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Cluster variation method, Padé approximants, and critical behavior

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In the present paper we show how nonclassical, quite accurate, critical exponents can be extracted in a very simple way from the Padé analysis of the results obtained by mean-field-like approximation schemes, and in particular by the cluster variation method. We study the critical behavior of the Ising model on several lattices (quadratic, triangular, simple cubic and face centered cubic) and two problems of surface critical behavior. Both unbiased and biased approximants are used, and results are in very good agreement with the exact or numerical ones.

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As is well known, mean-field-like approximations are very useful tools in the investigation of phase transitions, but they fail completely in predicting critical exponents of low-dimensional systems, giving results which are independent of the model and the dimensionality. This is due to neglecting long range correlations, and thus they are completely unreliable if one is interested in the behavior of a model near critical or multicritical points.

On the other hand, there are some mean-field-like approximations which describe very accurately the low- and/or high-temperature behavior of statistical mechanical models. In particular, the cluster variation method (CVM) introduced by Kikuchi [1] and reformulated several times [2] has been shown [3] to reproduce exactly many terms of the high- and low-temperature expansions of thermodynamical quantities like specific heat, magnetization, and susceptibility.

In the present paper we show how this property of the CVM (and also of other schemes, as we shall see) can be used to build up a very simple procedure for determining quite accurately the critical temperature and critical exponents of a given model, which relies on the Padé analysis of low- and high-temperature results obtained by the CVM. The plan of our presentation is as follows: we first review the main ideas of the CVM and of Padé approximants, then we describe in detail our technique and several test applications and finally we discuss results and possible generalizations.

The cluster variation method in its modern formulation [2] can be seen as a truncation of a cumulant expansion of the functional to be minimized in the variational principle of statistical mechanics. The latter states that the free energy F of a model system described by the Hamiltonian $\mathcal{H}$ on a lattice Λ can be obtained by minimizing the functional

$$F[\rho_\Lambda] = \mathrm{Tr}(\rho_\Lambda \mathcal{H} + k_B T \rho_\Lambda \ln \rho_\Lambda), \tag{1}$$

where k_B and T are, as customary, Boltzmann's constant and absolute temperature, with respect to the density matrix ρ_Λ, subject to the constraint $\mathrm{Tr}\rho_\Lambda = 1$. Upon introducing the cluster density matrices $\rho_\alpha = \mathrm{Tr}_{\Lambda\setminus\alpha}\rho_\Lambda$, where α is a cluster of n_α sites and the trace is performed over all variables out of α, Eq. (1) is approximated by a restricted variational principle for the functional

$$F[\{\rho_\alpha, \alpha \in P\}] = \sum_{\alpha\in P} \mathrm{Tr}(\rho_\alpha h_\alpha) + k_B T \sum_{\alpha\in P} a_\alpha \mathrm{Tr}(\rho_\alpha \ln \rho_\alpha), \tag{2}$$

where P is a set of "maximal" clusters and all their subclusters, h_α is the n_α-body interaction contribution due to the cluster α (maximal clusters should be taken large enough to contain all kind of interactions present in $\mathcal{H}$), the coefficients a_α obey [2]

$$\sum_{\beta\subseteq\alpha\in P} a_\alpha = 1 \quad \forall\beta \in P \tag{3}$$

and the ρ_α's are subject to the constraints

$$\mathrm{Tr}\rho_\alpha = 1 \quad \forall\alpha \in P, \quad \rho_\alpha = \mathrm{Tr}_{\beta\setminus\alpha}\rho_\beta \quad \forall\alpha \subset \beta \in P. \tag{4}$$

Local minima of F can be obtained in a simple way by means of an iteration scheme devised by Kikuchi [4], the natural iteration method (NIM) which, for maximal clusters up to 8-9 sites as those we used, does not require large amounts of CPU time.

It should be clear that an approximation in this scheme is uniquely defined by the choice of the maximal clusters (so if the maximal clusters are all the elementary cells of a simple cubic lattice, we will speak of the cube approximation, and so on), and it will not be accurate near critical points, where the correlation length of the system becomes larger than the size of the maximal clusters. Generally speaking, taking larger maximal clusters will narrow the region in which the approximation is not accurate.

