Shape dependent finite-size effect of critical two-dimensional Ising model on a triangular lattice

Xintian Wu, 1,* Nickolay Izmailian, 2† and Wenan Guo 1,‡

1Department of Physics, Beijing Normal University, Beijing, 100875, China
2A.I. Alikhanyan National Science Laboratory, Alikhanian Br.2, 375036 Yerevan, Armenia.

(Dated: May 5, 2014)

Abstract

Using the bond-propagation algorithm, we study the finite-size behavior of the critical two-dimensional Ising model on a finite triangular lattice with free boundaries in five shapes: triangle, rhombus, trapezoid, hexagon and rectangle. The critical free energy, internal energy and specific heat are calculated. The accuracy of the free energy reaches $10^{-26}$. Based on accurate data on several finite systems with linear size up to $N = 2000$, we extract the bulk, surface and corner parts of the free energy, internal energy and specific heat accurately. We confirm the conformal field theory prediction of the corner free energy to be universal and find logarithmic corrections in higher order terms in the critical free energy for the rhombus, trapezoid, and hexagon shaped systems, which are absent for the triangle and rectangle shaped systems. The logarithmic edge corrections due to edges parallel or perpendicular to the bond directions in the internal energy are found to be identical, while the logarithmic edge corrections due to corresponding edges in the free energy and the specific heat are different. The corner internal energy and corner specific heat for angles $\pi/3$, $\pi/2$ and $2\pi/3$ are obtained, as well as higher order corrections. Comparing with the corner internal energy and corner specific heat previously found on a rectangle of the square lattice (Phys. Rev. E. 86 041149 (2012)), we conclude that the corner internal energy and corner specific heat for the rectangle shape are not universal.

PACS numbers: 02.70.-c, 05.50.+q, 75.10.Nr, 75.10.Hk

*wuxt@bnu.edu.cn
†izmail@yerphi.am
‡waguo@bnu.edu.cn
I. INTRODUCTION

The finite-size scaling theory, introduced by Fisher, finds extensive applications in the analysis of experimental, Monte Carlo, and transfer-matrix data, as well as in recent theoretical developments related to conformal invariance [1–4]. It becomes of practical interest due to the recent progresses in fine processing technologies, which has enabled the fabrication of nanoscale materials with novel shapes [5–7]. Exact solutions have been playing a key role in determining the form of finite-size scaling. Ferdinand and Fisher [8] pioneered on the two-dimensional (2D) Ising model on a finite size square lattice, which extended Onsager’s exact solution [9] and stimulated the ideas of finite-size scaling. Since then, exact results of the model on finite size lattices with various boundaries have been studied intensively [8–18]. Detailed knowledge has been obtained for the torus case [12], for the helical boundary condition [13], for the Brascamp-Kunz boundary condition [14, 15] and for an infinitely long cylinder [16]. The exact solution on the triangular lattice has also been studied intensively [17, 18].

However for the 2D Ising model the exact solution with free boundaries, i.e. free edges and sharp corners, is still missed. As we know, the Bethe ansatz is a powerful technique to solve the 2D Ising model, but this technique would not allow to place the system on a rectangle with free boundary conditions on top and bottom, since the expression of the boundary state in terms of the Bethe eigenvectors is unknown, which is a famous unsolved problem in statistical mechanics. Although there are Monte Carlo and transfer matrix studies on this problem [19, 20], the accuracy or the system sizes of the results are not enough for extracting the finite size corrections. Meanwhile, for 2D critical systems, a huge amount of knowledge has been obtained by the application of the powerful techniques of integrability and conformal field theory (CFT) [3, 4, 21, 23]. Cardy and Peschel predicted that the next subdominant contribution to the free energy on a square comes from the corners [3], which is universal, and related to the central charge $c$ in the continuum limit. Kleban and Vassileva [21] extended the result to a rectangle. These results are consistent with the conjectured exact analytic formula for the Ising model on a square lattice [24].

Several years ago an efficient bond propagation (BP) algorithm was developed for computing the partition function of the Ising model with free edges and corners in two dimensions [25, 26]. Making use of this algorithm, we recently determined numerically the exact
partition function of the Ising model on the square lattice with rectangle shape and free boundaries [27]. We not only confirmed the CFT predictions, but also found logarithmic corrections due to corners in the internal energy and specific heat.

