Further extensions of the high-temperature expansions for the two-dimensional classical XY model on the triangular and the square lattices

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(Dated: June 9, 2008)

Abstract

The high-temperature expansions of the spin-spin correlation function of the two-dimensional classical XY (planar rotator) model are extended by two terms, from order 24 through order 26, in the case of the square lattice, and by five terms, from order 15 through order 20, in the case of the triangular lattice. The data are analyzed to improve the current estimates of the critical parameters of the models. We determine $\beta_c = 0.5599(7)$ and $\sigma = 0.499(5)$ in the case of the square lattice. For the triangular lattice case, we estimate $\beta_c = 0.3412(4)$ and $\sigma = 0.500(5)$.

PACS numbers: PACS numbers: 05.50+q, 11.15.Ha, 64.60.Cn, 75.10.Hk

Keywords: XY model, planar rotator model, N-vector model, high-temperature expansions
We have recently extended, from the 21th to the 24th order, the high-temperature (HT) expansions for the spin-spin correlation function of the classical two-dimensional XY Berezinskii-Kosterlitz-Thouless (BKT) lattice model with nearest-neighbor interactions on the square (sq) lattice and briefly updated the series analysis for the susceptibility and the second-moment correlation-length. Here we present a further extension of the HT expansions from the 24th order through the 26th order for the sq lattice and from the 15th order to the 20th order in the case of the triangular (tr) lattice. In our derivation of the series coefficients, we have used a non-graphical recursive algorithm based on the Schwinger-Dyson equations for the spin-spin correlations of the XY-model. The necessary computations were performed using a few nodes of a pc cluster for an equivalent single-processor CPU-time of seven weeks in the case of the tr lattice and a CPU-time ten times as long in the case of the sq lattice. Arguing as in Ref. \[5\] that the "effective length" (namely the ability to provide accurate numerical information) of the HT expansions of a given system on different lattices, is proportional to the computer time used in the series generation, we expect that the "effective length" of our expansions for the tr lattice, is only slightly smaller than that of the sq lattice series and moreover that their convergence will be faster, because the tr lattice is closely-packed.

Let us recall that the lattice XY spin model with nearest-neighbor interactions is described by the Hamiltonian

$$H\{v\} = -2J \sum_{<nn>} \vec{v}(\vec{r}) \cdot \vec{v}(\vec{r}')$$  \hspace{1cm} (1)

where \(\vec{v}(\vec{r})\) is a two-component classical unit vector at the site \(\vec{r}\) and the sum extends to the nearest-neighbor sites of the lattice.

We have calculated the spin-spin correlation function

$$C(\vec{0}, \vec{x}; \beta) = \langle \vec{v}(\vec{0}) \cdot \vec{v}(\vec{x}) \rangle,$$  \hspace{1cm} (2)

as series expansion in the variable \(\beta = 2J/kT\), with \(T\) the temperature and \(k\) the Boltzmann constant, for all values of \(\vec{x}\) for which the HT expansion coefficients are non-trivial within the maximum order reached. In terms of these quantities, we can form the expansions of the \(l\)-th order spherical moments of the correlation function:

$$m^{(l)}(\beta) = \sum_{\vec{x}} |\vec{x}|^l \langle \vec{v}(\vec{0}) \cdot \vec{v}(\vec{x}) \rangle$$  \hspace{1cm} (3)

and, in particular, of the reduced ferromagnetic susceptibility \(\chi(\beta) = m^{(0)}(\beta)\).

The second-moment correlation length is defined, as usual, in terms of \(m^{(2)}(\beta)\) and \(\chi(\beta)\):

$$\xi^2(\beta) = m^{(2)}(\beta)/4\chi(\beta).$$  \hspace{1cm} (4)

After completing our computations, we have been kindly informed by H. Arisue\[6\] that, in the particular case of the sq lattice, he has recently obtained, using the "finite lattice" method, remarkably longer HT expansions: through the 38th order for the nearest-neighbor spin-spin correlation \(C(0, 0; 1, 0; \beta)\) and through the 34th order for the susceptibility and the second and fourth moment of the correlation function.

When also these further extended data will be published, the agreement, through their common extent, between both sets of results independently obtained by completely different
methods, will be a significant check of correctness in consideration of the notoriously intricate nature of the high-order HT computations.

In order to determine the critical parameters of the models, the HT expansions of the above defined quantities should be confronted to the following main predictions of the BKT renormalization-group analysis of the XY system.

