High-temperature study of the Kosterlitz-Thouless phase transition in the XY model on the triangular lattice

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High-temperature series expansions of the spin-spin correlation function for the XY (or plane rotator) model on the triangular lattice are extended by two terms up to order β^{14}. Tables of the expansion coefficients are reported for the correlation function spherical moments of order $l = 0$ and 2. 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

In the last two decades since the seminal papers by Berezinski and by Kosterlitz and Thouless, the critical behavior of the two-dimensional XY (or plane rotator) model has been much studied numerically, mainly on the square lattice,[1–13] but, sometimes, also on the triangular lattice.[2,5] The steady increase of the computers power, important recent progress in Monte Carlo (MC) algorithms[14] and the calculation of $O(\beta^{20})$ high temperature expansions (HTE's) on the square lattice,[8] have produced increasingly accurate verifications of the Kosterlitz and Thouless (KT) theory.[15,16] However, since on reasonable grounds it has been disputed[6,11] that these studies are really conclusive, further quantitative evidence is still valuable.

Here we present an extension (by two terms up to order β^{14}) and a new analysis, by the methods of Ref. 8, of HTE's for the XY model on the triangular lattice. Our study gives further support to the KT picture and leads to fairly precise estimates of the KT critical parameters. On the contrary, our results appear not to be consistent with a conventional power-law critical behavior unless the exponents are very large, namely $\gamma \gtrsim 3.2$ and $\gamma+2\nu \gtrsim 5.4$. If this is the case, our $O(\beta^{14})$ series do not seem to be sufficiently long to yeld accurate estimates of the critical exponents.

In the second section, we recall briefly the main predictions of the KT theory. The third section is devoted to an analysis of the series by ratio extrapolation, and by rational and differential approximants techniques. The last section contains our conclusions.

II. THE MODEL AND THE HT SERIES

The Hamiltonian of the two-dimensional XY model is

$$H\{s\} = -\frac{1}{2}\sum_{\langle x,x'\rangle} s(x)s(x'). \qquad (1)$$

Here $s(x)$ is a two-component classical spin of unit length associated to the site with position vector x of a two-dimensional triangular lattice and the sum extends over all nearest-neighbor lattice pairs $\langle x, x'\rangle$.

Our series have been computed by a FORTRAN code which solves recursively the Schwinger-Dyson equations for the correlation functions.[7,17]

Here we shall analyze the HTE of the spherical moments of the correlation function $m^{(l)}(\beta)$ for $l = 0$ (reduced susceptibility) and $l = 2$.

Table I shows the HTE coefficients through β^{14} of the nearest-neighbor spin-spin correlation function. In Tables II and III, we have reported the expansion coefficients for the moments $m^{(l)}(\beta)$ with $l = 0$ and 2.

The main predictions of the nonrigorous renormalization group analysis of the plane rotator model[15,16] can be summarized as follows.

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

$$\xi(\beta) \propto \xi_{as}(\beta) = \exp\left(\frac{b}{\tau^{\sigma}}\right)[1 + O(\tau)], \qquad (2)$$

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

The value of the exponent σ predicted in Ref. 15 is $\sigma = 1/2$ and b is a nonuniversal positive constant.

TABLE I. HTE coefficients of the nearest-neighbor correlation function.

Order	Coefficient
1	0.50000000000000000000000000000
2	0.50000000000000000000000000000
3	0.43750000000000000000000000000
4	0.31250000000000000000000000000
5	0.18229166666666666666666666667
6	0.07291666666666666666666666667
7	-0.03955078125000000000000000000
8	-0.20448133680555555555555555556
9	-0.44802788628472222222222222222
10	-0.76376953125000000000000000000
11	-1.13934388337311921296296296296 2
12	-1.58150900381582754629629629629 6
13	-2.11418561178540426587301587301 6
14	-2.76027832004338555445326278659 6

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

Order	Coefficient
0	1.000000000000000000000000
1	3.000000000000000000000000
2	7.500000000000000000000000
3	16.8750000000000000000000
4	35.6250000000000000000000
5	72.0625000000000000000000
6	141.2734375000000000000000
7	270.1728515625000000000000
8	506.3834635416666666666666
9	933.5703776041666666666666
10	1697.512101236979166666666
11	3050.264278496636284722222
12	5424.862119886610243055555
13	9561.162654477074032738095
14	16716.55156094636866655299

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

$$\langle s(0)s(x)\rangle \propto \frac{[\ln(r)]^{2\theta}}{r^{\eta}}[1 + O(\ln\{\ln(r)\}/\ln(r))]. \quad (3)$$

The values predicted[15,18] for η and θ are, respectively, $\eta = 1/4$, $\theta = 1/16$.

