

High-temperature expansions through order 24 for the two-dimensional classical XY model on the square lattice

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The high-temperature expansion of the spin-spin correlation function of the two-dimensional classical XY (planar rotator) model on the square lattice is extended by three terms, from order 21 through order 24, and analyzed to improve the estimates of the critical parameters.

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Tests of increasing accuracy¹ of the Berezinskii-Kosterlitz-Thouless (BKT) theory² of the two-dimensional XY model critical behavior have been made possible by the steady improvements of the computer performances and the progress in the numerical approximation algorithms. However, the critical parameters of this model have not yet been determined with a precision comparable to that reached for the usual power-law critical phenomena due to the complicated and peculiar nature of the critical singularities. Therefore, any effort at improving the accuracy of the available numerical methods by stretching them toward their (present) limits should be welcome. After extending the high-temperature (HT) expansions of the model in successive steps³ from order β^{10} to β^{21} , we present here a further extension by three orders for the expansions of the spin-spin correlation on the square lattice and perform a first brief analysis of our data for the susceptibility and the second-moment correlation length. More results and further extensions both for the square and the triangular lattice⁴ will be presented elsewhere. Our study strengthens the support of the main results of the BKT theory already coming from the analysis of shorter series and suggests a closer agreement with recent high-precision simulation studies^{1,5} of the model.

The Hamiltonian

$$H\{v\} = -2J \sum_{nn} \vec{v}(\vec{r}) \cdot \vec{v}(\vec{r}'), \quad (1)$$

with $\vec{v}(\vec{r})$ a two-component unit vector at the site \vec{r} of a square lattice, describes a system of XY spins with nearest-neighbor interactions.

Computing the spin-spin correlation function,

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

(for all values of \vec{x} for which the HT-expansion coefficients are nontrivial within the maximum order reached), as series expansion in the variable $\beta = J/kT$, enables us to evaluate the expansions of the l th order spherical moments of the correlation function,

$$m^{(l)}(\beta) = \sum_{\vec{x}} |\vec{x}|^l \langle s(\vec{0}) \cdot s(\vec{x}) \rangle, \quad (3)$$

and, in particular, the reduced ferromagnetic susceptibility $\chi(\beta) = m^{(0)}(\beta)$. In terms of $m^{(2)}(\beta)$ and $\chi(\beta)$, we can form the second-moment correlation length:

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

Our results for the susceptibility are

$$\begin{aligned} \chi = & 1 + 4\beta + 12\beta^2 + 34\beta^3 + 88\beta^4 + \frac{658}{3}\beta^5 + 529\beta^6 + \frac{14\,933}{12}\beta^7 + \frac{5737}{2}\beta^8 + \frac{389\,393}{60}\beta^9 + \frac{2\,608\,499}{180}\beta^{10} + \frac{3\,834\,323}{120}\beta^{11} \\ & + \frac{1\,254\,799}{18}\beta^{12} + \frac{84\,375\,807}{560}\beta^{13} + \frac{6\,511\,729\,891}{20\,160}\beta^{14} + \frac{66\,498\,259\,799}{96\,768}\beta^{15} + \frac{1\,054\,178\,743\,699}{725\,760}\beta^{16} \\ & + \frac{39\,863\,505\,993\,331}{13\,063\,680}\beta^{17} + \frac{19\,830\,277\,603\,399}{3\,110\,400}\beta^{18} + \frac{8\,656\,980\,509\,809\,027}{653\,184\,000}\beta^{19} + \frac{2\,985\,467\,351\,081\,077}{108\,864\,000}\beta^{20} \\ & + \frac{811\,927\,408\,684\,296\,587}{14\,370\,048\,000}\beta^{21} + \frac{399\,888\,050\,180\,302\,157}{3\,448\,811\,520}\beta^{22} + \frac{245\,277\,792\,666\,205\,990\,697}{1\,034\,643\,456\,000}\beta^{23} \\ & + \frac{83\,292\,382\,577\,873\,288\,741}{172\,440\,576\,000}\beta^{24} + O(\beta^{25}). \end{aligned} \quad (5)$$

