Partition function zeros and leading order scaling correction of the 3D Ising model from multicanonical simulations

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October 27, 2018

Abstract

The density of states for the three-dimensional Ising model is calculated with high-precision from multicanonical simulations. This allows us to estimate the leading partition function zeros for lattice sizes up to \( L = 32 \). Combining previous statistics for smaller lattice sizes, we have evaluated the correction to scaling and the critical exponent \( \nu \) throughout an analysis of a multi-parameter fit and of Bulirsch-Stoer (BST) extrapolation algorithm. The performance of the BST algorithm is also explored in case of the 2D Ising model, where the exact partition function zeros are known.

Keywords: Ising model, scaling exponent, multicanonical simulation, partition function zeros

PACS-No.: 05.50.+q, 05.70.-a, 64.60.Fr

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1 Introduction

In recent years there has been a persistent interest in obtaining accurate estimates of critical parameters of the three-dimensional (3D) Ising-like systems through high performance simulations and perturbative expansions. Our aim here is to enlarge the knowledge about critical behavior of Ising-like 3D systems by calculating not only the critical exponent of the correlation length \( \nu \), but also by tackling the much harder problem of calculating the first correction to scaling \( w \).

A common way to extract information on phase transitions from Monte Carlo simulations is by means of finite-size scaling (FSS), for instance by analyzing the partition function zeros in the complex temperature plane. This approach is not restricted to Ising-like systems and was recently even used to study structural transitions in bio-molecules. However, separation of universality classes can be tricky for 3D systems, and requires high-precision data. An important tool for obtaining such data was provided by Ferrenberg and Swendsen who revived reweighting techniques introduced by Salsburg et al. forty years ago. In the sequence, multiple-histogram and multicanonical simulations were proposed for a reliable numerical determination of the density of states and extensively checked in two-dimensions where exact results are available. Only by combining one of these sophisticated new simulation techniques (exhaustive multicanonical Monte Carlo simulations for \( L \leq 32 \)) with Itzykson’s finite-size scaling relation for the partition function zeros, we were able to obtain the results presented in this article.

Before proceeding further, we give the outline of the paper. In the next section we describe the numerical evaluation of the partition function. Section 3 is concerned with the crucial task of data analysis. There we calculate the critical exponent \( \nu \) and the correction to scaling. The exponent \( \nu \) was first obtained by a four-parameter fitting. Next, we used the Bulirsch-Stoer algorithm to extrapolate results from finite lattices to the thermo-
dynamical limit. That algorithm has a free-parameter $w$ which is exactly the wanted correction to scaling. We further corroborate on results recently obtained by other techniques. Finally, we test the performance of our approach, and specially the BST algorithm, for the 2D Ising model where the exact zeros are known.

2 Multicanonical simulation and partition function zeros

In the multicanonical algorithm \cite{18} conformations with energy $E$ are assigned a weight $w_{mu}(E) \propto 1/n(E)$. Here, $n(E)$ is the density of states. A simulation with this weight will lead to a uniform distribution of energy:

$$P_{mu}(E) \propto \rho(E) w_{mu}(E) = \text{const}.$$  \hspace{1cm} (1)

This is because the simulation generates a 1D random walk in the energy, allowing itself to escape from any local minimum. Since a large range of energies are sampled, one can use the reweighting techniques \cite{14} to calculate thermodynamic quantities over a wide range of temperatures by

$$< A >_T = \frac{\int dx \ A(x) w^{-1}(E(x)) e^{-\beta E(x)}}{\int dx \ w^{-1}(E(x)) e^{-\beta E(x)}},$$  \hspace{1cm} (2)

where $x$ stands for configurations.

It follows from equation \cite{4} that the multicanonical algorithm allows us to calculate estimates for the spectral density:

$$\rho(E) = P_{mu}(E) w_{mu}^{-1}(E).$$  \hspace{1cm} (3)

We can therefore construct the partition function of the three-dimensional Ising model

$$Z(\beta) = \sum_{E} \rho(E) u^E,$$  \hspace{1cm} (4)
where we define $u = e^{-4\beta}$.

In the present article, the estimates of the partition function rely on averages over NRUN simulations of NSWEEP Monte Carlo updates for 3D Ising models of linear size $L$. In order to allow the system to thermalize, additional sweeps in the beginning were performed and discarded. Table 1 lists the respective values for NSWEEP and NRUN.