From Eqs. (2) and (3), together with the usual scaling ansatz, it follows that, for $l > \eta - 2$, the correlation moment $m^{(l)}(\beta)$ should diverge as $\beta \uparrow \beta_c$ with the singularity

$$m^{(l)}(\beta) \propto \tau^{-\theta}\xi_{as}(\beta)^{2-\eta+l}[1 + O(\tau^{1/2}\ln(\tau))]. \quad (4)$$

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, it is worth mentioning the rigorous bound[19]

$$\beta_c \geq 2\beta_c^I = \frac{1}{2}\ln 3 = 0.5493..., \quad (5)$$

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

Order	Coefficient
0	0.000000000000000000000000000
1	3.000000000000000000000000000
2	18.00000000000000000000000000
3	72.37500000000000000000000000
4	239.6250000000000000000000000
5	703.7500000000000000000000000
6	1902.406250000000000000000000
7	4835.969726562500000000000000
8	11719.07975260416666666666666
9	27326.64085286458333333333333
10	61726.45278320312500000000000
11	135743.4609174940321180555555
12	291741.0660864935980902777777
13	614640.8839340452163938492063
14	1272465.830598210733403604497

where β_c^I is the inverse critical temperature of the Ising model on the triangular lattice.

III. AN ANALYSIS OF THE HT SERIES

We estimate the critical parameters by simple modifications of current methods of series analysis.[7,8,20–23]

In Refs. 7 and 8 we have shown that the ratios $r_n(m^{(l)}) = a_n^{(l)}/a_{n+1}^{(l)}$ of the successive HTE coefficients of the correlation moment $m^{(l)}(\beta)$ for large n behave as

$$r_n(m^{(l)}) = \beta_c + \frac{C_l}{(n+1)^{\epsilon}} + O(1/n^{\lambda}), \quad (6)$$

with $\epsilon = \frac{1}{1+\sigma}$, $C_l = -[(2-\eta+l)\sigma b\beta_c]^{\epsilon}$, and $\lambda = \min(1, 2\epsilon)$. According to the KT prediction we should have $\epsilon = 2/3$. This is a clear signature of the KT singularity and it should be detected in a ratio analysis of the HTE's.

On the other hand if, instead of (2) and (4), we had conventional power-law critical behavior so that, as $\beta \uparrow \beta_c$,

$$m^{(l)}(\beta) \sim \tau^{-\gamma-l\nu}[A_l + B_l\tau^{\Delta} + \cdots], \quad (7)$$

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. (6) with $\epsilon = 1$ and $\lambda = 1 + \Delta$, namely

$$r_n(m^{(l)}) = \beta_c + \frac{\beta_c(1-\gamma-l\nu)}{n} + O(1/n^{1+\Delta}). \quad (8)$$

In Fig. 1, we have plotted versus $1/n$ the sequences of ratios $r_n(m^{(l)})$ for $l = 0$ and 2. These ratio plots exhibit a residual curvature and an increasing slope for

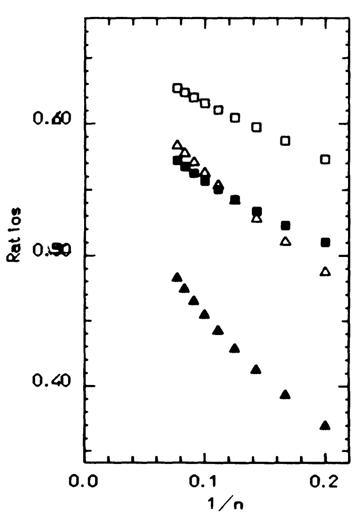

FIG. 1. The successive ratios of the HTE coefficients of various moments are plotted versus $1/n$. The ratios $r_n(\chi)$ are represented by solid squares; $r_n(m^{(2)})$ by solid triangles. We have also plotted the linearly extrapolated ratio sequences $r_n^{(1)}(\chi)$ (open squares), and $r_n^{(1)}(m^{(2)})$ (open triangles).

large n. If Eq. (8) were a correct representation of the asymptotic behavior of $r_n(m^{(l)})$, the $O(1/n)$ terms in (8) should be suppressed by forming the linearly extrapolated sequences

$$\begin{aligned} r_n^{(1)}(m^{(l)}) &= n r_n(m^{(l)}) - (n-1) r_{n-1}(m^{(l)}) \\ &= \beta_c + O(1/n^{1+\Delta}), \end{aligned} \tag{9}$$

which, for large n, should approach with vanishing slope their common limit β_c. This does not happen (at least up to $n = 14$), as it is shown in Fig. 1 where we have also plotted the sequences $r_n^{(1)}(m^{(l)})$ versus $1/n$. The estimates of β_c obtained from $r_n^{(1)}(m^{(l)})$ still increase rapidly with order.

