Quantitative study of the Kosterlitz-Thouless phase transition in a system of two-dimensional plane rotators (XY model): High-temperature expansions to order β^{20}

P. Butera and M. Comi
Istituto Nazionale di Fisica Nucleare, Dipartimento di Fisica, Università di Milano, Via Celoria 16, 20133 Milano, Italy
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High-temperature series expansions of the spin-spin correlation function for the plane rotator (or XY) model on the square lattice are extended by three terms through order β^{20}. Tables of the expansion coefficients are reported for the correlation function spherical moments of order $l = 0, 1, 2$. The expansion coefficients through β^{15} for the vorticity are also tabulated. Our analysis of the series supports the Kosterlitz-Thouless predictions on the structure of the critical singularities and leads to fairly accurate estimates of the critical parameters.

I. INTRODUCTION

The critical behavior of the two-dimensional (2D) plane rotator (or XY) model, has long been studied numerically by high-temperature expansions (HTE's),[1–3] by Hamiltonian strong-coupling expansions,[4] by Monte Carlo (MC) simulations,[5,6] and by other techniques. In spite of these considerable efforts, a really accurate verification of the Kosterlitz and Thouless (KT) theory[7,8] remained out of reach before recent technical advances such as the recent invention of MC algorithms with reduced critical slowing down,[10] the calculation of long high-temperature expansions, and the availability of a greater computing power. In the last few years many extensive numerical studies of an increasing accuracy have appeared,[9,11–15] part of which have been also stimulated by a challenge to the KT approach issued in Ref. 6. These works generally favor the essential singularity structure predicted by KT arguments over the power-law structure of usual critical phenomena. However, one more warning for caution on the actual scope and limits of MC results came from Ref. 13, reporting an exemplary analysis of a multigrid MC simulation and a critical review of previous MC works. This paper sets higher qualitative standards for future MC studies and, like Ref. 6, again questions the possibility of discriminating between the KT and the power-law scenarios, only by fits to MC data with the present level of accuracy and extension. On the other hand, we had stressed[9] that, even in the absence of a detailed rigorous theoretical treatment of the XY model, the general attitude in favor of the KT picture can be convincingly justified, already now, if all available numerical evidence both from the simulations and from the newly computed HTE's is properly taken into account.

Here we present a further extension (by three terms up to order β^{20}) and a new analysis of HTE's for the 2D plane rotator model on the square lattice. A HTE approach is always a necessary complement to the statistical simulations since it provides detailed and extensive information, but in this case it also improves significantly our chances to distinguish numerically between the KT and the power-law behaviors and leads us to exclude this latter possibility. Once the question concerning the nature of the critical singularity is settled, we can get reliable estimates of the critical parameters, although, in this case, perhaps less precise than it could be expected from series of such a length.

The paper is organized as follows: In Sec. II the definitions of the quantities that have been computed are briefly recalled and their HTE coefficients are tabulated. Section III is devoted to an analysis of the series by ratio extrapolation and by rational and differential approximants techniques. Section IV contains some discussion of previous work and our conclusions.

II. HIGH-TEMPERATURE SERIES

The Hamiltonian of the two-dimensional plane rotator (or XY) model is

$$H\{s\} = -\sum_{x} \sum_{\mu=1,2} s(x) \cdot s(x+e_\mu). \tag{1}$$

Here $s(x)$ is a two-component classical spin of unit length associated to the site with position vector $x = n_1 e_1 + n_2 e_2 = (n_1, n_2)$ of a two-dimensional square lattice, and e_1, e_2 are the two elementary lattice vectors. The sum over x extends over all lattice sites.

Our series have been computed by a FORTRAN code which solves iteratively the Schwinger-Dyson equations for the correlation functions.[9,16,17] The algorithm has been described in full detail in Ref. 9. Here it is enough to mention that we have computed the HTE coefficients of the two-point correlation function

$$C(x;\beta) = \langle s(0) \cdot s(x) \rangle \tag{2}$$

for the 120 inequivalent sites x for which the expansion is nontrivial to order β^{20}. In this approach the main obstacle to a further extension of our results is not computational time which is still definitely modest (of the order of 20 h for a 3500 VAX station), but the increasing demand of fast memory. Our work has been made

TABLE I. HTE coefficients of the nearest-neighbor correlation $C(0,x)$ with $x=(0,1)$.

Order	Coefficient
1	0.500000000000000000000000000000
3	0.187500000000000000000000000000
5	0.010416666666666666666666666666
7	-0.005045572916666666666666666666
9	-0.011897786458333333333333333333
11	-0.009914482964409722222222222222
13	-0.006428721594432043650793650793
15	-0.003556433509266565716455853174
17	-0.001900080568517583644836294214
19	-0.000804827256075995542618566322

TABLE III. HTE coefficients of the next-nearest-neighbor correlation $C(0,x)$ with $x=(1,1)$.

Order	Coefficient
2	0.500000000000000000000000000000
4	0.125000000000000000000000000000
6	0.005208333333333333333333333333
8	-0.012695312500000000000000000000
10	-0.016959635416666666666666666666
12	-0.012420654296875000000000000000
14	-0.007721207633851066468253968253
16	-0.004255058809562965675636574074
18	-0.002158290178150189710135275818
20	-0.000850845285942630162314763144

possible by a laborious segmentation of the computing procedure.

The object of our analysis are the series for the spherical moments of the correlation function $m^{(l)}(\beta)$ defined as follows:

$$m^{(l)}(\beta)=\sum_{x}|x|^{l}C(x;\beta)=\sum_{r=1}^{\infty}a_{r}^{(l)}\beta^{r} \tag{3}$$

(here $|x|=\sqrt{n_1^2+n_2^2}$), $l\geq 0$, and the sum extends over all lattice sites. The zeroth-order spherical moment $m^{(0)}(\beta)$ is also called (reduced) susceptibility and denoted by $\chi(\beta)$. The data we are presenting augment significantly our earlier work.[9]

In Tables I, II, and III we have reported the HTE coefficients through β^{20} of the spin-spin correlation functions $\langle s(0)\cdot s(x)\rangle$ with $x=(1,0)$, $x=(2,0)$, and $x=(1,1)$, respectively.

In Tables IV, V, and VI we have reported the expansion coefficients for the moments $m^{(l)}(\beta)$ with $l=0$, 1, 2.

