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

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Abstract. The density of states for the three-dimensional Ising model is calculated with high precision by means of multicanonical simulations. This allows us to estimate the leading partition function zeros for lattice sizes up to $L = 32$. We have evaluated the critical exponent ν and the correction to scaling through an analysis of a multi-parameter fit and of the 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.

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 [1–10]. Our aim here is to enlarge the knowledge about critical behaviour of Ising-like 3D systems not only by calculating the critical exponent of the correlation length ν, 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 analysing the partition function zeros in the complex temperature plane [11, 12]. This approach is not restricted to Ising-like systems and was recently even used to study structural transitions in bio-molecules [13]. However, separation of universality classes can be tricky for 3D systems, and it requires high-precision data. An important tool for obtaining such data was provided by Ferrenberg and Swendsen [14], who revived reweighting techniques introduced by Salsburg *et al* [15] 40 years ago. In sequence, multiple-histogram [16, 17] and multicanonical simulations [18] 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 $L \leqslant 32$) with Itzykson's FSS relation for the partition function zeros [11] and a convenient algorithm of extrapolation due to Bulirsch–Stoer (BST) were we able to obtain the results presented in this paper.

Before proceeding further, we give the outline of the paper. In the next section we describe the numerical evaluation of the multicanonical density of states $\rho(E)$. Section 3 is concerned with the crucial task of data analysis. There we calculate the critical exponent ν and the

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correction to scaling. The exponent ν was first obtained by a four-parameter fitting. Next, we used the BST algorithm [19,20] to extrapolate results from finite lattices to the thermodynamical limit. That algorithm has a free parameter w, which is exactly the desired correction to scaling. The performance of our approach and the usefulness of the BST algorithm is checked for the 2D Ising model where the exact zeros are known. Finally, we extend this analysis to the 3D Ising model and compare our estimate of w with results recently obtained by other techniques.

2. Multicanonical simulation and partition function zeros

The multicanonical algorithm and other generalized-ensemble techniques [21] were originally developed to overcome the supercritical slowing down of first-order phase transitions [18] and they were afterwards also used for simulations of systems with a rough energy landscape such as spin glasses [22] and proteins [23]. Here, we present a short introduction to the multicanonical algorithm [18], which by now has become a standard simulation technique. A more detailed review of multicanonical sampling and related methods can be found in [24,25]. Multicanonical sampling [18] is defined by the condition that conformations with energy E are assigned a weight

$$w_{mu}(E) \propto 1/\rho(E). \tag{1}$$

Here, $\rho(E)$ is the density of states. Note, that unlike in canonical simulations the multicanonical weight (equation (1)) is not *a priori* known and one needs its estimator for a numerical simulation. In our case it was obtained by a common iterative procedure first introduced in [26,27].

Once estimators for the multicanonical weight are determined, a standard update scheme such as the Metropolis algorithm will realize a Markov chain and a simulation with this weight will lead to a uniform distribution of energy:

$$P_{mu}(E) \propto \rho(E) w_{mu}(E) = \text{const}. \tag{2}$$

This is because the simulation generates a 1D random walk in the energy, allowing itself to overcome any energy barrier and to escape from any local minimum. Hence, the whole range of possible energies is sampled in a multicanonical simulation, and one can use equation (2) to calculate estimates for the spectral density:

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

We can therefore construct the partition function of the 3D Ising model from a multicanonical simulation through

$$Z(\beta) = \sum_E \rho(E)\, \mathrm{e}^{-\beta E} = \sum_E \rho(E) u^E \tag{4}$$

where we define $u = \mathrm{e}^{-\beta}$, and β is the inverse temperature $\beta = 1/k_{\mathrm{B}}T$.

In this paper, the estimates of the partition function rely on averages over N_{run} simulations of N_{sweep} Monte Carlo updates for 3D Ising models of linear size L. In order to allow the system to thermalize, additional sweeps at the beginning were performed and discarded. Table 1 lists the respective values for N_{run} and N_{sweep}.

