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24-th Order High Temperature Expansion for the 3-d Ising Model

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We present the series for the free energy and our estimate for the critical exponent α, as computed by a recursive bookkeeping algorithm on the CM5.

1. TRANSFER-MATRIX ALGORITHM

We begin with a discussion of the algorithm to compute the High-Temperature(HT) expansion on finite 3-d Ising lattices. Starting from the action

$$E\{s\} = -\sum_{<i,j>} s_i s_j \ , \tag{1}$$

the partition function is expanded in a HT series

$$Z = \sum_{\{s\}} \exp\left(-\beta E\right) = (2\cosh^3\beta)^V \sum_k p(k) t^k, \tag{2}$$

with the expansion parameter $t = \tanh\beta$. V is the volume of the system. The free energy per spin is defined as

$$f = -\frac{1}{\beta V}\log Z = -\frac{2\cosh^3\beta}{\beta} - \frac{1}{\beta}\sum_k f_k t^k \ . \tag{3}$$

For simplicity, consider a finite simple cubic lattice which, in the recursion algorithm, is built up by adding one site after the other, layer by layer. This procedure defines the recursion step, which requires knowledge only of those spin states that are contained in the exposed two-dimensional surface layer. To minimize finite size effects, it is best to use helical boundary conditions [1,2]. One can visualize helical boundary conditions by imagining all spins in the layer laid out along a straight line. In this picture, the nearest neighbours to a given site in the sequence in the ith direction can be chosen to be h_i sites away, with $i = x, y, z$. It is convenient to assume $h_x < h_y < h_z$. It is easy to see that as spins are added, one needs only to keep track of the states of spins on the topmost h_z sites. Let these spins be denoted $s_1, \ldots, s_{h_z}$. Then the partition function can be rewritten as

$$Z \propto \sum_k \sum_{s_1,\ldots,s_{h_z}} p(k; s_1, \ldots, s_{h_z}) t^k \ . \tag{4}$$

The recursion step, which consists of adding another spin s_0 to the system, can be can be carried out by performing the following updating procedure for the coefficients p [4]

$$\begin{aligned}
& 2p'(k; s_0, s_1, \ldots, s_{h_z-1}) \\
= \ & p(k-0; s_1, \ldots, s_{h_z-1}, s_0) \\
+ \ & p(k-0; s_1, \ldots, s_{h_z-1}, \bar{s_0}) \\
+ \ & p(k-1; s_1, \ldots, s_{h_z-1}, s_0)(s_0 s_{h_x} + s_0 s_{h_y} + 1) \\
+ \ & p(k-1; s_1, \ldots, s_{h_z-1}, \bar{s_0})(s_0 s_{h_x} + s_0 s_{h_y} - 1) \\
+ \ & p(k-2; s_1, \ldots, s_{h_z-1}, s_0)(s_{h_x} s_{h_y} + s_0 s_{h_x} + s_0 s_{h_y}) \\
+ \ & p(k-2; s_1, \ldots, s_{h_z-1}, \bar{s_0})(s_{h_x} s_{h_y} - s_0 s_{h_x} - s_0 s_{h_y}) \\
+ \ & p(k-3; s_1, \ldots, s_{h_z-1}, s_0)(s_{h_x} s_{h_y}) \\
+ \ & p(k-3; s_1, \ldots, s_{h_z-1}, \bar{s_0})(-s_{h_x} s_{h_y}) \ .
\end{aligned} \tag{5}$$

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Table 1
Structures and weights w of the lattices used

h_x	9	1	9	5	7	10	5	14	11	14	9	9	5	5	16	10	16	1	17
h_y	11	12	14	15	15	13	15	15	16	16	17	16	17	19	17	19	20	18	21
h_z	13	14	16	16	16	17	17	17	17	17	19	20	20	20	21	21	21	22	22
w	-3	3	-3	-3	3	-3	3	-3	3	3	-1	-2	-1	1	-2	5	2	-2	2

Table 2
Free energy up to 24th order

order k	free energy f_n
0	0
2	0
4	3
6	22
8	375/2
10	1980
12	24044
14	319170
16	18059031/4
18	201010408/3
20	5162283633/5
22	16397040750
24	266958797382

It is crucial to remove finite-size errors by combining the results of different lattice structures as described in refs. [1,2]. We use the set of lattices listed in table 1 and obtain the free energy coefficients up to 24th order as given in table 2. In order to eliminate the contribution from (unphysical) loops with an odd number of links in any direction, we use the cancellation technique of ref. [2]. Possible contributions of higher-order finite-size-loops are at least of order 25 for this set of lattices. Since we use open boundary conditions, the coefficients p are invariant under the global transformation $s_i \rightarrow -s_i$. This Z(2) symmetry enables us to reduce memory requirements by a factor of two. Unlike refs. [1–3] we use multiple-word arithmetic to account for the size of the coefficients. This implementation needs about 100% more memory but leads to a doubling in performance. Since the number of words can be adjusted separately for every order, the computational effort can be reduced accordingly. On a 32 node Connection Machine CM-5 the total time for all computations was about 50 hours.