In present paper we apply the BP algorithm to study the Ising model on finite triangular lattices with free boundaries in five different shapes, focusing on how the shape affects the finite-size scaling. The five shapes are triangle, rhombus, trapezoid, hexagon and rectangle, as shown in Fig. 1. Based on accurate data on a sequence of finite systems with linear size up to \( N = 2000 \), we extract the bulk, surface and corner parts of the free energy, internal energy and specific heat accurately. We verify the conformal field theory prediction of the corner free energy and find logarithmic corrections in higher order terms in the critical free energy for the rhombus, trapezoid, and hexagon shaped systems, which are absent for the triangle and rectangle shaped systems. The logarithmic edge corrections due to edges parallel or perpendicular to the bond direction in the internal energy are found to be identical, while the logarithmic edge corrections due to the corresponding edges in the specific heat are different. The corner internal energy and corner specific heat for angles \( \pi/3, \pi/2 \) and \( 2\pi/3 \) are obtained, as well as higher order corrections. Comparing with the previous found corner internal energy and corner specific heat on a rectangle of the square lattice [27], we conclude that the corner internal energy and corner specific heat for the rectangle shape are not universal.

Our paper is organized as follows: In section II we briefly describe the BP algorithm used here. We present in sec. III our main results and discussion. We conclude in sec. IV.

II. METHOD

The partition function of the Ising model on the 2D triangular lattice is

\[
Z = \sum_{\{\sigma_i\}} \exp (\beta \sum_{(i,j)} \sigma_i \sigma_j),
\]

where the nearest neighbor couplings are dimensionless and \( \beta \) is the inverse temperature. This partition function for finite triangular lattice with five different shapes and open boundaries is calculated with the BP algorithm [25] at the exact critical point \( \beta_c = \frac{1}{4} \ln(3) = 0.274653072167 \cdots \). Figure 1 shows the five shapes: triangle, rhombus, trapezoid, hexagon and rectangle. The linear size \( N \) of a finite lattice is defined as the length of edges in the tri-
FIG. 1. (a) The triangle-shaped triangular lattice with \( N = 4 \). (b) The rhombus-shaped lattice with \( N = 4 \). (c) The trapezoid-shaped lattice with \( N = 3 \). (d) The hexagon-shaped lattice with \( N = 3 \). (e) The rectangle-shaped lattice with \( N = 5 \). Three bond directions and the perpendicular direction are shown (see text).

angle, rhombus and hexagon cases, of which the length of edges are equal. For the trapezoid shape, \( N \) is the shortest edge, of which the lengths of the three short edges are required to be equal. For the rectangle, \( N \) is defined as the length of the bottom edge, and the number of layers is required to be \( N \), which means the actual geometrical vertical length is \( N\sqrt{3}/2 \). According to the finite-size scaling [1], the system size should be the actual geometrical length, not the number of layers. Therefore the aspect ratio of the rectangle, we consider here, is \( \sqrt{3}/2 \) rather than 1.

The BP algorithm for the Ising model on the triangular lattice has been described in detail in [26]. For the triangle-shaped and rhombus-shaped lattice, this algorithm can be applied directly. However, for the trapezoid-shaped, hexagon-shaped and rectangle-shaped lattice, the inverse of the BP series reduction should be introduced, which corresponds to generating a new spin between two spins such that

\[
e^{J_{12}\sigma_1\sigma_2} \equiv \sum_{\sigma_0} e^{\delta F + J\sigma_0(\sigma_1 + \sigma_2)},
\]

as illustrated in Fig. 2(a). It is convenient to use variables \( j \equiv e^{-J} \), \( j_{12} \equiv e^{-J_{12}} \) and \( \delta f \equiv e^{\delta F} \). Then we get the solution \( \delta f = j_{12}/2 \) and \( j = \sqrt{j_{12}^2 - \frac{1}{j_{12}^2}} - 1 \).

In each step of the BP algorithm the transformation is exact. The numerical accuracy is only limited by the machine’s precision, which is the round-off error \( 10^{-32} \) in the quadruple
FIG. 2. (a) Inverse of the BP series reduction. See the formulation for this transformation in text. (b)-(g) are schematic of the algorithm for the trapezoid-shaped lattice. From (b) to (c), the inverse of BP series reduction is applied to the diagonal bond (thick line) at the bottom of the trapezoid. From (c) to (d), this operation is applied to another diagonal bond (thick line). From (d) to (e) bond propagation operations are applied. From (e) to (f), the inverse of BP series reduction is applied again. (f) to (g) Those diagonal bonds are eliminated by the usual BP procedure.