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, which also grows with lattice size. Since our aim is to obtain with high precision the leading complex partition function zeros $u_1^0(L)$, we need to avoid any truncation of polynomial in equation (4). For this reason we use the method presented in [28] to obtain those complex zeros from our multicanonical simulations. The so calculated zeros are collected in table 1.

Table 1. Leading partition function zeros for the 3D Ising model on L^3 lattices from multicanonical simulations.

L	$N_{\rm run}$	$N_{\rm sweep}$	Re (u_1^0)	Im (u_1^0)	Re (β_1^0)	Im (β_1^0)
6	2048	100 000	0.397 586(18)	0.045 435(17)	0.228 964(11)	0.028 445(11)
8	1024	600 000	0.402 723(11)	0.028 596(10)	0.226 748(07)	0.017 722(06)
12	512	900 000	0.407 018(12)	0.014 925(12)	0.224 557(07)	0.009 163(08)
16	512	1200 000	0.408 814(11)	0.009 422(11)	0.223 557(07)	0.005 761(07)
24	256	1800 000	0.410 341(14)	0.004 935(12)	0.222 674(09)	0.003 006(07)
32	256	1800 000	0.410 991(15)	0.003 124(14)	0.222 289(09)	0.001 900(08)

3. FSS analysis

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

$$u_1^0(L) = u_{\rm c} + AL^{-1/\nu}[1 + {\rm O}(L^{-w})]. \tag{5}$$

Since we are interested in analysing ν as a function of the correction to the scaling exponent w, we first follow [17, 29] and fit our data to a four-parameter scaling relation,

$$|u_1^0(L) - u_{\rm c}| = a_1 L^{-1/\nu} + a_2 L^{-a_3}. \tag{6}$$

In view of present precision for the estimates $u_1^0(L)$ ($\sim$0.5% for the largest lattice $L = 32$) this approach is adequate to obtain the parameter ν, but not to estimate the correction to scaling w. In order to make this four-parameter fit more stable and to study the behaviour of ν as a function of L, we include additional statistics already available in the literature for smaller lattice sizes. In [17], table 1, zeros for the 3D Ising model are presented for $L = 3, 4, 6, 8, 10$ and 14, together with data from [29] for $L = 5, 6, 8$ and 10. We utilized that information and combined it with our new results (table 1), taking into account the corresponding precision of each datum. The final estimate for each lattice is a linear combination of available data with normalized weight factors, i.e. the reciprocals of the corresponding empirical variances for each datum [30].

To explain this procedure in more detail we consider a set of P independent measurements, $\overline{f}_i$, $(i = 1, 2, \ldots, P)$ with statistical error $\triangle\overline{f}_i$ for the quantity f. Our final estimate is the linear combination

$$\overline{f} = \sum_{i=1}^{P} w_i \overline{f}_i \tag{7}$$

with the normalization condition $\sum_{i=1}^{P} w_i = 1$, where the weight factors w_i correspond to the inverse variance of $\overline{f}_i$, $w_i \propto 1/(\triangle\overline{f}_i)^2$. Such an approach has proven to be useful in combining multiple histograms [31, 32].

In figure 1 we show the corresponding fit for all lattice sizes, whose parameters are found by monitoring the goodness of fit Q [33]. Here we choose the recently obtained critical value $u_{\rm c} = 0.412\,046\,84(25)$ [8], to apply the least-squares method to equation (6), although the fit is not very sensitive to the precision in the value of critical temperature $u_{\rm c}$. The error bar of these 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 $\nu = 0.628\,53(35)$ 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 [2, 7, 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.

