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High-temperature series analyses of the classical Heisenberg and *XY* models

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Although there is now a good measure of agreement between Monte Carlo and high-temperature series expansion estimates for Ising ($n = 1$) models, published results for the critical temperature from series expansions up to 12th order for the three-dimensional classical Heisenberg ($n = 3$) and *XY* ($n = 2$) models do not agree very well with recent high-precision Monte Carlo estimates. In order to clarify this discrepancy we have analyzed extended high-temperature series expansions of the susceptibility, the second correlation moment, and the second field derivative of the susceptibility, which have been derived a few years ago by Lüscher and Weisz for general O(n) vector spin models on D-dimensional hypercubic lattices up to 14th order in $K \equiv J/k_B T$. By analyzing these series expansions in three dimensions with two different methods that allow for confluent correction terms, we obtain good agreement with the standard field theory exponent estimates and with the critical temperature estimates from the new high-precision Monte Carlo simulations. Furthermore, for the Heisenberg model we also reanalyze existing series for the susceptibility on the BCC lattice up to 11th order and on the FCC lattice up to 12th order using the same methods.

1. Introduction

In the past few years considerable progress has been made in developing very efficient Monte Carlo (MC) simulation techniques (for reviews, see, e.g., [1]). This allows high-precision computations of the critical coupling and the critical exponents of continuous phase transitions with an accuracy that is comparable with the widely accepted estimates derived from field theory [2, 3]. The third and oldest approach to extract information about the critical properties of those systems are analyses of high-temperature series expansions. For some standard models (with notable exceptions including the three-dimensional Ising model [4, 5] and certain two-dimensional systems), however, the critical coupling and the critical exponents calculated by this method have much larger error bars and are more vulnerable to systematic errors. In order to improve this situation two points are important. First, more refined methods of analysis than in the pioneering works must be employed, and second it is obvious that longer series are needed. The first point should cause no problem anymore for continuous phase transitions since over the years many greatly refined methods have been developed that take into account various confluent correction-to-scaling terms and are now available on a routine basis [6, 7]. Confluent corrections to scaling arise from irrelevant operators and their neglect can bias critical coupling and critical exponent estimates. The generation of longer series, however, is still a very demanding numerical and computational problem, even though it appears to be trivial in principle.

Significant progress in series generation has been made with star graph [8] and no-free-end (NFE) graph [9–11] enumerations which lead to medium length series in general dimensions for many systems. However, these approaches are limited by the order of the existing graph table and not all problems have star or NFE formulations; even when these exist, the implementation can be quite complex. For the classical $O(n)$ vector spin models an important step forward has been made by Lüscher and Weisz [12], who applied linked cluster expansion techniques to compute the expansion coefficients of the susceptibility, the second correlation moment and the second field derivative of the susceptibility on D-dimensional hypercubic lattices up to the 14th order in the expansion parameter $K = J/k_B T$ and provided explicit tables for $1 \leq n \leq 4$, $2 \leq D \leq 4$. Moreover, Butera et al. [13] observed that the symmetry of these models implies (Schwinger–Dyson) identities between correlation functions that allow a recursive computation of the series expansion coefficients and reveal their structure as function of n. Combining their result with those of Lüscher and Weisz they were able to give the expansion coefficients in general form as ratios of polynomials in n. Although still one term shorter than the NFE tables [9, 10], and three terms below the star graph series of Singh and Chakravarty [8], these methods can be used to generate longer series directly, requiring only larger computer memory and not preexisting graph tables.

The motivation to analyze the extended high-temperature series expansions of the Heisenberg model comes from two recent high-precision MC simulation studies [14, 15] of this model on simple cubic (SC) lattices which gave significantly larger values for the critical coupling than previous estimates based on analyses of series expansions up to 12th order [16–19], and transfer matrix

Table I
Estimates of the critical coupling K_c of the Heisenberg ($n = 3$) model on a simple cubic lattice from various sources (HTS: high-temperature series analysis, TMMC: transfer-matrix Monte Carlo simulation, MC: Monte Carlo simulation).