In Table VII we have reported the HTE coefficients through β^{15} of the expectation value of the squared vorticity $v(\beta)^2$, a quantity built in terms of two-, three-, and four-spin correlation functions[18] which probes the vortex pair dissociation mechanism of the phase transition. In the definition of the vorticity it is convenient to refer to the representation $s(x)=(\cos\theta(x),\sin\theta(x))$, and then we have

$$\begin{aligned}\langle v(\beta)^2\rangle=\frac{1}{3}&+\frac{4}{\pi^2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n^2}\langle e^{in(\theta_1-\theta_2)}\rangle\\&-\frac{2}{\pi^2}\sum_{n,m\neq 0}\frac{(-1)^{n+m}}{nm}\langle e^{in(\theta_1-\theta_2)+im(\theta_2-\theta_3)}\rangle\\&-\frac{1}{\pi^2}\sum_{n,m\neq 0}\frac{(-1)^{n+m}}{nm}\langle e^{in(\theta_1-\theta_2)+im(\theta_3-\theta_4)}\rangle.\end{aligned} \tag{4}$$

Here $\theta_1,\theta_2,\theta_3,\theta_4$ are the angular variables associated with the four sites defining an elementary square on the lattice. We shall only tabulate this series, since it has already been extensively discussed in Ref. 18, where our HTE has been compared to a Langevin simulation.

Finally, we remind the interested reader that a list of the presently available HT data for this model also includes a series[9] through β^{12} for the "true correlation length"[20] and a series through β^{14} for $\chi^{(4)}(\beta)$, the sec-

TABLE II. HTE coefficients of the next-nearest-neighbor correlation $C(0,x)$ with $x=(0,2)$.

Order	Coefficient
2	0.2500000000000000000000000000000
4	0.3125000000000000000000000000000
6	0.0455729166666666666666666666666
8	-0.0239257812500000000000000000000
10	-0.0236504448784722222222222222222
12	-0.0180172390407986111111111111111
14	-0.0109599196721637059771825396825
16	-0.00643771678156743394424465388007
18	-0.00331282301929834284736622835219
20	-0.00150452549535034334988961284262

TABLE IV. HTE coefficients of the susceptibility $m^{(0)}$.

Order	Coefficient
0	1.000000000000000000000000
1	2.000000000000000000000000
2	3.000000000000000000000000
3	4.250000000000000000000000
4	5.500000000000000000000000
5	6.854166666666666666666667
6	8.265625000000000000000000
7	9.722005208333333333333333
8	11.205078125000000000000000
9	12.675553385416666666666667
10	14.152012803819444444444444
11	15.601900227864583333333333
12	17.019300672743055555555556
13	18.392466299874441964285714
14	19.714506515624031187996032
15	20.971455838629808375444362
16	22.163650634196279751140184
17	23.280944825182959960064373
18	24.320568285114725921379686
19	25.279185763955802490448171
20	26.153731926768238512226443

TABLE V. HTE coefficients of the first correlation moment $m^{(1)}$.

Order	Coefficient
0	0.000000000000000000000000
1	2.000000000000000000000000
2	4.828427124746190097603377
3	8.958203932499369089227521
4	14.774302788642591334803698
5	22.405537350785873843406389
6	32.018311604539175300778647
7	43.776633965886723037276578
8	57.804795726728279225339368
9	74.171223440617174956388203
10	92.948162559177956624043786
11	114.170878181118055761226873
12	137.820848184699262000940865
13	163.889685030219313242632769
14	192.312469972536223823702791
15	223.008032736766111405219191
16	255.881465307579934186740726
17	290.805253343564738390269085
18	327.634680720388208255919862
19	366.217176852355184083122429
20	406.375299064909623959197097

ond derivative of the susceptibility with respect to the magnetic field at zero field.[19]

III. ANALYSIS OF THE HT SERIES

In this section we present the estimates of the critical parameters obtained by simple methods of series analysis[9,21–23] which, after some numerical experimenting both with appropriate model series and with our series, turned out to be best suited for extracting the expected behavior of the correlation moments in the critical region.

TABLE VI. HTE coefficients of the second correlation moment $m^{(2)}$.

Order	Coefficient
0	0.0000000000000000000000000
1	2.0000000000000000000000000
2	8.0000000000000000000000000
3	20.2500000000000000000000000
4	42.0000000000000000000000000
5	76.8541666666666666666666666
6	129.020833333333333333333333
7	203.222005208333333333333333
8	304.671875000000000000000000
9	438.956803385416666666666666
10	612.005447048611111111111111
11	830.037403700086805555555556
12	1099.39771050347222222222222
13	1426.589506772964719742063492
14	1818.089718954903738839285714
15	2280.298322941197289360894097
16	2819.491738309136984419780644
17	3441.674843107074259683802248
18	4152.534972385628279951911521
19	4957.398607418558360103903951
20	5861.100409957330553479786132

TABLE VII. HTE coefficients of the expectation of the squared vorticity $\langle v(\beta)^2 \rangle$.

Order	Coefficient
0	0.33333333333333333333333333333333
1	-0.20264236728467554288775892641946
2	-0.13931662750821443573533426191338
3	-0.00093815910779942380966555058527
4	-0.01391846988836801417621000438623
5	0.02145616787492672223895597466054
6	0.00395517130108460209757177042318
7	0.00626571732016345480145945834089
8	0.00498164199972076876178153427788
9	0.00188487896531662245169702329601
10	0.00506374324797059743179508168123
11	-0.00016501166685598670821344313122
12	0.00321456708015923485554342658920
13	-0.00038482795295650133767225429558
14	0.00167133027095100840999836256202
15	-0.00028727125412299355443537746859

Let us first recall briefly the main results of the nonrigorous renormalization-group analysis of the plane rotator model.[7,8]

The correlation length $\xi(\beta)$ is expected to diverge as $\beta \uparrow \beta_c$ with the unusual singularity

$$\xi(\beta) \propto \xi_{as}(\beta) = \exp\left(\frac{b}{\tau^{\sigma}}\right)[1 + O(\tau)], \qquad (5)$$

where $\tau = \beta_c - \beta$.

The value of the exponent σ predicted in Ref. 7 is $\sigma = 1/2$ and b is a nonuniversal positive constant.

At the critical temperature, the asymptotic behavior of the two-spin correlation function as $r = |x| \to \infty$ is expected to be

$$\langle s(0) \cdot s(x) \rangle \propto \frac{[\ln(r)]^{2\theta}}{r^{\eta}}[1 + O(\ln[\ln(r)]/\ln(r))]. \qquad (6)$$

The values predicted[7,24] for η and θ are, respectively, $\eta = 1/4$, $\theta = 1/16$.

