High-temperature expansion of the magnetic susceptibility and higher moments of the correlation function for the two-dimensional XY model

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We calculate the high-temperature series of the magnetic susceptibility and the second and fourth moments of the correlation function for the XY model on the square lattice to order $\beta^{33}$ by applying the improved algorithm of the finite lattice method. The long series allow us to estimate the inverse critical temperature as $\beta_c = 1.1200(1)$, which is consistent with the most precise value given previously by the Monte Carlo simulation. The critical exponent for the multiplicative logarithmic correction is evaluated to be $\theta = 0.054(10)$, which is consistent with the renormalization group prediction of $\theta = \frac{1}{16}$.

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I. INTRODUCTION

It is believed that the XY model in two dimensions exhibits a phase transition of the Kosterlitz-Thouless (K-T) type[1], which is driven by the condensation of vortices. From the renormalization group arguments, it was predicted that the correlation length has an essential singularity at the transition temperature $T_c$ as

$$\xi \sim \exp \left( \frac{b}{t^\sigma} \right),$$

with $\sigma = \frac{1}{2}$ where $t = T/T_c - 1$ is the reduced temperature and $b$ is a non-universal constant. At the critical temperature the correlation function behaves like

$$G(r) \sim \frac{(\ln r)^{2\theta}}{r^\eta} \left[ 1 + O \left( \frac{\ln \ln r}{\ln r} \right) \right],$$

with $\eta = \frac{1}{4}$ and $\theta = \frac{1}{16}$, and the $j$-th moment $m_j$ of the correlation function behaves like

$$m_j \sim \xi^{2+j-\eta(\ln \xi)^{2\theta}} \left[ 1 + O \left( \frac{\ln \ln \xi}{\ln \xi} \right) \right].$$

The free energy and its temperature derivatives (i.e., the internal energy and the specific heat) were also predicted to behave like

$$f \sim \xi^{-2} + \text{non-singular term}.$$

At the critical temperature, the first term on the right-hand side of Eq. (4) has an essential singularity with itself and its derivatives going to zero, while the second term stays nonzero.

The behavior in Eq. (1) for the correlation length has been well established both by numerical simulations and the high-temperature expansion. The standard Monte Carlo simulation[2, 3] gave $\beta_c = 1.130(15)$ with $b = 2.15(10)$ and $\beta_c = 1.118(5)$ with $b = 1.70(20)$ for the square lattice. (Here $\beta_c$ is the critical inverse temperature, which will be defined below.) More precise values $\beta_c = 1.1208(2)$ with $b = 1.800(2)$[4] and $\beta_c = 1.1199(1)$ with $b = 1.776(4)$[4] were obtained using the finite-size scaling technique and the renormalization group finite-size scaling method, respectively. In the latter approach, the renormalization group flow of the observable was matched with that of the exactly solvable BCSOS model. The latter value of $\beta_c$ was recently confirmed by a large scale Monte Carlo simulation on a $2048 \times 2048$ lattice using the finite-size scaling method[4]. On the other hand the high-temperature expansion for the magnetic...
susceptibility and higher moments of the correlation function to order $\beta^{31}$ \cite{12} and $\beta^{26}$ \cite{14} gave less precise value $\beta_c = 1.118(3)$ with $b = 1.67(4)$ and $\beta_c = 1.1198(14)$ with $b = 1.77(1)$, respectively. It seems that the available high-temperature series is not long enough to give the estimation of the values for the critical temperature and other critical parameters in the same precision as the Monte Carlo simulation. So it is desirable to extend the high-temperature series to much higher order.

As for the critical exponent $\theta$ for the multiplicative logarithmic correction in the moments of the correlation function, there has been controversial arguments. Negative values ranging from $\theta = -0.077$ to $\theta = -0.056$ \cite{5, 8, 9} were given by the analysis of the numerical simulation based on the thermal scaling formula \cite{14}, while the finite size scaling analysis gave positive values in the range of $\theta = 0.02 - 0.035$ \cite{8, 10, 11}. The large scale Monte Carlo simulation by Hasenbusch \cite{6} gave a value $\theta = 0.056(7)$, which is consistent with the renormalization group prediction, assuming a modified finite-size-scaling behavior

$$m_0 \sim L^{2-\eta} (C + \ln L)^{\theta},$$

where $L$ is the size of the lattice used in the simulation and $C$ is a constant. On the other hand, the high-temperature expansion series to order $\beta^{21}$ \cite{12} gave negative values of $\theta = -0.042(5)$ and $\theta = -0.05(2)$ assuming the thermal scaling \cite{6}. We should note that these values from the high-temperature series are obtained only for the Dlog-Padé approximants and the general inhomogeneous differential approximants do not give convergent result to this order. Higher order series would be needed again to resolve the discrepancy between the result of the high-temperature series analysis and the renormalization group prediction.