K_c	Method	Authors
0.692	8 terms HTS	Wood and Rushbrooke (1966) [16]
0.692(4)	9 terms HTS	Joyce and Bowers (1966) [17]
0.6916(2)	9 terms HTS	Ritchie and Fisher (1972) [18]
0.6924(2)	12 terms HTS (Padé)	McKenzie et al. (1982) [19]
0.6925(1)	12 terms HTS (ratio)	
0.6922(2)	TMMC ($n \geq 5$)	Nightingale and Blöte (1988) [20]
0.6925(3)	TMCC ($n \geq 6$)	
0.6929(1)	Metropolis MC	Peczak et al. (1991) [14]
0.6930(1)	1 cluster MC	Holm and Janke (1992) [15]
0.693035(37)	multiple 1 cluster MC	Chen et al. (1993) [21]
0.6929(1)	14 terms HTS	this work

MC studies [20]; see table I (also included is newer MC data [21], which was obtained after completion of our work). There are two sources for the expected improvement. First, on hypercubic lattices two more terms of the series are known and second, more refined methods taking into account confluent correction terms are available. For the latter reason we also reanalyze the long-known but shorter series for the susceptibility on the body centered cubic (BCC) and face centered cubic (FCC) lattices. Finally, we present analyses of the new longer series for the XY ($n = 2$) model on the SC lattice.

2. Model and observables

We consider the classical O(n) symmetric Heisenberg model with partition function

$$Z = \prod_i \left(\int \mathrm{d}\Omega_i \right) \exp\left(K \sum_{\langle i,j \rangle} \boldsymbol{s}_i \cdot \boldsymbol{s}_j \right) , \tag{1}$$

where $K = J/k_\mathrm{B}T$ is the reduced inverse temperature, $\langle i, j\rangle$ denotes nearest-neighbor pairs, and Ω_i is the surface of the n-dimensional unit sphere associated with the degrees of freedom of the n-dimensional unit spins $\boldsymbol{s}_i$ at each site of a regular three-dimensional lattice. In this paper we investigate the new longer series for the Heisenberg ($n = 3$) model on an SC lattice, and reanalyze existing series for the BCC and FCC lattices. Further we also study the new longer series for the XY ($n = 2$) model on an SC lattice. In order to estimate the critical couplings and exponents we concentrate on three observables, the susceptibility

$$\begin{aligned}\chi &= \sum_i \langle s_0 \cdot s_i \rangle = \lim_{V\to\infty} \left\langle V\left(\frac{1}{V}\sum_i s_i\right)^2\right\rangle \\ &= A_\chi t^{-\gamma}(1 + a_\chi t^{\Delta_1} + b_\chi t + \cdots)\,, \end{aligned} \tag{2}$$

the second correlation moment

$$\begin{aligned} m^{(2)} &= \sum_i i^2 \langle s_0 \cdot s_i \rangle = \chi \frac{\Sigma_i\, i^2 \langle s_0 \cdot s_i \rangle}{\Sigma_i \langle s_0 \cdot s_i \rangle} \\ &= A_{m^{(2)}} t^{-(\gamma+2\nu)}(1 + a_{m^{(2)}} t^{\Delta_1} + b_{m^{(2)}} t + \cdots)\,, \end{aligned} \tag{3}$$

and the second field derivative of the susceptibility

$$\begin{aligned} \chi^{(4)} &= \frac{3}{n(n+2)} \sum_{i,j,k} \langle s_0 \cdot s_i\, s_j \cdot s_k \rangle_c \\ &= A_{\chi^{(4)}} t^{-(3\gamma+2\beta)}(1 + a_{\chi^{(4)}} t^{\Delta_1} + b_{\chi^{(4)}} t + \cdots)\,, \end{aligned} \tag{4}$$

where $\langle \cdots \rangle$ denotes expectation values with respect to the partition function (1) and the subscript c in (4) stands for the connected part. The second lines in (2)–(4) give the assumed critical behavior where $t \equiv K_c - K > 0$ is the distance from the critical point in the high-temperature phase, γ, ν and β are the standard critical exponents of the susceptibility, correlation length and magnetization, respectively, and the terms in parentheses describe the leading confluent and analytic correction terms. In (4) we have made use of the relation $\Delta = \gamma + \beta$, where Δ is the gap exponent. In the high-temperature phase these observables can be expanded as

$$\chi(n, K) = 1 + \sum_{r=1}^{\infty} a_r(n)\, K^r\,, \tag{5}$$

$$m^{(2)}(n, K) = \sum_{r=1}^{\infty} b_r(n)\, K^r\,, \tag{6}$$

$$\chi^{(4)}(n, K) = \frac{3}{n(n+2)} \left(-2 + \sum_{r=1}^{\infty} d_r(n)\, K^r \right), \tag{7}$$

defining the coefficients $a_r(n)$, $b_r(n)$ and $d_r(n)$, computed in refs. [12, 13]. For the convenience of the reader we have compiled their numerical values for $n = 2$ and $n = 3$ in tables II and III.