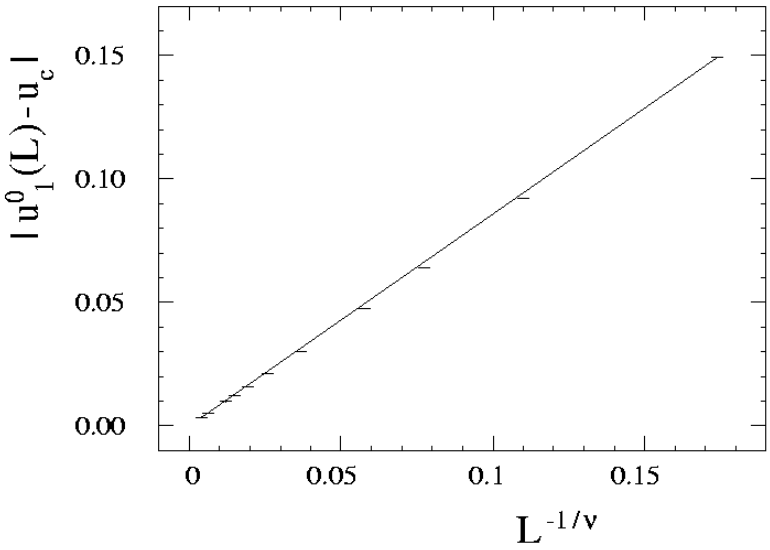

Figure 1. Four-parameter fit for $|u_1^0(L) - u_c|$ as a function of $L^{-1/\nu}$ in the range $L = 3$–32. The least-squares method gives $\nu = 0.628\,53(35)$ with $Q = 0.89$.

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 [34] (which in turn was based on Nightingale's finite-size RG transformation [35] for the correlation length ξ_L). Our method to evaluate w was previously used in [28] 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 ν is given by [36, 37]

$$1 + \frac{1}{\nu_{L,L'}} = \ln\left(\frac{\partial\xi_{L'}/\partial\beta}{\partial\xi_L/\partial\beta}\right)_{\beta_c} \Bigg/ \ln\left(\frac{L'}{L}\right). \tag{8}$$

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

$$\xi_L = LY_\xi((\beta - \beta_c)L^{1/\nu}, hL^{y_H}, \tilde{u}L^{y_3}). \tag{9}$$

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

From equations (8) and (9) one obtains, for $h = 0$,

$$\frac{1}{\nu_{L,L'}} = \frac{1}{\nu} + a_0\frac{L'^{y_3} - L^{y_3}}{\ln(L'/L)} + b_0\frac{L'^{2y_3} - L^{2y_3}}{\ln(L'/L)} + \cdots \tag{10}$$

where a_0 and b_0 include derivatives such as $\partial Y_\xi(y, z)/\partial y|_{y=0,z=0}$. With the introduction of the rescaling factor $s = L'/L$ in equation (10), we now can evaluate y_3 [34].

However an important point remains to be answered: how to estimate the finite-size dependence of ν on lattice sizes L and L'? This can be achieved from large enough pairs of

Table 2. Sequences of estimates for $\nu_{L,2L}$. The second column contains estimates from pairs of lattices $(L, 2L)$ according to equation (11), while in the third column these estimates are obtained by replacing $|u_1^0(2L) - u_c|/|u_1^0(L) - u_c|$ by $\mathrm{Im}\, u_1^0(2L)/\mathrm{Im}\, u_1^0(L)$. The corresponding zeros $u_1^0(L)$ for the smallest lattices $L = 3$, 4 and 5 were obtained in [17], whereas for $L = 6$ and 8 they were estimated from our values (table 1) combined with the ones also quoted in [17].

L	$\nu_{L,2L}$	$\nu_{L,2L}$
3	0.607 13(10)	0.609 16(11)
4	0.619 86(13)	0.618 31(14)
5	0.624 51(31)	0.621 81(33)
6	0.625 77(44)	0.622 72(46)
8	0.627 19(64)	0.624 29(67)
12	0.627 8(14)	0.626 3(14)
16	0.627 0(25)	0.627 9(26)

lattices L and L', with $L' > L$, through the following expression for the partition function zeros:

$$\frac{1}{\nu_{L,L'}} = \ln\left(\frac{|u_1^0(L') - u_c|}{|u_1^0(L) - u_c|}\right) \Big/ \ln\left(\frac{L}{L'}\right). \tag{11}$$

This equation defines our finite-size estimators $\nu_{L,L'}$ from the complex zeros $u_1^0(L)$. A second estimate can be obtained with the replacement of $|u_1^0 - u_c|$ by its imaginary part $\mathrm{Im}\,(u_1^0)$ in equation (11). For large enough systems we have $\mathrm{Re}\,(u_1^0) \sim u_c$, and the two approaches should lead to the same result.

