[11] Indeed, five-fit analysis (a confluent-correction method) of the twelfth-order spin-S series produces results in agreement with the renormalization-group results ($\gamma \sim 1.24$). however, the Ising and Heisenberg cases differ on several points.

(1) The larger range of disagreement, i.e., $1.38 < \gamma < 1.42$ for the Heisenberg model, is to be contrasted with that for the Ising model, $1.24 < \gamma < 1.25$.

(2) The role of confluent singularities is somewhat different in the two cases. In the Ising case where workers relied on the longer spin-$\frac{1}{2}$ series, the amplitude of the confluent correction is almost certainly negative, which causes standard analysis to overestimate the indices.[9-11] In the Heisenberg case, workers relied more heavily on the longer spin-infinity series. Here, the amplitude is positive, resulting in an underestimate from standard analysis.

Our new longer, zero-field series (see Table II) have been derived for the classical Heisenberg model in which unit vectors (classical "spins") $\mathbf{S}_i$ occupy each site i of a fcc lattice and interact with their nearest neighbors through the Hamiltonian

$$-\beta H = K \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \ ,$$

TABLE I. Various series and renormalization-group results for the indices.

	γ	ν
	Series	
This work	$1.40\ ^{+0.03}_{-0.01}$	0.720 ± 0.010
Ref. 1	1.405 ± 0.020	0.717 ± 0.007
Ref. 3	1.375 ± 0.010	0.702 ± 0.005
Ref. 4	$1.42\ ^{+0.02}_{-0.01}$	0.725 ± 0.015
Ref. 5	$1.39\ \pm 0.01$	
	Renormalization group	
Ref. 7	$1.39\ \pm 0.01$	0.705 ± 0.005
Ref. 8	1.386 ± 0.004	0.705 ± 0.003

TABLE II. Our twelfth-order high-temperature series for the susceptibility and correlation function.

Susceptibility $3\chi = 3\mu_0$	Correlation function $\xi^2 = \mu_2/\mu_0$
1.0	$4.0K$
$4.0K$	$16.0K^2$
$14.6666666666666K^2$	$58.8444444444443K^3$
$51.7333333333333K^3$	$208.355555555554K^4$
$178.459259259259K^4$	$721.352804232797K^5$
$606.745396825394K^5$	$2460.68524397408K^6$
$2042.10041152261K^6$	$8306.72269018206K^7$
$6821.95284028997K^7$	$27825.0321783441K^8$
$22659.3609292753K^8$	$92648.9229054439K^9$
$74921.3032135086K^9$	$307025.400683868K^{10}$
$246802.546214377K^{10}$	$1013490.72770326K^{11}$
$810503.233705947K^{11}$	$3334737.54661336K^{12}$
$2654791.75915185K^{12}$	

where $\langle i,j \rangle$ restricts the sum to nearest neighbors and where $K=J/kT$. To derive twelfth-order correlation function series, we have modified an existing program which correctly derives tenth-order series for Ising, XY, and Heisenberg models on a variety of lattices, by adding the 35 "elementary" diagrams which contribute in eleventh and twelfth orders. The extended program correctly reproduces Ising susceptibility and specific-heat series through twelfth order showing that all diagrams have been included correctly.[11] To derive XY and Heisenberg series, the program decorates each line in the diagrams with the appropriate Cartesian indices in a routine fashion. As discussed in the Appendix, checks have been performed supporting the correctness of our decoration subprograms. Even though several of the higher-order coefficients in Refs. 5 and 6 disagree with ours in the sixth or seventh significant figure, as discussed in the Appendix, we are confident that our coefficients are correct given the routine way that the decorations are performed coupled with the checks.

In Sec. II we discuss the standard analysis of our twelfth-order classical Heisenberg series for the susceptibility and for the correlation length. we find results which agree with the standard analyses of Refs. 3, 5, and 6, but disagree with our previous results[1] where we tried to account for confluent-correction effects by relying heavily on trends in the extrapolation procedures. The twelfth-order series studied here show that the series are too irregular for such trends to be reliable.

In Sec. III we present the results of an unbiased five-fit analysis which show the following.

(1) The amplitude of the confluent correction is relatively large and positive.

(2) Past experience has shown that a standard analysis will underestimate the leading indices, when the confluent-correction amplitude is positive. Indeed the five-fit determination of the leading indices, shown to be more reliable, leads to values larger than those from Sec. II.

