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Extended High-Temperature Series for the Spin- $\frac{1}{2}$ Heisenberg Ferromagnet

M. D. Kuz'min

Aix-Marseille Université, IM2NP, UMR CNRS 7334, 13397 Marseille, France

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ABSTRACT

High-temperature series for the magnetic susceptibility and hypersusceptibility of the $S = 1/2$ Heisenberg ferromagnet have been extended to 14th order in $x = J/kT$ for four common lattices. Hence improved estimates have been deduced for the critical points, $x_c = 0.2491(1)$ (fcc), 0.3968(2) (bcc), 0.596(1) (sc), 1.124(2) (diamond), as well as for the critical exponents, $\gamma = 1.428(3)$ and $\Delta = 1.814(6)$. The latter are distinct from the respective values for the classical ($S = \infty$) Heisenberg model, $\gamma \approx 1.40$ and $\Delta \approx 1.77$.

KEYWORDS

High-temperature series; Heisenberg model; magnetic susceptibility

1. Introduction

The Heisenberg model is widely believed to be the most realistic model of ferromagnetism. The corresponding Hamiltonian is given by

$$\hat{\mathcal{H}} = -2J \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + g\mu_B H \sum_{i=1}^N \hat{S}_i^z \quad (1)$$

Here J is the exchange integral, $J > 0$, $\hat{\mathbf{S}}_i$ stands for the spin operator for the i^{th} lattice site, and the summation in the first instance is over all pairs of nearest-neighbor sites. Our consideration is limited to three-dimensional (3D) lattices; only such systems can order ferromagnetically. No exact solution has been found for the problem of statistical treatment of the Hamiltonian (1) in 3 dimensions. Among the approximate techniques it is particularly worth to mention the high-temperature series (HTS) expansion proposed by Kramers and put to practice by Opechowski [1]. In the Kramers-Opechowski method a ferromagnet is viewed from a remote paramagnetic temperature range, high above the Curie point, $T \gg T_C \sim J/k$. The magnetic equation of state, $M(H, T)$, is constructed in two stages.

(I) The magnetization is expanded in powers of applied magnetic field,

$$M = \chi H - \chi_3 H^3 + \dots, \quad (2)$$

where χ is magnetic susceptibility, χ_3 is (magnetic) hypersusceptibility, etc. Only odd

powers of H may enter, due to the time-reversal symmetry. The minus sign before χ_3 is introduced for convenience, in order to have $\chi_3 > 0$. The term 'magnetic hypersusceptibility' is not widely used in the physics literature, but there is no better, more generally accepted name for χ_3 .

(II) Temperature dependence of χ , χ_3 , ... is presented as HTS,

$$\chi = \frac{Ng^2\mu_B^2}{4kT} \sum_{n=0}^{\infty} \frac{a_n}{2^n n!} x^n \quad (3)$$

$$\chi_3 = \frac{Ng^4\mu_B^4}{48(kT)^3} \sum_{n=0}^{\infty} \frac{b_n}{2^n n!} x^n \quad (4)$$

Here $x = J/kT$, a_n and b_n are integers obtainable exactly for any n , and the consideration has been restricted to $S = 1/2$ for the rest of this work. In reality, finding a_n and b_n involves much computational effort and a_n are known for $n \leq 14$ in the best-studied cases ($S = 1/2$ on the simple cubic and bcc lattices [2]), whereas the only information on b_n was published more than half-a-century ago and limited to $n \leq 8$ [3].

My attention was drawn to χ_3 as I was seeking to evaluate Landau's coefficient [4], $b = \chi_3/\chi^4$, employed in a model equation of state proposed some time ago [5]. This project necessitated an extension to $n \leq 14$ of all HTS for χ_3 , as well as of that for χ on the fcc lattice, previously known to 12th order [2]. I added to that 14th-order series for the little studied diamond lattice.

After the extended HTS had been obtained, it became clear that $b \rightarrow 0$ as $T \rightarrow T_C$ and so my original intention could not be realized. The thrust of this work was then redirected toward the outstanding problems of Heisenberg ferromagnets.