As $\beta \to \beta_c$, the divergence of the correlation length is expected to be dominated by the characteristic singularity

$$\xi(\beta) \sim \xi_{as}(\beta) = \exp(b\tau^{-\sigma})[1 + O(\tau)]$$

where $\tau = 1 - \beta/\beta_c$ and the universal exponent $\sigma$ is expected to take the value $\sigma = 1/2$, while $b$ is a non-universal (and thus lattice dependent) positive constant.

The critical behavior of the susceptibility is predicted to be

$$\chi(\beta) \sim \xi_{as}^{2-\eta}(\beta) = \exp \left( (2-\eta)b\tau^{-\sigma} \right)[1 + O(\tau)]$$

The parameter $\eta$ represents the correlation-function exponent and is predicted to take the value $\eta = 1/4$.

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

$$<\vec{v}(0) \cdot \vec{v}(x)> \sim \frac{(\ln r)^{2\theta}}{r^\eta}[1 + O(\ln(\ln r)/\ln r)]$$

The value $\theta = 1/16$ is predicted for the second universal exponent characterizing the critical correlation function.

Following a recent renormalization-group analysis of the two-dimensional $O(2)$ nonlinear $\sigma$-model, which should belong to the same universality class as the XY model, we shall assume that the critical behavior of $\chi(\beta)$ does not contain singular multiplicative corrections by powers of $\ln(\xi)$ (or equivalently singular multiplicative corrections by powers of $\tau$). The possible existence of such corrections has long been numerically investigated with conflicting and essentially inconclusive results. As we will indicate below, our series analysis is completely consistent with the conclusions of Ref.[9].

Let us now come to our results for the $sq$ lattice: we have added the two terms

$$\chi(\beta) = \ldots + \frac{376988970189597090587}{384296140800} \beta^{25} + \frac{6233737838591540773643}{3138418483200} \beta^{26} + \ldots$$

(8)

to the expansion of the susceptibility.

To the expansion of the second moment of the correlation function, we have added the terms

$$m^{(2)}(\beta) = \ldots + \frac{5412508223507386985733313}{13450364928000} \beta^{25} + \frac{7139182711315236460182251}{7846046208000} \beta^{26} + \ldots$$

(9)

The lower-order coefficients of the $sq$-lattice expansions of $\chi(\beta)$ and of $m^{(2)}(\beta)$ have been recently tabulated in Ref.[1] and therefore they will not be reproduced here.

On the contrary, we have listed in Table[1] also the coefficients already known through 15th order in the case of the $tr$ lattice, in addition to the five coefficients that we have
recently calculated for the nearest-neighbor spin-spin correlation, the susceptibility and the second moment of the correlation function.

Let us now update the analysis of Refs.\[1,4\] for the sq lattice expansions by including all coefficients that we have so far derived. The expected form eq. (5) of the critical singularity suggests that the critical parameters should be conveniently obtained by an inhomogeneous-differential-approximant (DA) study of the location and the exponent of the leading singularity of the quantity $\ln^2(\chi)$. This conclusion is supported also by a simple comparison of the distribution of the singularities on the real $\beta$-axis for the DAs of $\chi(\beta)$ and of $\ln^2(\chi)$ which, independently of theoretical prejudice, suggests that the analytic structure of the latter form is more suitable to a study by DAs. Notice that the choice of this inhomogeneous-differential-approximant (DA) study of the location and the exponent of the leading singularity of $\ln^2(\chi)$ is more suitable to a study by DAs. Notice that the choice of this particular function of $\chi(\beta)$ does not imply any biasing of $\sigma$, as long as we do not make any selection of the singularities of the DAs for $\ln^2(\chi)$ on the basis of their exponents. In our previous note, we had already observed that a possibly more accurate analysis might be based on the obvious remark that, near the critical point, by eq. (6), we have to expect $\ln(\chi) = c^sq_1/\tau^\sigma + c^sq_2 + \ldots$. Assuming $\sigma \simeq 1/2$, a simple fit to the asymptotic form of $\ln(\chi)$, can determine $c^sq_2 \simeq -1.5$. We are then led to study also the simple generalization of the function $\ln^2(\chi)$, defined by $L(a, \chi) = (a + \ln(\chi))^2$, where $a$ is some constant. The relative strength of the $\tau^{-\sigma}$ and $\tau^{-2\sigma}$ singularities in the function $L(a, \chi)$ is determined by the value of $a$. Therefore it might be numerically convenient to analyze the function $L(a, \chi)$ with $a \simeq -c^sq_2$, rather than simply $\ln^2(\chi)$, because the dominant singularity of $L(-c^sq_2, \chi)$ should then be $\tau^{-2\sigma}$, with a small or vanishing $\tau^{-\sigma}$ contribution and thus approximately a simple pole, if $\sigma \simeq 1/2$. We can therefore expect that analyzing the DAs of $L(-c^sq_2, \chi)$ will make it possible to determine with good accuracy not only the position, (which is not very sensitive to the choice of $a$), but also the exponent of the critical singularity.