A commonly known method for series expansions is the graphical method \cite{15}. However, in this method, one must list all the graphs that contribute to the desired order of the series. An alternative and powerful method to generate the expansion series is the finite lattice method \cite{16, 17, 18}. It avoids listing up all the graphs and it reduces the problem to the calculation of the partition functions for the relevant finite-size lattices, which is a rather straightforward procedure if we use the transfer matrix formulation. In many cases, the finite lattice method generates longer series than the graphical method \cite{19, 20, 21, 22, 23, 24, 25, 26}. Unfortunately, in the case of the XY model in two dimensions, the original finite lattice method can generate a high-temperature series that is at most as long as the series that can be obtained by the graphical method.

In order to generate long series for the the XY model in two dimensions, we here apply an improved algorithm of the finite lattice method developed by the author and Tabata \cite{27, 28}. This improved algorithm is powerful in the case of models in which the spin variable at each site takes more than two values, including an infinite number of values. This algorithm was applied to generate a low-temperature series for the solid-on-solid model \cite{27} and high- and low-temperature series for the $q$-state Potts model in two dimensions \cite{29}. In both cases, it generates much longer series than the original finite lattice method. The XY model in two dimensions can be mapped to a kind of solid-on-solid model, and the improved algorithm of the finite lattice method in fact enabled us to obtain the high-temperature series for the free energy of this model on the square lattice to order $\beta^{33}$ \cite{29}, which is two times longer than the series previously derived. From the analysis of the obtained long series we confirmed that the free energy of the two-dimensional XY model behaves like Eq. (3), with values of the critical temperature and the non-universal constant $b$ that are close to the values obtained in the study of the correlation length. We apply this improved algorithm of the finite lattice method to generate the high-temperature series to order $\beta^{33}$ for the magnetic susceptibility and the second and fourth moments of the correlation function. The obtained long series will provide the value of the critical temperature in the same precision as the latest large scale Monte Carlo simulations and the value of the critical exponent $\theta$ which is consistent with the renormalization group prediction.

In section 2, we describe how to apply the improved algorithm of the finite lattice method to generate the high-temperature series for the moments of the correlation function. In section 3, the high-temperature series to order $\beta^{33}$ are given. Section 4 is devoted to the analysis of the obtained series to evaluate the critical parameters.

II. ALGORITHM

We consider the XY model defined on the square lattice. The Hamiltonian of this system is

$$H = -\sum_{\langle i,j \rangle} J \vec{s}_i \cdot \vec{s}_j,$$

where $\vec{s}_i$ is a two-dimensional unit vector located at the lattice site $i$, and the summation is taken over all pairs $\langle i, j \rangle$ of nearest neighbor sites. The correlation function is given by

$$< \vec{s}_x \cdot \vec{s}_0 > = \frac{\Gamma_{x,0}}{Z},$$
where $Z$ is the partition function

$$Z = \int \prod_i d\theta_i \exp \left( -\frac{H}{kT} \right),$$

and

$$\Gamma_{x,0} = \int \prod_i d\theta_i \bar{s}_x \bar{s}_0 \exp \left( -\frac{H}{kT} \right).$$

Here $T$ is the temperature and $\theta_i$ is the angle variable of the spin $\bar{s}_i = (\cos \theta_i, \sin \theta_i)$.

This model can be mapped exactly to a solid-on-solid model and the numerator and denominator of Eq. (10) can be rewritten as

$$Z = \sum_{\{h \mid -\infty \leq h \leq +\infty\}} \prod_{(i,j)} I_{|h_i - h_j|} (\beta),$$

and

$$\Gamma_{x,0} = \sum_{\{h \mid -\infty \leq h \leq +\infty\}} \prod_{(i,j)} I_{|h_i - h_j + \Delta_{i,j;x,0}|} (\beta),$$

where $\beta = J/kT$, $I_n$ is the modified Bessel function, the product is taken with respect to all the pairs of neighboring plaquettes, and the variable $h_i$ at each plaquette $i$ takes integer value ranging from $-\infty$ to $+\infty$. In Eq. (11) the $\Delta_{i,j;x,0}$ is defined as

$$\Delta_{i,j;x,0} = \begin{cases} 1 & \text{for } b_{i,j} \in L_{x,0}, \\ 0 & \text{otherwise}, \end{cases}$$

where $b_{i,j}$ is the bond sandwiched by the neighboring plaquettes $i$ and $j$, and $L_{x,0}$ is the set of bonds on an arbitrary shortest path connecting the sites $0 = (0,0)$ and $x = (x_1, x_2)$ along the bonds, for which we adopt here the path that starts from the site 0 and go straight first in 1 direction and then in 2 direction reaching the site $x$ when $x_1 x_2 \geq 0$, and first in 2 direction and then in 1 direction when $x_1 x_2 < 0$.