Turning to critical exponents, we have computed a sequence of (unbiased) estimates of $\gamma + l\nu$ by the formula

$$(\gamma + l\nu)_n = \frac{(n-1)^2 r_n(m^{(l)}) - n(n-2) r_{n-1}(m^{(l)})}{n r_{n-1}(m^{(l)}) - (n-1) r_n(m^{(l)})}. \tag{10}$$

The sequences of estimates so obtained for γ and $\gamma + 2\nu$ are plotted versus $1/n$ in Fig. 2. We conclude that, under the assumption of power-law scaling, the simplest extrapolations suggest $\gamma \gtrsim 3.2$ and $\gamma + 2\nu \gtrsim 5.4$. These estimates for the exponents are larger than those obtained from a fit[6] of (square lattice) MC data to power-law critical behavior.

Let us assume now that Eq. (6) is valid instead of Eq. (8), then by reporting the $r_n(m^{(l)})$ sequences versus $1/n^{2/3}$, we should obtain nice straight plots, as indeed is observed in Fig. 3. We can suppress the $O(1/n^{2/3})$ terms in the sequences $r_n(m^{(l)})$ by forming the (nonlinearly) extrapolated sequences

$$\begin{aligned} s_n(m^{(l)}) &= \frac{n^{2/3} r_n(m^{(l)}) - (n-1)^{2/3} r_{n-2}(m^{(l)})}{n^{2/3} - (n-1)^{2/3}} \\ &= \beta_c + O(1/n). \end{aligned} \tag{11}$$

Unfortunately the sequences obtained are not regular enough to give a much more precise estimate of β_c by a further extrapolation in $1/n$. The results are reported

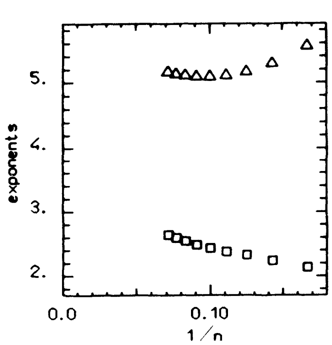

FIG. 2. Unbiased estimates of the critical exponent γ of the susceptibility under the assumption of a power-law critical singularity obtained from the ratios $r_n(\chi)$ (open squares). Analogous estimates of the exponent $\gamma + 2\nu$ as obtained from $r_n(m^{(2)})$ (open triangles).

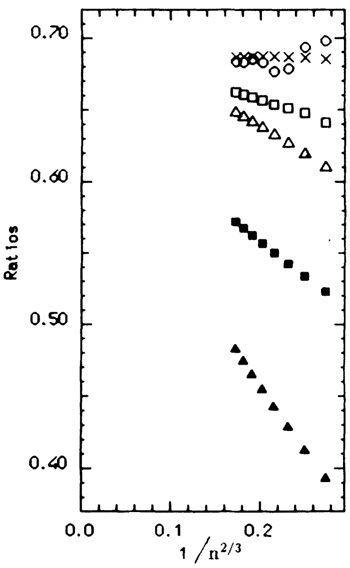

FIG. 3. Ratio plots for the HTE coefficients versus $1/n^{2/3}$. The ratios $r_n(\chi)$ are represented by solid squares; $r_n(m^{(2)})$ by solid triangles. The ratio sequences have been extrapolated in $1/n^{2/3}$ obtaining the sequences $s_n(\chi)$ (open squares), $s_n(m^{(2)})$ (open triangles). A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

in Fig. 3. We can infer that $\beta_c = 0.683 \pm 0.004$.