The BP algorithm needs about $N^3$ steps to calculate the free energy of a $N \times N$ lattice (much faster than other numerical method). Therefore the total error is approximately $N^{3/2} \times 10^{-32}$. This estimation has been verified in the following way: We compared the results obtained using double precision, in which there are 16 effective decimal digits, and those using quadruple precision. Because the latter results are much more accurate than the formal, we can estimate the error in double precision results by taking the quadruple results as the exact results. We thus found that the error is about $N^{3/2} \times 10^{-16}$. In our calculation, the largest size reached is $N = 2000$, the round-off error is less than $10^{-26}$.

The free energy density, internal energy per spin and specific heat density are calculated at the critical point according to

$$\begin{align*}
    f &= \ln \frac{Z}{S}, \quad u = \frac{\partial f}{\partial \beta}, \quad c = \beta^2 \frac{\partial^2 f}{\partial \beta^2},
\end{align*}$$

respectively, where $S$ is the number of spins on the lattice, which is $S = N(N + 1)/2$, $N^2$, $N(3N - 1)/2$, $3N^2 - 3N + 1$, $N^2 - (N - 1)/2$ for the triangle, rhombus, trapezoid, hexagon and rectangle shaped system, respectively. One can alternatively define the free
energy density according to the actual geometrical area, which is different from the present definition by a trivial constant.

With the BP algorithm, we obtain the free energy density $f$ directly. The internal energy and specific heat are calculated by using a differentiation method

$$u \approx -\frac{f(\beta_c + \Delta \beta) - f(\beta_c - \Delta \beta)}{2\Delta \beta},$$

$$c \approx \beta_c^2 \frac{f(\beta_c + \Delta \beta) + f(\beta_c - \Delta \beta) - 2f(\beta_c)}{(\Delta \beta)^2}.$$  

(4)

In our calculation, $\Delta \beta = 10^{-7}$ is used. The analysis of error in the calculations of $u$ and $c$ has been discussed in [27]. The final estimation of the accuracy of the free energy, internal energy and specific heat is $10^{-26}, 10^{-11}, 10^{-9}$, respectively.

The calculations were carried out for $10^5, 10^4, 10^3, 85, 127$ systems, with linear size $N$ varying from 30 to 2000, for the triangle, rhombus, trapezoid, hexagon and rectangle shaped triangular lattice, respectively.

III. RESULTS

A. Critical free energy density

By fitting the finite size data, we find that the exact expansion of the critical free energy can be written in the following form, with $k$ from 3 to 12 for the triangle and rectangle, $k$ from 3 to 9 for the other shapes:

$$f = f_\infty + f_{\text{surf}} \frac{p(N)}{S} + \frac{f_{\text{corn}} \ln N + f_2}{S} + \sum_{k=3} f_k + l_k \ln N S^{k/2},$$  

(5)

where $p(N)$ is the perimeter, which equals to $3N, 4N, 5N - 1, 6N, (2 + \sqrt{3})N$ for the triangle, rhombus, trapezoid, hexagon and rectangle, respectively. This expansion is different from that for the triangular lattice with periodic boundary conditions [18], in which there’s no surface, corner terms, logarithmic corrections, and only even $k$ presents.

The fitting method is the standard Levenberg-Marquardt method for nonlinear fit. The standard deviation (SD) is defined by $\sigma = \sqrt{\sum (f_i - f_i^{(\text{fit})})^2 / (n_d - n_f)}$ with $f_i$ the numerical data, $f_i^{(\text{fit})}$ the value given by the fitting formula, $n_d$ the number of data used and $n_f$ the number of fitting parameters. For all cases, $\sigma$ reaches $10^{-25}$. The accuracy is seen from the fitted bulk free energy density $f_\infty$: the worst fit among the five cases is for the rhombus,
which yields \( f_\infty = 0.879585386161571570938962(7) \), and the best one is for the triangle yielding \( f_\infty = 0.8795853861615715709389605(3) \). These results coincide with the exact value \( f_\infty = 0.879585386161571570938960283 \ldots \) in more than 24 decimal numbers.

\[
\begin{array}{|c|c|c|c|}
\hline
\text{shape} & f_{\text{surf}} & f_{\text{corn}} & f_2 \\
\hline
\text{triangle} & -0.103077638834090655343(2) & 0.1666666666666666667(4) & 0.00680483246685952(4) \\
\text{rhombus} & -0.103077638834090655343(2) & 0.14583333333333333333(2) & 0.1839728334687587(1) \\
\text{trapezoid} & -0.103077638834090655343(1) & 0.14583333333333333333(2) & 0.2213952601428039(1) \\
\text{hexagon} & -0.103077638834090655343(2) & 0.1041666666666666668(3) & 0.4758271527774812(2) \\
\text{rectangle} & -0.10907840733730539239(2) & 0.125000000000000000001(2) & 0.22549835683994714(1) \\
\hline
\end{array}
\]

TABLE I. The fitted edge, corner free energy and \( f_2 \) in Eq. (5).