The improved algorithm of the finite lattice method to generate the high-temperature expansion series for the correlation function of this model is essentially the same as that for the free energy described in Ref. [29]. We first calculate the correlation function for each of the finite-size rectangular lattice $\Lambda(l_1 \times l_2, p)$ with a restricted range of the value of the plaquette variable

$$< \bar{s}_x \bar{s}_0 >_{\Lambda; h_+, h_-} = \frac{\Gamma_{x,0}(\Lambda, h_+, h_-)}{Z(\Lambda; h_+, h_-)}.$$

Here the finite size lattice $\Lambda(l_1 \times l_2, p)$ is specified by its size $|\Lambda| = l_1 \times l_2$ and its position $p$, and each plaquette variable $h_i$ is restricted so that $h_- \leq h_i \leq h_+$ (where $h_- \leq 0$ and $h_+ \geq 0$) both in the calculation of the numerator and the denominator. We define the size of the finite lattice so that the $l_1 \times l_2$ lattice involves $l_1 \times l_2$ plaquettes, including the bonds and sites on their boundary. For instance, the $1 \times 1$ lattice consists of a single plaquette, including 4 bonds and 4 sites. We take into account finite-size lattices with $l_1 = 0$ and/or $l_2 = 0$. An $l_1 \times 0$ lattice consists of $l_1$ bonds and $l_1 + 1$ sites with no plaquette. The $0 \times 0$ lattice consists only of one site with no bond or plaquette. The boundary condition is taken such that all the plaquette variables outside the $l_1 \times l_2$ lattice are fixed to zero. The numerator and the denominator of Eq. (13) can be calculated efficiently by the transfer matrix method using a procedure in which a finite-size lattice is built one plaquette at a time [30, 31].

We then define $\phi_{x,0}(\Lambda, h_+, h_-)$ of the finite size lattice $\Lambda$ and of the restricted range of the plaquette variables recursively as

$$\phi_{x,0}(\Lambda, h_+, h_-) = < \bar{s}_x \bar{s}_0 >_{\Lambda; h_+, h_-} - \sum_{\Lambda' \subseteq \Lambda, 0 \leq h_+ \leq h_+, h_- \leq h'_+ \leq 0 \quad (\Lambda', h'_+, h'_-) \neq (\Lambda, h_+, h_-)} \phi_{x,0}(\Lambda', h'_+, h'_-).$$

It should be noted that $\phi_{x,0}(\Lambda, h_+, h_-) = 0$ if the site $x$ or 0 is not included in $\Lambda$. 
The correlation function in the thermodynamic limit is then given by

\[
< \vec{s}_x \vec{s}_0 > \equiv \lim_{|\Lambda| \to \infty, h_+ \to \infty, h_- \to -\infty} < \vec{s}_x \vec{s}_0 >_{\Lambda; h_+, h_-} = \sum_{\Lambda, h_+, h_-} \phi_{x,0}(\Lambda, h_+, h_-). \tag{15}
\]

In the last line of Eq. (15) the summation should be taken for all the lattice size and all of its position and all integer values of \( h_+ \) and \( h_- \) with \( 0 \leq h_+ \leq \infty, -\infty \leq h_- \leq 0 \).

In the standard (graphical) cluster expansion of the correlation function for the SOS model, a cluster is composed of polymers: one main polymer that consists of the set of bonds \( L_{x,0} \) and connected plaquettes attaching to it and possible sub-polymers that consists of connected plaquettes. An example of the main polymer and sub-polymer can be seen in Fig. 1. A value \( h_i (\neq 0) \) is assigned to each plaquette \( i \) of the polymer. We can assign to each cluster two numbers, \( h_{\text{max}} (\geq 0) \) and \( h_{\text{min}} (\leq 0) \), which are the maximum and the minimum, respectively, of the plaquette variable \( h_i \) in all the plaquettes of the polymers of which the cluster consists. Then, we can prove that \( \phi_{x,0}(\Lambda, h_+, h_-) \) includes the contributions to \( < \vec{s}_x \vec{s}_0 > \) from all the clusters of polymers in the standard cluster expansion for which \( h_{\text{max}} = h_+ \) and \( h_{\text{min}} = h_- \) and that can be embedded into the lattice \( \Lambda \) but cannot be embedded into any of its rectangular sub-lattices.
Now we consider from what order the series expansion of $\phi_{x,0}(\Lambda, h_+, h_-)$ with respect to $\beta$ starts. It is enough to give the order for the position $x = (x_1, x_2)$ so that $x_1 \geq 0$ and $x_2 \geq 0$. The order for the other cases is known by the 90° rotational symmetry of the model. Any cluster that contributes to the lowest-order term of the series expansion for $\phi_{x,0}(\Lambda, h_+, h_-)$ consists only of a main polymer. Hence the series expansion of $\phi_{x,0}(\Lambda, h_+, h_-)$ begins from order $\beta^{n_{x,0}(\Lambda, h_+, h_-)}$ in the case of $h_+ \geq 1$ and $h_- \leq -1$ with

$$n_{x,0}(\Lambda, h_+, h_-) = \begin{cases} 
2l_1 + 2l_2 - x_1 - x_2 + 4h_+ & \text{for } (p_1, p_2) = (0, 0) \text{ and } (p_1', p_2') \neq (0, x_2), \\
2l_1 + 2l_2 - x_1 - x_2 + 4h_+ - 2 & \text{for } p_2 = 0, \ p_1' = x_1, \text{ and } (p_1, p_2) \neq (0, x_2) \\
2l_1 + 2l_2 - x_1 - x_2 + 4h_+ - 4 & \text{for the others.} 
\end{cases}$$