In our analysis of the HT series, we have restricted to a class of quasi-diagonal second-order DAs quite similar to that used in Ref.\[1\], namely to the $[k, l, m; n]$ DAs defined by the conditions: $20 \leq k + l + m + n \leq 24$ with $k \geq 6; l \geq 6; m \geq 5$ and such that $|k - l|, |l - m| \leq 2$, and $1 < n < 7$. For the shorter $tr$ lattice series, these conditions have to be modified in an obvious way. We have always made sure that our final estimates, within a small fraction of their spread, are independent of the precise definition of the DA class examined.

In the case of the sq lattice, from an unbiased DA analysis of $\ln^2(\chi)$ we obtain $\beta_c = 0.5599(7)$, in complete agreement with the results of our previous analysis of the 24-th order series and also with the MonteCarlo analysis of Ref.\[11\] which yielded $\beta_c = 0.55995(15)$. Notice that the uncertainty of this estimate was not given explicitly in Ref.\[11\], and that the value that we have nevertheless indicated is only a reasonable guess. We have obtained the estimate $\sigma = 0.499(5)$ for the singularity exponent by DAs of $L(-c^sq_2, \chi)$, chosen in the same class defined above and biased with the value of $\beta_c = 0.55995$ given in Ref.\[11\]. Its uncertainty accounts also for the spread in the estimate of the critical temperature used to bias the DA calculation. These results are illustrated in Fig.\[10\].

In Fig.\[2\] we have compared how the estimate of $\sigma$ depends on the value $\beta^bias_c$ used to bias the DAs, when either the quantity $L(-c^sq_2, \chi)$ or $\ln^2(\chi)$ is analyzed in a vicinity of $\beta^bias_c = \beta_c = 0.55995$. Clearly the results obtained from the analysis of $\ln^2(\chi)$ are much more sensitive to the bias value.

Taking advantage of our extension of the HT series, we can also get some hint of the analytic structure of the susceptibility in a vicinity of the origin of the complex $\beta$ plane. In Fig.\[8\] we have reported a scatter-plot showing the distribution of the nearby complex singularities for a large class of inhomogeneous first-order DAs of $L(-c^sq_2, \chi)$. We have
discarded only a few spurious real singularities with modulus less than \(0.9\beta_c\). We can notice that, in addition to the physical singularities at \(\pm\beta_c\) and to many randomly scattered complex singularities, which we believe to represent only numerical noise, there is evidence of five pairs of complex-conjugate singularities, located just beyond the convergence disc of the series. They are indicated by clusters of DA singularities, which are likely to coalesce around tips of cuts with increasing series order. These results, which do not essentially depend on the value of the constant \(a\) in \(L(a,\chi)\), are reminiscent of the regular pattern of the nearby unphysical singularities (cuts) which were exactly determined for the \(sq\)-lattice two-dimensional \(O(N)\) \(\sigma\)-model\textsuperscript{14} in the large \(N\) limit and conjectured\textsuperscript{15} to exist also for finite \(N\geq 3\).

Let us now perform a similar update of the analysis for the \(tr\) lattice series. As shown in Fig\textsuperscript{4} an unbiased DA study of \(\ln^2(\chi)\) yields a critical inverse-temperature \(\beta_c = 0.3412(4)\), sizably improving the precision of our 14th-order estimate \(\beta_c = 0.340(1)\) reported in Ref.\textsuperscript{4}, but disagreeing with the DA estimate \(\beta_c = 0.33986(4)\) obtained in the 15th-order study of Ref.\textsuperscript{12}. From an analysis of DAs of \(\ln^2(\chi)\) biased with the critical temperature \(\beta_c = 0.3412(4)\), we are led to the estimate \(\sigma = 0.53(2)\). If, however, in analogy with the \(sq\)-lattice analysis, we consider the quantity \(L(a,\chi)\) with \(a = -c_r^2 \approx 1.1\), obtained from a fit of the asymptotic behavior of \(\ln(\chi)\) as indicated above, we arrive at the estimate \(\sigma = 0.500(4)\). It is also particularly interesting to notice that the pattern of the singularities of \(L(a,\chi)\) in the complex \(\beta\)-plane is much simpler than that observed in the case of the \(sq\) lattice and consists of a single pair of complex-conjugate clusters, located farther from the border of the convergence disc than in the case of the \(sq\) lattice. This is an indication that the convergence of the \(tr\)-lattice HT series will be faster than in the \(sq\) lattice case, and so the argument that the effective lengths of the HT series for the two lattices are comparable, receives further support.