Once, we have calculated reliable estimates for the partition function we can calculate the zeros. In the polynomial form, equation (4) has a large number of coefficients for large lattice sizes. For this reason we apply the method presented in [21] to obtain the leading complex zeros $u_1^0(L)$. In table 1 we collect the so calculated zeros as obtained from our multicanonical simulations.

### 3 Finite size scaling analysis

The standard FSS approach for the zero $u_1^0(L)$ closest to the real positive axis neglects, for sufficiently large $L$, corrections to scaling [11],

$$u_1^0(L) = u_c + AL^{-1/\nu} \left[ 1 + O(L^{-w}) \right].$$

(5)

Since we are interested in analysing $\nu$ in function of the correction to scaling exponent $w$, we follow ref. [17, 22] and fit our data to a four parameter scaling relation,

$$|u_1^0(L) - u_c| = a_1 L^{-1/\nu} + a_2 L^{-a_3}.$$  

(6)

However, due to the small number of available lattices, such a multi-parameter fit is not appropriate. To circumvent this difficulty we proceed including statistics already available for smaller lattice sizes. In ref. [17], table 1, zeros for 3D Ising model are presented for $L = 6, 8, 10$ and 14, together with data from ref. [22] for $L = 3, 4, 5, 6, 8$ and 10. In addition, we decided to take into account that information and our results in table 1, weighted with the corresponding available precision. The final estimates for each lattice is a
linear combination of available data with normalized weight factors which are taken as the reciprocals of the corresponding empirical variances for each data [23].

In figure 1 we show the corresponding fit for all lattice sizes, whose parameters are found by monitoring the goodness of fit $Q$ [24]. Here we choose the recently obtained critical value $u_c = 0.41204684(25)$ [8], to apply the least-square method to equation (1), although the fit is not very sensible to the precision in the value of critical temperature $u_c$. The error bar of those data is included, but it is hardly seen in that scale. The goodness of fit ($Q = 0.89$) reveals a very good agreement with the data. We obtain $\nu = 0.62853(35)$ and $a_3 = 4.861(84)$.

If we discard the smallest sizes $L = 3, 4$ and 5, we obtain $\nu = 0.6280(15)$ ($Q = 0.84$), corresponding to $y_t = 1/\nu = 1.5924(38)$, which is in remarkable agreement with previous results [4, 1, 8]. However, this fit is less stable with relation to the parameters in the second term. This is because of the presence of rather large lattice sizes.

3.1 Correction to scaling from RG transformation

In this section we now evaluate the correction to scaling by a method which is similar to the “finite size phenomenological renormalization group (RG)” analysis by Binder [23] (which in turn was based on Nightingale’s finite size RG transformation [26] for the correlation length $\xi_L$). Our method to evaluate $w$ was previously used [21] to analyse the 2D Ising model, and it is briefly recalled here.

In order to consider the scaling relation for the longitudinal correlation length $\xi_L(\beta)$, we assume that the system is of finite length scale $L$ in one direction and infinite in all other directions. The standard expression for the correlation exponent $\nu$ is now given by [27, 28]

$$1 + \frac{1}{\nu, L'} = \ln \left( \frac{\partial \xi_{L'}/\partial \beta}{\partial \xi_{L}/\partial \beta} \right)_{\beta_c} / \ln \left( \frac{L'}{L} \right).$$

(7)
This expression is obtained from a linearization around the fixed critical point $\beta_c$ for fixed scaling transformation $L \to L'$. The scaling equation for the finite size longitudinal correlation length is given by

$$\xi_L = L Y_\xi((\beta - \beta_c)L^{1/\nu}, hL^{y_H}, \tilde{u}L^{y_3}).$$  \hspace{1cm} (8)

This differentiable equation includes corrections due to the leading bulk irrelevant scaling field $\tilde{u}$ with exponent $y_3 < 0$, and a magnetic field dependence for the sake of completeness.

From equation (7) and equation (8) one obtains, for $h = 0$,

$$\frac{1}{\nu_{L,L'}} = \frac{1}{\nu} + a_0 \frac{L^{y_3} - L^{y_3}}{\ln(L'/L)} + b_0 \frac{L'^{2y_3} - L^{2y_3}}{\ln(L'/L)} + ...$$  \hspace{1cm} (9)

where $a_0$ and $b_0$ include derivatives like $\partial Y_\xi(y, z)/\partial y|_{y=0, z=0}$. With the introduction of the rescaling factor $s = L'/L$ in equation (9), we can now evaluate $y_3$.