From Eqs. (5) and (6) it follows that, for $l > \eta - 2$, the correlation moment $m^{(l)}(\beta)$ should diverge as $\beta \uparrow \beta_c$ with the singularity

$$m^{(l)}(\beta) \propto \tau^{-\theta} \xi_{as}(\beta)^{2-\eta+l}[1 + O(\tau^{\frac{1}{2}} \ln(\tau))]. \qquad (7)$$

At β_c a line of critical points should begin which extends to $\beta = \infty$, so that for $\beta > \beta_c$ both ξ and the correlation moments remain infinite.

Finally, we must recall that the existence of a transition of the system from a vortex-dominated high-temperature phase to a spin-wave low-temperature phase has been proved[25] and that the lower bound $\beta_c \geq \ln(1 + \sqrt{2}) \approx 0.88$ has been established[26] for the critical inverse temperature.

In Ref. 9 we used a theorem of Darboux[27] to point out that the leading asymptotic behavior for large order of the HTE coefficients of ξ (and of the correlation moments) may be estimated by saddle-point approximation of a contour integral, if it is determined by the singularity (5). Consider, for example, $\xi(\beta) = \sum_n c_n\beta^n$; then, for large n, we have

$$c_n = \frac{1}{2\pi i}\oint \xi(\beta)\frac{d\beta}{\beta^{n+1}} \propto \frac{1}{2\pi i}\oint \xi_{as}(\beta)\frac{d\beta}{\beta^{n+1}}. \quad (8)$$

For general $b, \sigma > 0$, the following asymptotic expression is obtained:[9]

$$c_n \propto \beta_c^{-n-1}\exp[B(n+1)^{\sigma\epsilon} + O(n^{(\sigma-1)\epsilon})], \quad (9)$$

with

$$\epsilon = \frac{1}{1+\sigma} \quad \text{and} \quad B = \frac{(\sigma+1)b^\epsilon}{(\sigma\beta_c)^{\sigma\epsilon}}. \quad (10)$$

Therefore for the ratios of the successive HTE coefficients $r_n(\xi) = c_n/c_{n+1}$ we have

$$r_n(\xi) = \beta_c + \frac{C}{(n+1)^\epsilon} + O(1/n^\lambda), \quad (11)$$

with $C = -(\sigma b\beta_c)^\epsilon$ and $\lambda = \min(1, 2\epsilon)$. A similar formula is valid for the ratios $r_n(m^{(l)}) = a_n^{(l)}/a_{n+1}^{(l)}$ of the successive HTE coefficients of the correlation moment $m^{(l)}(\beta)$ if C is replaced by $C_l = -[(2-\eta+l)\sigma b\beta_c]^\epsilon$. The correction terms $O(1/n^\lambda)$ in (11) also account for the subdominant singularities in (5). According to the KT prediction we should have $\epsilon = 2/3$. This is a neat signature of the KT singularity in the HTE approach.

On the other hand, if, instead of (5) and (7), we had conventional power-law critical singularities so that, as $\beta \uparrow \beta_c$,

$$m^{(l)}(\beta) \sim \tau^{-\gamma-l\nu}[A_l + B_l\tau^\Delta + \cdots], \quad (12)$$

where $\Delta > 0$ and, as usual, γ and ν denote the susceptibility and the correlation length exponents, respectively, we would obtain a formula analogous to Eq. (11) with $\epsilon = 1$ and $\lambda = 1 + \Delta$, namely,

$$r_n(m^{(l)}) = \beta_c + \frac{\beta_c(1-\gamma-l\nu)}{n} + O(1/n^{1+\Delta}). \quad (13)$$

A complication for the series analysis is due to the occurrence of an antiferromagnetic singularity at $-\beta_c$ which is typical of loose lattices. It should, however, affect only the higher correction terms in (11) [or in (13)], usually introducing oscillations in the ratio plots. A simple prescription to reduce this inconvenience in numerical extrapolations consists in studying the ratios of alternate coefficients, for example, $\bar{r}_n(m^{(l)}) = \sqrt{a_{n-1}^{(l)}/a_{n+1}^{(l)}}$ instead of the usual ratios $r_n(m^{(l)}) = a_n^{(l)}/a_{n+1}^{(l)}$.

In view of the above considerations consistent evidence that $\sigma \neq 0$ is evidence against simple power-law behavior and therefore our analysis should begin by trying to estimate σ or, equivalently, ϵ.

Let us first perform the simplest tests on the ratio sequences.

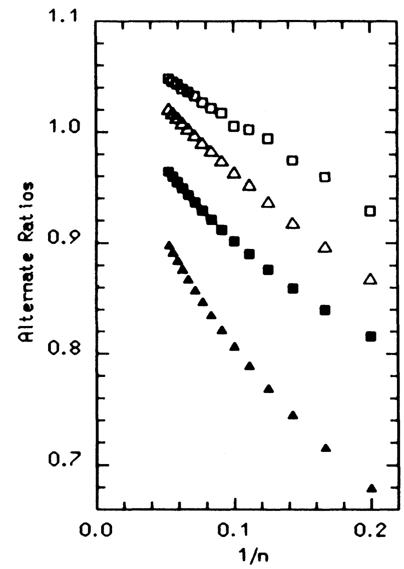

FIG. 1. Alternate ratios of HTE coefficients of various moments are plotted vs $1/n$. The alternate ratios $\bar{r}_n(\chi)$ are represented by solid squares, $\bar{r}_n(m^{(1)})$ by solid triangles. We have also plotted the linearly extrapolated sequences $\bar{r}_n^{(1)}(\chi)$ (open squares) and $\bar{r}_n^{(1)}(m^{(1)})$ (open triangles).

In Fig. 1 we have plotted vs $1/n$ the sequences of alternate ratios $\bar{r}_n(m^{(l)})$ for $l = 0, 1, 2$. These ratio plots exhibit a sizable curvature and an increasing slope for large n. If Eq. (13) were an adequate representation of the asymptotic behavior of $\bar{r}_n(m^{(l)})$, we should be able to suppress the $O(1/n)$ terms in (13) by forming the linearly extrapolated sequences

$$\bar{r}_n^{(1)}(m^{(l)}) = n\bar{r}_n(m^{(l)}) - (n-1)\bar{r}_{n-1}(m^{(l)}) = \beta_c + O(1/n^{1+\Delta}), \quad (14)$$

which, for large n, should approach with vanishing slope their common limit β_c. However, this does not happen, as is shown in Fig. 1, where we have also plotted the extrapolated sequences $\bar{r}_n^{(1)}(m^{(l)})$ vs $1/n$. The estimates of β_c thus obtained are still rapidly increasing with order.