Table II

Expansion coefficients for the *XY* ($n = 2$) model high-temperature series for a simple cubic lattice. Given are the expansion coefficients a_r of the susceptibility χ, the expansion coefficients b_r of the second correlation moment $m^{(2)}$, and the expansion coefficients d_r of the second field derivative of the susceptibility $\chi^{(4)}$ up to 14th order (for details compare text).

Order r	a_r	b_r	d_r
1	3.0000000000	3.0000000000	−24.0000000000
2	7.5000000000	18.0000000000	−160.5000000000
3	18.3750000000	72.3750000000	−822.0000000000
4	43.5000000000	247.5000000000	−3576.8125000000
5	102.3437500000	770.5937500000	−13971.7500000000
6	237.0546875000	2261.3437500000	−50454.9648437500
7	546.9462890625	6360.6650390625	−171739.3593750000
8	1252.0048828125	17343.7773437500	−557978.9429687500
9	2858.8175292969	46158.4210449219	−1746304.9972656250
10	6496.1514078776	120515.3193033854	−5299323.3505303277
11	14735.3746412489	309746.4250318739	−15671446.8761067708
12	33314.7537746853	785831.2964274089	−45336965.5964835394
13	75222.2566392081	1971809.9920579093	−128702556.1244287884
14	169444.4882359232	4901417.5916496216	−359396456.8541712222

3. Methods of analysis

We analyze the series given in tables II and III with two different methods [22] that allow for confluent and analytic correction terms. Taking the susceptibility as a generic example (and suppressing subscripts) we thus assume a critical behavior of the form

Table III

Expansion coefficients for the classical Heisenberg ($n = 3$) model high-temperature series for the simple cubic lattice. Given are the expansion coefficients a_r of the susceptibility χ, the expansion coefficients b_r of the second correlation moment $m^{(2)}$, and the expansion coefficients d_r of the second field derivative of the susceptiblity $\chi^{(4)}$ up to 14th order (for details compare text).

Order r	a_r	b_r	d_r
1	2.0000000000	2.0000000000	−16.0000000000
2	3.3333333333	8.0000000000	−71.7333333333
3	5.4222222222	21.4222222222	−246.0444444444
4	8.5185185185	48.7111111111	−716.4486772487
5	13.2670194004	100.7336860670	−1870.2019047619
6	20.3359905938	196.1285831864	−4508.3329617872
7	30.9989637468	365.7050425240	−10232.2542817950
8	46.8673402574	660.4991803514	−22145.7412271162
9	70.6067866595	1163.5584276550	−46128.4203352476
10	105.8320214871	2009.6315902889	−93088.6148720584
11	158.2324753396	3414.9732182123	−182932.5061463846
12	235.7598652836	5725.3717946474	−351440.3272602895
13	350.6189575427	9489.5939248535	−662121.9818887996
14	520.1310140421	15575.4527177723	−1226410.1925173962

$$\chi = At^{-\gamma}(1 + at^{\Delta_1} + bt + \ldots)\,, \tag{8}$$

where $\Delta_1 = \nu\omega$ (≈ 0.55) is the confluent correction exponent and bt a (subleading) analytic correction term. The non-universal amplitudes A, a, b are assumed to be constant. The ... inside the parentheses indicate further higher order corrections of the form t^{Δ_m}, $t^{m+n\Delta_1}$, which we neglect in our analysis.

In the method referred to as M1, first the leading singularity is removed by forming

$$B = \gamma\chi + t\frac{\partial\chi}{\partial t} = At^{-\gamma}(\Delta_1 at^{\Delta_1} + bt + \cdots)\,. \tag{9}$$

Then Padé approximants are applied to the logarithmic derivative of B,

$$\frac{\partial \ln B}{\partial t} = \frac{\Delta_1(\gamma - \Delta_1)at^{\Delta_1 - 1} + (\gamma - 1)b}{t(\Delta_1 at^{\Delta_1 - 1} + b)}\,, \tag{10}$$

yielding for given K_c the confluent correction exponent Δ_1 as function of γ, $\Delta_1 = \Delta_1(\gamma)$. The optimal set of values for the parameters K_c, γ and Δ_1 is determined visually from the best intersection of different Padé approximants.

