Finite size behaviors of critical Ising model on a rectangle with free boundaries

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(Dated: May 2, 2014)

Using the bond-propagation algorithm, we study the Ising model on a rectangle of size $M \times N$ with free boundaries. For five aspect ratios $\rho = M/N = 1, 2, 4, 8, 16$, the critical free energy, internal energy and specific heat are calculated. The largest size reached is $M \times N = 64 \times 10^6$. The accuracy or the system sizes of the results are not enough to extract the finite size corrections. Meanwhile, for 2D quantum systems with open boundaries, in 2D it is the natural one to consider in the case of quenches for one dimensional quantum systems with open boundaries. In 2D it is the simplest geometry to study transport properties for Anderson localization. Although there are Monte Carlo and transfer matrix studies on this problem [14, 15], the accuracy or the system sizes of the results are not enough to extract 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) [16–18]. Cardy and Peschel predicted that the next subdominant contribution to the free energy on a square comes from the corners [17], which is universal, and related to the central charge $c$ in the continuum limit. Kleban and Vassileva [18] extended the study of the free energy on a rectangle. They further derived a geometry dependent term to the free energy. However, they did not determine a geometry independent additive constant in the coefficient. Till now there is few evidence for these predictions from exact solutions or numerical calculations. Furthermore, as far as we know, there is no detailed study of the internal energy and the specific heat on a rectangle neither by CFT nor by exact solutions/numerical calculations.

Recently an efficient bond propagation (BP) algorithm was developed for computing the partition function of the Ising model in two dimensions, which is exact to machine precision and works for any planar network of Ising spins with arbitrary bond strengths [19, 20]. It is also much faster than Monte Carlo simulation, and costs quite moderate memory comparing with the transfer matrix method. Very large system size can be reached. The BP algorithm is thus a powerful tool to study the Ising model on a rectangle with free edges and corners. In this letter we apply the BP algorithm to study the Ising model on an $M \times N$ rectangle. We obtain finite size data of the critical free energy $f$, internal energy $U$ and specific heat $c$. By fitting these data we find that the exact expansion of the critical free energy, internal energy and specific heat can be written in the following form

\begin{equation}
    f = f_\infty + f_{\text{surf}} \frac{M + N}{S} + f_{\text{corn}} \frac{\ln S}{S} + \sum_{k=1}^{\infty} \frac{A_k}{S^{(k+1)/2}},
\end{equation}

\begin{equation}
    U = U_\infty + U_{\text{surf}} \frac{M \ln N + N \ln M}{S} + U_{\text{corn}} \frac{\ln S}{S} + \sum_{k=1}^{\infty} \frac{B_k}{S^{k/2}},
\end{equation}
\[ f = A_0 \ln N + c_0 + c_{\text{surf}} \frac{M \ln N + N \ln M}{S} + c_{\text{corn}} \ln S + \sum_{k=1}^{\infty} \frac{D_k}{S^{k/2}}. \]

where \( S = M \times N \) is the area of the system. \( f_\infty, U_\infty \) are the bulk term, \( f_{\text{surf}}, U_{\text{surf}} \) the surface coefficient, \( f_{\text{corn}}, U_{\text{corn}} \) the corner coefficient for the free energy, internal energy respectively. \( c_{\text{surf}}, c_{\text{corn}} \) are the corresponding coefficients for the specific heat. We find the fitted values \( f_\infty, f_{\text{surf}}, f_{\text{corn}}, f_{\text{corn}}, A_0 \) are excellently consistent to the exactly known results \[11,10,11\]. The corner free energy \( f_{\text{corn}} = c/8 \) \[17,18\] is proved. More over the geometry independent constant, which is ignored in Kleban and Vassileva work \[18\], is determined. We also find the corner contributions \( U_{\text{corn}} \) and \( c_{\text{corn}} \), which are independent of aspect ratio. As far as we know, no previous studies predict such terms. We start by introducing the BP algorithm briefly. Then we present our numerical results and analysis.

Method. The schematic of the BP algorithm is shown in Fig. 1. In this algorithm BP series reduction, BP \( \Delta - Y \) transformation and its inverse are the building blocks. By successively integrating in and then integrating out spin degrees of freedom in a way that only introduces local changes to the network, this algorithm progressively moves degrees of freedom to an open edge of the network, where they are eliminated. The transformation in each step is exact. The numerical accuracy is limited by machine's precision, which is the round-off error \( 10^{-32} \) in the quadruple precision. The BP algorithm needs about \( N^3 \) steps to calculate the free energy of an \( N \times N \) 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 \( M = N = 8000 \), the round-off error is less than \( 10^{-26} \). The partition function of the Ising model on a 2D square 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. The free energy density, internal energy per spin and specific heat density are defined by

\[ f = \frac{\ln Z}{MN}, \quad U = \frac{\partial f}{\partial \beta}, \quad c = \beta^2 \frac{\partial^2 f}{\partial \beta^2}. \]