For a test function which mimics the correlation length, i.e., it has the same leading exponent and confluent correction suggested by the five-fit analysis of the correlation length, standard analysis predicts a result for the leading exponent of the test function indistinguishable from the value determined in Sec. II. This convincingly supports the reliability of the five-fit results over those from standard methods. As a result of all our analysis, we assert $T_c=3.1757\pm0.0020$, $2\nu=1.44\pm0.03$, and $\gamma=1.40^{+0.03}_{-0.01}$.

Contrary to experience with the Ising model, an unbiased confluent-correction analysis of correct twelfth-order series for the Heisenberg model worsens (rather than improves) agreement with the renormalization-group results. We hope to undertake the partial differential approximant analysis of Gaussian to Heisenberg crossover using the method of Chen, Fisher, and Nickel,[10] to more reliably account for the effect of confluent corrections.

II. STANDARD ANALYSIS

Table III presents both the Neville table extrapolations of the ratio and log-derivative sequences for T_c as well as

TABLE III. Standard analysis of susceptibility series for T_c. The column labeled 0 gives the unextrapolated sequence, the column labeled 1 gives the linear extrapolant, the column labeled 2 gives the quadratic extrapolant, etc.

N	χ $(N-1,N)$	(N,N)	$(N,N-1)$
2	3.1880	3.1805	3.2071
3	3.1837	3.1839	3.1852
4	3.1838	3.1790	3.1890
5	3.1772	3.1776	3.1775
6	3.1776		3.1776

	Ratio				Log-derivative		
N	0	1	2	N	0	2	3
2	3.3333			2	3.3333		
3	3.2485	3.2061		3	3.2400	3.1933	
4	3.2166	3.1847	3.1775	4	3.2071	3.1743	3.1679
5	3.2012	3.1780	3.1736	5	3.1925	3.1706	3.1682
6	3.1944	3.1810	3.1839	6	3.1877	3.1779	3.1852
7	3.1906	3.1811	3.1812	7	3.1853	3.1793	3.1810
8	3.1877	3.1790	3.1755	8	3.1831	3.1768	3.1726
9	3.1855	3.1777	3.1750	9	3.1814	3.1755	3.1729
10	3.1838	3.1772	3.1762	10	3.1803	3.1755	3.1756
11	3.1826	3.1771	3.1768	11	3.1795	3.1759	3.1768
12	3.1817	3.1770	3.1769	12	3.1789	3.1761	3.1769

the near-diagonal Padé estimates of T_c using the susceptibility $\chi \equiv \mu_0$ series. It is instructive to compare these Neville tables with those from Ref. 1 where we estimated $T_c = 3.1753 \pm 0.0020$. Omitting the eleventh and twelfth rows of Table III reproduces the corresponding part of Table XII from Ref. 1. The lower-order entries of these tables show trends approaching a value less than 3.176 which led us to conclude $T_c = 3.1753 \pm 0.0020$; e.g., consider the downward trend in the second column from the log-derivative susceptibility sequence. These trends, which suggest a value of T_c smaller than 3.176, change in eleventh or twelfth order leading us to favor a value of T_c slightly greater than 3.176. Our Padé estimates are consistent with the suggestion of Fisher and Ritchie,[3] $T_c = 3.178 \pm 0.003$, although the new terms and downward trends lead us to favor a value closer to 3.177. On the basis of this and additional analysis, we assert $T_c = 3.177 \pm 0.002$.

This slightly larger value of T_c is expected to lead to values of the indices lower than those of Ref. 1. Table IV presents the Neville table extrapolations of ratio and log-derivative sequences for the critical indices, γ from the susceptibility, and ν from the correlation length.

As expected the entries in Table IV are smaller than the corresponding entries in Table XV of Ref. 1, reflecting the use of a larger T_c. For example, when one considers the Neville extrapolations of the susceptibility sequences, Table XV of Ref. 1 showed upward trends to a value of γ above 1.40 which led us to predict $\gamma = 1.405 \pm 0.020$; now there are downward trends to a value below 1.396. Estimates of $\gamma \sim 1.39$ and $2\nu \sim 1.416$ from this ratio analysis are consistent with the Padé estimates given the apparent upward trends in the near-diagonal Padé terms. Including the effect of our uncertainty in T_c, we estimate $\gamma = 1.39 \pm 0.02$ and $\nu = 0.708 \pm 0.010$.