For the second moment of the correlation function we have

$$\begin{aligned}
m_2 = & 4\beta + 32\beta^2 + 162\beta^3 + 672\beta^4 + \frac{7378}{3}\beta^5 + \frac{24\,772}{3}\beta^6 + \frac{312\,149}{12}\beta^7 + 77\,996\beta^8 + \frac{13\,484\,753}{60}\beta^9 + \frac{28\,201\,211}{45}\beta^{10} \\
& + \frac{611\,969\,977}{360}\beta^{11} + \frac{202\,640\,986}{45}\beta^{12} + \frac{58\,900\,571\,047}{5040}\beta^{13} + \frac{3\,336\,209\,179}{112}\beta^{14} + \frac{1\,721\,567\,587\,879}{23\,040}\beta^{15} \\
& + \frac{16\,763\,079\,262\,169}{90\,720}\beta^{16} + \frac{5\,893\,118\,865\,913\,171}{13\,063\,680}\beta^{17} + \frac{17\,775\,777\,329\,026\,559}{16\,329\,600}\beta^{18} + \frac{1\,697\,692\,411\,053\,976\,387}{653\,184\,000}\beta^{19} \\
& + \frac{41\,816\,028\,466\,101\,527}{6\,804\,000}\beta^{20} + \frac{206\,973\,837\,048\,951\,639\,371}{14\,370\,048\,000}\beta^{21} + \frac{721\,617\,681\,295\,019\,782\,781}{21\,555\,072\,000}\beta^{22} \\
& + \frac{79\,897\,272\,060\,888\,843\,617\,033}{1\,034\,643\,456\,000}\beta^{23} + \frac{2\,287\,397\,511\,857\,949\,924\,319}{12\,933\,043\,200}\beta^{24} + O(\beta^{25}). \tag{6}
\end{aligned}$$

The coefficients of order less than 22 were already tabulated in Refs. 3, but for completeness we report all known terms. As implied by Eq. (1), the normalization of these series reduces to that of our earlier papers³ by the change $\beta \rightarrow \beta/2$.

Let us now list briefly the main predictions² of the BKT renormalization-group analysis to which the HT series should be confronted in order to extract the critical parameters.

As $\beta \rightarrow \beta_c$, the correlation length $\xi^2(\beta) = m^{(2)}(\beta)/4\chi(\beta)$ is expected to diverge with the characteristic singularity

$$\xi^2(\beta) \propto \xi_{as}^2(\beta) = \exp(b/\tau^\sigma)[1 + O(\tau)], \tag{7}$$

where $\tau = 1 - \beta/\beta_c$. The exponent σ takes the universal value $\sigma = 1/2$, whereas b is a nonuniversal positive constant. At the critical inverse temperature $\beta = \beta_c$, the asymptotic behavior of the two-spin correlation function as $|\vec{x}| = r \rightarrow \infty$ is expected⁶ to be

$$\langle s(\vec{0}) \cdot s(\vec{x}) \rangle \propto \frac{(\ln r)^{2\theta}}{r^\eta} \left[1 + O\left(\frac{\ln \ln r}{\ln r}\right) \right]. \tag{8}$$

Universal values $\eta = 1/4$ and $\theta = 1/16$ are predicted also for the correlation exponents.

A simple nonrigorous argument based on Eqs. (7) and (8) suggests that for $l > \eta - 2$, the spherical correlation moment $m^{(l)}(\beta)$ diverges as $\tau \rightarrow 0^+$ with the singularity

$$m^{(l)}(\beta) \propto \tau^{-\theta} \xi_{as}^{2-\eta+l}(\beta) [1 + O(\tau^{1/2} \ln \tau)]. \tag{9}$$

This argument was challenged⁷ by a recent renormalization-group analysis implying that the logarithmic factor in Eq. (8) gives rise to a less singular correction in the correlation moments, taking, for example, in the case of the susceptibility, the form

$$m^{(0)}(\beta) \propto \xi_{as}^{2-\eta}(\beta) [1 + cQ], \tag{10}$$

where $Q = \frac{\pi^2}{2[\ln(\xi+u)]^2} + O[\ln(\xi)^{-5}]$ and u is a nonuniversal parameter.

By Eqs. (7) and (9), the ratios $r_n(m^{(l)}) = a_n^{(l)}/a_{n+1}^{(l)}$ of the successive HT-expansion coefficients of the correlation moment $m^{(l)}(\beta)$ for large n should behave³ as

$$r_n(m^{(l)}) = \beta_c + C_l/(n+1)^\zeta + O(1/n), \tag{11}$$

with $\zeta = 1/(1+\sigma)$, to be contrasted with the value $\zeta = 1$ which is found for the usual power-law critical singularities.

To begin with, let us assume that $\sigma = 1/2$ as expected, so that $\zeta = 2/3$. Figure 1 gives a suggestive visual test of the asymptotic behavior of some ratio sequences $r_n(m^{(l)})$ by comparing them with Eq. (11). The four lowest continuous curves interpolating the data points are obtained by separate three-parameter fits of the ratio sequences $r_n(\chi)$, $r_n(m^{(1/2)})$, $r_n(m^{(1)})$, and $r_n(m^{(2)})$ to the asymptotic form $a + b/(n+1)^{2/3} + c/(n+1)$ of Eq. (11). In the same figure, the two upper sets of points are obtained by extrapolating the alternate-ratio sequence for the susceptibility, first in terms of $1/(n+1)^{2/3}$ and then in terms of $1/(n+1)$. The values of β_c indicated by the fits of the ratio sequences range between 0.5592 and 0.5611.

