Cluster-variation–Padé-approximant method for the simple cubic Ising model

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The cluster-variation–Padé-approximant method is a recently proposed tool, based on the extrapolation of low- and high-temperature results obtained with the cluster-variation method, for the determination of critical parameters in Ising-like models. Here the method is applied to the three-dimensional simple cubic Ising model, and new results, obtained with an 18-site basic cluster, are reported. Other techniques for extracting nonclassical critical exponents are also applied and their results compared with those by the cluster-variation–Padé-approximant method.

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The cluster-variation method (CVM) [1–3] is a hierarchy of approximations that generalizes the well-known mean-field approximation and has been widely applied in the last decades, mainly to study the equilibrium properties of classical, discrete lattice models with short-range interactions. The CVM results are more and more accurate as the size of the clusters considered increases (at least in a specific way, see below), but the critical exponents always take the mean field (classical) values. The issue of extracting nonclassical critical exponents from mean field approximations has been the subject of a certain amount of research work in recent years. As far as the CVM is concerned, a few schemes have been proposed in recent years to give estimates of critical exponents from the CVM results. One of these schemes, the cluster-variation–Padé-approximant method (CVPAM) [4,5], was specifically devised for the CVM and exploits its great accuracy at high and low temperatures by means of an extrapolation of the thermodynamic quantities based on Padé approximants.

In the present paper I report on an investigation on the CVM approximation for the Ising model on the simple cubic lattice with the largest basic cluster (18 sites) ever considered. The results of this approximation are used to give nonclassical estimates of the three-dimensional Ising critical exponents, using mainly the cluster-variation–Padé-approximant method (CVPAM). Other schemes, like the coherent anomaly method (CAM) [6] and an approach by Tomé and de Oliveira [7] are also considered.

I shall study the Ising model on the simple cubic lattice, with nearest-neighbor (NN) interactions only, described by the reduced Hamiltonian

$$\frac{\mathcal{H}}{k_B T} = -K \sum_{\langle ij \rangle} s_i s_j , \tag{1}$$

where K is the (reduced) interaction energy, $s_i = \pm 1$ is the usual Ising variable at site i, the summation runs on NN pairs, and k_B and T are, as customary, Boltzmann's constant and absolute temperature, respectively.

The CVM is a variational method based on the minimization of a free energy density which is obtained [2,3] by truncating the cumulant expansion of the exact variational principle of equilibrium statistical mechanics. The approximate free energy density depends on the density matrix (matrices) of the largest cluster(s) entering the expansion, which completely determines the approximation. The simple cubic Ising model has been investigated, using the CVM, by Kikuchi [1] in the NN pair, square and cube approximations, and by the present author [8] in the star-cube approximation. Here I shall use the 18-point approximation which is obtained by choosing as the basic cluster the $3\times3\times2$ cluster obtained by joining four cubes as in Fig. 1, which is the largest cluster ever considered for this lattice. The choice of this cluster is motivated by Schlijper's observation [9] that, due to the existence of a transfer matrix for the model, accuracy can be increased by enlarging the basic clusters in $d-1$ dimensions only, where d is the lattice dimensionality. One could imagine a series (the generalization of the so-called C series by Kikuchi and Brush [10]) of basic clusters made of $L\times L\times2$ sites, where for $L=2$ one has the cube approximation, for $L=3$ the present one, and for $L>3$ approximations that cannot be dealt with using current computers.

Following An [2], the (reduced) free energy density to be minimized can be written in the form

$$\begin{aligned} f(\rho_{18}) = &-3K\,\mathrm{Tr}(s_1 s_2 \rho_4) + \mathrm{Tr}(\rho_{18}\ln\rho_{18}) - 2\,\mathrm{Tr}(\rho_{12}\ln\rho_{12}) \\ &- \mathrm{Tr}(\rho_9\ln\rho_9) + \mathrm{Tr}(\rho_8\ln\rho_8) + 2\,\mathrm{Tr}(\rho_6\ln\rho_6) \\ &- \mathrm{Tr}(\rho_4\ln\rho_4), \end{aligned} \tag{2}$$