In conclusion, this standard analysis of our twelfth-order series is more consistent with the results of Refs. 3, 5, and 6 than with those of Ref. 1. It seems clear that an overreliance on trends in the Neville extrapolations of Ref. 1 led to slight overestimates of standard analysis results for the indices. However, as we shall see, the presence of confluent corrections causes the standard methods to underestimate the indices, with the result that all the evidence favors values of the indices close to or above the estimates of Ref. 1.

III. FIVE-FIT ANALYSIS

The existence of confluent corrections and their effect on the standard analysis for the indices has been well documented. One of the several nearly equivalent methods for including the effect of these confluent corrections is the q-fit method.[11,12] The logic behind the q-fit method is similar to that of the ratio method.[11,13] In this application, the assumed form of the leading singularity includes one confluent correction, i.e.,

$$\chi = At^{-\gamma}(1+Bt^{\Delta_1}) = \sum_{j=0}^{\infty} b_j K^j \; , \quad t = 1 - KT_c \; . \tag{3.1}$$

To estimate the values of the five undetermined parameters characterizing this singularity, one equates the $q=5$ consecutive coefficients in the expansion of this singularity to the corresponding coefficients in the high-temperature series, $\chi = \sum_{j=0}^{\infty} a_j K^j$, i.e., $a_j = b_j$ for $j = n$, $n-1$, $n-2$, $n-3$, and $n-4$. These five equations in the five undetermined parameters can be solved numerically providing nth estimates of the parameters. In principle, the sequence of these successive estimates should approach the true value of the parameter in the limit of large n. For T_c and the leading index, the test-function analysis shows that the five-fit estimates are significantly improved over ratio or Padé estimates even though Δ and B are poorly estimated. Test-function analysis indicates that, for reasonable higher-order confluent corrections, an improvement in the B and Δ estimates that are presently available (from 12th- to 21st-order series), requires inaccessibly long series (greater than 50th order).

TABLE IV. Ratio analysis for the indices from the susceptibility series and from the correlation length series using $T_c = 3.177$.

	γ				ν		
N	0	1	2	N	0	1	2
1	1.2590						
2	1.3083	1.3575		2	0.7590		
3	1.3308	1.3758	1.3849	3	0.7364	0.6912	
4	1.3432	1.3806	1.3854	4	0.7290	0.7067	0.7222
5	1.3508	1.3812	1.3822	5	0.7244	0.7058	0.7044
6	1.3563	1.3837	1.3887	6	0.7212	0.7051	0.7038
7	1.3606	1.3863	1.3927	7	0.7190	0.7059	0.7079
8	1.3640	1.3875	1.3913	8	0.7174	0.7066	0.7086
9	1.3666	1.3879	1.3894	9	0.7163	0.7071	0.7086
10	1.3688	1.3881	1.3886	10	0.7154	0.7073	0.7084
11	1.3705	1.3881	1.3884	11	0.7147	0.7074	0.7080
12	1.3720	1.3881	1.3882	12	0.7141	0.7075	0.7075

TABLE V. The sequence from a five-fit analysis of the susceptibility and correlation length for the parameters in Eq. (3.1).

		χ			
N	T_c	γ	A	Δ_1	B
4	3.1579	1.526	0.512	0.53	0.95
5	3.1656	1.472	0.614	0.55	0.63
6	3.1835	1.358	0.876	1.07	0.28
7	3.1807	1.374	0.838	0.82	0.23
8	3.1661	1.682	0.181	0.47	4.32
9	3.1693	1.581	0.300	0.41	2.22
10	3.1749	1.423	0.709	0.57	0.42
11	3.1764	1.398	0.790	0.77	0.33
12	3.1766	1.394	0.799	0.82	0.34

		$\xi^2=\mu_2/(\mu_0 K)$			
N	T_c	γ	A	Δ_1	B
4	3.1309	0.853	0.849	0.64	2.01
5	3.1697	0.733	1.672	0.63	0.53
6	3.1812	0.698	2.045	0.89	0.30
7	3.1771	0.713	1.867	0.69	0.37
8	3.1758	0.720	1.772	0.62	0.42
9	3.1756	0.721	1.757	0.61	0.43
10	3.1749	0.727	1.668	0.56	0.50
11	3.1752	0.724	1.714	0.59	0.46