In table 2 we present sequences of these two possible estimates $\nu_{L,sL}$ as a function of the fixed rescaling factor $s = 2$. The second column contains the results of equation (11) and the third one the replacement of $|u_1^0(sL) - u_c|/|u_1^0(L) - u_c|$ by $\mathrm{Im}\, u_1^0(sL)/\mathrm{Im}\, u_1^0(L)$.

As L increases, the values obtained by matching pairs of lattices are expected to converge to a limiting value. In particular, if we match our largest lattices $L = 24$ and 32 we obtain from equation (11) $\nu = 0.6260(66)$, 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 still not precise enough and render a non-monotonic sequence of estimates towards its critical value ν as $L \to \infty$. On the other hand, estimates based only on the imaginary part of the zeros exhibit the monotonic behaviour.

Since equations (10) and (11) are valid only for large enough lattice sizes, we have to discard the smallest values from table 2. For this reason we prefer not to follow the usual procedure: to evaluate equation (10) by a multi-parameter fit. Instead, we note that equation (10) can be written with $L' = sL$ (for a given fixed s) as

$$T(h) = T + a_1 h^w + a_2 h^{2w} + \cdots \tag{12}$$

where we identify

$$\begin{aligned} y_3 &= -w \\ h &= 1/L \\ T(h) &= 1/\nu_{L,2L} \end{aligned} \tag{13}$$

and with

$$T = 1/\nu.$$

Equation (12) is in the proper form to be analysed in the asymptotic limit $h \to 0$ 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 $T(h_N)$, $(N = 0, 1, 2, \ldots)$ converging to zero as $N \to \infty$. See also [38] for a recent discussion on the 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

$$\begin{aligned} T_{-1}^{(N)} &= 0 \\ T_{0}^{(N)} &= T(h_N) \end{aligned} \tag{14}$$

and

$$T_m^{(N)} = T_{m-1}^{(N+1)} + (T_{m-1}^{(N+1)} - T_{m-1}^{(N)}) \left[\left(\frac{h_N}{h_{N+m}} \right)^w \left(1 - \frac{T_{m-1}^{(N+1)} - T_{m-1}^{(N)}}{T_{m-1}^{(N+1)} - T_{m-2}^{(N+1)}} \right) - 1 \right]^{-1}. \tag{15}$$

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 that $|T_m^{(i)} - T| \leqslant \varepsilon_m^{(i)}$ in the limit $i \to \infty$. The above remark gives a criterion [20] for choosing w in order to have a fast and reliable convergence: as the value to minimize $\varepsilon_m^{(i)}$.

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, for which exact values for $\nu_{L,2L}$ are presented in [28].

For illustrative purposes, we display in figures 2–4 the BST extrapolants for different sets of sequences $T(h_N)$ obtained by gradually discarding smallest lattice sizes. In figure 2 we show the BST estimates of the critical exponent ν^{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 behaviour at $w \sim 1.580$ for the extrapolated results (full curves) to $h \to 0 (L \to \infty)$ for the above sequence. In the neighbourhood of that pole we note the corresponding large values for the systematic error (dashed curves) according to the scale on the right-hand side of that figure. Here we define the error as the difference between the extrapolated value T and the value of the 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, ν^{BST} is weakly dependent on w. For instance, we obtain ν 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, $h = 1/12, 1/16, 1/20, 1/24$ and $1/32$. In this 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 $h = 1/16, 1/20, 1/24$ and $1/32$, and we obtain $w \in [0.411, 1.3220]$, with a pole at $w \sim 1.3871$.