Let us now turn to a brief review of some basic facts about Padé approximants [5]. An $[L,M]$ Padé approximant to a function $F(z)$ is defined by

$$[L,M] \equiv \frac{P_L(z)}{Q_M(z)} = \frac{p_0 + p_1 z + p_2 z^2 + \cdots + p_L z^L}{1 + q_1 z + q_2 z^2 + \cdots + q_M z^M}. \tag{5}$$

The usefulness of these approximants in statistical mechanics derives from the fact that a function with a power-law singular behavior

$$F(z) \approx A(z)\left(1 - \frac{z}{z_c}\right)^{-\lambda}, \qquad z \to z_c^-, \tag{6}$$

with $A(z)$ analytic at z_c, will have a logarithmic derivative of the form

$$D(z) \equiv \frac{d}{dz}\ln F(z) \approx -\frac{\lambda}{z - z_c}[1 + O(z - z_c)], \quad z \to z_c^-, \tag{7}$$

and a simple pole like that in Eq. (7) can be represented exactly by Padé approximants. Clearly, z_c and $-\lambda$ are given respectively by the pole and the corresponding residue of the Padé approximant. Furthermore, if the exact value (and this is sometimes the case) or a very accurate estimate is available for z_c, better estimates of λ can be obtained by approximating the function

$$\lambda^*(z) \equiv (z_c - z)D(z) \approx \lambda + O(z - z_c), \qquad z \to z_c^-. \tag{8}$$

In this case λ is estimated directly as the value of the approximant at z_c. If no estimate of z_c is given as an input one speaks of *unbiased* approximants, otherwise the approximants are called *biased*.

We can now turn to the description of our technique. To fix ideas, let us consider the Ising model on a face centered cubic (fcc) lattice. The Hamiltonian is

$$\frac{\mathcal{H}}{k_B T} = -J\sum_{\langle ij\rangle} s_i s_j - h\sum_i s_i, \tag{9}$$

where J and h are the (reduced) interaction strength and magnetic field, $s_i = \pm 1$ is the z component of a spin 1/2 operator at the lattice site i and the first summation is over nearest neighbors (NN's). Our first step consists in choosing two CVM approximations (i.e., two sets of maximal clusters) M_1 and M_2 in such a way that M_2 can be regarded as an improvement with respect to M_1. To be concrete, in the following M_1 will be the octahedron plus tetrahedron approximation proposed by Aggarwal and Tanaka [3], while M_2 will be the *oriented rhombohedron* approximation (to be described in detail in a separate paper [6]). This approximation is obtained by selecting as maximal clusters all the primitive rhombohedral unit cells of an fcc lattice with a given orientation (an fcc lattice can be decomposed into primitive cells of this shape in four different ways, corresponding to different orientations). Since a rhombohedron is made up of an octahedron with two tetrahedra attached on opposite faces, we can expect this approximation to improve with respect to M_1. Indeed, this can be easily verified by comparing different estimates for the critical temperature: one obtains $T_c = 1/J_c \simeq 10.03$ from the CVM tetrahedron approximation, 10.01 from M_1, 9.97 from M_2 and 9.83 from high-temperature expansions [7].

The next step is to compare results from M_1 and M_2 to determine the temperature (or, equivalently, interaction strength) range in which M_1 is accurate in some sense. Let us consider first the low-temperature region, in order to obtain estimates for the critical temperature and the critical exponent β associated with the vanishing of the order parameter $m = \langle s_i\rangle$. We have chosen as a measure of the accuracy of M_1 the quantity $\delta m(J) = |m_1(J) - m_2(J)|$, where $m_k(J)$ is the value of the order parameter (in zero field) as given by approximation M_k, which, not too close to the critical point, should be a good approximation to the absolute error of $m_1(J)$ with respect to the exact (unknown) value (it can be checked on two-dimensional problems that this is a very reasonable assumption). Then we define a value $J_{\min}$ of the interaction strength such that $\delta m(J) < \epsilon$ for $J > J_{\min}$, where ϵ is a small positive number, and say that M_1 (and consequently also M_2) is *accurate* for $J > J_{\min}$. Of course it would be desirable to take ϵ very small, since large values of ϵ cause poor values of the order parameter to be treated as accurate, but, on the other hand, reducing ϵ narrows the temperature range on which the Padé analysis will be made. A good compromise, which we have used throughout this paper, is $\epsilon = 10^{-5}$, which for M_1 and M_2 as above yields $J_{\min} = 0.14$.