Here we denote $(p_1, p_2)$ as the position of the bottom-left corner and $(p_1', p_2')$ as the position of the top-right corner, respectively, of the lattice $\Lambda$ with its size $l_1 \times l_2$ ($p_1' - p_1 = l_1$ and $p_2' - p_2 = l_2$). Examples of the main polymer are given in Fig. 2 (a) (b) (c), which correspond to the three cases in Eq.\(16\), respectively. In the case of $h_+ \geq 1$ and $h_- = 0$ we have

$$n_{x,0}(\Lambda, h_+, h_-) = \begin{cases} 
2l_1 + 2l_2 - x_1 - x_2 + 4h_+ & \text{for } p_1 = 0, \ p_2' = x_2 \text{ and } (p_2, p_1') \neq (0, x_1), \\
2l_1 + 2l_2 - x_1 - x_2 + 4h_+ - 2 & \text{for } p_1 = 0, \ p_2 < 0 \text{ and } (p_2' > x_2 \text{ or } p_1' = x_1), \\
2l_1 + 2l_2 - x_1 - x_2 + 4h_+ - 4 & \text{for the others,} 
\end{cases}$$

and in the case of $h_+ = 0$ and $h_- \leq -1$

$$n_{x,0}(\Lambda, h_+, h_-) = \begin{cases} 
2l_1 + 2l_2 - x_1 - x_2 + 4|h_-| & \text{for } (p_1, p_2) = (0, 0) \text{ and } (p_1', p_2') = (x_1, x_2), \\
2l_1 + 2l_2 - x_1 - x_2 + 4|h_-| + 4 & \text{for } p_2 = 0, \ p_1' = x_1 \text{ and } (p_1, p_2') \neq (0, x_2), \\
2l_1 + 2l_2 - x_1 - x_2 + 4|h_-| & \text{for } p_2 = 0, \ p_1 < 0 \text{ or } p_1' = x_1, \ p_2' > x_2, \\
2l_1 + 2l_2 - x_1 - x_2 + 4|h_-| - 4 & \text{for the others.} 
\end{cases}$$

Examples of the main polymer are given in Fig. 3 (a) and (b), which correspond to the last case in Eq.\(17\) and the last case in Eq.\(18\), respectively. In the case of $h_+ = 0$ and $h_- = 0$ we have

$$n_{x,0}(\Lambda, h_+, h_-) = \begin{cases} 
l_1 + l_2 & \text{for } (p_1, p_2) = (0, 0) \text{ and } (p_1', p_2') = (x_1, x_2), \\
\infty & \text{for the others.} 
\end{cases}$$

Here $n_{x,0}(\Lambda, h_+, h_-) = \infty$ implies that $\phi_{x,0}(\Lambda, h_+, h_-) = 0$.

Thus, in order to obtain the expansion series for the correlation function $< \tilde{s}_{x} \tilde{s}_{0}>$ to order $\beta^N$, we have only to take into account all combinations of the rectangular lattice $\Lambda$ and the range of the plaquette variable $(h_+, h_-)$ that satisfy the relation $n_{x,0}(\Lambda, h_+, h_-) \leq N$ in the summation of Eq.\(15\) and to evaluate each of the $\phi_{x,0}(\Lambda, h_+, h_-)$ to order $\beta^N$.

The $j$-th moment of the correlation function is given by

$$m_j = \sum_x |x|^j < \tilde{s}_{x} \tilde{s}_{0}>$$

where $|x|$ is the distance between the site $x$ and 0. The moment can be calculated more efficiently in the following way. First we calculate $\tilde{\Gamma}_j(l_1, l_2, h_+, h_-)$ defined by

$$\tilde{\Gamma}_j(l_1, l_2, h_+, h_-) = \sum_{x, y \leq \Lambda} \frac{|x-y|^j \Gamma_{x,y}(\Lambda, h_+, h_-)}{Z(\Lambda)}$$

where $\Gamma_{x,y}(\Lambda, h_+, h_-)$ is the correlation function between sites $x$ and $y$ on the lattice $\Lambda$ with plaquette variables $(h_+, h_-)$.
TABLE I: Coefficients of the high-temperature series for the magnetic susceptibility $m_0$. 