(I) The availability of two independent quantities, χ and χ_3 , enables one to determine all critical exponents as well as the critical point $x_c = J/kT_C$. The last complete revision of the critical exponents of the $S = 1/2$ Heisenberg ferromagnet was undertaken more than half-a-century ago [3]; it was based on 10th-order HTS for χ (9th-order in the case of the fcc lattice) and 8th-order HTS for χ_3 . The latest partial revision, involving γ and x_c , is nearly a quarter of a century old [2]; the analyzed HTS were of order 14 (sc and bcc lattices) and 12 (fcc). I emphasize the lag of the fcc series because they provide the better-converged estimates.

(II) The lack of agreement between the critical exponents of the $S = 1/2$ and the classical ($S = \infty$) Heisenberg models requires clarification.

This paper is organized as follows: after a brief description of the calculation of the coefficients (Section 2), the series are analyzed at some length in Section 3, followed by a Discussion (Section 4) and a Conclusion (Section 5).

2. Calculation of series coefficients

Table 1 contains the integers a_n and b_n entering in the HTS for χ and χ_3 , Eqs. (3) and (4), respectively, for four different lattice types and $n \leq 14$. (The trivial zeroth-order factors, $a_0 = b_0 = 1$, are not included.) The calculations were performed by using the finite cluster technique as described by Baker et al. [3]. The advantage of Baker's formulation of the method is that it is immediately suitable for the calculation of χ and χ_3 , as well as higher-order hypersusceptibilities, χ_5 , χ_7 etc. It should be noted

that the calculation of b_n , in addition to a_n , involves no extra computational cost but a certain programming effort. The algorithm of Ref. [3] consists of six stages, two of which (Nos. 4 and 6) are trivial.

(1) Generation of 603,927 free connected graphs with ℓ bonds and up to $\ell + 1$ vertices, $\ell \leq 14$. This task was carried out by running sequentially the programs `gen.f` and `sort.f` provided by J. Oitmaa as a supplement to his book [6]. Both programs were used essentially unchanged and only took a short time to run. The only modification was to extend the format of the symmetry number to 12 characters; this was necessary for the so-called star graphs, whose symmetry number equals $\ell!$

(2) Computing the expansion coefficients A_n and B_n for each graph (leading to a_n and b_n , respectively). This proved to be the most time-consuming part of the entire project because an own, rather inefficient program had to be used. On the positive side, this stage of the calculation is carried out independently for each graph and is therefore massively parallelizable.

(3) Embedding all smaller graphs into a given graph. This was also done by using an own program that took about two months to run.

(5) Embedding all graphs into a crystal lattice was carried out by using J. Oitmaa's programs `count.f` and `treecnt.f`. The latter accelerates considerably the calculation in the case of tree graphs, as explained in Chapter 2.2 of Ref. [6]; it was used (together with `count.f` and my own program selecting the non-tree graphs) for the lattices having high coordination numbers, bcc and fcc, where `count.f` is too slow. For the diamond structure, which is not a Bravais lattice, the program `count.f` was modified so as to allow for two differently coordinated sites.

Some of the values presented in Table 1 were compared and found consistent with earlier results. This concerns a_n with $n \leq 14$ (sc and bcc) and $n \leq 12$ (fcc) previously computed by Oitmaa and Bornilla [2] as well as b_n with $n \leq 8$ (sc, bcc, and fcc) obtained by Baker et al. [3]. For the diamond structure, a test calculation of a_n ($n \leq 12$) was performed by J. Richter and R.O. Kuzian who used the Magdeburg HTS code [7], now extended to 12th order; the result was in agreement with Table 1.

3. Analysis of the Series

3.1. Padé approximants method: critical points x_c

The technique has been known since the 1960s, a recent concise description can be found, e.g., in Ref. [6]. It is based on the assumption that near T_C the quantity of interest (in this case the susceptibility χ) depends on temperature as

$$\chi \sim (T - T_C)^{-\gamma}, \quad T \approx T_C, \quad T > T_C, \quad (5)$$

or, in terms of x , as

$$\chi \sim (x_c - x)^{-\gamma}, \quad x \approx x_c, \quad x < x_c, \quad (6)$$

where γ is a constant called critical exponent. The symbol ' \sim ' in the above expressions implies the presence of a prefactor that is nonzero at T_C (or x_c) and may depend smoothly on T or x .