According to finite-size scaling, the surface correction term \( f_{\text{surf}}p(N)/S \) stems from free edges. As shown in Fig. (1(e)), there are three bond directions for the triangular lattice. For the triangle, rhombus, trapezoid, and hexagon shapes, the edges are all along one bond direction. The edge free energy per unit length on these edges should be equal. For the rectangle shape, there are two edges along one bond direction and two other edges perpendicular to that bond direction in a zigzag way. Therefore the edge free energy per unit length along the two different directions can be different in principle. To be clear, we denote the surface free energy per unit length (the straight length, not the total length of the zigzag line) along and perpendicular to the bond direction as \( f_{\parallel}\text{surf} \) and \( f_{\perp}\text{surf} \), respectively. The surface free energy is thus \( f_{\text{surf}}p(N) = f_{\parallel}\text{surf}p(N) \) for the triangle, rhombus, trapezoid, and hexagon shape, respectively. For the rectangle shape, it is \( f_{\text{surf}}p(N) = \bar{f}_{\text{surf}}(2 + \sqrt{3})N \), with \( \bar{f}_{\text{surf}} = (2f_{\parallel}\text{surf} + \sqrt{3}f_{\perp}\text{surf})/(2 + \sqrt{3}) \), which is the mean surface free energy per unit perimeter, considering the straight length of the edges along the perpendicular direction is \( \sqrt{3}N/2 \), which is used to define the perimeter. The fitted values of \( f_{\text{surf}} \) is given in Tab. I.

For the rectangle case, we obtain

\[
f_{\parallel}\text{surf} = -0.103077638834090655343(2), \quad f_{\perp}\text{surf} = -0.116007497958656704304(2). \tag{6}
\]

Cardy and Peschel showed in [3] that the presence of a corner of interior angle \( \gamma \) along boundaries of typical size \( N \) give rise to a logarithmic correction to the critical free energy density

\[
f_{\text{corn}} \frac{\ln N}{S} = -\frac{c_\gamma}{24\pi}(1 - (\frac{\pi}{\gamma})^2)\frac{\ln N}{S}, \tag{7}
\]
where $c$ is the conformal anomaly. The total corner free energy is

\[
f_{\text{corn}} = \begin{cases} 
3f_{\text{corn}}^{(\pi/3)} = \frac{1}{6} = 0.1666666... & \text{for triangle} \\
2 \left( f_{\text{corn}}^{(\pi/3)} + f_{\text{corn}}^{(2\pi/3)} \right) = \frac{7}{48} = 0.14583333... & \text{for rhombus and trapezoid} \\
6f_{\text{corn}}^{(2\pi/3)} = \frac{5}{48} = 0.10416666... & \text{for hexagon} \\
4f_{\text{corn}}^{(\pi/2)} = \frac{1}{8} = 0.125 & \text{for rectangle}
\end{cases}
\]

The fitted corner free energy $f_{\text{corn}}$ for the five shapes are listed in Tab. I, from which one can see that our results reproduces the CFT result very accurately.

TABLE II. The fitted parameters for order $k \geq 3$ in Eq. (5) for the critical free energy of the triangle and rectangle shaped triangular lattices. There is no logarithmic corrections except for the corner term, i.e., all $l_k = 0$.

| shape  | triangle                 | rectangle                  |
|--------|--------------------------|----------------------------|
| $f_3$  | 0.117851130197757931(2)  | -0.0144959340650645(9)     |
| $f_4$  | 0                        | 0.0180683705511(1)         |
| $f_5$  | -0.00245523187923(4)     | -0.01237101066(1)          |
| $f_6$  | 0.001247090597(1)        | 0.0168641489(1)            |
| $f_7$  | -0.0016255469(3)         | 0.00302743(4)              |
| $f_8$  | 0.00124715(1)            | 0.001335(1)                |
| $f_9$  | -0.0005633(2)            | -0.03133(3)                |
| $f_{10}$| -0.000553(3)             | 0.0701(4)                  |
| $f_{11}$| 0.00159(2)               | -0.161(2)                  |
| $f_{12}$| -0.050(4)                |                           |