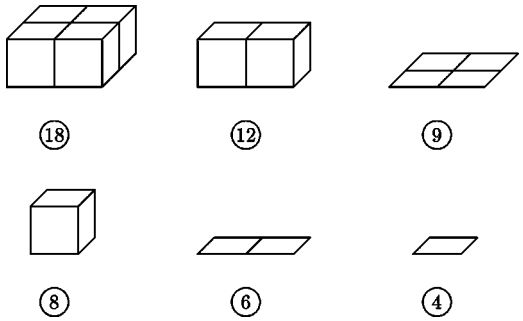

FIG. 1. The 18-point basic cluster and its subclusters.

TABLE I. Comparison of various CVM estimates for the critical point with the best estimates.

Method	Pair [1]	Square [1]	Cube [1]	Star cube [8]	18 point (present)	Best estimates [13–17]
K_c	0.20273	0.21693	0.21829	0.2187	0.2199	0.22165

where ρ_n denotes the density matrix of the n-point cluster (see Fig. 1), while $\mathrm{Tr}(s_1 s_2 \rho_4)$ is the NN correlation (s_1 and s_2 being any NN sites on the square plaquette).

The free energy density can be regarded as dependent on ρ_{18} only, because the subcluster density matrices can be defined as suitable partial traces of ρ_{18}. Since the Hamiltonian is classical, the density matrices are diagonal, and hence our free energy density depends, in principle, on the 2^{18} diagonal elements of ρ_{18} corresponding to the spin configurations of the 18-point cluster. These elements are, however, not all independent. First of all, the density matrices must be normalized according to $\mathrm{Tr}\,\rho_{18}=1$. In addition, many elements are degenerate because of the lattice symmetries. The nondegenerate ρ_{18} elements turn out to be 17676, a rather small number if compared with $2^{18}=262144$. Taking into account lattice symmetries the size of the problem is reduced by a factor slightly smaller than 16, which is the number of elements of the symmetry group of our 18-point basic cluster. Finally, it must be observed that ρ_{12} can be defined in different ways as a partial trace of ρ_{18}. In order to ensure that these different traces yield the same density matrix one has to impose 1134 constraints on the elements of ρ_{18}. Once these constraints are satisfied no ambiguity is left in the definition of the other subcluster density matrices. Therefore, one is left with the problem of finding the minimum of a function of 17676 variables, with 1134 (leaving apart the trivial normalization constraint) linear constraints among them. The problem can be easily treated in the framework of the natural iteration method (NIM) [11,12], developed by Kikuchi for the solution of the CVM variational problem. The solution for a single value of K (not too close to the critical point) can be found on a modern personal computer in a time of the order of ten minutes.

The accuracy of the present approximation can be assessed in several ways. For instance, I have compared in Table I the present K_c value with those from other CVM approximations and with the best estimates [13–17]. Another interesting check is the comparison, in Table II, of our magnetization values $m=\langle s_i \rangle$ with those given by the formula by Talapov and Blöte [17], determined on the basis of high precision simulations and finite size scaling. It is interesting to observe that the best agreement between the two methods occurs in the middle of the temperature range considered [which lies within the temperature range $t=1-K_c/K \in (0.0005;0.26)$, where Talapov and Blöte regard their result as very accurate]. For $T=1/K=3.7$ the two magnetizations differ only by 10^{-7}. For larger temperatures our results are certainly less accurate than those by Talapov and Blöte, while the inverse must be true for smaller temperatures (the result by Talapov and Blöte is significantly smaller than 1 at very low temperatures and has a maximum around $T=1.85$).

TABLE II. Comparison of our estimate of the magnetization with that by Talapov and Blöte.