However an important point remains to be answered: how to estimate finite size dependence of $\nu$ on lattice sizes $L$ and $L'$? This can be achieved from large enough pairs of lattices $L$ and $L'$, with $L' > L$, through the following expression for the partition function zeros:

$$\frac{1}{\nu_{L,L'}} = \ln \left( \frac{|u_0^1(L') - u_c|}{|u_0^1(L) - u_c|} \right) / \ln \left( \frac{L}{L'} \right).$$  \hspace{1cm} (10)

This equation defines our finite size estimators $\nu_{L,L'}$ from data in table 1. A second estimate can be obtained with the replacement $|u_0^1(L') - u_c|$ by its imaginary part $\text{Im}(u_0^1)$ in equation (10). For large enough systems we have $\text{Re}(u_0^1) \sim u_c$, and both approaches should lead to the same result.

In table 2 we present sequences of those two possible estimates $\nu_{L,sL}$ as a function of the fixed rescaling factor $s = 2$, where the second column stands for the results of equation (10) and the third one for the replacement $|u_0^1(sL) - u_c| / |u_0^1(L) - u_c|$ by $\text{Im}(u_0^1(sL)) / \text{Im}(u_0^1(L))$.

As $L$ increases, the values obtained by matching pairs of lattices are expected to converge to a limiting value. If we match our largest lattices
\( L = 24 \) and 32 we obtain from equation (10) \( \nu = 0.6260(66) \) whereas \( \nu = 0.6292(70) \) is obtained by using only the imaginary part of the zeros.

Looking at the values for the crossings \((L, 2L)\) with \((12, 24)\) and \((16, 32)\) in the second column of table 2, we realize that our values for the real part of the corresponding zeros are not precise enough to obtain an ordered sequence towards its critical value \( \nu \) as \( L \to \infty \). On the other hand the estimate based on the imaginary part of zeros seems to preserve this trend.

Since equations (9) and (10) are valid only for large enough lattice sizes, we have to discard the smallest values in table 2. For this reason we prefer not to evaluate equation (9) by a multi-parameter fit. On the other hand, we note that this relation with \( L' = sL \), is an equation of type

\[
T(h) = T + a_1 h^w + a_2 h^{2w} + \cdots,
\]

(11)

where we identify,

\[
y_3 = -w \\
h = 1/L \\
T(h) = 1/\nu_{L,2L}
\]

(12)

and \( T = 1/\nu \) the asymptotic limit for \( h \to 0 \). Hence, equation (11) is in the proper form to be analysed by the so called BST approximants, on which we elaborate in the next section.

### 3.2 BST extrapolation

Bulirsch and Stoer [19] developed an algorithm to extrapolate a sequence \( h_N \), \((N = 0, 1, 2, \ldots)\) converging to zero as \( N \to \infty \). See also ref. [29] for a recent discussion on BST algorithm.

The BST algorithm approximates tabulated data \( T(h) \) by a sequence of rational functions [19, 20]. The limiting value \( T \) is computed from a table of
recurrent relations defined from:

\[ T_{-1}^{(N)} = 0 \]
\[ T_{0}^{(N)} = T(h_N) \] \hspace{1cm} (13)

and

\[ T_{m}^{(N)} = T_{m-1}^{(N+1)} + (T_{m-1}^{(N+1)} - T_{m-1}^{(N)}) \]
\[
\left[ \left( \frac{h_N}{h_{N+m}} \right)^w \left( 1 - \frac{T_{m-1}^{(N+1)} - T_{m-1}^{(N)}}{T_{m-1}^{(N+1)} - T_{m-1}^{(N+2)}} \right) \right]^{-1}.
\] \hspace{1cm} (14)

Here \( w \) plays the role of a free parameter. If one defines \( \varepsilon_m^{(i)} = 2(T_{m}^{(i+1)} - T_{m}^{(i)}) \), it is expected \( |T_{m}^{(i)} - T| \leq \varepsilon_m^{(i)} \) in the limit \( i \to \infty \). The above remark gives a criterion [20] for choosing \( w \) as the value to minimize \( \varepsilon_m^{(i)} \), in order to have a fast and reliable convergence.

Our aim is to extrapolate the finite size sequence in table 2 by the BST algorithm. However, before proceeding with our analysis, we would like to explore first how the BST extrapolant approach performs for exact data. For this end, we come to the 2D Ising model. In ref. [21] the exact values for \( \nu_{L,2L} \) are presented. We show in figures 2, 3, and 4 the BST extrapolants obtained from different sets of sequences \( T(h_N) \).