A more accurate analysis can be based on the simple remark that near the critical point, by Eqs. (7) and (9) [or Eq. (10)], one has $\ln(\chi) = c_1/\tau^\sigma + c_2 + \dots$. Therefore, if $\sigma = 1/2$, the relative strength of the $1/\sqrt{\tau}$ and $1/\tau$ singularities in the function $L(a, \beta) = [a + \ln(\chi)]^2$ is determined by the value of the constant a . If we choose $a \approx 1.19$, the function $L(a, \beta)$ is approximately dominated by a simple pole and we can expect that the differential approximants (DAs)⁸ will be able to determine with higher accuracy not only the position but also the exponent of the critical singularity. Using inhomogeneous second-order DAs of $L(a, \beta)$, we can locate the critical singularity at $\beta_c = 0.5598(10)$. By analyzing in the same way the series data truncated to order 21 which were previously available, we would get the estimate $\beta_c = 0.5588(15)$. A consistent estimate $\beta_c = 0.558(2)$ had been obtained in earlier independent^{3,9} studies of the same series using Padé approximants or first-order DAs. Older studies³ of slightly shorter series also indicated values of β_c in the same range, but with notably larger uncertainty. Thus, the results of the series in this study indicate a stabilization and a sizable reduction of the spread for the β_c estimates. Our uncertainty estimates are generally taken as the width of the distribution of the values of β_c in the appropriate class of DAs. Figure 2 shows the singularity distribution (open histogram) of the set of quasi-diagonal DAs which yield our estimate. These are chosen

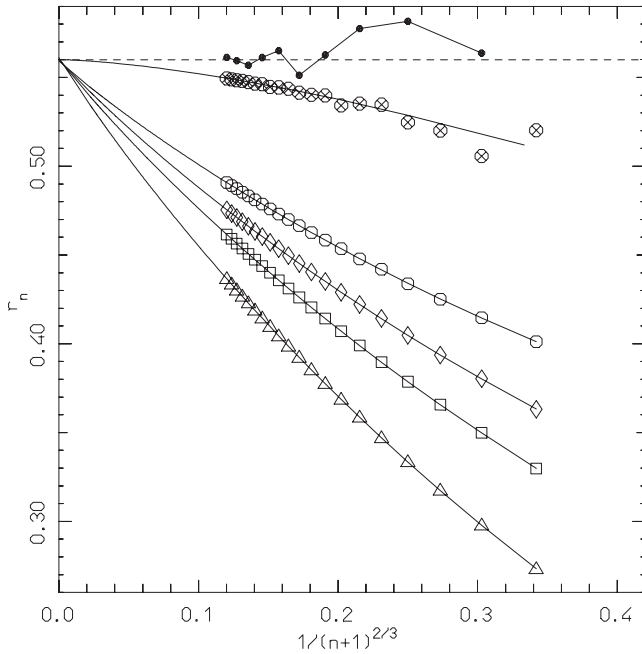


FIG. 1. Ratios of the successive HT-expansion coefficients vs $1/(n+1)^{2/3}$: for the susceptibility χ (open circles), for $m^{(1/2)}$ (rhombs), for $m^{(1)}$ (squares), and for $m^{(2)}$ (triangles). The four lowest continuous curves are obtained by separate three-parameter fits of each ratio sequence to its leading asymptotic behavior [Eq. (11)]. The data points represented by crossed circles are obtained by extrapolating the sequence of the susceptibility alternate ratios with respect to $1/n^{2/3}$, and the continuous line interpolating them is the result of a two-parameter fit of the last few points to the expected asymptotic form $a+b/n$. The small black circles are obtained by a further extrapolation of the latter quantities with respect to $1/n$. The continuous line interpolating the black circles is drawn only as a guide for the eye. The horizontal broken line indicates the critical value $\beta_c=0.559\,95$ suggested by the simulation of Ref. 5.

as the approximants $[k, l, m; n]$ with $17 < k+l+m+n < 22$. Moreover, we have taken $|k-l|, |l-m|, |k-m| < 3$ with $k, l, m > 3$ and $1 < n < 7$. The class of DAs can be varied with no significant variation of the final estimates, for example, by further restricting the extent of off-diagonality or by varying the minimal degree of the polynomial coefficients in the DAs. No limitations have been imposed on the exponents of the singular terms or on the background terms in the DAs in order to avoid biasing the β_c estimates. Should we require that the exponent of the most singular term in the approximants differs from -1 , for example, by less than 20%, we would obtain $\beta_c=0.560\,2(5)$, well within the uncertainty of our previous unrestricted estimate. The vertical dashed line in Fig. 2 shows the value $\beta_c=0.559\,95$ suggested by the simulation of Ref. 5. Although no explicit indication of an uncertainty comes with this estimate, an upper bound to its error might be guessed from the statement⁵ that the simulation can exclude values larger than or equal to $\beta_c=0.560\,45$ for the inverse critical temperature.