$T=1/K$	m (present work)	m (Talapov and Blöte [17])
3.4	0.8972562	0.8972440
3.5	0.8806417	0.8806366
3.6	0.8616750	0.8616735
3.7	0.8399256	0.8399255
3.8	0.8148173	0.8148161
3.9	0.7855490	0.7855416
4.0	0.7509519	0.7509251
4.1	0.7092094	0.7091249
4.2	0.6572414	0.6569722
4.3	0.5891051	0.5881361
4.4	0.4905811	0.4859045
4.5	0.3067063	0.2378014

In order to obtain nonclassical estimates of the critical exponents, I shall now apply the CVPAM according to the rules outlined in [4,5]. In the CVPAM one computes a thermodynamical function F for a set of temperature values in a range where the CVM approximation can be regarded as very accurate. These values are then used as a basis for extrapolation by means of Padé approximants and their generalizations.

As a first step I shall consider the low-temperature magnetization as a function of the variable $x=e^{-K}$. In order to determine a temperature range $x<x_{\max}$ in which the 18-point CVM is very accurate, I compare it with a lower order CVM approximation. Although the star-cube approximation is slightly more accurate, I choose the cube approximation for this purpose, since, as I mentioned above, the cube and 18-point approximations can be thought of as belonging to the same series. Requiring that the magnetization difference is less than the empirically determined [5] threshold $\epsilon=10^{-5}$, I obtain $x_{\max}=0.75$. The function $m(x)$ now has to be extrapolated to estimate its singular properties, taking into account also confluent singularities, which is corrections to scaling. To this end I use Adler's generalizations [18–20], usually denoted by $M1$ and $M2$, of the ordinary Padé-approximant method (I recall that an $[L,M]$ Padé approximant is simply the ratio of two polynomials of degree L and M [21,22]). Given a function $F(x)$ with a singularity that can be assumed of the form $(x_c-x)^{-\lambda}[1+a(x_c-x)^{\Delta_1}]$, method $M1$ considers Padé approximants to the logarithmic derivative of the function

$$B(x)=\lambda F(x)-(x_c-x)\frac{dF}{dx} \tag{3}$$

for assigned x_c and λ. The dominant singularity in $(d/dx)\ln B(x)$ is a pole at x_c with residue $\lambda-\Delta_1$ if $\Delta_1<1$

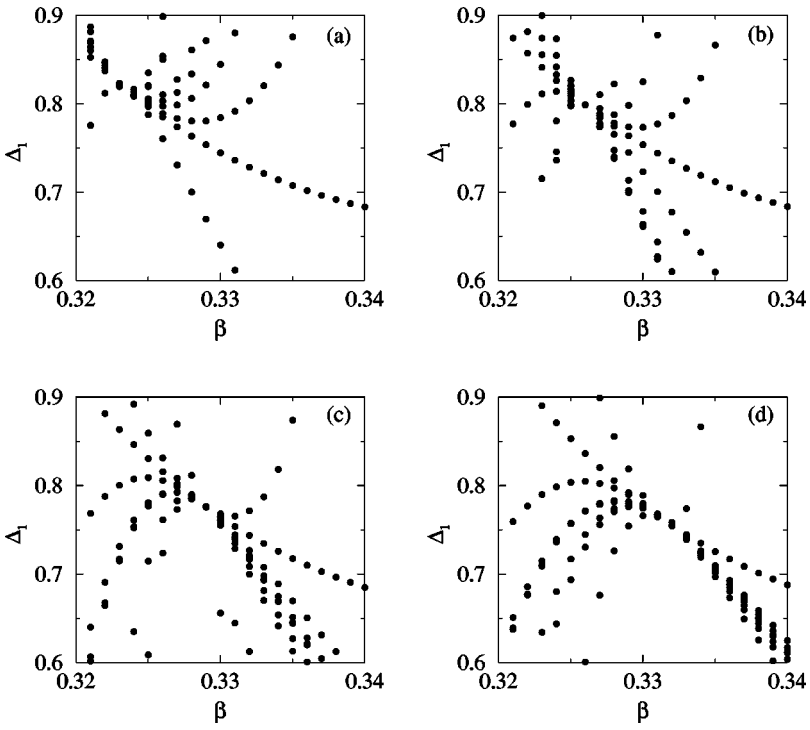

FIG. 2. Δ_1 vs β plot obtained by method $M1$, for $T_c=4.512$ (a), 4.513 (b), 4.514 (c), and 4.515 (d), using $[L,M]$ approximants with $3\leqslant L\leqslant 5$, $L-1\leqslant M\leqslant L+1$.