Table V gives the five-fit estimates of the parameters in Eq. (3.1) from our susceptibility and correlation length series. The susceptibility sequences are quite irregular, with perhaps two ($n=8$ and 9) defective entries. From the far more regular correlation length sequences, we estimate $T_c=3.1757\pm0.0020$ and $\nu=0.722\pm0.010$, where ranges of values include the last five terms in these sequences. In what follows, we will argue that this five-fit estimate of ν is more reliable than the lower estimate from standard analysis. From χ, we estimate $\gamma=1.40^{+0.03}_{-0.01}$, ignoring the eighth and ninth entries.

The test-function analysis of Ref. 11 tried to estimate the effect of higher-order confluent corrections on the results of a five-fit analysis. Using test functions of the form

$$\chi=t^{-\gamma}(1+B\sqrt{t}+Ct)\,, \tag{3.2}$$

this analysis suggested several rules of thumb, three of which prove useful here:

(i) When $BC>0$, Δ_1 is overestimated.

(ii) When Δ_1 is overestimated, there is a slight underestimate of the leading index.

(iii) When $B>0$, the standard methods result is a much grosser underestimate of the leading index than the five-fit underestimate mentioned in (ii).

Since the best determination indicates $\Delta_1\sim0.55$,[7,8,10] the values for Δ_1 in Table V are overestimates. Coupled with our experience of test functions [(ii) above], this leads us to expect that the five-fit estimates of the leading indices are, if anything, underestimates, however slight. These differences between the five-fit estimates of the leading indices $\gamma=1.40$ and $\nu=0.722$ and the previous ratio and Padé estimates are fully consistent with standard analysis misestimates effected by confluent corrections of the kind observed.

To demonstrate this assertion, we have performed ratio and Padé analyses of the twelfth-order series obtained by expanding the test function

$$\xi^2=t^{-1.44}(1+0.47\sqrt{t})\,,\quad t=1-K \tag{3.3}$$

in which the leading index and confluent correction approximate what is observed for the correlation length, i.e., $\nu\sim0.72$, $\Delta_1\sim0.5$, and $B\sim0.47$. Table VI presents the ratio analysis for the critical temperature and leading exponent of this test function; the ratio analysis is typical of all the standard analyses. The critical temperature, $T_c=1.0$, is overestimated by a few hundredths of a percent while the index determinations, formed using the correct critical temperature (not the standard analysis value) underestimate the correct value by 1 to 2%. The striking agreement between these misestimates of the lead-

TABLE VI. Ratio analysis for the test function [Eq. (3.3)] showing the effect of a confluent correction approximating the one in the correlation length.

	Index equals 1.44				$T_c\equiv1.0000$		
N	0	1	2	N	0	1	2
1	1.2801						
2	1.3226	1.3651		2	1.0425		
3	1.3420	1.3806	1.3884	3	1.0193	1.0078	
4	1.3537	1.3891	1.3976	4	1.0118	1.0042	1.0031
5	1.3619	1.3947	1.4031	5	1.0082	1.0028	1.0018
6	1.3681	1.3988	1.4069	6	1.0061	1.0020	1.0013
7	1.3729	1.4019	1.4097	7	1.0048	1.0016	1.0009
8	1.3769	1.4044	1.4119	8	1.0039	1.0013	1.0007
9	1.3801	1.4065	1.4137	9	1.0033	1.0010	1.0006
10	1.3830	1.4082	1.4152	10	1.0028	1.0009	1.0005
11	1.3854	1.4097	1.4164	11	1.0024	1.0007	1.0004
12	1.3875	1.4110	1.4175	12	1.0021	1.0006	1.0004

ing index, $\nu=0.71$, and our previous estimate of the correlation length exponent from ratio and Padé analyses, $\nu=0.708$, support our contention that the correct exponent is larger, with standard analysis misestimates due to a confluent correction approximating that indicated in Table V. Note that use of the standard analysis overestimate of T_c would have lowered the standard analysis value of ν even further.