Table 1. Numerators of the coefficients of the series (3) and (4).

	n	a_n	b_n
fcc	1	12	48
	2	240	2616
	3	6624	160 560
	4	234 720	11 002 752
	5	10 208 832	835 122 048
	6	526 810 176	69 686 304 768
	7	31 434 585 600	6 349 093 780 224
	8	2 127 785 025 024	627 660 411 821 568
	9	161 064 469 168 128	66 948 437 049 348 096
	10	13 483 480 670 745 600	7 666 174 328 536 528 896
	11	1 237 073 710 591 635 456	938 215 064 459 053 977 600
	12	123 437 675 536 945 410 048	122 232 651 377 642 004 885 504
	13	13 308 034 251 238 570 770 432	16 892 421 264 218 383 510 585 344
	14	1 541 580 126 710 320 881 573 888	2 468 497 065 918 097 771 353 243 648
bcc	1	8	32
	2	96	1104
	3	1664	42 656
	4	36 800	1 829 888
	5	1 008 768	86 898 432
	6	32 626 560	4 536 371 712
	7	1 221 399 040	258 696 566 272
	8	51 734 584 320	16 010 149 161 984
	9	2 459 086 364 672	1 069 341 645 185 024
	10	129 082 499 311 616	76 689 197 386 625 024
	11	7 432 690 738 003 968	5 879 364 215 165 460 480
	12	464 885 622 793 134 080	479 898 240 528 262 455 296
	13	31 456 185 663 820 136 448	41 557 856 836 061 600 710 656
	14	2 284 815 238 218 471 260 160	3 805 742 298 941 631 538 200 576
sc	1	6	24
	2	48	588
	3	528	15 576
	4	7920	451 584
	5	149 856	14 443 584
	6	3 169 248	506 983 488
	7	77 046 528	19 391 190 528
	8	2 231 209 728	803 563 967 232
	9	71 938 507 776	35 917 588 432 896
	10	2 446 325 534 208	1 722 930 773 726 208
	11	92 886 269 386 752	88 283 216 264 288 256
	12	3 995 799 894 239 232	4 813 925 139 748 448 256
	13	180 512 165 153 832 960	278 435 490 119 778 459 648
	14	8 443 006 907 441 565 696	17 025 958 848 008 604 254 208
diamond	1	4	16
	2	16	232
	3	64	3280
	4	736	49 408
	5	11 584	858 496
	6	43 072	16 479 232
	7	-607 232	323 727 616
	8	50 435 584	6 921 055 744
	9	1 264 185 088	176 780 333 056
	10	-38 340 475 904	4 611 877 660 672
	11	-563 767 881 728	106 623 185 145 856
	12	73 927 460 466 688	3 130 312 628 383 744
	13	311 178 505 633 792	133 547 209 652 518 912
	14	-151 984 023 599 341 568	3 703 926 000 353 837 056

One considers the inverse logarithmic derivative of $\chi(x)$,

$$\frac{\chi(x)}{\chi'(x)} = \frac{1}{\gamma} (x_c - x), \quad (7)$$

and notes that this quantity has a simple zero at $x = x_c$, where its derivative equals $-1/\gamma$.

Computationally, one proceeds from Eq. (3), omitting the prefactor of the sum. (This prefactor is nonzero at $T = T_C$ and smooth in the vicinity of T_C .) Now the left-hand side of Eq. (7) — a ratio of two polynomials of orders 14 and 13 — is re-expanded in powers of x . The result is a polynomial of order 13. One constructs a number of Padé approximants $[n, d]$ to this result, $n + d \leq 13$, and seeks for each of them the least positive root, x_c . (A Padé approximant $[n, d]$ is a ratio of two polynomials of orders n (numerator) and d (denominator); the reason for using Padé approximants is that they converge better than power series.)