Still under the assumption of power-law critical singularities, we might also compute a sequence of (unbiased) estimates of $\gamma + l\nu$ by the formula

$$(\gamma + l\nu)_n = \frac{(n-1)^2\bar{r}_n(m^{(l)}) - n(n-2)\bar{r}_{n-1}(m^{(l)})}{n\bar{r}_{n-1}(m^{(l)}) - (n-1)\bar{r}_n(m^{(l)})}. \quad (15)$$

We have reported the sequences of estimates so obtained for γ and $\gamma + \nu$ vs $1/n$ in Fig. 2. If any conclusion at all may be drawn from these standard computations it is that, under the assumption of power-law scaling, a ratio analysis might suggest that $\beta_c > 1.06$, $\gamma > 2.9$, and $\gamma + \nu > 4$. The simplest extrapolations would suggest $\beta_c > 1.09$, $\gamma > 3.4$, and $\gamma + \nu > 4.8$. As we shall discuss later, these estimates are inconsistent with the significantly smaller estimates resulting from fits of MC

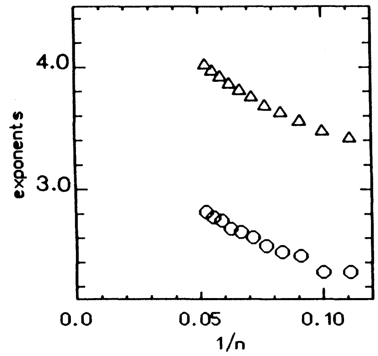

FIG. 2. Unbiased estimates of the critical exponent γ of the susceptibility under the assumption of a power-law critical singularity obtained from the alternate ratios $\bar{r}_n(\chi)$ (open circles). Analogous estimates of the exponent $\gamma+\nu$ as obtained from $\bar{r}_n(m^{(1)})$ (open triangles).

data to power-law critical behavior.

Let us observe now that, if Eq. (11) is valid instead of Eq. (13), then by reporting the $\bar{r}_n(m^{(l)})$ sequences versus $1/n^{2/3}$, we should obtain nicely straight plots. Figure 3 appears to be a convincing illustration of this statement. The next obvious step of suppressing the $O(1/n^{2/3})$ terms in the sequences $\bar{r}_n(m^{(l)})$ by forming the (nonlinearly) extrapolated sequences

$$\bar{s}_n(m^{(l)}) = \frac{n^{2/3}\bar{r}_n(m^{(l)}) - (n-2)^{2/3}\bar{r}_{n-2}(m^{(l)})}{n^{2/3}-(n-2)^{2/3}} = \beta_c + O(1/n) \quad (16)$$

does not result in a sequence regular enough to warrant a further extrapolation in $1/n$ and therefore a more precise estimate of β_c. We have, however, computed also the linearly extrapolated sequence $\bar{s}_n^{(1)}(m^{(l)})$ and reported the results in Fig. 3. From these we can infer that $\beta_c = 1.120 \pm 0.005$. A possible improvement of this procedure should be based on Euler-transformed moment series, as we have discussed at length in Ref. 9, where the results and the conclusions of this kind of analysis on a shorter series can be found. Since this procedure might be questioned,[22] we will not insist on the details here.

We can give a direct unbiased estimate of ϵ in terms of ratios as follows. Introduce the quantity

$$t_n = \frac{\bar{r}_n(\chi^2)}{\bar{r}_n(\chi)}; \quad (17)$$

then, if the ratios $\bar{r}_n(\chi)$ and $\bar{r}_n(\chi^2)$ have the asymptotic behavior (11), the sequence

$$\epsilon_n = n \ln\left(\frac{t_n - 1}{t_{n+1} - 1}\right) \quad (18)$$

will provide estimates of ϵ. Quantities u_n and v_n analogous to t_n may be defined in terms of the moments $m^{(1)}$ and $m^{(2)}$ and their squares, and, via Eq. (18), the corresponding sequences ϵ_n' and ϵ_n'' may be formed. All these sequences have been plotted vs $1/n$ in Fig. 4. They are slightly irregular so that it is not easy to get precise extrapolations to $n=\infty$. The figure, however, clearly sug-

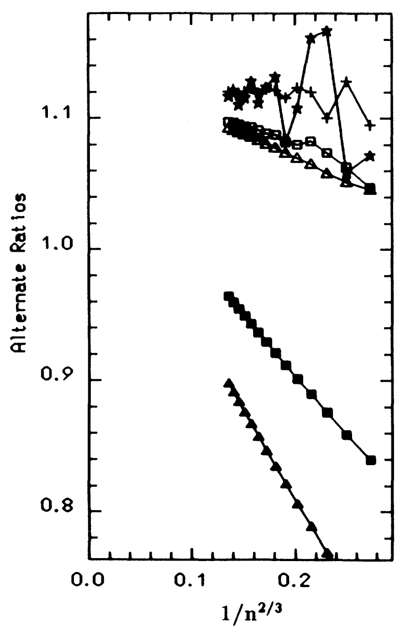

FIG. 3. Ratio plots for alternate HTE coefficients vs $1/n^{2/3}$. The alternate ratios $\bar{r}_n(\chi)$ are represented by solid squares, $\bar{r}_n(m^{(1)})$ by solid triangles. The alternate ratio sequences have been extrapolated in $1/n^{2/3}$ obtaining the sequences $\bar{s}_n(\chi)$ (open squares), $\bar{s}_n(m^{(1)})$ (open triangles). A further extrapolation in $1/n$ of the sequences s_n gives $\bar{s}_n^{(1)}(\chi)$ (stars), $\bar{s}_n^{(1)}(m^{(1)})$ (crosses).

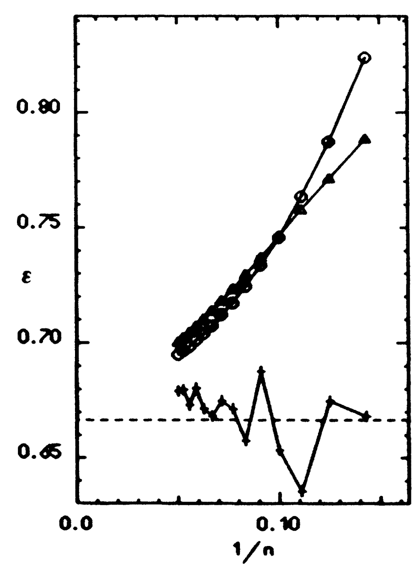

FIG. 4. Sequences ϵ_n (crosses), ϵ_n' (open triangles), ϵ_n'' (open circles), as computed from the quantities t_n introduced in (17), and from the analogous ones u_n and v_n, are plotted vs $\frac{1}{n}$. The dashed line indicates the KT prediction for the value of ϵ.

gests that the sequences have a common limiting value somewhere around 0.67. This result definitely excludes a power-law singularity (in that case, of course, the limiting value should be 1) and compares very nicely with the KT prediction $\epsilon = 2/3$.