In the previous study on the finite square lattice in a rectangle shape[27], we estimated the corner free energy $f_{\text{corn}} = 0.125 \pm 2.0^{-10}$ for the rectangle shape with various aspect ratios. Here we find the same result $f_{\text{corn}} = 0.125 \pm 2.0 \times 10^{-18}$ on the rectangle-shaped triangular lattice. This indicates that the corner term of the free energy is independent of the microscopic properties of the lattice. Therefore we proved the CFT prediction that the corner free energy is universal [3]. However, our calculations are for the aspect ratio fixed as $\rho = 2/\sqrt{3}$ at present work. Thus it is not enough to further verify Kleban’s CFT predictions on the effect of the aspect ratio of the rectangle-shaped lattice [21].
TABLE III. The fitted parameters of Eq. (5) for the critical free energy. The third and fourth order logarithmic correction $l_3, l_4$ are zero.

| shape   | rhombus                        | trapezoid                    | hexagon                     |
|---------|--------------------------------|------------------------------|-----------------------------|
| $f_3$  | $0.0486111111111112(2)$        | $-0.00210692865756(2)$       | $-0.06014065304055(7)$     |
| $f_4$  | $-0.00810185186(2)$            | $0.01363281706(2)$           | $0.03472222217(7)$         |
| $f_5$  | $0.00381144(6)$               | $-0.00686168(6)$             | $-0.0180976(4)$            |
| $f_6$  | $-0.00215(1)$                 | $0.00894(1)0$                | $0.0150(1)$                |
| $f_7$  | $-0.0008(5)$                  | $0.0316(6)$                  | $-0.018(7)$                |
| $f_8$  | $-0.026(4)$                   | $-0.113(5)$                  | $-0.56(9)$                 |
| $f_9$  | $0.032(2)$                    | $0.097(3)$                   | $0.21(3)$                  |

| $l_5$  | $0.00346339(1)$               | $0.00494874(1)$              | $0.00999797(6)$            |
| $l_6$  | $-0.003461(2)$                | $-0.008767(3)$               | $-0.00863(2)0$            |
| $l_7$  | $0.0024(1)$                   | $0.0117(2)$                  | $0.011(2)0$               |
| $l_8$  | $0.006(2)$                    | $0.011(3)$                   | $0.17(5)$                  |
| $l_9$  | $0.007(5)$                    | $0.070(8)$                   | $0.9(2)$                   |

For higher order terms, we give fitted coefficients in Tab. III and IV. For the critical free energy of the triangle and rectangle shaped triangular lattices, there is no logarithmic corrections except for the corner term, i.e., all $l_k = 0$. For the triangle shape, the coefficient $f_4$ is determined to be zero since it is extremely small in our fits if this term is present, and the fitting result changes little if we discard this term. In contrast to the triangle and rectangle shape, for the other three shaped triangular lattices, we find higher order ($k \geq 5$) logarithmic corrections besides the corner term. Although these logarithmic corrections are very weak, with very small coefficients, our high accurate data indicate their existence.

B. Critical internal energy density

We fit the data on the critical internal energy with the following formula

$$u = u_\infty + u_{surf} \frac{p(N) \ln N}{S} + u_{corn} \frac{\ln N}{S} + \sum_{k=1}^{\infty} \frac{u_k}{S^{k/2}},$$

where $p(N)$ is again the perimeter. In our fits, $k$ is truncated to 4. Again, this formula is different from that for the triangular lattice with periodic boundary conditions [18], in
which there’s no logarithmic surface term, no corner term, and only odd \(k\) presents. The bulk value \(u_\infty\) is known to be 2 \[17\]. Our fit of \(u_\infty\) is \(2.0 \pm 1.0 \times 10^{-10}\) for the five shapes. The other fitted parameter are given in Tab. IV.