Table 2. Padé matrices of the critical point x_c .

lattice	d	$n = 4$	5	6	7
fcc	4	0.24921	0.24894	0.24903	0.24907
	5	0.24367	0.24903	0.24910	0.24909
	6	0.24897	0.24907	0.24909	0.24914
	7	0.24918	0.24908	0.24908	—
bcc	4	0.3953	0.3958	0.3969	0.3968
	5	0.3971	0.3968	0.3968	0.3969
	6	0.3967	0.3968	0.3968	0.3968
	7	0.3969	0.3970	0.3968	—
sc	4	0.5964	0.5956	0.5950	0.5948
	5	0.5950	0.5949	0.5955	0.5957
	6	0.5949	0.5950	0.5957	0.5950
	7	0.5973	0.5965	0.5963	—
diamond	4	1.107	1.054	1.107	1.142
	5	1.073	1.098	1.125	1.123
	6	1.333	1.149	1.123	1.124
	7	1.815	1.074	1.125	—

The so obtained approximate values of x_c , for $4 \leq n \leq 7$ and $4 \leq d \leq 7$, are collected in Table 2. One can see them converge as n and d increase. The limits are estimated as follows:

$$x_c = \begin{cases} 0.2491(1), & \text{fcc,} \\ 0.3968(2), & \text{bcc,} \\ 0.596(1), & \text{sc,} \\ 1.124(2), & \text{diamond.} \end{cases} \quad (8)$$

From this point on x_c will be regarded as a known quantity.

The Padé technique also offers the possibility to find the critical exponent γ . To this end, derivatives of the just constructed approximants $[n, d]$ should be evaluated at $x = x_c$, cf. Eq. (7). The resulting Padé tables converge slowly and do not yield but rough estimates of γ (an example for the bcc lattice was given in Ref. [6], Table 7.9). Several more sophisticated techniques allowing for a confluent correction term in $\chi(x)$

were tried out by Oitmaa & Bornilla [2]. These attempts resulted in no improvement and it was concluded that the amplitude of the confluent term was small. I therefore chose to use the more direct ratios method for the determination of γ (and Δ).

3.2. Ratios method: critical exponents γ and Δ

This a yet older technique dating back to the 1950s; a modern description can be found in Ref. [6]. We begin with stating the method aimed at the determination of γ and regarding x_c as already known. A central quantity here is the ratio of the n^{th} coefficient in the HTS for χ , Eq. (3), to the preceding coefficient,

$$r_n = \frac{1}{2n} \frac{a_n}{a_{n-1}}. \quad (9)$$

If $\chi(x)$ obeys Eq. (6), the asymptotic behavior of r_n for n large is given by

$$r_n = \frac{1}{x_c} \left[1 + \frac{\gamma - 1}{n} + O\left(\frac{1}{n^2}\right) \right]. \quad (10)$$

That is, for $1/n$ small, the r_n -vs- $1/n$ dependence is a straight line having an intercept of $1/x_c$ and a slope of $(\gamma - 1)/x_c$. Thus, the slope yields γ immediately, since x_c is already known. Graphic evidence for the fcc lattice is presented in Fig. 1a. The solid line is a linear fit through all the points, including the isolated point in the bottom-left corner, $(0, x_c^{-1})$, $x_c = 0.2491$. The other points are $(1/n, r_n)$, $n \geq 6$, as found from Eq. (9) with a_n from Table 1.

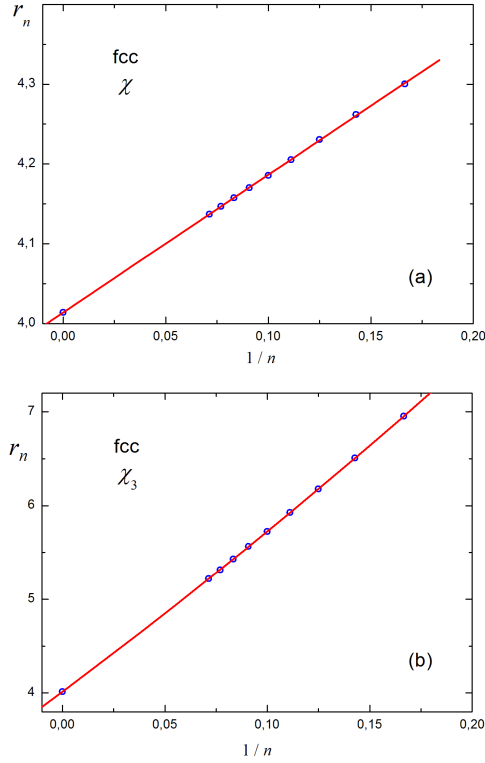


Figure 1. Ratios plots for the face-centered cubic lattice.