| $n$  | $a_{n(0)}$ |
|------|------------|
| 0    | 1          |
| 1    | 4          |
| 2    | 12         |
| 3    | 34         |
| 4    | 88         |
| 5    | 658        |
| 6    | 529        |
| 7    | 14933      |
| 8    | 5737       |
| 9    | 389393     |
| 10   | 2608499    |
| 11   | 3834323    |
| 12   | 1254799    |
| 13   | 8437807    |
| 14   | 6511279891 |
| 15   | 66498259799|
| 16   | 105417874699|
| 17   | 3986350599331|
| 18   | 19830277603399|
| 19   | 8656980509809027|
| 20   | 2985676751081077|
| 21   | 811927408684296587|
| 22   | 39988050180302157|
| 23   | 24527779266620395990697|
| 24   | 8129233625778753288741|
| 25   | 376988970895790950587|
| 26   | 62337378385195430773643|
| 27   | 480555032864478422139959|
| 28   | 80636988313579215330647|
| 29   | 19240186460979407757812460721|
| 30   | 34266867760374182894222566317|
| 31   | 986429202328615891762212069959|
| 32   | 93607376428024822547086555709|
| 33   | 6658861878626519703173982149291449|

for each finite size lattice $\Lambda$. We note that the numerator and the denominator of Eq. [21] depend only on the lattice size $|\Lambda| = l_1 \times l_2$ and on $h_+, h_-$ and that they are independent of the position of the lattice after the summation is taken for $x$ and $y$. They can be calculated efficiently again by the transfer matrix method using the procedure in which a finite-size lattice is built one plaquette at a time not only for $j = 0$ but also for $j \geq 2$ ($j$ : even), the detail of which was described in the application of the finite lattice method to the calculation of the low-temperature series for the second moment of the correlation function in the simple cubic Ising model \[23\]. The moment is then given by

$$m_j = \sum_{l_1,l_2,h_+,h_-} \tilde{\phi}_j(l_1,l_2,h_+,h_-)$$

(22)

where $\tilde{\phi}_j(l_1,l_2,h_+,h_-)$ is defined recursively as

$$\tilde{\phi}_j(l_1,l_2,h_+,h_-) = \Gamma_j(l_1,l_2,h_+,h_-) - \sum_{(l_1',l_2',h_+',h_-')\neq(l_1,l_2,h_+,h_-)} (l_1 - l_1' + 1)(l_2 - l_2' + 1)\tilde{\phi}_j(l_1',l_2',h_+',h_-')$$

(23)

From Eq.\[(16)\] - \[(19)\] we know that $\tilde{\phi}_j(l_1,l_2,h_+,h_-)$ starts from order $\beta^{n_j}(l_1,l_2,h_+,h_-)$ with

$$\hat{n}(l_1,l_2,h_+,h_-) = \begin{cases} l_1 + l_2 & \text{for } h_+ = h_- = 0, \\ l_1 + l_2 + 4h_+ - 4 & \text{for } h_+ > 0 \text{ and } h_- = 0, \\ l_1 + l_2 + 4|h_-| - 3 & \text{for } h_+ = 0 \text{ and } h_- < 0, \\ l_1 + l_2 + 4h_+ + 4|h_-| - 7 & \text{for } h_+ > 0 \text{ and } h_- < 0. \end{cases}$$

(24)

III. SERIES

We have calculated the high-temperature expansion series to order $\beta^{33}$ for the $j$-th moments $m_j$ ($j = 0, 2, 4$) of the correlation function for the XY model on the square lattice ($m_0$ is the magnetic susceptibility). The obtained
TABLE II: Coefficients of the high-temperature series for the second moment \( m_2 \) of the correlation function.

| \( n \) | \( a_n^{(2)} \) |
|---|---|
| 0 | 0 / 1 |
| 1 | 4 / 1 |
| 2 | 32 / 1 |
| 3 | 162 / 1 |
| 4 | 672 / 1 |
| 5 | 7378 / 3 |
| 6 | 24772 / 3 |
| 7 | 312149 / 12 |
| 8 | 202640986 / 45 |
| 9 | 58900571047 / 5040 |
| 10 | 28201211 / 45 |
| 11 | 611969977 / 360 |
| 12 | 202640986 / 45 |
| 13 | 5893118865913171 / 1306368000 |
| 14 | 172156758787 / 23040 |
| 15 | 167630792610 / 90720 |
| 16 | 3336209179 / 112 |
| 17 | 172407619209131397294126152343 / 1694759809280000 |
| 18 | 54125082235073698573313 / 14370048000 |
| 19 | 721617681295019782781 / 112 |
| 20 | 19775777329026559 / 16329600 |
| 21 | 5893118865913171 / 1306368000 |
| 22 | 2287397511857949924319 / 23040 |
| 23 | 167630792610 / 90720 |
| 24 | 3336209179 / 112 |
| 25 | 5893118865913171 / 1306368000 |
| 26 | 721617681295019782781 / 112 |
| 27 | 19775777329026559 / 16329600 |
| 28 | 5893118865913171 / 1306368000 |
| 29 | 721617681295019782781 / 112 |
| 30 | 19775777329026559 / 16329600 |

The expansion coefficients are listed in Table I, II and III, where the coefficient \( a_n^{(j)} \) is defined as

\[
m_j = \sum_{n=1}^{N} a_n^{(j)} \left( \frac{\beta}{2} \right)^n.
\]

We have checked that each of the \( \tilde{\phi}_j(l_1, l_2; h_+, h_-) \)'s in Eq. (23) starts from the correct order in \( \beta \), as given by Eq. (24). Our series coincide exactly with the series to order \( \beta^{21} \) for \( j = 0 \), 2 and 4 given by Campostrini et al. \[12\] and to order \( \beta^{26} \) for \( j = 0 \) and 2 given by Butera and Pernici \[13, 14\], which was obtained by a graphical method and a non-graphical recursive algorithm based on the Schwinger-Dyson equations, respectively.