| TABLE IV. The fitted parameters of Eq. (8) for the critical internal energy per spin. |
|---------------------------------|-----------------|-----------------|-----------------|-----------------|
| shape              | triangle | rhombus | trapezoid | hexagon | rectangle |
| \(u_{surf}\)   | -0.55132891(2) | -0.551328867(8) | -0.55132888(1) | -0.55132891(2) | -0.5513290(7) |
| \(u_{corn}\)   | -1.653995(3) | -0.735055(7) | -0.73506(1) | 1.10268(2) | 0.147707(6) |
| \(u_1\)         | 0.1358131(3) | -0.7286080(2) | -1.4553110(3) | -3.4498392(7) | -1.1246224(2) |
| \(u_2\)         | -1.42006(1) | -1.09359(3) | -0.55400(4) | 1.71014(4) | -0.95485(2) |
| \(u_3\)         | -0.70291(8) | -0.2154(3) | 0.0302(4) | -0.372(1) | 0.1049(2) |
| \(u_4\)         | -0.0243(4) | 0.113(2) | 0.044(4) | 0.49(1) | -0.030(2) |

The leading correction is due to the edges (or surface), which is unknown to our knowledge. We denote the surface internal energy per unit length of the edge along one bond direction by \(u_{surf}^{\parallel}\), and that perpendicular to that direction by \(u_{surf}^{\perp}\). For the triangle, rhombus, trapezoid, and hexagon shapes, we have \(u_{surf} = u_{surf}^{\parallel}\). For the rectangle we have \(u_{surf} = (2u_{surf}^{\parallel} + \sqrt{3}u_{surf}^{\perp})/(2 + \sqrt{3})\), and

\[
\begin{align*}
    u_{surf}^{\parallel} &= -0.55132889(2), \\
    u_{surf}^{\perp} &= -0.55132895(7).
\end{align*}
\]

This is an interesting result because it means that the surface internal energy per unit length is symmetric for an edge along or perpendicular to an arbitrary bond direction. Comparing this result with \(u_{surf}\) for the rectangle shaped square lattice in our previous work\[27\], where \(u_{surf} = 0.6366198(1)\), we find that the ratio is 1.1547005, which is very close to \(2/\sqrt{3} = 1.154700538\cdots\). Because the exact value of \(u_{surf}\) for the square lattice is \(2/\pi\) \[11\], we conjecture that the exact value of the surface internal energy for the triangular lattice is given by

\[
    u_{surf}^{\parallel} = u_{surf}^{\perp} = -\sqrt{3}/\pi.
\]

Following the convention for the critical free energy, we write the coefficient of \((\ln N)/S\) as \(u_{corn}\). We denote the corner correction by \(u_{corn}^{(\gamma)}\), where \(\gamma\) is the angle of the corner. Under
the assumption that \( u_{\text{corn}} \) is the sum of the corner’s contributions, we have

\[
  u_{\text{corn}} = \begin{cases} 
    3u_{\text{corn}}^{(\pi/3)} & \text{for triangle} \\
    2 u_{\text{corn}}^{(\pi/3)} + u_{\text{corn}}^{(2\pi/3)} & \text{for rhombus and trapezoid} \\
    6u_{\text{corn}}^{(2\pi/3)} & \text{for hexagon} \\
    4u_{\text{corn}}^{(\pi/2)} & \text{for rectangle}
  \end{cases}
\]

From the Tab. IV, we obtain the corner term for the three angles

\[
  u_{\text{corn}}^{(\pi/3)} = -0.551332(1), \quad u_{\text{corn}}^{(\pi/2)} = 0.036927(2), \quad u_{\text{corn}}^{(2\pi/3)} = 0.183781(3). \quad (11)
\]

In the previous study on the square lattice [27], we obtained the corner term \( u_{\text{corn}} = -0.4502(1) \) for the rectangle with various aspect ratios. It is different from the present result \( u_{\text{corn}} = 0.147707(6) \) for the rectangle-shaped triangular lattice, which indicates that the corner term of the internal energy depends on the microscopic structure of the lattice, thus is not universal.

The other parameters \( B_1, B_2, B_3, B_4 \) are also estimated and listed in Tab. IV. We have tried other forms of formula to fit the critical internal energy. The terms \( \ln S/S^{3/2}, \ln S/S^2 \) are excluded considering the coefficients are extremely small. Moreover the standard deviations of the fits with these terms included are much larger than those without them.

C. Critical specific heat

The data of the critical specific heat are fitted using the following formula

\[
  c = A_0 \ln N + c_0 + c_{\text{surf}} \frac{p(N) \ln N}{S} + c_{\text{corn}} \frac{\ln N}{S} + \sum_{k=1}^{\infty} \frac{c_k}{S^{k/2}}, \quad (12)
\]

where \( p(N) \) is the perimeter. \( k \) is from 1 to 4 in our fits. Compared with the expansion for the triangular lattice with periodic boundary conditions [18], there are additional logarithmic surface term and corner term.