and $\lambda-1$ otherwise. Method $M2$ considers instead, for assigned x_c and Δ_1, Padé approximants to

$$G(y)=-\Delta_1(y-1)\frac{d\ln F}{dy},\quad y=1-\left(1-\frac{x}{x_c}\right)^{\Delta_1},\quad (4)$$

which should converge to λ for $y=1$. In the CVPAM, the function $d\ln B/dx$ or $G(y)$ is evaluated at $L+M+1$ equally spaced points $x_n=x_{\max}-n\,\delta x$, $x=0,1,\ldots L+M$ and then an $[L,M]$ Padé approximant is determined by interpolation. The value of the spacing δx must be adjusted empirically so that the sets of linear equations which must be solved for the interpolation are not badly conditioned. For the magnetization, the best conditioned sets of equations are obtained for $\delta x=0.015$.

Applying method $M1$ to our magnetization estimates we have obtained the correction to scaling exponent Δ_1 as a function of the critical exponent β for several values of the trial critical temperature $T_c=1/K_c$. It is known [20] that the plots given by $M1$ have a different curvature above and below the critical temperature. In the ordered phase the Δ_1 versus β plot is bent upward, while in the disordered phase it is bent downward. Using this criterion we can locate the critical temperature in the range $4.512\leqslant T_c\leqslant 4.515$, which corresponds to $0.22148\leqslant K_c\leqslant 0.22163$, in agreement with the most recent estimates [13–17]. From the corresponding plots, reported in Fig. 2, one reads the estimates $0.323<\beta<0.332$ for the magnetization critical exponent and $0.75<\Delta_1<0.82$ for the correction to scaling exponent. As in the case of the face-centered-cubic lattice [5], the critical exponent result is consistent with recent estimates [13,17], while the correction to scaling one is substantially higher. Method $M2$ does not provide a clearcut way to estimate T_c, but using the result by $M1$ as an input we get (see Fig. 3) $0.322<\beta<0.331$ and $0.79<\Delta_1<0.87$.

I tried to analyze the high-temperature susceptibility data (which typically give much better results than the low-temperature one) in the same way. I considered the susceptibility as a function of the variable $w=\tanh K$ and determined a region $w<w_{\max}$ of the disordered phase in which the 18-point CVM approximation can be regarded as very accurate by comparing the NN correlation (which is bounded, and hence is better than the susceptibility for such a test) with that given by the cube approximation. The two estimates differ by less than $\epsilon=10^{-5}$ when $w<w_{\max}=0.13$. Unfortunately, both methods $M1$ and $M2$ failed to converge and I had to resort to ordinary Padé approximants for the logarithmic derivative of the susceptibility. The points for the interpolation were chosen as described previously, with a spacing $\delta w=0.003$. Results for the critical exponent γ from $[L,L]$ approximants biased with the above estimates for T_c are reported in Table III. Also including results from $[L,L\pm1]$ approximants I can conclude $1.237<\gamma<1.248$, which again is consistent with the most recent estimates.

Finally, I have tried to analyze the magnetization data by means of other techniques, namely the CAM [6] and a similar approach by Tomé and de Oliveira [7].

TABLE III. Critical exponent γ from biased $[L,L]$ approximants.