Compared to the finite-lattice approach of Enting and Guttmann [3], our method appears to require more CPU-time since we need to cancel unphysical loops. It should be noted, however, that helical lattices are very naturally implemented in data parallel software environments and thus lead to better performance. In the usual finite lattice method [3] on the other hand, the HT expansion can only be extended in fairly coarse steps, using lattices with (4×5) cross-section for 22nd order and (5×5) cross-section for 26th order. Thus a 24th order computation would not have been feasible with out 1 Gbyte machine.

2. CRITICAL EXPONENT

The specific heat is defined as

$$c|_{h=0} = \beta^2 \frac{\partial^2}{\partial \beta^2} \log Z = \sum_k c_{2k} t^{2k} \qquad (6)$$

and is expected to behave near T_C as

$$c|_{h=0} = A|T - T_C|^{-\alpha} \left[1 + B|T - T_C|^{\theta} + \ldots\right], \qquad (7)$$

with A and B being analytic near T_C [7].

We find for the critical exponent using inhomogeneous differential Padé-approximants (IDPs) [8]

$$\begin{aligned} \alpha_1 &= 0.102 \pm 0.008 \qquad (8) \\ \alpha_2 &= 0.109 \pm 0.016\,, \end{aligned}$$

at the value $t_C = 0.218092$ obtained from Monte-Carlo simulations [9]. The first value is obtained using a linear fit to the unbiased approximants [4], whereas the second value is the mean value from directly biased approximants.

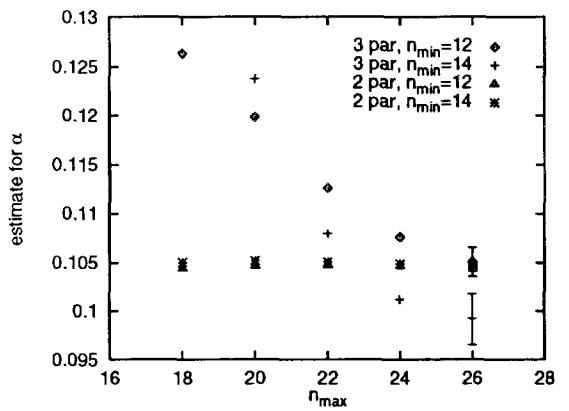

Figure 1. Estimates of α using 2- and 3-parameter-fits. Each point represents the results of a fit to the set of values $\{s_{n_{min}}, \ldots, s_{n_{max}}\}$. The error bars of the rightmost values represent the uncertainty of the extrapolated 26th term.

IDPs can also be used to predict the most significant digits of the next term in the specific heat series [3]. The estimate of the 24th order term as obtained in ref. [3] agrees perfectly with our exact result. In the same manner we can estimate the 26th order term in the expansion to be

$$f_{26} = 443762(4) \times 10^7 \ , \qquad (9)$$

where the error quoted refers to two standard deviations.

The ratio $r_n = c_n/c_{n-2}$ of successive coefficients of the specific-heat series is expected to behave as [7]

$$r_n = \frac{1}{t_C^2}\left(1 + \frac{\alpha - 1}{n} + \frac{c}{n^{1+\theta}} + \frac{d}{n^{1+2\theta}} + \ldots\right) . \qquad (10)$$

Assuming that the correction-to-scaling exponent θ is close to 0.5 [9,10], the following sequence s_n is expected to converge towards α like

$$s_n := \left(t_C^2 r_n - 1\right) n + 1 = \alpha + \frac{c}{n^{1/2}} + \frac{d}{n} + \ldots \ . \qquad (11)$$

We performed 3-parameter fits to the set of values $\{s_{12}, \ldots, s_{26}\}$ to obtain estimates for α. The results of these fits are shown as diamonds in fig. 1. To get an estimate of the uncertainties of our results, we investigate the stability of the fits by eliminating the point s_{12} from the data. As a result we obtain sizeable changes for α shown as crosses in fig. 1.

Since we find that the correction-to-scaling coefficient c vanishes within error we also performed 2-parameter fits to the same data set. The results of these fits are also shown in fig. 1

Finally we investigate the influence of the uncertainty in the correction-to-scaling exponent θ on our results. Repeating the analysis with $\theta = 0.53$ [9] we find that the error in α is smaller than 0.0005.

Taking into account the fact that omitting the $\frac{c}{n^{1/2}}$ term gives rise to an additional systematic error, we endup with the estimate for the critical exponent

$$\alpha = 0.104(4) \ . \qquad (12)$$

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