The leading term \( A_0 \ln N \) is known from the exact result [18], which reads \( A_0 = \frac{3\sqrt{3}}{4\pi} (\ln 3)^2 \approx 0.4990693780 \cdots \). Our fit yields \( A_0 \approx 0.499069374(5) \). The other fitted parameters are listed in Tab. IV.

The leading correction \( p(N) \ln N/S \) is caused by the edges. We denote the surface specific heat per unit length of the edge along one bond direction by \( c_{\text{surf}}^\parallel \), and that perpendicular
to the direction by $c_{\text{surf}} \perp$. For the triangle, rhombus, trapezoid, and hexagon shape, we have $c_{\text{surf}} = c_{\parallel \text{surf}}$, for the rectangle, we set $c_{\text{surf}} = (2c_{\parallel \text{surf}} + \sqrt{3}c_{\perp \text{surf}})/(2 + \sqrt{3})$, and find

$$
c_{\parallel \text{surf}} = 0.166354(2), \quad c_{\perp \text{surf}} = 0.105462(2).
$$

Note that this term is absent in the torus case [8] and not mentioned in the long strip case [11], but exists in the cylinder case with Brascamp-Kunz boundary conditions [14, 15].

**TABLE V. The fitted parameters of Eq. (12) for the critical specific heat of the five shapes.**

| shape     | triangle | rhombus | trapezoid | hexagon | rectangle |
|-----------|----------|---------|-----------|---------|-----------|
| $c_0$     | $-0.80424237(1)$ | $-0.60510331(1)$ | $-0.51995011(1)$ | $-0.2673395(1)$ | $-0.573388895(9)$ |
| $c_{\text{surf}}$ | $0.1663558(3)$ | $0.1663531(5)$ | $0.1663520(5)$ | $0.166338(9)$ | $0.1380941(8)$ |
| $c_1$     | $-0.187862(5)$ | $-0.036692(3)$ | $-0.10391(2)$ | $-0.2749(2)$ | $-0.08529(9)$ |
| $c_{\text{corn}}$ | $0.7484(1)$ | $0.3864(2)$ | $0.3857(3)$ | $-0.343(6)$ | $-0.1510(2)$ |
| $c_2$     | $0.6410(4)$ | $0.6443(8)$ | $0.615(1)$ | $0.58(2)$ | $0.6833(7)$ |
| $c_3$     | $0.339(2)$ | $0.177(6)$ | $0.04(1)$ | $-0.09(3)$ | $-0.057(5)$ |
| $c_4$     | $0.024(8)$ | $-0.12(4)$ | $-0.00(7)$ | $1.8(3)$ | $0.17(3)$ |

Following the convention for the critical free energy, we write the coefficient of $(\ln N)/S$ as $c_{\text{corn}}$. We denote the corner correction by $c_{\gamma \text{corn}}$ where $\gamma$ is the angle of the corner. Again, under the assumption that the total correction is the sum of the corners, we have

$$
c_{\text{corn}} = \begin{cases} 
3c_{\gamma \text{corn}}^{(\pi/3)} & \text{for triangle} \\
2 \left(c_{\gamma \text{corn}}^{(\pi/3)} + c_{\gamma \text{corn}}^{(2\pi/3)}\right) & \text{for rhombus and trapezoid} \\
6c_{\gamma \text{corn}}^{(2\pi/3)} & \text{for hexagon} \\
4c_{\gamma \text{corn}}^{(\pi/2)} & \text{for rectangle}
\end{cases}
$$

From Tab. IV we obtain the corner contribution of the three angles,

$$
c_{\gamma \text{corn}}^{(\pi/3)} = 0.24948(3), \quad c_{\gamma \text{corn}}^{(\pi/2)} = -0.03775(5), \quad c_{\gamma \text{corn}}^{(2\pi/3)} = -0.057(1).
$$

In the previous study on the square lattice [27], we obtained the corner term $c_{\text{corn}} = 0.368(1)$ for the rectangle with various aspect ratios. It is different from the present result $c_{\text{corn}} = -0.1510(2)$ for the rectangle-shaped triangular lattice, which indicates that the corner term of the specific heat depends on the microscopic structure of the lattice, thus is not universal.
We have also tried other forms of fitting formula to fit the critical specific heat data. For example, we added the terms \((\ln S)^3/S\), \((\ln S)^2/S\) in the fitting formula and found that their coefficients are extremely small.