L \ T_c	4.512	4.513	4.514	4.515
4	1.24748	1.24520	1.24296	1.24076
5	1.24748	1.24519	1.24289	1.24058
6	1.24748	1.24502	1.24217	1.23895
7	1.24749	1.24505	1.24228	1.23922
8	1.24748	1.24482	1.24155	1.23769
9	1.24749	1.24483	1.24156	1.23769
10	1.24746	1.24487	1.24207	1.23905

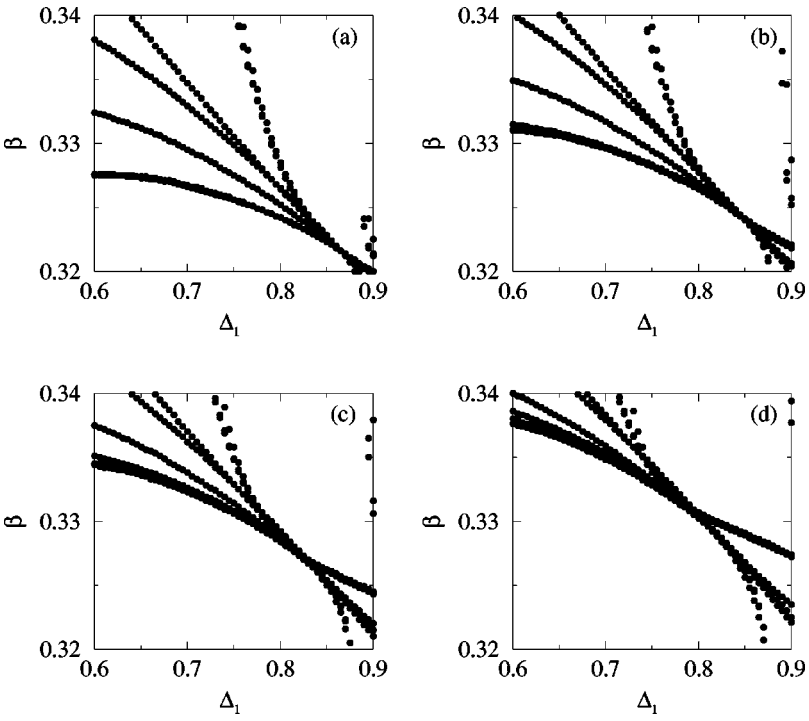

FIG. 3. β vs Δ_1 plot obtained by method $M2$, for $T_c=4.512$ (a), 4.513 (b), 4.514 (c), and 4.515 (d), using $[L,M]$ approximants with $3\leqslant L\leqslant 5$, $L-1\leqslant M\leqslant L+1$.

The CAM scaling hypothesis for the magnetization [6] is that its critical amplitude, defined by $m(T)\simeq B^*(T^*-T)^{1/2}$ must diverge as $B^*\sim(T^*-T_c)^{\beta-1/2}$, where T_c is the true critical temperature and T^* and B^* are the estimates for the critical temperature and the critical amplitude in a given approximation. Using the above-mentioned best estimate $K_c=0.221\,65$ for the critical temperature, a fit on the results from the pair, cube, star cube, and 18-point CVM approximation (the plaquette approximation was discarded since it was clearly out of the curve) I got $\beta=0.351$. Poorer results were obtained discarding, in addition to the plaquette approximation, the pair approximation or the star-cube approximation ($\beta=0.415$ and 0.212, respectively).

The approach by Tomé and de Oliveira [7] is based on the scaling assumption $m(T_c)\sim(T^*-T_c)^{\beta}$. The best results with this approach have been found by fitting the results from the pair, cube, and 18-point approximations ($\beta=0.312$) and those from the cube and 18-point approximations only ($\beta=0.344$).

In conclusion, I have developed an 18-point (the largest maximal cluster ever considered) CVM approximation for the simple cubic lattice and applied it to the Ising model. The results from this approximation have been used to extract nonclassical estimates for the critical exponents. Among the three methods considered for this purpose, namely the CVPAM, the CAM, and the method by Tomé and de Oliveira, the CVPAM is the only one which gives critical exponents which are (except for the correction to scaling exponent) consistent with the most recent estimates. The CVPAM is therefore to be preferred when extrapolating CVM results to the critical region. The effort needed was essentially the same in all cases, since most of the labor and computer time go into the development and solving of the CVM approximation. In particular, the computer resources needed are remarkably small if compared with the requirements of extensive Monte Carlo simulations or series expansions, and the results are only slightly poorer, a feature which makes the CVPAM an interesting technique whenever powerful computers are not available and/or very high accuracy is not needed.

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