Other prescriptions to compute ϵ, as well as to obtain a first estimate of the exponent θ, involve Padé approximants (PA's).

Before entering into the PA analysis, let us recall that PA's are known to converge well to (locally) meromorphic analytic functions. In order to take advantage of this property, it would be convenient to work with suitable functions of the given HT series for which the critical singularity is a simple pole. Because of the structures (5) and (7), this is not possible in general, and, at best, one can form functions of the HT series having a simple pole accompanied by subdominant confluent singularities. As a consequence, whenever high-precision estimates are pursued from expansions of limited length, one should keep in mind that the convergence properties and the accuracy of the PA estimates may be different, not only for different quantities, but also for different functions of the same quantity, according to the nature and relative strength of the subdominant singularities. For instance, estimates of β_c or σ obtained from different moments (or different functions of the same moment) may differ more than the (statistical) quantity (see below) we shall adopt as an estimate of the error. In order to reduce this "systematical" error in the analysis, one should resort to differential approximants (DA's), a natural generalization[23] of the rational approximants which, unlike PA's, can make allowance numerically for the confluent subdominant singularities. Occasionally, we have also computed DA's, restricting for simplicity to first-order inhomogeneous DA's. These are probably not flexible enough, so that only partial improvements are gained and therefore the analysis ought to be properly extended to second-order DA's.

One should also note that it is necessary to analyze various moments in order to compute all critical parameters of interest, but not all moments (at a given fixed order of HTE) are expected to be equally reliable. Indeed, for higher values of l, the moment $m^{(l)}(\beta)$ receives a larger contribution from correlations between distant spins for which a smaller number of HTE coefficients is available, so that it might be slower in reaching the asymptotic regime. In this connection we have also explored the consequences of a prescription of least sensitivity of the results to the choice of l. As we shall discuss later, in an estimate of the critical exponent η which involves two different moments, it seems convenient to use $m^{(0)}(\beta)$ and another moment $m^{(l)}(\beta)$ with small l chosen such that the estimate of η is stationary in l.

Let us now specify our way of presenting the results.

Given the first $n+1$ terms of a power series in β, we will form all $[N/D]$ PA's with $N+D \leq n$. We will always take $N, D \geq 5$. The quantities of interest for each approximant, such as the location of the "critical" pole, the residue at that pole, or simply the value at β_c of the PA, will be displayed in a triangular array, denoted as a Padé table, with N labeling the columns and D the rows. Whenever some entry is followed by an asterisk ("defective entry") we will mean that there might be convergence problems indicated by the presence in the corresponding approximant of more than a single pole in the range $0 \leq \beta \leq 1.2\beta_c$ or in a narrow complex strip containing this segment. A blank is left in the table whenever no value in the numerical range of interest exists for the corresponding approximant.

The indications coming from a PA analysis using $n+1$ coefficients will be summarized by an estimate, obtained by averaging over a "sample" including all nondefective entries of the PA table with $N, D \geq 5$ and $n-2 \leq N+D \leq n$ and qualified by a conventional "error," defined as twice the standard deviation of the mean value. Whenever, for sufficiently large $N+D$, the entries of the PA table are not too scattered and the successive averages show no residual trend, these are sensible definitions which may be slightly refined by excluding from our sample occasional entries differing from the mean more than 5 standard deviations and then recomputing the mean value and the standard deviation on the smaller sample. Sometimes we shall find it suggestive to visualize by a histogram the spread of the entries of a Padé table.

Let us now evaluate ϵ by a Padé technique.

Computing the PA's to $D\ln[\ln(\chi)/\beta]$, the logarithmic derivative of $\ln(\chi)/\beta$ should enable us to discriminate between the structures (7) and (12) of the critical singu-

TABLE VIII. Location of the critical poles of the PA's to $D\ln[\ln(\chi)/\beta]$. The degree N of the PA numerator labels the columns, and the degree D of the denominator labels the rows. Asterisks indicate the "defective entries"; blanks indicate the lack of an acceptable entry.

D	N 5	6	7	8	9	10	11	12	13
5	1.1408	1.1277	1.1129		1.1312	1.1319*	1.1029	1.1087	1.1133
6	1.1476*		1.1193	1.1261	1.1169	1.1231	1.1094	1.0996*	
7		1.1431	1.1225	1.1223	1.1219	1.1202	1.1174		
8	1.1142	1.1271	1.1223*	1.1226*	1.1225*	1.1116			
9	1.1208	1.1242	1.1218	1.1225*	1.1225*				
10	1.1265	1.1233	1.1375*	1.1029*					
11	1.1185	1.1218	1.1068*						
12	1.1236	1.1208							
13	1.1611*								

TABLE IX. Residues at the critical poles of the PA's to $D\ln[\ln(\chi)/\beta]$. Same conventions as in the previous table.

D	N 5	6	7	8	9	10	11	12	13
5	0.611	0.563	0.504		0.596	0.600*	0.420	0.458	0.488
6	0.630*		0.531	0.564	0.516	0.549	0.463	0.400*	
7		0.620	0.545	0.545	0.542	0.533	0.516		
8	0.512	0.567	0.545*	0.546*	0.545*	0.470			
9	0.540	0.554	0.542	0.545*	0.546*				
10	0.566	0.550	0.549*	0.364*					
11	0.526	0.543	0.408*						
12	0.553	0.537							
13	0.740*								

larity, since the residues at the critical poles have either to approach σ, if (7) holds, or to vanish, if (12) holds.

Table VIII is the Padé table for the location of the critical pole of the approximants to $D\ln[\ln(\chi)/\beta]$, and Table IX is the Padé table for the residues. From this (unbiased) analysis we get the estimates $\beta_c = 1.118 \pm 0.003$ and $\sigma = 0.52 \pm 0.03$.

By a similar argument it should be convenient to study the residue at the critical pole for the PA's to $D\ln[D\ln(\chi)]$, the double-logarithmic derivative of $\chi(\beta)$. The residue should tend either to 1, if (12) holds, or to $1+\sigma$, if (7) holds.