In spite of the sizable extension of the series, both in the \(sq\) and in the \(tr\) lattice cases, the study of the indicator function \(H(\beta) = \ln(1 + m(2)/\chi^2)/\ln(\chi) = \frac{\eta}{2-\eta} + O(\rho^\infty)\) (or of analogous functions of different correlation-moments), does not show very sharp improvements in the accuracy of the determination of the exponent \(\eta\), for which we consistently obtain the estimate \(\eta = 0.25(2)\).

Assuming \(\sigma = 1/2\), essentially the same estimate of \(\eta\) is obtained from a DA analysis of the series expansions of \(\tau^\sigma\ln(\chi) = (2 - \eta)b + O(\tau^\sigma)\) and of \(\tau^\sigma\ln(\xi^2/\beta) = 2b + O(\tau^\sigma)\) both in the case of the \(sq\) and of the \(tr\) lattices. Assuming \(\eta = 1/4\), we can estimate the non-universal parameters \(b_{sq} = 1.77(1)\) and \(b_r = 1.70(1)\).

In order to get alternative estimates of \(\eta\), we may also try to analyze directly the large-order behavior of the expansion coefficients of \(\chi(\beta)\) and of \(\xi^2(\beta)\). Assuming \(\sigma = 1/2\) and using the known value of \(\beta_c\), we can fit the series coefficients of these quantities to their expected asymptotic behavior \(c_n \sim \beta^{-n-1}\exp[\mathcal{B}(n + 1)^{1/3} + O(n^{-1/3})]\) with \(\mathcal{B} = B_\chi = 3/2(2\pi)^{1/3}b^{1/3}/(\beta - 1)^{1/4}\) in the case of the susceptibility, while \(B = B_\xi^2 = 3/2(2\pi)^{1/3}b^{1/3}/(\beta - 1)^{1/4}\) in the case of \(\xi^2(\beta)\). Both in the case of the \(sq\) and of the \(tr\) lattices, using the sets of coefficients of the susceptibility and of the correlation length, we can estimate \(\eta = 0.25(1)\) from the ratio \(B_\chi/B_\xi^2\). This estimate is however suspect because, assuming \(\eta = 0.25\), we can consistently estimate \(b = 1.46(10)\) in the case of the \(sq\) lattice and \(b = 1.36(10)\) in the case of the \(tr\) lattice. Thus we must suppose that the series coefficients are not yet near enough to their asymptotic values that the value of \(b\) can be reliably estimated by this direct analysis, in spite of the fact that the ratio \(B_\chi/B_\xi^2\) already takes the expected value.

Finally, it is also interesting to notice that, as indicated in our previous analysis, a study
of the function \( R(\beta) = \frac{\chi(\beta)}{\xi^2 - \eta(\beta)} \), of its logarithm and of its log-derivative, supports the arguments of Ref.\cite{9} concerning the absence of singular multiplicative corrections by powers of \( \ln(\xi) \) to the critical behavior of \( \chi \) and gives results completely consistent with the assumption that \( \eta = 1/4 \). Indeed if \( \eta \neq 1/4 \) or if \( \eta = 1/4 \), but there were in \( \chi \) singular multiplicative corrections, either Padé approximants or DAs of the above quantities should detect some singular behavior as \( \beta \to \beta_c \), which, at the present orders of expansion, is not seen at all.

In conclusion, our recent HT series data confirm the BKT predictions for the critical behavior of the XY system and confirm or improve the existing estimates of the critical parameters for both the \( sq \) and the \( tr \) lattices.

I. ACKNOWLEDGEMENTS

We thank H. Arisue for informing us about his recent results. Our computations have been performed on the pc cluster Turing of the Milano-Bicocca INFN Section. We thank the Physics Depts. of Milano-Bicocca University and of Milano University for their hospitality and support. Our work was partially supported by the MIUR.