In the second method, referred to as M2, Padé approximants in a new variable

$$y = 1 - (-K/K_c)^{\Delta_1} = 1 - (t/K_c)^{\Delta_1} \tag{11}$$

are applied to

$$\begin{aligned} t\frac{\partial \ln x}{\partial t} &= -\gamma + \frac{\Delta_1 at^{\Delta_1} + bt}{1 + at^{\Delta_1} + bt} \\ &= -\gamma - \frac{\Delta_1 K_c a(y-1) + K_c b(y-1)^{1/\Delta_1}}{1 - K_c a(y-1) - K_c(y-1)^{1/\Delta_1}}\,, \end{aligned} \tag{12}$$

yielding for given K_c the exponent γ as function of Δ_1, $\gamma = \gamma(\Delta_1)$. Again the intersection of different Padé approximants is used to select the optimal set of parameters.

The two methods are complementary and as stressed in appendix D of ref. [22] should always be used in conjunction to avoid spurious results due to so-called resonances at values of Δ_1/n, $n = 2, 3, \ldots$, in the otherwise more accurate method M2. The analysis was made with the help of the recently developed VGS program package [7], which makes extensive use of the graphic features of an X-window environment and allows easy and efficient scanning of the three-dimensional parameter space.

4. Results

4.1. Heisenberg ($n = 3$) model

SC lattice: As mentioned in the introduction our main emphasis was on the Heisenberg model on an SC lattice since recent high-precision MC simulation studies [14, 15] were at odds with previous high-temperature series expansion analyses [16–19]. In particular the critical coupling K_c turned out to be significant larger than widely accepted series estimates based on expansions up to 12th order; see table I. Our main result from analyses of the longer 14 terms series using methods M1, M2 is that we can clearly confirm the MC estimates of K_c. More precisely for all three series we get consistent results from methods M1 and M2, and the three estimates for K_c vary only weakly: $K_c = 0.6928$ from analyses of χ, $K_c = 0.6930$ from $m^{(2)}$ and $K_c = 0.6928$ from $\chi^{(4)}$. Taking the average of these three values as the final result we get

$$K_c = 0.6929 \pm 0.0001 \qquad \text{(SC lattice)}\,. \tag{13}$$

To illustrate the method of analysis we show for the susceptibility in fig. 1 graphs of the highest near diagonal Padé approximants to the critical exponent γ in the three-parameter space K_c, Δ_1 computed according to method M2. A two-dimensional plot of the central slice at $K_c = 0.6928$ is shown in fig. 2b. The corresponding plot for method M1 is displayed in fig. 2a. From the point of the best intersection of the different Padé approximants shown in fig. 2 we read off

$$\gamma = 1.400 \pm 0.010\,, \tag{14}$$

and $\Delta_1 = 0.7 \pm 0.2$. Similar analyses of the series for $m^{(2)}$ yield $\gamma + 2\nu = 2.825 \pm 0.020$ or inserting (14),

$$\nu = 0.712 \pm 0.010\,, \tag{15}$$

and from $\chi^{(4)}$ we get $3\gamma + 2\beta = 4.925 \pm 0.020$ or using (14)

$$\beta = 0.363 \pm 0.010\,. \tag{16}$$

Using the scaling relation $\alpha + 2\beta + \gamma = 2$ and the estimates (14), (16) we calculate