In this case, however, the convergence is less good, probably due to subdominant singularities stronger than in the previous case, but again the KT structure is clearly favored. We find $\beta_c = 1.114 \pm 0.0035$ and $\sigma = 0.4 \pm 0.02$. We can try to reduce the influence of the confluent singularities by a simple modification of this analysis, namely, by computing PA's to $\tau D\ln[\tau D\ln(\chi)]$ at $\beta = \beta_c$. Of course, this is a biased test since a previous knowledge of β_c is required. If we take $\beta_c = 1.118$, we get $\sigma = 0.48 \pm 0.03$, in good agreement with the results obtained from the study of $D\ln[\ln(\chi)/\beta]$. Repeating these tests on higher-order moments we get consistent results although with slightly higher central values for β_c. For instance, a study of $D\ln[\ln(1+m^{(1)})/\beta]$ yields $\beta_c = 1.127 \pm 0.005$ and $\sigma = 0.55 \pm 0.03$; however, the successive averages show a residual decreasing trend.

Another simple (biased) test of the singularity structure (7) is performed by computing the quantity

$$T(\chi) = \frac{D\ln[D\chi(\beta)]}{D\ln[\chi(\beta)]} \tag{19}$$

or analogous quantities formed from other correlation moments. If $\chi(\beta)$ has the KT singularity structure (7), then, as $\beta \uparrow \beta_c$, we find $T(\chi) = 1 + O(\tau^\sigma)$. If, on the contrary, $\chi(\beta)$ has a power-law singularity, then $T(\chi) = 1 + \frac{1}{\gamma} + O(\tau)$. We can therefore distinguish the two cases by evaluating PA's of $T(\chi)$ at the critical inverse temperature β_c and thus obtaining some "effective value" for γ. We have taken $\beta_c = 1.118$. The histogram in Fig. 5 shows the distribution of the values of $\frac{1}{T-1}$ in the PA table. Analogously computing $T(m^{(1)})$ we can obtain an "effective value" for $\gamma+\nu$. The results of this computation are also reported in Fig. 5 as a hatched histogram. The data suggest that $\gamma > 4.5$ and $\gamma+\nu > 6.5$, showing complete consistency with the indications from the ratio tests. These conclusions remain essentially unmodified if we evaluate $T(\chi)$ and $T(m^{(1)})$ at the smaller value $\beta_c = 1.09$ which, under the assumption of power-law behavior, seems to be indicated by ratio extrapolations and by PA's to the logarithmic derivative of $\chi(\beta)$ (see below). Finally, taking the value $\beta_c = 1.01$, as indicated by a recent power-law fit to MC data,[6,13] yields $\gamma > 3.5$ and $\gamma+\nu > 6.5$. Needless to mention, we may also compute $T(\ln(\chi))$ or $T(D\ln(\chi))$ and check that $\ln(\chi)$ [respectively $D\ln(\chi)$] exhibit the power singularities expected from (7).

Another biased computation which gives fairly good estimates for some critical parameters is the following. Let us fix a value for the constant σ' and compute PA's for the quantity

$$[\ln(\chi)/\beta]^{1/\sigma'} = \left(\frac{(2-\eta)b}{\beta_c\tau^\sigma}\right)^{1/\sigma'} [1 + O(\tau^\sigma \ln(\tau))] \tag{20}$$

under the assumption (7).

We have varied σ' in small steps from 0.49 to 0.51. The results are summarized in Fig. 6 showing how the estimate of β_c depends on σ'. By the same procedure we

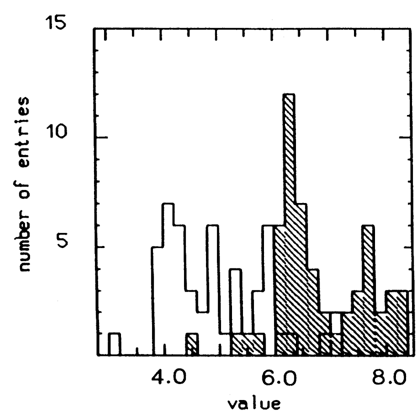

FIG. 5. Distribution of the values in the PA table of the quantity $[T(\chi)-1]^{-1}(\beta_c)$ defined by (19) (unhatched histogram). The same for the quantity $[T(m^{(1)})-1]^{-1}(\beta_c)$ (hatched histogram).

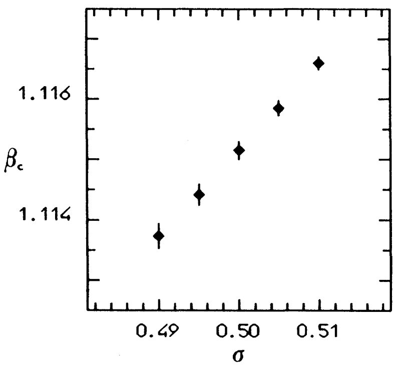

FIG. 6. Estimates of the inverse critical temperature β_c, obtained from a study of the "critical pole" of the PA's to $(\frac{\ln(\chi)}{\beta})^{\frac{1}{\sigma'}}$, are plotted vs σ'.

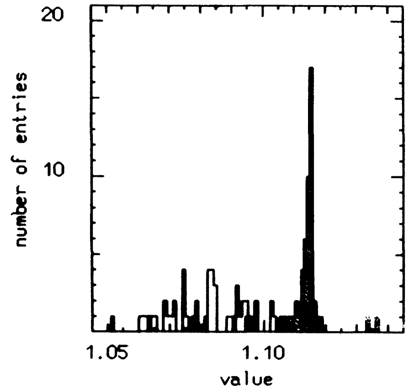

FIG. 7. Histogram of the distribution of the values of β_c in the table of PA's to $D\ln(\chi)$ ($N, D \geq 5$ and $N+D \leq 19$) with a resolution of 10^{-3}. For contrast the narrow distribution of the values of β_c in the PA table for $[\ln(\chi)/\beta]^2$ is also reported (hatched histogram on the right).

may get the quantity $(2-\eta)b$ as a function of σ' from the residue at the critical pole of the PA's. For the particular value $\sigma' = 1/2$, the PA table for the position of the critical singularity is reported as Table X. The distribution of the values of β_c in the PA table is displayed in the histogram of Fig. 7. The values of b computed from the residues at the poles (assuming moreover $\eta = 1/4$) are reported in Table XI. From this analysis final estimates for β_c and b are $\beta_c = 1.1151 + 0.14(\sigma' - 0.5) \pm 0.0002$ and $b = 1.672 - 3.4(\sigma' - 0.5) \pm 0.004$.