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FIG. 1: XY model on the $sq$ lattice. Distribution of the singularities of a class of second-order DAs of $\ln^2(\chi)$ vs their position on the $\beta$ axis (open histogram). The central value of the open histogram is $\beta_c = 0.5599(7)$. The bin width is 0.0007. The vertical dashed line shows the critical value $\beta_c = 0.55995$ indicated by the simulation of Ref. [11], for which one can guess an uncertainty somewhat smaller than ours. The hatched histogram represents the distribution of the exponent $\sigma$ obtained from DAs of $L(-c_{2}^s, \chi)$, biased with $\beta_c = 0.55995$, vs their position on the $\sigma$ axis. The central value of the hatched histogram is $\sigma = 0.499(5)$ and the bin width is 0.003.
FIG. 2: A comparison of the estimates of the exponent $\sigma$ obtained from a class of DAs of $\ln^2(\chi)$ and of $L(-c_2, \chi)$, biased with the inverse critical temperature. Results are shown for both the $sq$ and the $tr$ lattices. We have varied the value of $\beta^\text{bias}_c$, used to bias the DAs, in a small vicinity of the values $\beta_c^\text{sq} = 0.55995$, in the case of the $sq$ lattice, and $\beta_c^\text{tr} = 0.3412$, in the case of the $tr$ lattice. The temperature-biased exponent estimates are plotted vs $x = \beta^\text{bias}_c/\beta^\text{sq}_c$ in the case of the $sq$ lattice and vs $x = \beta^\text{bias}_c/\beta^\text{tr}_c$ in the case of the $tr$ lattice. The black squares (resp. black triangles) show the results obtained from the analysis of $\ln^2(\chi)$ in the case of the $sq$ lattice (resp. $tr$ lattice) and the open squares (resp. open triangles) those obtained from the study of $L(-c_2, \chi)$ in the case of the $sq$ lattice (resp. $tr$ lattice).
FIG. 3: XY model on the $sq$ lattice. A scatter plot of the singularities of a class of first-order DAs for $L(-c^sq_2, \chi)$ in the complex $\beta$ plane. Here $x = Re(\beta)$ and $y = Im(\beta)$. The central circle has radius $\beta_c$. The small circles are drawn to enclose clusters of singularities which are likely to coalesce around tips of cuts.

FIG. 4: XY model on the $tr$ lattice. Distribution of the singularities of a class of second-order inhomogeneous DAs of $\ln^2(\chi)$ versus their position on the $\beta$ axis. The central value of the distribution is $\beta_c = 0.3412(4)$. The bin width is 0.0003.
**TABLE I:** XY model on the *tr* lattice. The series expansion coefficients for the nearest-neighbor spin-spin correlation $C(0, 0; 1, 0; \beta)$, the reduced susceptibility $\chi(\beta)$ and the second moment of the correlation function $m^{(2)}(\beta)$.

| order | $C(0, 0; 1, 0; \beta)$ | $\chi(\beta)$ | $m^{(2)}(\beta)$ |
|-------|-----------------|--------------|---------------|
| 0     | 0               | 1            | 0             |
| 1     | 1               | 6            | 6             |
| 2     | 2               | 30           | 72            |
| 3     | $\frac{7}{2}$   | 135          | 579           |
| 4     | 5               | 570          | 3834          |
| 5     | $\frac{35}{6}$  | 2306         | 22520         |
| 6     | $\frac{11}{2}$  | 18083        | 121754        |
| 7     | $\frac{16}{3}$  | 27667        | 4952033       |
| 8     | 2               | 777805       | 36001013      |
| 9     | $-\frac{1}{2}$  | 1433961      | 83947407      |
| 10    | 20              | 20850087     | 1264157753    |
| 11    | 10              | 30           | 20            |
| 12    | 320             | 144          | 12688548065393|
| 13    | $-\frac{87289819}{2}$ | 65793037351 | 12068548065393|
| 14    | 5400            | 840          | 2520          |
| 15    | $-\frac{10256893919}{2}$ | 165647319078571 | 315223835174739 |
| 16    | 2268000         | 904800       | 151200        |
| 17    | $-\frac{3357272555039}{2}$ | 46008457500392489 | 41132310524237321 |
| 18    | $-\frac{1400375733941}{2}$ | 1983863997387623 | 826713976281365323 |
| 19    | 4583400         | 403800       | 211200        |
| 20    | $-\frac{2643137055251}{2}$ | 24492999075345043 | 422063820244829129 |
| 21    | 35249000        | 21772091     | 310400        |
| 22    | $-\frac{55206137402197}{2}$ | 1671043050049640293 | 662836750489256035 |
| 23    | 32659200        | 43545600     | 124416        |
| 24    | $-\frac{6827447251427903}{2}$ | 3781762635592705657 | 2575741048252225529833 |
| 25    | 14148240000     | 2903040000   | 124100000     |
| 26    | $-\frac{40824970393676669}{2}$ | 40259236103219767249 | 72876383936358221619671 |
| 27    | 54867456000     | 9144576000   | 9144576000    |