$$\alpha = -0.125 \pm 0.020\,. \tag{17}$$

Since we have three independent estimates of critical exponents this result can

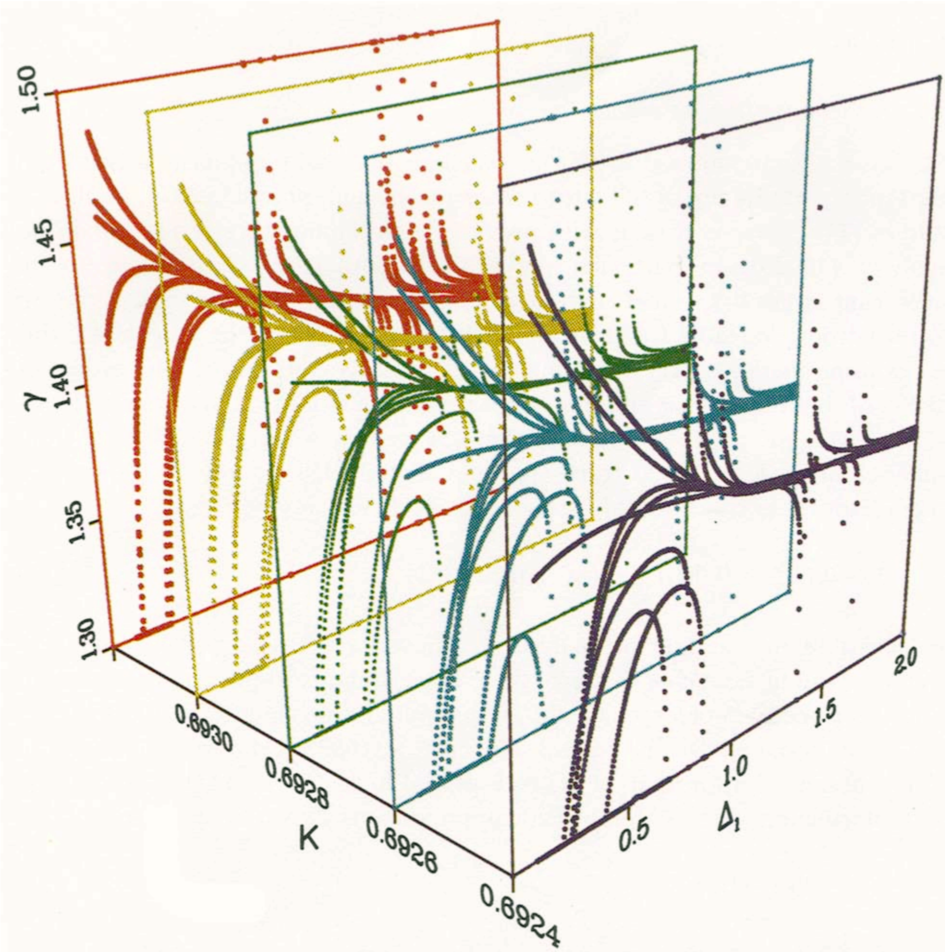

Fig. 1. Graphs of highest near diagonal Padé approximants to γ in the three-parameter space K_c, Δ_1, γ for method M2. A two-dimensional plot of the central slice at $K_c = 0.6928$ is shown in fig. 2b.

be used to test the hyperscaling relation $\alpha = 2 - D\nu$. Using the estimate (15) we obtain

$$\alpha = -0.136 \pm 0.030\,, \tag{18}$$

in good agreement with (17), thus supporting the hyperscaling hypothesis. Similarly, the scaling relation $\delta = 1 + \gamma/\beta$ gives

$$\delta = 4.86 \pm 0.10\,, \tag{19}$$

while the hyperscaling relation $\gamma/\nu = 2 - \eta = D(\delta - 1)/(\delta + 1)$ yields a com-

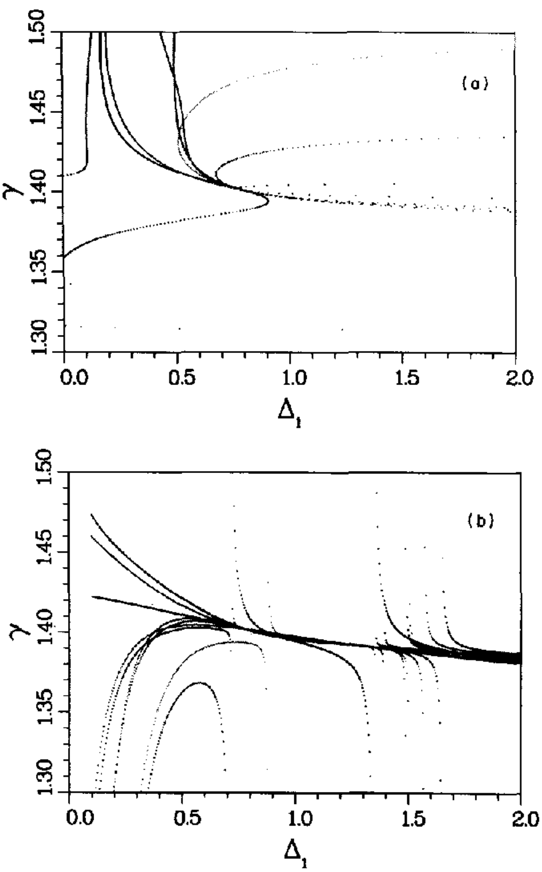

Fig. 2. Graphs of highest near diagonal Padé approximants to γ plotted against Δ_1 at fixed $K_c = 0.6928$ for (a) method M1 and (b) method M2.

parison between central estimates of $\gamma/\nu = 1.966$ from the values quoted above and the rhs of the scaling relation

$$D(\delta - 1)/(\delta + 1) = 1.975 , \tag{20}$$

again in good agreement with each other. Our results for the critical exponents are summarized in table IV, where they are compared with the standard field theory values and the results from recent MC simulations.