To obtain the large numerators and denominators of the coefficients exactly, we have used the same technique as in the calculation of the free energy series \[29\]. In each step of the calculation the series expansion of a function \( f(\beta) \) is expressed as

\[
f(\beta) = \sum_n \frac{a_n}{n!} \left( \frac{\beta}{2} \right)^n,
\]

then the product of the two functions is given by

\[
f(\beta)g(\beta) = \sum_n \frac{c_n}{n!} \left( \frac{\beta}{2} \right)^n,
\]

with

\[
c_n = \sum_{n'=0}^{n} \frac{n!}{n'(n-n')!} a_{n-n'} b_{n-n'},
\]

and, if \( a_n \)'s and \( b_n \)'s are integers, \( c_n \)'s are also integers.

The calculations were carried out on a PC cluster at the Information Processing Center at OPCT and on an Altix3700 BX2 at Yukawa Institute of Kyoto University.
TABLE III: Coefficients of the high-temperature series for the fourth moment $m_4$ of the correlation function.

| $n$ | $a_n^{(4)}$ |
|-----|-------------|
| 0   | 0 / 1       |
| 1   | 4 / 1       |
| 2   | 96 / 1      |
| 3   | 930 / 1     |
| 4   | 6112 / 1    |
| 5   | 96850 / 3   |
| 6   | 147648 / 1  |
| 7   | 7305173 / 12|
| 8   | 2319540 / 9 |
| 9   | 498173873 / 60|
| 10  | 1271029508 / 45|
| 11  | 2210163319 / 24|
| 12  | 2606525954 / 9 |
| 13  | 444953438647 / 5040|
| 14  | 147648 / 1  |
| 15  | 81597010130527 / 10752|
| 16  | 1271029508 / 45|
| 17  | 7305173 / 12 |
| 18  | 2319540 / 9  |
| 19  | 498173873 / 60|
| 20  | 1271029508 / 45|
| 21  | 2210163319 / 24|
| 22  | 2606525954 / 9 |
| 23  | 444953438647 / 5040|
| 24  | 147648 / 1  |
| 25  | 81597010130527 / 10752|
| 26  | 1271029508 / 45|
| 27  | 7305173 / 12 |
| 28  | 2319540 / 9  |
| 29  | 498173873 / 60|
| 30  | 1271029508 / 45|
| 31  | 2210163319 / 24|
| 32  | 2606525954 / 9 |
| 33  | 444953438647 / 5040|

IV. SERIES ANALYSIS

From Eq. (3) the logarithm of the moment of the correlation function is expected to behave near the critical temperature like

$$\ln m_j \sim \frac{(2 + j - \eta)b}{\tau^\sigma} + O(\ln \tau), \quad (29)$$

where $\tau = 1 - \beta/\beta_c$ and $\beta_c = J/kT_c$ is the critical inverse temperature. Here we analyze it by the first order inhomogeneous differential approximation (IDA), in which the differential equation for $f(\beta) = \ln m_j$ is satisfied as

$$Q_m(\beta) f'(\beta) + P_l(\beta) f(\beta) + R_k(\beta) = O(\beta^{m+l+k+2}), \quad (30)$$

where $Q_m(\beta)$, $P_l(\beta)$ and $R_k(\beta)$ are polynomials of order $m$, $l$ and $k$ respectively and $Q_m(0) = 1$. The critical inverse temperature $\beta_c$ is given by the zero of $Q_m(\beta)$ and the exponent $\sigma$ is evaluated by

$$\sigma = -\frac{P_l(\beta_c)}{Q_m'(\beta_c)}. \quad (31)$$

In the analysis by the first order IDA here and below, we restrict $m + l + k + 2$ to be the maximum order of the analyzed series with $-1 \leq k \leq 9$ and $|m - l| \leq 4$, and exclude the approximants that have another zero of $Q_m(\beta)$ with $|\beta - \beta_c|/\beta_c < 0.10$, which is called near-by singularity.