The differences between the results from our confluent singularity analysis and those of Refs. 4 and 5 seem to arise because of the value of T_c used in their T_c biased methods. Both references rely most heavily on T_c or index biased methods favoring that value which gives them the smoothest sequences. Camp and VanDyke favor a value of T_c only slightly smaller than ours which leads them to favor slightly larger indices.[4] Note that part of the difference in the susceptibility index may be due to our preference (perhaps erroneous) for values closer to the standard analysis values based on the smaller confluent correction amplitude. McKenzie, Domb, and Hunter favor a value of T_c close to our standard analysis value and find index values similar to those in Sec. III.[5] We doubt that their index estimate is correct, since given a positive amplitude for the confluent correction, standard methods underestimate the indices.

IV. CONCLUSIONS

For the correlation length index, the five-fit estimates (supported by the size of the ratio and Padé analysis underestimates due to the predicted confluent correction) lead us to assert $2\nu=1.44\pm0.02$, where conservative uncertainties include the ratio and Padé estimates as a lower bound. Arriving at a best estimate of the susceptibility index is rather more problematic because of irregularities in the five-fit tables. Excluding the apparently defective $n=8$ and 9 entries, the values for B are smaller than observed for the correlation length; hence, the ratio and Padé estimates of γ will be closer to the correct value than was the case with the correlation length index. The last three entries are fairly consistent and produce values for T_c near our estimate $T_c=3.1757\pm0.0020$. On these bases, we estimate $\gamma=1.40^{+0.03}_{-0.01}$; by doing this, we have tried to err, if at all, in underestimating the index and overestimating the uncertainties.

As a result, we believe that there does exist a discrepancy between the series and renormalization-group values of the indices for the Heisenberg model; the renormalization-group values agree with ours to within uncertainties only because of our generous uncertainties. Unlike the situation with the Ising model where the confluent singularity analysis had little effect on the most reliable standard analysis (for the $s=\frac{1}{2}$ Ising model),[9–11] confluent singularity analysis of the classical Heisenberg series shows that the results of standard analysis, in seemingly good agreement with the renormalization-group results, underestimate the indices.

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APPENDIX: CHECKING THE CORRECTNESS OF OUR SERIES

There are bothersome discrepancies between our coefficients and those of Refs. 5 and 6. Specifically, our eleventh- and twelfth-order susceptibility coefficients differ in the seventh significant figure from those of Ref. 5, which are

$$810503.9650K^{11}+2654798.191K^{12}\ ;$$

the corresponding terms from our Table II are

$$810503.233705947K^{11}+2654791.759151855K^{12}\ .$$

Furthermore, of our two new free-energy coefficients not discussed previously,

$$376.43549526607K^{12}+926.26155555729K^{13}\ ,$$

the twelfth-order coefficient agrees with the general D expansion of Ref. 6; the thirteenth-order term differs from that of Ref. 6 in the sixth significant figure.

We are confident that there is no error in our coefficients. The program which derived the series is a twelfth-order extension of a program used in the late 1960s to derive the tenth-order series of Ref. 1 among others. Our extended program correctly derives twelfth-order Ising susceptibility series,[11] which demonstrates that all diagrams (elementary diagrams[14]) have been correctly included. To derive Heisenberg series, the same program decorates, in a routine fashion, all bonds with the x, y, and z Cartesian labels and then sums over all decorated graphs. We are convinced that this is done correctly for all twelve orders in the correlation function for several reasons.

(i) All diagrams contributing to the nearest-neighbor correlation function are correctly decorated through eleventh order because of the agreement between our free-energy series through twelfth order and the previously mentioned, general D series of Ref. 6.

(ii) The on-site correlation function is exactly $\frac{1}{3}$, i.e., all higher-order coefficients are zero to within round-off. This suggests that all diagrams contributing to the on-site correlation function (specifically all elementary diagrams where the two fixed vertices can occupy the same lattice site) are correctly decorated (or the unlikely possibility) that errors accidentally cancel. This check is also satisfied for the ($n=2$) plane rotator model.

(iii) We believe that the most convincing check is our derivation of the $n=3$ cubic model in the limit of infinite cubic anisotropy where the model reduces to three Ising models and the susceptibility is just the Ising susceptibility.[15] The correctness of our series for this model is convincing proof that the elementary diagrams are decorated correctly, because although this model has the same vertex weights (semi-invariants) as an Ising model the decorations of the elementary diagrams are labeled very differently. We are convinced that an error in decorating procedure could not allow correct derivation of both Ising and infinite cubic model series.

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