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

We are finally at the 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 to utilize equations (10) and (11), we are left with the sequence displayed in the third column of table 2. Figure 5 presents our obtained BST estimates for the critical exponent ν from a sequence of lengths $h = 1/6, 1/8, 1/12$ and $1/16$. 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

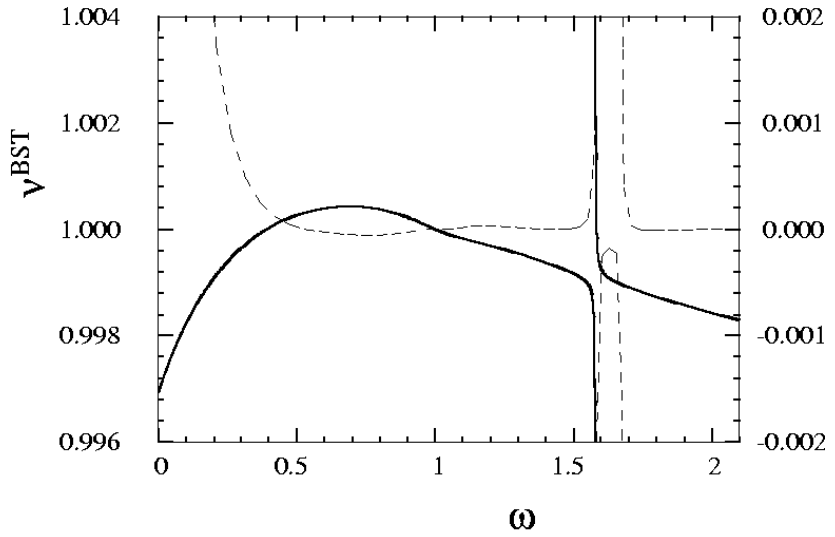

Figure 2. BST estimates of the critical exponent ν (full curves) and systematic error (dashed curves), as a function of the free parameter w, for the 2D Ising model. The extrapolation is obtained from the finite-size sequence with lattice sizes from $L = 4$ up to 32. The right-hand scale refers to the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

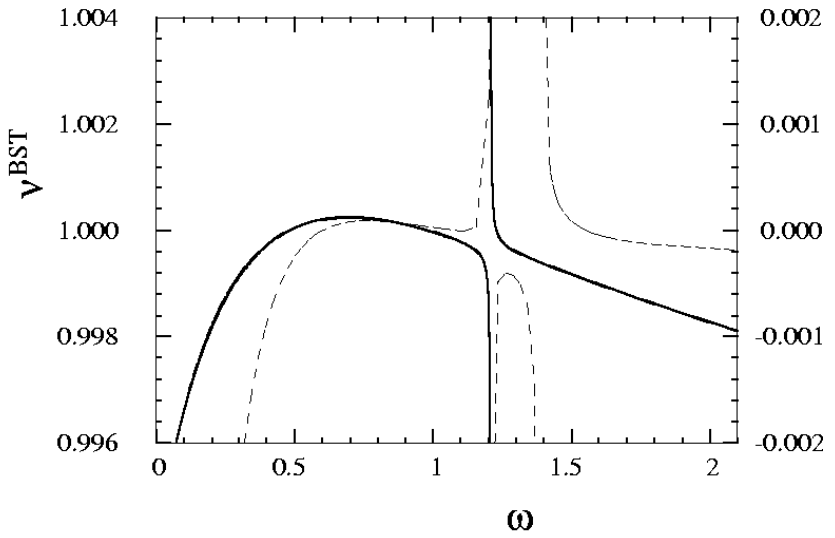

Figure 3. As in figure 2, BST estimates of the critical exponent ν (full curves) and systematic error (dashed curves) for the 2D Ising model, with lattice sizes from $L = 12$ up to 32. The right-hand scale refers to the systematic error.

0.0015 as our input condition to find w, as exemplified for the 2D Ising model. This statistical error leads to the range $[0.671, 0.819]$ for w, marking the region of minimum systematic error. We translate that range into $w = 0.745(74)$ as our best estimate for the correction to the scaling exponent.