Two factors contribute to the error in the determination of the slope of the fit: (i) imperfect alignment of the points, treated statistically even though the coordinates of all but one of them are known exactly; (ii) uncertainty in the ordinate of the bottom-left point, x_c^{-1} , known approximately. At a later stage, as the slope is converted to γ , $\gamma = 1 + x_c \times \text{slope}$, the uncertainty in x_c results in extra error (iii). The procedure used to determine γ in this work took into account all three sources of error.

First, the upper limit for γ was found by shifting the bottom-left point to its lowest possible position, by taking $x_c = 0.2492$ instead of 0.2491. The standard least-squares technique was then applied, which yielded a slope of 1.7322 ± 0.0065 , or a maximum slope of 1.7387. Finally, γ_{\max} was obtained by taking the maximum slope and the highest x_c ,

$$\gamma_{\max} = 1 + 1.7387 \times 0.2492 = 1.433 .$$

To find the lower bound for γ , x_c was reduced to 0.2490, so that the bottom-left point in Fig. 1a rose to its highest possible position. The linear-fit slope was determined to be 1.7155 ± 0.0076 , the minimum slope 1.7079. Hence

$$\gamma_{\min} = 1 + 1.7079 \times 0.2490 = 1.425 .$$

Both estimates are summarized as

$$\gamma = 1.429(4) . \tag{11}$$

Figure 1b is a ratios plot for χ_3 of the fcc lattice. In that case the ratios r_n were de-

fined by Eq. (9) with a_n replaced by b_n . Two modifications to Eq. (10) were necessary: (i) $\gamma + 2\Delta$ had to be substituted for γ and (ii) a term in $1/n^2$ had to be included to allow for a non-negligible upward curvature. The latter fact bore little on the determination of Δ : a standard parabolic least-squares fitting routine was employed; the only output information used for further processing was the factor of $1/n$ (initial slope) and its standard deviation. The procedure of finding the mean value and error bar was essentially the same as the one described above for γ and resulted in

$$\gamma + 2\Delta = 5.062(13) ,$$

whence, by Eq. (11),

$$2\Delta = 3.633(17) . \tag{12}$$

Ratios plots for the bcc lattice are shown in Fig. 2. The fit is a straight line in the upper panel, representing r_n for χ , while it is a parabola in the lower panel, relevant to χ_3 . The determination of γ and Δ was quite similar to that for the fcc lattice, albeit rather less accurate. The results are as follows:

$$\gamma = 1.420(11) , \tag{13}$$

$$2\Delta = 3.613(26) . \tag{14}$$

Ratios plots for the lattices with lower coordination numbers (simple cubic and diamond) were too erratic to be reproduced here.

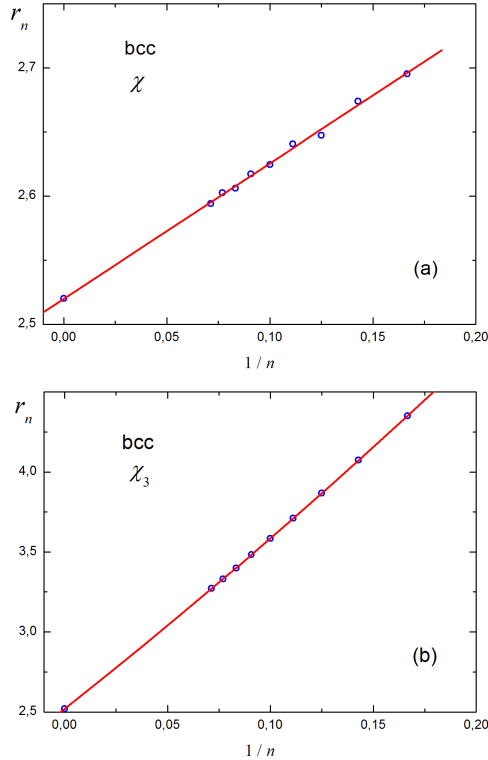


Figure 2. Ratios plots for the body-centered cubic lattice.