We then determine Padé approximants for the logarithmic derivative of the magnetization

$$D(z) = \frac{d}{dz}\ln m(z), \tag{10}$$

where (as customary for low-temperature approaches)

$z = e^{-J}$ is a variable which vanishes at zero temperature and $m(z)$ is given by approximation M_1 (or M_2, if this is not very time-consuming), by requiring that, for a given pair of positive integers L and M,

$$[L,M](z_n) = D(z_n), \qquad z_n = \exp(J_{\min} + n\Delta J),$$

$$n = 0, 1, 2, \ldots, L + M. \quad (11)$$

The choice of ΔJ is constrained, since the above linear system becomes ill-conditioned as the interpolation points become too close, either in the z direction (ΔJ small) or in the $D(z)$ direction (ΔJ large). In Table I we report estimates of T_c and β obtained by unbiased $[L, M]$ approximants for $\Delta J = 0.03$. They indicate clearly that $T_c \simeq 9.79$ (a strong improvement with respect to the M_2 estimate) and $\beta \simeq 0.31$, which are in good agreement with the high-temperature expansion critical temperature and with $\beta = 0.3258 \pm 0.0044$ (Monte Carlo simulations for the simple cubic lattice, Ref. [8]) respectively. Different values of ΔJ in the neighborhood of 0.03 give similar results.

Once an estimate for T_c has been obtained, it can be used to construct biased approximants for the logarithmic derivative of the high-temperature susceptibility. In the disordered phase, we measure the accuracy of CVM approximations by means of $\delta c(J) = |c_1(J) - c_2(J)|$, where $c_k(J)$ is the NN correlation function $\langle s_i s_j \rangle$ as given by approximation M_k. Requiring $\delta c(J) < 10^{-5}$ for $J < J_{\max}$ we obtained $J_{\max} = 0.048$. $[L, M]$ approximants have then been determined for the function

$$\gamma^*(w) = (w_c - w)\frac{d}{dw}\ln\chi(w), \quad (12)$$

where $w = \tanh(J)$ and $\chi(w)$ is the uniform zero field magnetic susceptibility. The $L + M + 1$ interpolation points have been defined by $w_n = \tanh(J_{\max} - n\Delta J), n = 0, 1, \ldots, L + M$. For $\Delta J = 0.002$, all the $[L, M]$ approximants with $2 \le L \le 5$ and $L - 1 \le M \le L + 1$, except the $[2, 1]$ one, give $\gamma = 1.26$, a result which is not far from the best estimate $\gamma = 1.2390 \pm 0.0071$ (Monte Carlo simulations for the simple cubic lattice, Ref. [8]). A similar analysis on the specific heat gives some indication for $\alpha \simeq 0.14$, but data do not accumulate very well. It should also be noted that biasing approximants with the high-temperature expansion estimate for the critical temperature improves results for the critical exponents: one obtains $\beta \simeq 0.33$ and $\gamma \simeq 1.24$.

We have done a similar analysis for the simple cubic lattice, choosing for M_1 the well-known cube approximation and for M_2 an approximation (again to be described in a separate paper [6]) which uses as maximal clusters both the elementary cubes and the "stars" formed by one site surrounded by its six nearest neighbors, which is a straightforward generalization of the approximation used by Finel and de Fontaine [9] in their investigation of the two-dimensional axial next-nearest-neighbor Ising (ANNNI) model. $J_{\min}$ and $J_{\max}$ are 0.28 and 0.13, respectively. Low-temperature unbiased approximants indicate clearly $T_c \simeq 4.51$, in very good agreement with $T_c = 4.511\,424 \pm 0.000\,053$ (Monte Carlo simulations, Ref. [8]), while β is between 0.30 and 0.31. Biased approximants for β, however, are in favor of $\beta \simeq 0.31$. Results from biased high-temperature approximants for the susceptibility suggest $\gamma \simeq 1.24$.

TABLE I. (T_c,β) for the fcc Ising model (unbiased approximants, $J_{\min} = 0.14$, $\Delta J = 0.03$).