A direct unbiased estimate of ϵ in terms of ratios is obtained from the sequence

$$\epsilon_n = n \ln\left(\frac{t_n - 1}{t_{n+1} - 1}\right), \tag{12}$$

where $t_n = \frac{r_n(\chi^2)}{r_n(\chi)}$. If the ratios $r_n(\chi)$ and $r_n(\chi^2)$ have the asymptotic behavior (6), the sequence ϵ_n will provide estimates of ϵ. A quantity u_n analogous to t_n may be defined in terms of the moment $m^{(2)}(\beta)$ and its square, and, via Eq. 12, the corresponding sequence ϵ'_n may be formed. The sequences ϵ_n and ϵ'_n have been plotted versus $1/n$ in Fig. 4. We have also reported the sequence $\bar{\epsilon}_n$ as computed from the susceptibility χ_I of the triangular lattice Ising model,[24] in order to emphasize the qualitatively different behavior of the two cases. These tests support the KT theory and are inconsistent with a power-law singularity: if that were the case, as it appears from the Ising model plot, the limit of the sequences should be 1. An extrapolation of ϵ_n and ϵ'_n to $n = \infty$ by the Barber-Hamer method[20] leads to the estimate $\sigma = 0.51 \pm 0.04$, while for the sequence $\bar{\epsilon}_n$ we get $\sigma = 0.02 \pm 0.04$. Note that this test is able to distinguish sharply powerlike singularities from KT singularities, unless asymptotic behaviors have not yet set in. This is true even if the critical exponents are large: for instance a reasonable model series, like χ_I^2 (having $\gamma = 3.5$), produces an ϵ sequence with the same qualitative behavior as $\bar{\epsilon}_n$.

The rest of our analysis uses differential approximants (DA's) or simply Padé approximants (PA's).

The expected singularity structure of $\ln(\chi)$, namely $\ln(\chi) = A(\beta)(\beta_c - \beta)^{-\sigma} + B(\beta)$ with $A(\beta)$ regular and

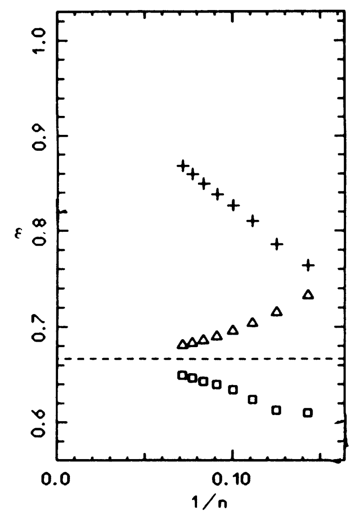

FIG. 4. The sequences ϵ_n (open squares), ϵ'_n (open triangles), as computed from the quantities t_n introduced in Eq. 12, and from the analogous ones u_n, are plotted versus $1/n$. The dashed line indicates the KT prediction for the value of ϵ. We have also reported the analogous sequence $\bar{\epsilon}_n$ (crosses) as computed from the susceptibility of the triangular lattice Ising model.

$B(\beta)$ at most weakly singular at β_c, should be reproduced with reasonable accuracy by inhomogeneous first order DA's. We have selected DA's $[n/l;m]$ with $1 \leq n \leq 6$, $2 \leq m \leq 5$, and $2 \leq l \leq 6$. From the nondefective approximants of the reduced sample that use at least 12 series coefficients, we get the unbiased estimates $\beta_c = 0.680 \pm 0.002$ and $\sigma = 0.49 \pm 0.03$. If we set $\sigma = \frac{1}{2}$, we get the biased estimate $\beta_c = 0.681 \pm 0.002$. Conservatively, we have estimated uncertainties as three times the standard deviation of the sample. The results remain essentially unchanged whether we use the Fisher-Au Yang-Hunter-Baker or the Guttmann-Joyce definitions[20] of the DA's.

We have also computed the PA's to the logarithmic derivative of $\ln(\chi)/\beta$. This quantity should discriminate between the structures (4) and (7) of the critical singularity, since the residues at the critical poles have either to approach σ, if (4) holds, or to vanish, if (7) holds. From the PA table for the location of the critical pole of the approximants to $D\ln[\ln(\chi)/\beta]$ and the PA table for the residues we get the estimates $\beta_c = 0.684 \pm 0.003$ and $\sigma = 0.54 \pm 0.04$. If we set $\sigma = \frac{1}{2}$, we get the biased estimate $\beta_c = 0.680 \pm 0.003$. The PA and the DA estimates are, therefore, consistent, the small difference in the central values being probably due to background effects.

Due to the slower convergence of the $m^{(2)}$ series a similar DA analysis of the correlation length [using $\ln(\frac{\xi^2}{\beta})$] is unsuccessful unless we assume $\sigma = \frac{1}{2}$. In this case we get the estimate $\beta_c = 0.684 \pm 0.004$ consistent with the previous ones from χ, but somewhat less accurate.