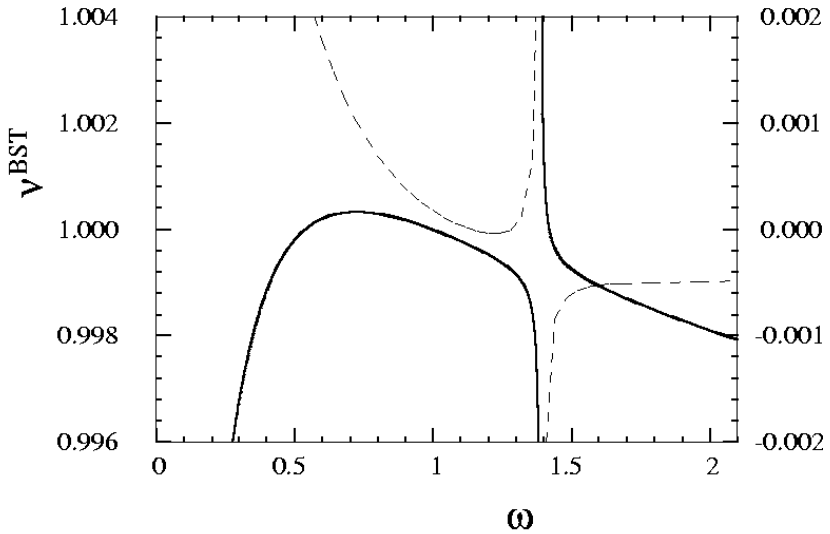

Figure 4. As in figure 2, BST estimates of the critical exponent ν (full curves) and systematic error (dashed curves) for the 2D Ising model, with lattice sizes from $L = 16$ up to 32. The right-hand scale refers to the systematic error.

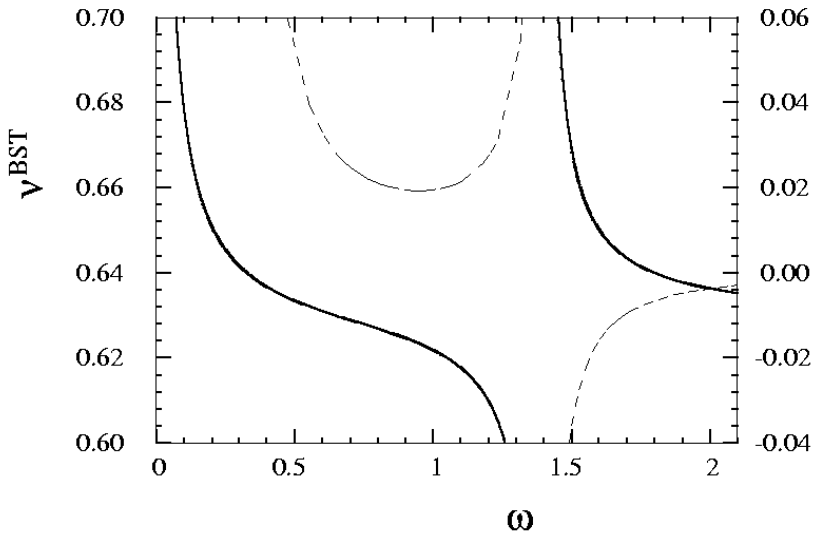

Figure 5. BST estimates of the critical exponent ν (full curves) and systematic error (dashed curves), as a function of the free parameter w for the 3D Ising model. The sequence is obtained with lattice sizes $L = 6$, 8, 12 and 16. The right-hand scale refers to the systematic error.

We remark that this approach yields a value for w which agrees within error bars with recent results from several other different approaches: by means of scaling relations of observables related to the magnetization [8] one finds $w = 0.87 \pm 0.09$, from perturbative expansion [7] at fixed dimension $D = 3$ follows $w = 0.799 \pm 0.011$, whereas $w = 0.814 \pm 0.018$ is estimated from ε-expansion.

4. Conclusions

In summary, we have described a new way to calculate the correction to the scaling exponent w for the 3D Ising model. The new approach combines a particular FSS relation (equation (10)) for the critical exponent ν (which is based on the behaviour of the leading partition function zeros) with a convenient algorithm (BST) to extrapolate sequences of polynomial form (equation (12)). Monte Carlo multicanonical simulations were performed to obtain high-precision estimates for the density of states and the leading partition function zeros for large lattices.

A four-parameter fitting was performed in order to find the correlation length critical exponent ν. Next, the results for ν including the statistical error were 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 (10) to few data points and rather large lattice sizes.

Our results for ν 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 ν 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 the 2D Ising model even $L = 64$ seems to be not large enough.

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