L	$[L, L-1]$	$[L, L]$	$[L, L+1]$
4	(9.75, 0.30)	(9.79, 0.31)	(9.78, 0.30)
5	(9.78, 0.31)	(9.78, 0.31)	(9.79, 0.31)
6	(9.78, 0.31)	(9.79, 0.31)	(9.79, 0.31)
7	(9.78, 0.31)	(9.79, 0.31)	(9.79, 0.31)
8	(9.79, 0.31)	(9.79, 0.31)	(9.79, 0.31)

In Table II we report results for two-dimensional lattices. In this case, due to the reduced dimensionality, the CVM is expected to be less accurate, but biasing the approximants with the exactly known critical temperature yields indeed very good results. We used the approximation B_{2N} proposed by Kikuchi and Brush [10] for the square lattice and a straightforward generalization of it for the triangular lattice, choosing $N = 3$ for M_1 and $N = 4$ for M_2.

Finally, we want to discuss two test applications of our method to surface problems. We have considered a semi-infinite Ising model with a (100) free surface and unmodified surface coupling, which is known [11] to exhibit a so-called *ordinary* transition, with the surface layer magnetization m_1 vanishing with an exponent β_1 which differs from the bulk exponent β and is estimated to be 0.78 ± 0.02 by Monte Carlo simulations [12] and 0.816 by second order ϵ expansion [13]. For this problem we have developed another CVM approximation (again described in detail in Ref. [6]), which we refer to as $4 \times N$, in which the semi-infinite system is approximated by a film of N layers, with the topmost layer representing the free surface, and the bottom layer constrained to the bulk, which in turn is studied in the cube approximation. In this system the maximal clusters for the CVM are chosen as those clusters with $4N$ sites, formed by a column of $N - 1$ elementary cubes. We used $N = 4$ for M_1 and $N = 5$ for M_2, obtaining $J_{\min} = 0.30$. Approximants biased with the previously determined bulk critical temperature for the simple cubic lattice indicate $\beta_1 \simeq 0.78$, in perfect agreement with Monte Carlo simulations.

Our last test application aims to illustrate that the CVM is not the unique classical approximation on which our method can be based. In particular, we have considered an approximation recently proposed by Lipowski and Suzuki [14] for two-dimensional systems (referred to as the LS approximation), which has been shown in Ref. [15] to yield the exact boundary magnetization of the square lattice Ising model. It is essentially a transfer matrix mean field approximation, where the boundary

TABLE II. Results for two-dimensional lattices (biased approximants, exact T_c).

Lattice	$J_{\min}$	β	$J_{\max}$	γ
Square	0.53	0.123	0.30	1.73
Triang.	0.35	0.125	0.17	1.74

magnetization is calculated by considering two strips of width N and $N-1$ with periodic boundary conditions along the infinite direction and applying the same effective field h_{eff} at one side of each strip, where h_{eff} is determined in such a way that the boundary magnetizations on the opposite sides of the strips be equal. The approximation is no more exact for more complicated models, but one can expect it to be quite accurate. We have applied it to the three-state Potts model in two dimensions, described by the Hamiltonian

$$\frac{\mathcal{H}}{k_B T} = -K \sum_{\langle ij \rangle} \delta_{s_i, s_j}. \tag{13}$$

We have taken $N = 4$ for M_1 and $N = 5$ for M_2 ($K_{\min} = 0.90$), and have estimated the boundary magnetization exponent β_1 using approximants biased with the exact critical temperature. Our results indicate clearly $\beta_1 \simeq 0.55$, in very good agreement with $\beta_1 = 5/9$, obtained combining Cardy's result $\beta_1 = \nu/(3\nu - 1)$ [16] with the conjecture $\nu = 5/6$, supported by many numerical results [17].

We have shown how quite accurate estimates of critical temperatures and critical exponents can be obtained by a Padé analysis of high- or low-temperature results of mean-field-like approximations, and especially of the cluster variation method. The method is quite simple (some analytical work can be needed to construct new CVM approximations, when necessary) and not at all time-consuming (all the calculations reported in this paper took a few hours of CPU time on a DEC Alpha machine), but nevertheless it yielded very satisfactory results in several test applications, also in surface problems. There are also several possible future developments, among which the calculation of critical amplitudes and the use of more sophisticated approximants like differential and partial differential approximants (the latter applying to the study of multicritical phenomena) are worth mentioning.

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