If we assume a power-law singularity such as in (12), from a study of the PA's to the logarithmic derivative of the susceptibility $D\ln(\chi)$, we should be able to estimate β_c, and from their residues, the critical exponent γ. As we have already discussed,[9] both the PA tables for the poles and for the residues (which we shall not report) contain many "defective entries" or blanks and do not show a good convergence. These features of the approximants suggest that the critical singularity is not a power. If we insist in producing anyway some estimate of the critical parameters, then, by averaging over all relevant entries of the PA tables for the poles and residues of the approximants to $D\ln(\chi)$ with $18 \leq N + D \leq 19$, we get $\beta_c = 1.08 \pm 0.02$ and $\gamma = 4.1 \pm 0.6$. Analogously by studying the PA's of $D\ln(m^{(2)}/m^{(1)})$, we get the estimates $\beta_c = 1.07 \pm 0.01$ and $\nu = 2.2 \pm 0.1$. These estimates are consistent with those obtained from ratio tests and from a study of $T(\chi)$ and $T(m^{(1)})$ but not with those obtained from recent power-law fits to MC data.[6,13] A histogram showing the broad distribution of the values of β_c in the PA table for $D\ln(\chi)$ is reported in Fig. 7. Note the contrast with the very narrow distribution of the values of β_c in the PA table for $[\ln(\chi)/\beta]^2$ displayed (as a hatched histogram) in the same figure.

The critical index η governing the large distance behavior of spin-spin correlation functions may be estimated observing that, by Eqs. (5) and (7),

$$2 - \eta = d\ln(\chi)/d\ln(m^{(2)}/m^{(1)}) \tag{21}$$

at $\beta = \beta_c$. Taking $\beta_c = 1.118$ yields $\eta = 0.293 \pm 0.015$, which is not too far from the value predicted by KT. A similar quantity has also been computed by MC simulations[11,14] in the range $0.73 < \beta < 0.94$, obtaining results completely consistent with ours. The exponent η may also be computed from PA's to the ratio

$$L(\beta, l) = \frac{\ln(\chi)}{\ln(1 + m^{(l)})} = \frac{2-\eta}{2-\eta+l} + O(\tau^{\sigma}\ln(\tau)). \tag{22}$$

We have taken $\beta_c = 1.118$ and have repeated the com-

TABLE X. Location of the critical poles of the PA's to $[\ln(\chi)/\beta]^2$. Same conventions as in the previous table.

D \ N	5	6	7	8	9	10	11	12	13	14
5		1.1088	1.1105	1.1106			1.1167	1.1154	1.1149	1.1149
6	1.1152	1.1132	1.1119	1.1079*		1.0811*	1.1151	1.1140	1.1149	
7	1.1136	1.0901*	1.1127	1.0944*	1.1091	1.1128	1.1145	1.1148		
8	1.1128	1.1130	1.1136	1.1153	1.1160	1.1155	1.1154			
9	1.1130	1.1127*	1.1059*	1.1164	1.1157	1.1154				
10	1.1142	1.1189*	1.1148	1.1147	1.1155					
11	1.1155	1.1155	1.1147	1.1148						
12	1.1155	1.1155	1.1152							
13	1.1173*	1.1151								
14	1.1157									

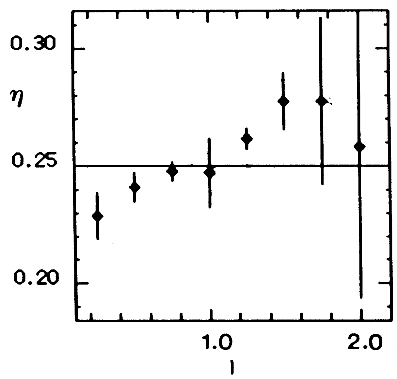

FIG. 8. Estimates of the exponent η obtained from the quantity $L(\beta_c, l)$ of Eq. (22) are plotted vs l for $\beta_c = 1.118$. The solid line indicates the KT prediction for the value of η.

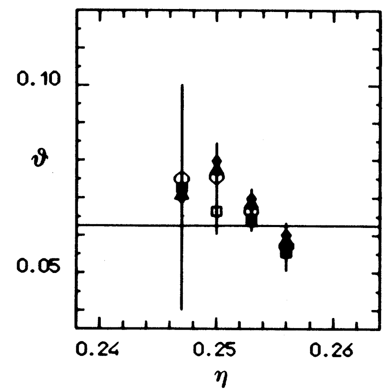

FIG. 9. Estimates (biased in η and β_c) of the exponent θ as computed from the quantity $\theta(\beta, \eta)$ defined in (24) are plotted vs η for various values of β_c: $\beta_c = 1.112$ (squares), $\beta_c = 1.115$ (triangles), $\beta_c = 1.118$ (triangles), $\beta_c = 1.121$ (rhombuses). The continuous line indicates the KT prediction for the value of θ.

putation for closely spaced values of l in the range [1/4, 7/4]. The estimates so obtained have been plotted vs l in Fig. 8. Since the results should not depend on l, it is reasonable to expect that the stationary value of $L(\beta_c, l)$ with respect to l is the best value of η. This gives $\eta = 0.27 \pm 0.02$.

Finally let us discuss briefly the small power correction $\tau^{-\theta}$ to the dominant singular behavior in (7) which has always eluded detection by any numerical method, including the HT series. By taking advantage of the three new HT coefficients available we can now give a first indication of its existence. We can isolate this singularity in a doubly biased analysis (with respect to η and β_c) by forming the quantity

$$S(\beta) = \chi(\beta)[m^{(1)}(\beta)/m^{(2)}(\beta)]^{2-\eta} = O(\tau^{-\theta}). \quad (23)$$

Then θ is obtained as the residue of the logarithmic derivative of $S(\beta)$ at $\beta = \beta_c$ or, equivalently, as the value at β_c of the quantity

$$\theta(\beta, \eta) = \tau[D\ln(\chi) + (2-\eta)D\ln(m^{(1)}/m^{(2)})]. \quad (24)$$

In Fig. 9 we have reported the quantity $\theta(\beta_c, \eta)$ vs η for various values of β_c in the range $1.112 < \beta_c < 1.121$. It is remarkable how precisely correlated are the expected values of θ and η.

IV. CONCLUSIONS

Let us now compare our results to those obtained in previous papers and state our conclusions.

The first MC works[5] were suggestive, but inconclusive. The size of the systems studied was too small and therefore the range of values of β explored in the simulations was still too far away from criticality, so that the data, although compatible or even strongly suggestive of a KT behavior, generally could be fitted as well in terms of a conventional power-law singularity. The limitations of these first-generation studies have been thoroughly described in Ref. 13, to which we address the interested reader.