BCC lattice: The susceptibility series [19] consists of only 11 terms, but the overall behavior is similar. We find optimal convergence at

$$K_c = 0.4867 \pm 0.0001 \qquad \text{(BCC lattice)} , \tag{21}$$

Table IV
Critical exponents for the three-dimensional classical Heisenberg ($n = 3$) model from various sources.

Method	ν	γ	β	α	δ
g-expansion [2]	0.705(3)	1.386(4)	0.3645(25)	−0.115(9)	4.802(37)
ϵ-expansion [3]	0.710(7)	1.390(10)	0.368(4)	−0.130(21)	4.777(70)
MC [14]	0.706(9)	1.390(23)	0.364(7)	−0.118(27)	4.819(36)
MC [15]	0.704(6)	1.388(14)	0.362(4)	−0.112(18)	4.837(11)
MC [21]	0.7036(23)	1.3896(70)	0.3616(31)	−0.1108(69)	–
This work	0.712(10)	1.400(10)	0.363(10)	−0.125(20)	4.86(10)

again with $\gamma \approx 1.4$ but with a lower correction-to-scaling exponent Δ_1 than was seen in the SC case. We quote central estimates of $\Delta_1 \approx 0.6$ from M1 and $\Delta_1 \approx 0.5$ from M2.

FCC lattice: For the FCC lattice the 12th order susceptibility series was analyzed, including corrections to scaling, in ref. [19]. It was found that the amplitude of the confluent correction (with $\Delta_1 = 0.55$ held fixed at the RG value [2]) was very small, and that the analytic correction was the dominant one. We find

$$K_c = 0.31475 \pm 0.00010 \qquad \text{(FCC lattice)} \tag{22}$$

and $\gamma \approx 1.39$, in good agreement with [19]. This γ is a little lower than our values on the other lattices, and closer to the values of other calculations. In contrast to [19], we saw clear evidence of a non-analytic correction to scaling at $\Delta_1 \approx 0.6$ from the M2 study of a first derivative of the susceptibility series.

4.2. *XY* ($n = 2$) *model*

SC lattice: For the *XY* model we have only analyzed the new longer series for the simple cubic lattice. In this case the series for the susceptibility turned out to be not well-behaved and it was very difficult to get precise estimates of the critical parameters. With this caveat in mind we estimate $K_c = 0.45407$ and $\gamma = 1.325$. On the other hand the series for $m^{(2)}$ and $\chi^{(4)}$ behaved similar to the Heisenberg model, i.e., both methods M1 and M2 gave consistent results and the estimates of K_c from both series agreed with each other,

$$K_c = 0.45414 \pm 0.00007 \qquad \text{(SC lattice)} . \tag{23}$$

While the previous estimate $K_c = 0.4539$ [23] from series analyses is again lower (and clearly below the error limits of the present study), our value (23) is consistent with recent Monte Carlo studies which gave $K_c = 0.45421(8)$ [24]

using multiple and $K_c = 0.4542(1)$ [25] using single cluster simulations. For the exponents we obtain central estimates of $\gamma + 2\nu = 2.67$ from the expansion of $m^{(2)}$, and $3\gamma + 2\beta = 4.67$ from the expansion of $\chi^{(4)}$. The exponents calculated from these estimates are $\nu = 0.673$, $\gamma/\nu = 1.970 = 2 - \eta$, and $\beta = 0.348$. These values are again consistent with field theoretical estimates [2, 3] The scaling relations yield $\alpha = -0.020$ and $\delta = 4.81$. The hyperscaling relations result in $\alpha = -0.018$, and $\gamma/\nu = D(\delta - 1)/(\delta + 1) = 1.968$, again in good agreement with our previous values.

5. Concluding remarks

Analyzing new longer series for the Heisenberg ($n = 3$) model using more refined methods than in early works we obtain for the SC lattice critical parameters that are in good agreement with completely independent results from two recent MC simulations. Our reanalysis of existing series for the FCC and BCC lattices indicate that the improvement comes mainly from the refined methods that are able to take into account confluent correction terms. With 14 (or even only 12 or 11) terms these series are, however, still too short to compete with the accuracy achieved by field theoretical methods for critical exponents, or with the precision claimed from simulations. However, the results clearly show that there remain no major discrepancies between series estimates and other calculations. Longer series clearly stabilize and thus increase the reliability of the estimates along the lines discussed here, and it therefore would be very desirable to have a few more terms available.

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Note added in proof

See also exponent estimates for the Heisenberg model given in ref. [26].

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