Biasing with $\beta_c=0.559\,8(10)$ the set previously specified of second-order DAs of $L(a, \beta)$ leads to the exponent estimate $\sigma=0.50(1)$. Figure 2 also shows the distribution of the

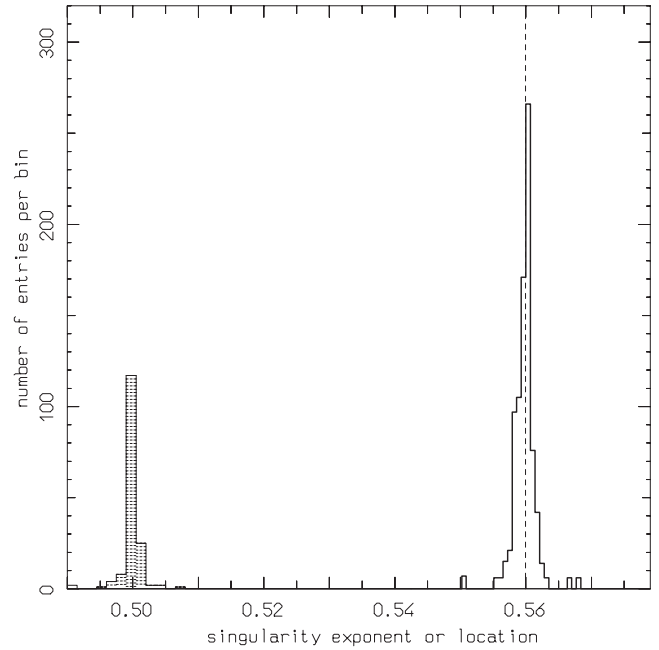


FIG. 2. Distribution of singularities for a class of second-order inhomogeneous DAs of $L(1.19, \beta)=(1.19+\ln \chi)^2$ vs their position on the β axis (open histogram). The central value of the open histogram is $\beta_c=0.559\,8(10)$. The bin width is 0.0007. The vertical dashed line shows the critical value $\beta_c=0.559\,95$ indicated by the simulation of Ref. 5 for which one can guess an uncertainty at least twice smaller than ours. The hatched histogram represents the distribution of the exponent σ obtained from DAs of $L(1.19, \beta)$ biased with $\beta_c=0.559\,8$ vs their position on the σ axis. The central value of the hatched histogram is $\sigma=0.500(1)$ and the bin width is 0.0015. The variation of the central value of σ as β_c varies in its uncertainty interval is 0.01. This value can be taken as a more reliable estimate of the uncertainty of σ .

exponent estimates (hatched histogram) from this biased set. The uncertainty we have reported for σ accounts not only for the width of its distribution shown in Fig. 2 but also for the variation of its central value as the bias value of β_c is varied in the uncertainty interval of the critical inverse temperature. Essentially the same value of σ would be obtained from the analysis of a series truncated to order 21.

While, as one should expect, the DA estimate of β_c is rather insensitive to the choice of a , the estimate of the exponent σ and the width of its distribution are fairly improved by our choice of a . Taking, for example, $a=0$, we would find $\sigma=0.53(4)$, which shows how the convergence of the exponent estimates is slowed down by the more complicated singularity structure of $L(0, \beta)$. Similar values of σ were found in previous studies of shorter series. Probably for the same reason, also the central values of the η estimates obtained from the usual indicators are still slightly larger than expected. For example, by studying the function $H(\beta)=\ln(1+m^{(2)}/\chi^2)/\ln(\chi)$ (or analogous functions of different moments), we can infer $\eta=0.260(10)$. The function⁷ $D(\beta)=\ln(\chi)-(2-\eta)\ln(\xi)$ and its first derivative are also interesting indicators of the value of η . Taking $\eta=1/4$, Padé approximants and DAs do not detect any singular behavior of

$D(\beta)$ or of its derivative as $\beta \rightarrow \beta_c$, thus confirming the complete cancellation of the leading singularity in $D(\beta)$. Moreover, this behavior seems to exclude the form [Eq. (9)] of the corrections which implies the presence of weak subleading singularities, while it is compatible with Eq. (10).

In conclusion, our analysis suggests that, in spite of their diversity, the HT extended series approach and the latest

most extensive simulation are competitive and lead to consistent numerical estimates of the highest accuracy so far possible.

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