In Fig. 4 we plot the zeros of $Q_m(\beta)$ in the complex plane of $\beta$. Besides clear accumulation of the points around $\beta = 1.12$ we see another accumulation around the nonphysical point $\beta = \beta_0 \sim -1.2 \pm 0.1i$. In order to remove the influence of this nonphysical critical point, we have made Euler transformation

$$\beta' = \frac{\beta}{1 - \beta/\beta_0}, \quad (32)$$

with $\beta_0 = -1.2$. In fact after this transformation the IDA gives a series of $(\beta_c, \sigma)$ which converges better onto a straight line. Biased analysis fixing $\sigma = \frac{1}{2}$ gives $\beta_c = 1.1200(4)$. Hence we apply this Euler transformation in all of the series analysis presented below.
The above analysis ignores the existence of the sub-leading correction terms to the leading power-law singularity of $\ln m_j$ in Eq.(29). So we have analyzed a combination of $m_0$ and $m_2$ as

$$\ln m_0 + c \ln \frac{m_2}{4\beta},$$

(33)

searching the parameter $c$ which will give more convergent result, anticipating that the sub-leading terms will be cancelled between the first and second terms in Eq.(33). In Fig. 5 we plot the estimated value of $\beta_c$ versus $c$ in the biased analysis fixing $\sigma = \frac{1}{2}$. We find that the choice of the parameter $c = 0.08 - 0.12$ gives nicely converging result of $\beta_c = 1.12007(4)$. We have also analyzed another combination as

$$\ln m_0 + c' \ln (1 + c'' m_2),$$

(34)

where $c''$ is an arbitrary parameter which should be chosen so that the combination will give the most convergent result. We have obtained the most convergent result of $\beta_c = 1.12003(5)$ for $c' = 0.05$ and $c'' = 0.58$ and $\beta_c = 1.11997(5)$ for $c' = 0.03$ and $c'' = 0.68$. Thus we can safely estimate $\beta_c = 1.1200(1)$. This value is quite consistent with the most precise value $\beta_c = 1.1199(1)$ obtained by Hasenbusch from the large-scale Monte Carlo simulation. Our value is much more precise than the value $\beta_c = 1.1198(14)$ by Butera and Pernici from the high-temperature series to order $\beta^{26}$.

Assuming the critical behavior of Eq.(11) and (3) we can estimate the non-universal parameter $b$ by the Padé
FIG. 6: Plot of the estimated value of $\theta$ by the 1st order IDA for the test function versus $B$.

approximation of

$$
\left(1 - \frac{\beta}{\beta_c}\right)^{\frac{1}{2}} \ln \left(1 + c \frac{m_2}{m_0}\right) \sim b
$$

(35)

and

$$
\left(1 - \frac{\beta}{\beta_c}\right)^{\frac{1}{2}} \ln \left(1 + c' \frac{m_4}{m_2}\right) \sim b.
$$

(36)

By searching the parameter $c$ or $c'$ that gives the most convergent estimation of $b$ keeping $\beta_c = 1.12000$ and $\sigma = \frac{1}{2}$, both of the two give the same result of $b = 1.758(1)$ for $c = 3.15 - 3.23$ and for $c' = 0.806 - 0.812$ respectively. Here we have used all of $[m, l]$ Padé approximants with $m \geq 14$ and $l \geq 14$. This value is a bit smaller than $b = 1.800(2)$ and $b = 1.776(4)$ obtained in the Monte Carlo simulations.

Unfortunately the long series do not improve the estimation of the exponent $\eta$ so much. For instance, the Padé approximation of the quantities

$$
\frac{\ln \left(1 + c \frac{m_2}{m_0}\right)}{\ln m_0} \sim \frac{2}{2 - \eta}
$$

(37)

and

$$
\frac{\ln \left(1 + c' \frac{m_4}{m_2}\right)}{\ln m_0} \sim \frac{\eta}{2 - \eta}
$$

(38)

give the most convergent result of $\eta = 0.256(2)$ for $c = 0.69$ and $\eta = 0.227(2)$ for $c' = 0.60$, respectively. The Padé approximation of

$$
\left(1 - \frac{\beta}{\beta_c}\right)^{\frac{1}{2}} \ln \left(1 + c' \frac{m_4}{m_2}\right) \sim \eta b
$$

(39)

gives $\eta b = 0.429(5)$ for $c'' = 0.83 - 0.89$ and, if we combine this with the above result $b = 1.758(1)$, gives $\eta = 0.244(3)$.

As for the exponent $\theta$, Dlog-Padé analysis of the 20th order series of the quantities

$$
\frac{m_0}{(m_2/m_0)^{2-\eta}} \sim \frac{m_4}{(m_2/m_0)^{6-\eta}} \sim \tau^{-2\sigma \theta} \{1 + O(\tau^\sigma \ln \tau)\}
$$

(40)
gave estimations $\theta = -0.042(5)$ and $\theta = -0.05(2)$, which have the sign opposite to the renormalization group prediction of $\theta = \frac{1}{16}$. The situation does not change even if our long series are used in the Dlog-\Pade analysis of these quantities. The series of the two quantities to 33rd order gives $\theta = -0.019(1)$ and $\theta = -0.015(9)$, respectively. The IDA with $k \geq 0$ gives rather convergent values within the same $k$ but quite scattered values for different $k$'s.