4. Discussion

Table 3 contains the values of x_c found in this work as well as those of earlier authors, deduced from shorter series. We observe that the estimates converge more rapidly and are more accurate — for a given number of terms in the HTS — for structures with higher coordination numbers, first and foremost, for the face-centered cubic lattice ($Z = 12$). This observation concerns to a yet higher extent the critical exponents and one may suggest that future efforts should be concentrated on the fcc lattice. To accelerate the convergence, one may even consider investigating lattices with yet higher Z , e.g., sc or fcc with equally strong exchange between first- and second-nearest neighbors ($Z = 18$) etc.

At the other end of the spectrum there is the diamond lattice, with $Z = 4$. A favorite object of study in the 1950s [9, 10], this lattice was later abandoned, apparently due to lack of convergence. Now armed with an HTS of order 14, we observe that convergence does set in and we obtain a reasonably accurate estimate of the Curie temperature. It would be interesting to go further in this direction and investigate a 3D structure having a still lower coordination number, $Z = 3$. This can be constructed on the basis of the simple cubic lattice by assuming that only one-half of the pairs of nearest neighbors are exchange-coupled — those connected with bold lines in Fig. 3. The system with $Z = 2$ is trivial; it can only be a linear chain, with no magnetic order. The case of $Z = 3$ is non-trivial: ferromagnetic ordering may or may not take place; this certainly merits a special study.

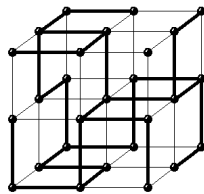
Table 3. Values of x_c from various sources.

lattice	Z	x_c [3]	x_c [2]	x_c (this work)
fcc	12	0.2492(10)	0.2490(4)	0.2491(1)
bcc	8	0.3963(10)	0.3968(2)	0.3968(2)
sc	6	0.5972(10)	0.5960(5)	0.596(1)
diamond	4	—	—	1.124(2)

The middle part of Table 3 is less interesting. Here we faithfully reproduce the results of Ref. [2], which is hardly surprising given that the authors already knew all a_n with $n \leq 14$.

Incidentally, the previous authors failed to appreciate the dependence of accuracy on Z . Thus, Baker et al. [3] believed their x_c to have the same 'error of perhaps 10^{-3} , for all lattices. In actual fact, their fcc result is clearly more accurate than that. Oitmaa and Bornilla did get a better precision for the bcc than for the simple cubic lattice,[2] both HTS being known to 14th order. Yet their fcc result was less accurate (because the HTS was of order 12) and so no clear trend could be observed.

Concluding the discussion of x_c , the most accurate result is obtained for the fcc lattice. A comparison of the values deduced from HTS of orders 9 [3], 12 [2], and 14 (this work) reveals no systematic shift of x_c , but rather a systematic decrease of the uncertainty. One can be reasonably confident of the result, $x_c = 0.2491(1)$.

**Figure 3.** Proposed semi-simple cubic structure, space group $I2_13 (T^5)$.

Turning now to the critical exponents γ and Δ , we note that the error intervals found for the fcc and bcc lattices (11-14) do overlap. Assuming that γ and Δ are lattice-independent, one can narrow down the uncertainty limits to the intersection of the intervals for both lattices:

$$\gamma = 1.428(3) \quad (15)$$

and

$$\Delta = 1.814(6). \quad (16)$$

Other critical exponents can be found from the scaling relations [8], e.g.,

$$\alpha = \gamma - 2(\Delta - 1) = -0.200(15), \quad (17)$$

$$\beta = \Delta - \gamma = 0.386(9), \quad \text{etc.} \quad (18)$$

The estimates (15, 16) respect both the fcc and the bcc error bars (11-14) and, indeed, those obtained for the simple cubic and diamond lattices — too broad to be