The new generation of MC studies,[11–14] taking decisive advantage both of the greater computing power presently available and of the newly invented algorithms with reduced critical slowing down, could be performed on rather large lattices, up to 512^2 sites[11] (or even 1200^2 sites in the case of Ref. 14 devoted, however, to the Villain model[28]). As a consequence, the recent MC data are either practically free from finite-size effects[11,12,14] or they have been carefully[13] analyzed in terms of finite-

TABLE XI. Residues at the critical poles of the PA's to $[\ln(\chi)/\beta]^2$. Same conventions as in the previous table.

	N									
D	5	6	7	8	9	10	11	12	13	14
5		1.609	1.623	1.623			1.692	1.675	1.668	1.668
6	1.670	1.649	1.636	1.607*		2.255*	1.671	1.655	1.669	
7	1.653	1.306*	1.644	1.676*	1.613	1.643	1.663	1.667		
8	1.646	1.648	1.654	1.674	1.685	1.677	1.676			
9	1.648	1.645*	1.636*	1.692	1.680	1.675				
10	1.660	1.738*	1.667	1.666	1.677					
11	1.676	1.677	1.665	1.667						
12	1.677	1.676	1.673							
13	1.698*	1.671								
14	1.680									

size scaling. As has been extensively discussed in Ref. 13, the recent simulations give more reliable, but, perhaps, not yet definitive indications in favor of the KT description. Indeed, the authors of Ref. 13 point out that a previous fit[6] to power-law behavior, which produced the estimates for the critical parameters, $\beta_c = 1.01 \pm 0.01$, $\gamma = 2.17 \pm 0.10$, $\nu = 1.34 \pm 0.04$, and $\eta = 0.386 \pm 0.02$, seems to be still consistent with their data, provided that the critical inverse temperature is increased to the value $\beta_c = 1.05$.

The data of Ref. 13, of course, may also be fitted to the KT behavior, and, assuming $\sigma = 1/2$, the estimates $\beta_c = 1.13 \pm 0.015$ and $b = 2.15 \pm 0.1$ are obtained.

We should also mention an overrelaxed MC study on a 512^2 lattice,[11] in which data have been taken up to $\beta = 1.02$. The conclusions of Ref. 11 are not essentially different: It is difficult to discriminate between the KT and the power-law fits (even) if only MC data for $\beta \geq 0.94$ ($\xi > 15$) are used. Moreover unconstrained independent (four parameter) best fits to KT behavior of the data for χ and ξ require somewhat different values for β_c (1.127 and 1.117, respectively) and for σ (0.57 and 0.47, respectively). (A safe estimate of the errors in this case is supposed to be given by the differences of these results rather than by the much smaller nominal uncertainties in the fit values.) If, however, σ is held fixed at 0.5, the best-fit values for the remaining critical parameters are $\beta_c = 1.118 \pm 0.005$ and $b = 1.7 \pm 0.2$, which agree with our own estimates. In these analyses some difficulties are met also with the determination of the exponent η: If its value is extracted directly from the parameters of the fits to χ and ξ, it turns out to be much larger than expected. It should be noted, however, that estimates near to the KT value are obtained either by resorting to MC renormalization group (as shown also in Ref. 15) or by using a discretized form of Eq. (21) (as shown also in Ref. 14). It is interesting to quote also a very recent "verification of the KT scenario"[29] by a method based on matching the renormalization-group flow of the dual of the XY model with the flow of the body-centered solid-on-solid model which has been exactly solved[30] to exhibit a KT transition. The method has to assume that $\sigma = 1/2$ and yields $\beta_c = 1.1197 \pm 0.0005$ and $b = 1.88 \pm 0.02$.

We can summarize the main limitations of these MC works as follows: The range of values of β covered, even in the most extensive among these studies,[11] is presently restricted to $\beta \leq 1.02$ (corresponding to $\xi \leq 70$) and, anyway, the estimates of the critical parameters have not yet reached a satisfactory level of precision. Finally, it should also be noted that there are arguments indicating that the KT critical region has a very small width,[31] and therefore it might have been explored only in its extreme periphery by these studies. Therefore all authors of MC works agree that further simulations much closer to β_c are still desirable.

Early HT studies,[1] based on ten-term series, were also inconclusive and unable to provide reasonably stable estimates of the critical parameters. Better suited methods of series analysis[2] were later proposed. A computation[3] of HTE's to order β^{12} on the triangular lattice gave a first valuable support to the KT scenario with the estimates $\sigma = 0.5 \pm 0.1$ and $\eta = 0.27 \pm 0.03$. Extensive calculations on highly asymmetric lattices[4] by Hamiltonian strong-coupling or finite-lattice techniques always gave indications in favor of the KT scenario.

As we made available substantially longer HT series,[9] it emerged not only that the KT critical behavior is favored by all tests (this conclusion was strengthened by the independent analysis of Ref. 32 by the four-fit method), but also that any series analysis designed to extract power-law scaling leads to estimates of the critical parameters definitely inconsistent with those coming from the corresponding fits to MC data. As we have observed above, the study of ratio plots, and of the PA's to the logarithmic derivative of χ and ξ, shows clear signs of a non-power-like nature of the critical singularity, and, if forced to produce estimates of the critical parameters, points to values of β_c, γ, and ν which are significantly larger than those derived from power-law fits to MC data and show a clear trend to increase with the number of HT coefficients used. This is precisely what one should see when trying to interpret an infinite-order singularity as a power singularity. It is then reasonable to expect that also future MC studies will still appear to be unable to decide between the two kinds of fits, but power-law fits will suggest embarassingly larger and larger values for γ and for ν. Conversely, extrapolations of the HT series by ratio, Padé, or differential approximant techniques, in a way consistent with the KT behavior, show a good stability, and agree with the KT fits to the MC data. They lead to the values of the critical parameters, $\beta_c = 1.118 \pm 0.003$, $b = 1.67 \pm 0.04$, $\sigma = 0.52 \pm 0.03$, and $\eta = 0.27 \pm 0.02$, and moreover make a first detection of the exponent θ possible. These are quite acceptable estimates, although they do not yet reach the high level of precision that is usually expected from so long a HT series probably because we are not yet using methods of series analysis which are entirely adequate to the complicated nature of the critical singularities. We conclude that a sufficient extension of the HT series has been achieved to enable us to assert that the critical behavior of the plane rotator model agrees only with the KT predictions[7] and that it is now possible, by various essentially different methods, to get consistent and fairly accurate estimates of the critical parameters.

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