High-Temperature Series Analyses of the Classical Heisenberg and XY Model

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Abstract

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 ($n = 2$) model 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 [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, 10, 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 $K \equiv J/k_BT$ 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 MC studies [20]; see Table 1 (also included is newer MC data [21], that 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

$$Z = \prod_i \left[ \int d\Omega_i \right] \exp \left[ K \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j \right],$$

where $K = J/k_BT$ is the reduced inverse temperature, $\langle i,j \rangle$ denotes nearest-neighbor pairs, and $\Omega_i$ is the surface of the $n$-dimensional unit sphere associated with the degrees of freedom of the $n$-dimensional unit spins $\vec{s}_i$ 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 a 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 a SC lattice. In or-
order to estimate the critical couplings and exponents we concentrate on three observables, the susceptibility

\[ \chi = \sum_i \langle \mathbf{s}_0 \cdot \mathbf{s}_i \rangle = \lim_{V \to \infty} V^{-\gamma} \left\langle \left( \frac{1}{V} \sum_i \mathbf{s}_i \right)^2 \right\rangle = A_\chi t^{-\gamma} \left[ 1 + a_\chi t^{\Delta_1} + b_\chi t + \ldots \right], \tag{2} \]

the second correlation moment

\[ m^{(2)} = \sum_i i^2 \langle \mathbf{s}_0 \cdot \mathbf{s}_i \rangle = \chi \frac{\sum_i i^2 \langle \mathbf{s}_0 \cdot \mathbf{s}_i \rangle}{\sum_i \langle \mathbf{s}_0 \cdot \mathbf{s}_i \rangle} = A_{m^{(2)}} t^{-(\gamma + 2\nu)} \left[ 1 + a_{m^{(2)}} t^{\Delta_1} + b_{m^{(2)}} t + \ldots \right], \tag{3} \]

and the second field derivative of the susceptibility

\[ \chi^{(4)} = \frac{3}{n(n+2)} \sum_{i,j,k} \langle \mathbf{s}_0 \cdot \mathbf{s}_i \mathbf{s}_j \cdot \mathbf{s}_k \rangle_c = A_{\chi^{(4)}} t^{-(3\gamma + 2\beta)} \left[ 1 + a_{\chi^{(4)}} t^{\Delta_1} + b_{\chi^{(4)}} t + \ldots \right], \tag{4} \]

where \( \langle \ldots \rangle \) denotes expectation values with respect to the partition function 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, \( \gamma, \nu \) and \( \beta \) are the standard critical exponents of the susceptibility, correlation length and magnetization, respectively, and the terms in square brackets describe the leading confluent and analytic correction terms. In (4) we have made use of the relation \( \Delta = \gamma + \beta \), where \( \Delta \) 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 2 and 3.
3 Methods of analysis

We analyze the series given in Tables 2 and 3 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

\[
\chi = At^{-\gamma} \left[ 1 + at^{\Delta_1} + bt + \ldots \right], \tag{8}
\]

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

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

\[
B = \gamma \chi + t \frac{\partial \chi}{\partial t} = At^{-\gamma} \left[ \Delta_1 at^{\Delta_1} + bt + \ldots \right]. \tag{9}
\]

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 \( \Delta_1 \) as function of \( \gamma \), \( \Delta_1 = \Delta_1(\gamma) \). The optimal set of values for the parameters \( K_c, \gamma \) and \( \Delta_1 \) is determined visually from the best clustering of different Padé approximants.

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

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

are applied to

\[
\frac{t \partial \ln \chi}{\partial t} = -\gamma + \frac{\Delta_1 at^{\Delta_1} + bt}{1 + at^{\Delta_1} + bt} = -\gamma - \frac{\Delta_1 K_c a(y - 1) + K_c b(y - 1)^{1/\Delta_1}}{1 - K_c a(y - 1) - K_c(y - 1)^{1/\Delta_1}}. \tag{12}
\]
yielding for given \( K_c \) the exponent \( \gamma \) as function of \( \Delta_1 \), \( \gamma = \gamma(\Delta_1) \). Again the clustering of different Padé approximants is used to select the optimal set of parameters.

The two methods are complementary and as stressed in App. D of ref. \[22\] should always be used in conjunction to avoid spurious results due to so-called resonances at values of \( \Delta_1/n \), \( n = 2, 3, \ldots \) in the otherwise more accurate method M2. The analysis was made with the help of the recently developed VGS program package \[7\] that 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 a 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 1. 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 \( \chi \), \( K_c = 0.6930 \) from \( m^{(2)} \) and \( K_c = 0.6928 \) from \( \chi^{(4)} \). Taking the average of these three values as the final result we get

\[
K_c = 0.6929 \pm 0.0001 \quad (SC\ lattice). \tag{13}
\]

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 \( \gamma \) in the three-parameter space \( K_c, \Delta_1, \gamma \) computed according to method M2. A two-dimensional plot of the central slice at \( K_c = 0.6928 \) is shown in Fig. 2(b). The corresponding plot for method M1 is displayed in Fig. 2(a). From the point of best clustering 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)

\[
\nu = 0.712 \pm 0.010,
\]