One possible reason why IDA for these quantities give scattered values for different $k$ may be the existence of the sub-leading logarithmically singular term in Eq.(40), which comes from the correction factor in Eq.(3). In fact the sub-leading logarithmic singularity can strongly disturb the correct evaluation of the leading power low exponent $2\sigma \theta$ if this exponent is as small as $\frac{1}{16}$. We plot in Fig. 6 the estimated value of $\theta$ by IDA for the expansion series to order $\beta^{33}$ for a test function

$$
\tau^{-2\sigma \theta} \left\{ 1 + \tau^\sigma (A + B \ln \tau) \right\}
$$

with $\theta = \frac{1}{16}$, $\sigma = \frac{1}{2}$, and $A = 0$ plotted versus $B$. We find that the estimated value of $\theta$ is quite sensitive to the amplitude $B$ of the logarithmic term, and although each approximant with the same $k$ gives rather convergent result for any fixed value of $B$, the approximants with different $k$ give the estimation of $\theta$ far from each other.

Thus we have evaluated $\theta$ using the combination of $m_0$, $m_2$ and $m_4$ as

$$
m_0^\alpha (1 + c'm_2)^{\alpha'} (1 + c''m_4)^{\alpha''}
$$

with

$$
\alpha(2 - \eta_0) + \alpha'(4 - \eta_0) + \alpha''(6 - \eta_0) = 0
$$

where

\[ \begin{align*}
\alpha & = 2 - \eta_0 \\
\alpha' & = 4 - \eta_0 \\
\alpha'' & = 6 - \eta_0
\end{align*} \]
and
\[ \alpha + \alpha' + \alpha'' = 1 \] (44)
and \( \eta_0 = \frac{1}{4} \), which is also considered to behave like Eq. [11] in general. We can however anticipate that, by taking the combination of the three quantities, the subleading logarithmic term may be cancelled if we choose appropriate values for the parameters \( \alpha \), \( \alpha' \) and \( \alpha'' \). We have used the biased 2nd order IDA:
\[ \tau^2 Q_{m_2}(\beta) f''(\beta) + \tau Q_{m_3}(\beta) f'(\beta) + P_1(\beta) f(\beta) + R_k(\beta) = O(\beta^m + m_1 + l + k + 3) \] (45)
with \( Q_{m_2}(0) = 1 \). The exponent \(-2\sigma \theta\) can be evaluated by the solution \( \gamma \) of
\[ \gamma(\gamma - 1) \frac{Q_{m_2}(\beta_c)}{\beta_c^2} - \gamma \frac{Q_{m_1}(\beta_c)}{\beta_c} + P_1(\beta_c) = 0. \] (46)

Here we adopt \( \beta_c = 1.1200 \). The 2nd order IDA can make more precise evaluation of \( \theta \) than the 1st order IDA for the function like Eq. [11]. Fig. 7 is the plot of the estimation of \( \theta \) by the 2nd order IDA for the 33rd order series of the test function [11] with \( \theta = \frac{1}{16} \), \( \sigma = \frac{1}{2} \), and \( A = 0.3 \). Of course the 2nd order IDA also gives different values of \( \theta \) for each of \( k \) if \( B \neq 0 \), but if \( B \) is small enough it can present precise estimation for the exponent of the leading singularity. By the analysis of the real combined quantity [12] we have found that the estimated values of \( \theta \) converge to \( \theta = 0.050(15) \) for all the range of \(-1 \leq k \leq 9 \) in a domain of the set of parameters \(-\alpha = 3.6 - 3.0 \), \( \alpha' = 2.8 - 4.0 \) and \( \alpha'' = 2.8 - 4.0 \). In the analysis we have restricted \( m_2 + m_1 + l + k + 3 = 32 \) with \(-1 \leq k \leq 9 \) and \( m_2 \geq 7 \), \( m_1 \geq 7 \), \( l \geq 7 \). The approximants that have near-by singularity (i.e. the zero of \( Q_2(\beta) \) or \( Q_1(\beta) \)) with \( |\beta - \beta_c|/\beta_c < 0.2 \) have been excluded. The most convergent result \( \theta = 0.054(10) \) is obtained for \( \alpha = -3.143 \), \( \alpha' = 3.134 \) and \( \alpha'' = 3.139 \). The values of \( \theta \) for each \( k \) in this set of parameters are shown in Fig. 8. We note that this value \( \theta = 0.054(10) \) is consistent with \( \theta = \frac{1}{16} \) predicted by the renormalization group.

V. SUMMARY

We calculated the high-temperature series for the zeroth moment (magnetic susceptibility) and the second and fourth moments of the correlation function in the XY model on the square lattice to order \( \beta^{12} \) by using the improved algorithm of the finite lattice method. The obtained long series have presented us an estimation for the value of the critical inverse temperature as \( \beta_c = 1.120(1) \), which is consistent with the most precise value given previously by the Monte Carlo simulation. The critical exponent \( \theta \) for the multiplicative logarithmic correction is evaluated using the combination of the three moments of the correlation function, giving \( \theta = 0.054(10) \), which is consistent with the value \( \theta = \frac{1}{16} \) predicted by the renormalization group argument.

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