Assuming $\sigma = \frac{1}{2}$, the nonuniversal parameter b may be obtained by computing PA's of the quantity

$$C(\beta) = \tfrac{1}{2}(\tau)^{\sigma}\ln(1 + m^{(2)}/\chi) = b + O(\tau^{\sigma}) \qquad (13)$$

at $\beta = \beta_c$. Taking β_c in the range [0.680–0.682], we estimate $b = 1.27 \pm 0.05$.

Finally, the critical index η governing the large distance behavior of spin-spin correlation function may be estimated (without bias on σ) by PA's of the ratio

$$H(\beta) = \frac{\ln(1 + m^{(2)}/\chi^2)}{\ln(\chi)} = \frac{\eta}{2-\eta} + O(\tau^{\sigma}) \qquad (14)$$

at $\beta = \beta_c$. Allowing as above for the uncertainty on β_c, we estimate $\eta = 0.27 \pm 0.01$.

If we assume a power-law singularity (7), from a study of the location of the singularities 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 observed in the case of the HTE's for the square lattice,[8] both the PA tables for the poles and for the residues contain many "defective entries" or blanks and show a very poor convergence. These features of the PA's suggest that the critical singularity is not a power or, at least, that our series are still too short. 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 $D\ln(\chi)$ we get $\beta_c = 0.655 \pm 0.008$ and $\gamma = 3.7 \pm 0.6$. This estimate for γ is consistent with those from ratio tests, but larger than those obtained in Ref. 6 from power-law fits to MC data.

IV. CONCLUSIONS

Let us finally compare our results to those obtained in previous studies of the model on the triangular lattice. To our knowledge, no MC simulation is available for the ferromagnetic XY model on the triangular lattice although, by virtue of the higher coordination number of this lattice, the approach to scaling behavior is expected to be faster than in the square lattice case, for the same lattice size. On the same grounds one can also argue[25] that, for a given number of HT coefficients, the triangular lattice series are "effectively longer" than the square lattice ones. In fact, we expect from our analysis that it would perhaps take only an $O(\beta^{16})$ triangular lattice series to reach the same precision as with our $O(\beta^{20})$ square lattice series.[8]

An extensive review of the square lattice numerical studies can be found in Refs. 8 and 11 and needs no duplication here. As to HT studies[1] on the triangular lattice, we recall that the early ones, based on ten term series, were essentially inconclusive and did not provide reasonably stable estimates of the critical parameters. When the HT series were extended to twelve terms,[5] an analysis by the four-fit method gave convincing indications of the validity of the KT predictions and yielded the estimates $\beta_c = 0.687 \pm 0.009$, $\sigma = 0.5 \pm 0.1$, and $\eta = 0.27 \pm 0.03$.

We believe that our extended series and our new tests further substantiate the KT picture and provide more precise estimates of the critical parameters, otherwise consistent with those of Ref. 5. We have pointed out that the study of ratio plots, and of the PA's to the logarithmic derivative of χ and ξ, are strongly suggestive that the critical singularity is not a power. If, however, we want to pursue a power-law interpretation, we should not overlook the unusual facts that, for a closely packed lattice, $O(\beta^{14})$ series do not seem long enough to determine with reasonable accuracy the critical parameters γ and ν and that the rough estimates obtained for these exponents are significantly larger than those observed in conventional critical phenomena and show a trend to increase with the number of coefficients used. These estimates are also larger than those obtained in the power-law fit of Ref. 6 to square lattice MC data. However we have reexamined the most recent and extensive MC simulation data[9,11] on the square lattice and we have observed that they are consistent with a power-law finite size scaling ansatz if we choose the larger exponents suggested by our series (it seems that this range of parameters has not been explored in the fits of Refs. 9 and 11). Our interpretation of all these facts has been already pointed out at the conclusion of our analysis of the square lattice series:[8] as the critical point is approached, larger and larger effective exponents are needed to fit an infinite order singularity by an ordinary power singularity.

We may conclude that, if we extrapolate the HT series consistently with the KT behavior, we find stable values of the critical parameters in good agreement with the KT fits to the MC data and with our previous studies of HTE's on square lattice. Our unbiased estimates of the critical parameters are $\beta_c = 0.680\pm0.002$, $\sigma = 0.49\pm0.03$, and $\eta = 0.27 \pm 0.01$.

If we set $\sigma = \frac{1}{2}$ we obtain the estimate $\beta_c = 0.681 \pm 0.002$ and by also fixing β_c at its central value we find $b = 1.27 \pm 0.05$.

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