In figure 2 we show the BST estimates of the critical exponent \( \nu_{\text{BST}} \) from a sequence for lattices of lengths \( L = h^{-1} \), with \( h = 1/4, 1/6, 1/8, 1/10, 1/12, 1/16, 1/20, 1/24 \) and \( 1/32 \). This figure presents a pole behavior at \( w \sim 1.580 \) for the extrapolated results (full lines) to \( h \to 0 \) (\( L \to \infty \)) for this sequence. In the neighbourhood of that pole we note the corresponding large values for the systematic error (dashed lines) according to the scale at the right hand side of that figure. Here we define the error as the difference between the extrapolated value \( T \) and a value of last but one interaction: \( T - T_{m-1}^{(2)} \).

We also observe that the known value \( \nu = 1 \) is obtained for \( w \simeq 1 \) with error \( \simeq 0 \). Moreover, it is remarkable that for this sequence of lengths \( h, \nu_{\text{BST}} \)
is weakly dependent on \( w \). For instance, we obtain \( \nu \) with 0.1% precision, \( \nu \in [0.999, 1.001] \) for a large range of \( w \) (\( w \in [0.1888, 1.5482] \)) before the pole.

In figure 3 we restrict the available sequence to higher lattice sizes, \( h = \frac{1}{12}, \frac{1}{16}, \frac{1}{20}, \frac{1}{24} \) and \( \frac{1}{32} \). In that case the extrapolation with 0.1% precision is also compatible with a still large range of values for \( w \): \( w \in [0.2816, 1.1969] \), before the pole at \( w \sim 1.2078 \). In figure 4, we restrict further the sequence to \( h = \frac{1}{16}, \frac{1}{20}, \frac{1}{24} \) and \( \frac{1}{32} \), and we obtain \( w \in [0.411, 1.3220] \), and a pole at \( w \sim 1.3871 \).

Therefore, as we restrict our sequences to higher lattice sizes, the effects of the correction to scaling term become more pronounced, leading to a smaller range for acceptable values of \( w \). This effect has a stronger counterpart in the criterium of minimum error: the acceptable range for \( w \) is actually narrower than stated above, mainly for figures 3 and 4.

We are finally now at a point where we can use the BST algorithm to analyse our 3D Ising model data of table 2. Since we have to discard smaller lattices in order to accomplish with the expected validity conditions to derive equations (8) and (9), we are left with the sequence in the third column in table 2. Figure 5 presents our so obtained BST estimates for the critical exponent \( \nu \) from a sequence for lengths \( h = \frac{1}{6}, \frac{1}{8}, \frac{1}{12} \), and \( \frac{1}{16} \). Since our sequences for \( 1/\nu L, 2L \) are restricted to lattice sizes from \( L = 6 \) up to 16 we take the four parameter fit estimate \( \nu = 0.6280 \) and its statistical error 0.0015 as our input condition to find out \( w \), as exemplified for the 2D Ising model. This statistical error leads to a range in \( w \) given by \( w = 0.745(74) \), marking the region of minimum systematic error.

Finally, we remark that this approach yields a value for \( w \) which is in full agreement with recent results from various other and different approaches: from scaling relations of observables related to the magnetization [8] it was estimated \( w = 0.87(9) \), from perturbative expansion at fixed \( D = 3 \) dimension followed \( w = 0.799(11) \), and \( w = 0.814(18) \) was estimated from \( \varepsilon \)-expansion [4].
4 Conclusions

In summary, we have described a new calculation of the correction to scaling exponent \( w \) based on Monte Carlo multicanonical simulations and finite size scaling theory for the partition function zeros. A four-parameter fitting was done in order to find out the correlation length critical exponent \( \nu \). Next, the result for \( \nu \) including the statistical error was used to obtain the acceptable values for the renormalization exponent \( y_3 = -w \) by means of the BST algorithm. This algorithm helped us to overcome the difficulties in the straight application of the multiparameter fit (9) to few data points and rather large lattice sizes.

Our results for \( \nu \) and \( w \) are in good agreement with recently obtained estimates by Ballesteros et al. [8] as well as perturbative expansion calculations by Guida and Zinn-Justin [7].

It is tempting to assume that an accurate value for \( w \) could be pursued by increasing the significant precision of the complex partition function zeros of the 3D Ising model. This would account for a more precise calculation of \( \nu_{L,L'} \), by evaluating crossings between lattice sizes \( L \) and \( L' \). However as we have seen from figures 2 to 4, where we used exact values for \( \nu_{L,L'} \), high precision in \( \nu \) does not necessarily lead to a smaller range in \( w \). Hence, as an overall conclusion, we note that the large range of \( w \) is not just a matter of a lack of statistical precision but demonstrates that it is necessary to go to much larger lattice sizes. In particular, for 2D Ising model even \( L = 64 \) seems to be not large enough.