**IV. CONCLUSION**

Using the BP algorithm, we have studied the 2D critical Ising model on a triangular lattice with free boundaries. For five shapes, triangle, rhombus, trapezoid, hexagon and rectangle, the critical free energy, internal energy and specific heat have been calculated. We have proved the conformal field theory prediction of the corner free energy and have shown that the corner free energy, which is proportional to the central charge \(c\), is indeed universal. For the edges parallel or perpendicular to the bond direction, the logarithmic edge corrections in the internal energy have been found to be almost identical, while these corrections in the free energy and in the specific heat have been found to be different. Comparing with the previous result on the square lattice in the rectangle shape, we have found that the corner internal energy \(u_{\text{corn}}\) and the corner specific heat \(c_{\text{corn}}\) for the rectangle shape are not universal, i.e., the coefficient in front of \(\ln N/S\) in the expansion of the internal energy and the specific heat are different for the square lattice and the triangular lattice.

We have also found that there exist logarithmic corrections in higher orders, say, there are terms \(\ln N/S^{5/2}\), \(\ln N/S^3\), \(\cdots\) in the critical free energy for the rhombus, trapezoid, and hexagon shapes. However these terms are absent for the triangle and rectangle shapes. This should be an interesting subject to be further investigated.

**ACKNOWLEDGMENTS**

This work is supported by the National Science Foundation of China (NSFC) under Grant No. 11175018.

---

[1] V. Privman and M. E. Fisher, Phys. Rev. B 30, 322 (1984).
[2] V. Privman, Phys. Rev. B 38, 9261 (1988).
[3] J. L. Cardy and I. Peschel, Nucl. Phys. B 300, 377 (1988).
[4] H. W. J. Blöte, J. L. Cardy, and M. P. Nightingale, Phys. Rev. Lett. 56, 742 (1986).
[5] S. Kawata, H.-B. Sun, T. Tanaka, K. Takeda, Nature 412, 697 (2001).
[6] V. F. Puntes, K. M. Krishnan, A. P. Alivisatos, Science 291, 2115 (2001).
[7] Y. Yin, R. M. Rioux, C. K. Erdonmez, S. Hughes, G. A. Somorjai, A. P. Alivisatos, Science 304, 711 (2004).
[8] A. E. Ferdinand and M. E. Fisher, Phys. Rev. 185, 832 (1969).
[9] L. Onsager, Phys. Rev. 65, 117 (1944).
[10] B. Kaufman, Phys. Rev. 76, 1232 (1949).
[11] H. Au-Yang and M. E. Fisher, Phys. Rev. B 11, 3469 (1975).
[12] E. V. Ivashkevich, N. Sh. Izmailian and C.-K. Hu, J. Phys. A 35 (2002) 5543.
[13] N. Sh. Izmailian and C.-K. Hu, Phys. Rev. E. 76, 041118 (2007).
[14] N. Sh. Izmailian, K. B. Oganesyan and C.-K. Hu, Phys. Rev. E 65 (2002) 056132.
[15] W. Janke and R. Kenna, Phys. Rev. B 65, 064110 (2002).
[16] N. Sh. Izmailian and C.-K. Hu, Phys. Rev. Lett. 86, 5160 (2001).
[17] G. F. Newell, Phys. Rev. 79, 876 (1950); R. M. F. Houttapel, Physica 16, 425 (1950).
[18] J. Salas, J. Phys. A: Math. Gen. 35, 1833 (2002).
[19] D. P. Landau, Phys. Rev. B 13, 2997 (1976).
[20] B. Stošić, S. Milošević and H. E. Stanley, Phys. Rev. B , 16, 11466 (1990).
[21] P. Kleban and I. Vassileva, J. Phys. A: Math. Gen. 24, 3407 (1991).
[22] R. Bondesan, J. Dubail, J. L. Jacobsen, and H. Saleur, Nucl. Phys. B 862, 555 (2012).
[23] R. Bondesan, J. L. Jacobsen, and H. Saleur, Nucl. Phys. B 867, 913 (2013).
[24] E. Vernier and J. L. Jacobsen, J. Phys. A: Math. Gen. 45, 045003 (2012).
[25] Y. L. Loh and E. W. Carlson, Phys. Rev. Lett. 97, 227205 (2006).
[26] Y. L. Loh, E. W. Carlson, and M. Y. J. Tan, Phys. Rev. B 76, 014404 (2007), in which a review of similar earlier algorithms is also presented.
[27] X.-T. Wu, N. Sh. Izmailian, and W.-A. Guo, Phys. Rev. E 86 041149 (2012).