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

\[
\beta = 0.363 \pm 0.010.
\]

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

\[
\alpha = -0.125 \pm 0.020.
\]

Since we have three independent estimates of critical exponents this result can be used to test the hyperscaling relation \( \alpha = 2 - D\nu \). Using the estimate (15) we obtain

\[
\alpha = -0.136 \pm 0.030,
\]

in good agreement with (14), thus supporting the hyperscaling hypothesis. Similarly, the scaling relation \( \delta = 1 + \gamma/\beta \) gives

\[
\delta = 4.86 \pm 0.10,
\]

while the hyperscaling relation \( \gamma/\nu = 2 - \eta = D(\delta - 1)/(\delta + 1) \) yields a comparison between central estimates of \( \gamma/\nu = 1.966 \) from the values quoted above and the r.h.s. of the scaling relation

\[
D(\delta - 1)/(\delta + 1) = 1.975,
\]

again in good agreement with each other. Our results for the critical exponents are summarized in Table 4, 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

\[
K_c = 0.4867 \pm 0.0001 \quad \text{(BCC lattice),}
\]

again with \( \gamma \approx 1.4 \) but with a lower correction-to-scaling exponent \( \Delta_1 \) 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 [3]) was very small, and that the analytic correction was the dominant one. We find

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

and $\gamma \approx 1.39$, in good agreement with [19]. This $\gamma$ 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,

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

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 $K_c = 0.4542(1)$ [23] 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 [4, 9]. 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 reanalyses of existing series for the FCC and BCC lattice 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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Table 1: 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, MC: Monte Carlo simulation).

| $K_c$       | method            | authors                        |
|------------|-------------------|--------------------------------|
| 0.692      | 8 terms HTS       | Wood and Rushbrooke (1966)     |
| 0.692(4)   | 9 terms HTS       | Joyce and Bowers (1966)        |
| 0.6916(2)  | 9 terms HTS       | Ritchie and Fisher (1972)      |
| 0.6924(2)  | 12 terms HTS (Padé) | McKenzie et al. (1982)    |
| 0.6925(1)  | 12 terms HTS (ratio) | Nightingale and Blöte (1988) |
| 0.6922(2)  | TMMC ($n \geq 5$) | Peczak et al. (1991)          |
| 0.6925(3)  | TMMC ($n \geq 6$) | Holm and Janke (1992)         |
| 0.6929(1)  | Metropolis MC     | Chen et al. (1993)            |
| 0.6930(1)  | 1 Cluster MC      | this work                     |
| 0.6930(37) | multiple 1 Cluster MC | this work                 |
| 0.6929(1)  | 14 terms HTS      |                                |
Table 2: 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 $\chi$, 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         | 3.000000000000| 3.000000000000| -24.000000000000|
| 2         | 7.500000000000| 18.000000000000| -160.500000000000|
| 3         | 18.375000000000| 72.375000000000| -822.000000000000|
| 4         | 43.500000000000| 247.500000000000| -3576.812500000000|
| 5         | 102.343750000000| 770.593750000000| -13971.750000000000|
| 6         | 237.054687500000| 2261.343750000000| -50454.964843750000|
| 7         | 546.946289062500| 6360.665039062500| -171739.359375000000|
| 8         | 1252.004882812500| 17343.777343750000| -557978.942968750000|
| 9         | 2858.817529296900| 46158.421044921900| -1746304.997265625000|
| 10        | 6496.151407877600| 120515.319303385400| -5299323.350530327700|
| 11        | 14735.374612489000| 309746.425031873900| -15671446.876106770800|
| 12        | 33314.753774685300| 785831.296427408900| -45336965.596483539400|
| 13        | 75222.256639208100| 1971809.992057909300| -128702556.12428788400|
| 14        | 169444.488235923200| 4901417.591649621600| -359396456.854171222200|
Table 3: 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 \(\chi\), 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).
### Table 4: Critical exponents for the three-dimensional classical Heisenberg ($n = 3$) model from various sources.

| method     | $\nu$   | $\gamma$ | $\beta$    | $\alpha$  | $\delta$   |
|------------|---------|----------|------------|-----------|------------|
| $g$-expansion [2] | 0.705(3) | 1.386(4) | 0.3645(25) | $-0.115(9)$ | 4.802(37)  |
| $\epsilon$-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 [13]    | 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)  | $-0.136(30)$ | 4.86(10)   |
Figure Headings

**Fig. 1**: Graphs of highest near diagonal Padé approximants to $\gamma$ in the three-parameter space $K_c$, $\Delta_1$, $\gamma$ for method M2. A two-dimensional plot of the central slice at $K_c = 0.6928$ is shown in Fig. 2(b).

**Fig. 2**: Graphs of highest near diagonal Padé approximants to $\gamma$ plotted against $\Delta_1$ at fixed $K_c = 0.6928$ for (a) method M1 and (b) method M2.