useful. The values (15, 16) are in perfect agreement with the results of Ref. [3], deduced from much shorter series,

$$\gamma = 1.43(1) \tag{19}$$

and

$$\Delta = 1.815(15). \tag{20}$$

From the comparison of respective values one can conclude that extending the series by 5 orders (for fcc, which is decisive) has not resulted in any significant shift of the uncertainty intervals; they have just become narrower. In other word, the lower bounds have risen and the upper ones decreased. As a result, values of γ under 1.425 can be ruled out for the spin- $\frac{1}{2}$ Heisenberg model.

It is rather surprising that a discrepant result,

$$\gamma = 1.41(2), \tag{21}$$

should be deduced from series of intermediate length [2]. The discrepancy is hard to understand, given the good agreement of the critical points in Table 3. A careful perusal of Ref. [2] makes an impression that the authors consciously sought agreement with what they believed to be the correct result, $\gamma = 1.39$ [11, 12], as confessed on p. 167 of Ref. [6], whereas their own data yielded $\gamma = 1.42$ and even $\gamma = 1.425$, with a much smaller uncertainty than ± 0.02 .

Our most solid piece of evidence is Fig. 1a. By Eq. (10), the slope of the plot equals $(\gamma - 1)x_c^{-1}$, where x_c is known rather precisely, cf. Table 3. In order to reconcile our slope, $0.43x_c^{-1}$, with the 'expected' one, $0.39x_c^{-1}$, one needs to account for the 10% discrepancy — a hard task because of the exact nature of the data plotted. Thus, the top-right point is at $(\frac{1}{6}, \frac{914601}{212684})$ and this is not likely to change in the centuries to come. The reader is invited to judge if he or she can see a 'considerable residual curvature' in the plot presented in Fig. 1a (the quotation is from Ref. [2]). In the absence of any reasonable explanation, one has to admit that the critical exponents of the spin- $\frac{1}{2}$ Heisenberg ferromagnet (15, 16) differ from those of the classical ($S = \infty$) Heisenberg model [13],

$$\gamma = \begin{cases} 1.404(4), & \text{sc,} \\ 1.396(3), & \text{bcc,} \end{cases} \tag{22}$$

and

$$\Delta = \begin{cases} 1.775(7), & \text{sc,} \\ 1.765(5), & \text{bcc.} \end{cases} \tag{23}$$

where the values of Δ (23) have been obtained from the ν 's of Ref. [13] by using the scaling relation, $\Delta = \frac{1}{2}(\gamma + 3\nu)$.

In other words, the critical exponents of the 3D Heisenberg model are not independent of the quantum number S . The importance of this statement is such that it should be put to a test as a matter of priority — by extending the HTS and concentrating on the fcc lattice. The only reason why the present series are limited to terms in x^{14} is the author's inexpert programming. An example of a 17th-order HTS was published

as long as 15 years ago [14], unfortunately, for the specific heat of a 2D lattice only. Nowadays, an expert calculation should be able to go still further.

5. Conclusion

High-temperature series for the susceptibility and hypersusceptibility of the spin- $\frac{1}{2}$ Heisenberg ferromagnet have been carried to 14th order in $x = J/kT$ for four common cubic lattices. Critical points x_c and critical exponents γ and Δ have been determined with improved precision. The accuracy is best for the lattice having the highest coordination number — fcc ($Z = 12$). There are realistic prospects of further improvement of the precision by way of (i) extending the series to order 18 and/or (ii) going over to lattices with higher coordination numbers, such as sc or fcc with 1st and 2nd nearest neighbors ($Z = 18$).

As regards the more loosely-packed structures, convincing evidence has been obtained that the diamond lattice orders ferromagnetically at $x_c = 1.124(2)$. It is proposed to extend the analysis to a yet more open structure ($Z = 3$) shown in Fig. 3.

Acknowledgements

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Note added in proof

After this Letter had been submitted, J. Oitmaa brought to my attention a recent paper of his [15] containing data equivalent to the a_n 's of Table 1 for the diamond lattice.

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