Acknowledgements

U. Hansmann gratefully acknowledges support by the National Science Foundation (CHE-9981874), and a generous travel grant by FAPESP (Brazil) which allowed him to visit the Ribeirão Preto Campus of the Universidade de São Paulo, Departamento de Física e Matemática. N.A. Alves and J.R.
Drugowich de Felicio acknowledge support by the brazilian agencies FAPESP, CAPES and CNPq.

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Table Captions:

**Table 1:** First partition function zeros for the 3D Ising model on a cubic lattice.

**Table 2:** Sequence of estimates for the critical exponent $\nu_{L,2L}$ from pairs of lattices $(L, 2L)$. The third column is obtained by replacing $|u_0^0(2L) - u_c| / |u_1^0(L) - u_c|$ by $\text{Im} u_1^0(2L) / \text{Im} u_1^0(L)$ in equation (10).
Table 1: First partition function zeros for the 3D Ising model on a cubic lattice.

| $L$ | NRUN | NSWEEP | Re($u^0_1$)   | Im($u^0_1$)   | Re ($\beta^0_1$) | Im ($\beta^0_1$) |
|-----|------|--------|---------------|---------------|------------------|------------------|
| 6   | 2048 | 100000 | 0.397 586(18) | 0.045 435(17) | 0.228 964(11)    | 0.028 445(11)    |
| 8   | 1024 | 600000 | 0.402 723(11) | 0.028 596(10) | 0.226 748(07)    | 0.017 722(06)    |
| 12  | 512  | 900000 | 0.407 018(12) | 0.014 925(12) | 0.224 557(07)    | 0.009 163(08)    |
| 16  | 512  | 1200000| 0.408 814(11) | 0.009 422(11) | 0.223 557(07)    | 0.005 761(07)    |
| 24  | 256  | 1800000| 0.410 341(14) | 0.004 935(12) | 0.222 674(09)    | 0.003 006(07)    |
| 32  | 256  | 1800000| 0.410 991(15) | 0.003 124(14) | 0.222 289(09)    | 0.001 900(08)    |
Table 2: Sequence of estimates for the critical exponent $\nu_{L,2L}$ from pairs of lattices $(L, 2L)$. The third column is obtained by replacing $|u_0^0(2L) - u_c| / |u_1^0(L) - u_c|$ by $\text{Im } u_0^0(2L) / \text{Im } u_1^0(L)$ in equation (10).

| $L$  | $\nu_{L,2L}$      | $\nu_{L,2L}$  |
|------|-------------------|----------------|
| 3    | 0.60713(10)       | 0.60916(11)    |
| 4    | 0.61986(13)       | 0.61831(14)    |
| 5    | 0.62451(31)       | 0.62181(33)    |
| 6    | 0.62577(44)       | 0.62272(46)    |
| 8    | 0.62719(64)       | 0.62429(67)    |
| 12   | 0.6278(14)        | 0.6263(14)     |
| 16   | 0.6270(25)        | 0.6279(26)     |
Figure Captions:

**Figure 1:** Four parameter fit for $|u_0^1(L) - u_c|$ in function of $L^{-1/\nu}$ in the range $L = 3 - 32$. The least square method gives $\nu = 0.62853(35)$ with $Q = 0.89$.

**Figure 2:** BST estimates of the critical exponent $\nu$ (full lines) and systematic error (dashed lines), as a function of the free parameter $w$, for 2D Ising model. The extrapolation is obtained from the finite size sequence with lattice sizes from $L = 4$ up to $L = 32$. The right side scale refers to the systematic error.

**Figure 3:** As in figure 2, BST estimates of the critical exponent $\nu$ (full lines) and systematic error (dashed lines) for 2D Ising model, with lattice sizes from $L = 12$ up to 32. The right side scale refers to the systematic error.

**Figure 4:** As in figure 2, BST estimates of the critical exponent $\nu$ (full lines) and systematic error (dashed lines) for 2D Ising model, with lattice sizes from $L = 16$ up to 32. The right side scale refers to the systematic error.

**Figure 5:** BST estimates of the critical exponent $\nu$ (full lines) and systematic error (dashed lines), as a function of the free parameter $w$ for 3D Ising model. The sequence is obtained with lattice sizes $L = 6, 8, 12$ and 16. The right side scale refers to the systematic error.
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