![Fig. 1.](image-url) (Color online) (a) and (b) are building blocks of the BP algorithm: BP series and BP \( \Delta - Y \) transformation, respectively. (c) The schematic of BP algorithm. (c1) The BP algorithm: BP series and BP \( \Delta - Y \) transformation, respectively. (c2) The \( \Delta - Y \) transformation is applied to the three spins and three bonds in red. (c3) The schematic of BP algorithm. (c4) The schematic of BP algorithm. (c5) The schematic of BP algorithm. (c6) Finally only two spins and one bond are left.

respectively. With the BP algorithm, we get the free energy density \( f \) at the critical \( \beta_c = \frac{1}{2} \ln(1 + \sqrt{2}) = 0.44068679 \cdots \) directly. The internal energy and specific heat are calculated by using a differentiation method

\[ U \approx -\frac{f(\beta_c + \Delta \beta) - f(\beta_c - \Delta \beta)}{2 \Delta \beta}, \]

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

In our calculation, \( \Delta \beta = 10^{-7} \) is used. The error in the calculation of \( U \) due to the finite \( \Delta \beta \) is approximately \( 4/(\Delta \beta)^2 \partial^2 f/\partial \beta^2 \), which is less than \( 10^{-11} \) for the lattice with \( N \leq 2000 \). The error in the calculation of \( c \) due to finite \( \Delta \beta \) is \( 4/(\Delta \beta)^3 \partial^3 f/\partial \beta^3 \), which is less than \( 10^{-9} \) for \( N \leq 2000 \). Another source of error is the accumulated error due to round-off, which is less than \( 10^{-26} \). This error is amplified by \( 1/\Delta \beta (1/\Delta \beta^2) \) times in the calculations of \( U \) (c), which is thus around \( 10^{-19} \) \((10^{-12})\). Therefore the errors of \( U, c \) are mainly caused by the finite \( \Delta \beta \) in the differentiation. In other words the accuracies of the free energy, internal energy and specific heat are \( 10^{-20}, 10^{-11}, 10^{-9} \) respectively.

The calculations have been carried out for various aspect ratios \( M/N = 1, 2, 4, 8, 16 \) on an \( M \times N \) rectangular lattice. For \( M = N \), the calculation was carried out from \( N = 30 \) to \( N = 8000 \). For \( M = 2, 4, 8, 16 \), the calculated lattice sizes are from \( N = 30 \) to \( N = 2000 \).

Critical free energy. We fit the data of free energy density with the formula given by Eq. 1 with \( k \) from 1 to 8. The fitting method is the Levenberg-Marquardt method \[21\] for nonlinear fit. The standard deviation (SD) is defined by

\[ SD = \sqrt{\sum_i (f_i - f_i^{(fit)})^2/(n_d - n_f)} \]
with $f_i$ the numerical data, $f_i^{(fit)}$ the value given by the fitting formula, $n_d$ the data number and $n_f$ the number of fitting parameters. For all $\rho$, $SD$ reaches $10^{-20}$.

The high accuracy can be seen from the bulk value $f_\infty$. For $\rho = 1$, the fitted values of $f_{\infty}$ is

$$0.92969539834161021499(1).$$

The asymptotic bulk value of the free energy density should be the same as the exact result given by Onsager, i.e.,

$$D_0 = \ln \sqrt{2} - \frac{2}{\pi} G = 0.92969539834161021506 \cdots$$

where $G = 1 - \frac{1}{\pi} + \frac{1}{\pi} - \frac{1}{\pi} + \cdots$. Our estimation is consistent to it in the accuracy of $10^{-20}$. For other $\rho$ the consistency is the same.

According to finite size scaling, the surface correction term stems from free edges. This correction for the model on an infinitely long strip with two free edges has been found through exact solution to be ($D_1 - \frac{1}{\pi} \ln(1 + \sqrt{2})/N$, where $D_1 = \int_0^\infty \ln[1 + \sqrt{2}(1 - \cos \theta)]^{1/2}(3 - \cos \theta)^{-1/2} \approx 0.2589553765253 \cdots$). Note the infinitely long strip can be considered as a rectangle with a aspect ratio $\rho \to \infty$. Thus the surface correction for a rectangle should be $f_{\text{surf}}(M + N)/S$ with $f_{\text{surf}} = D_1 - \frac{1}{\pi} \ln(1 + \sqrt{2}) = -0.1817314169844187569 \cdots$. Our fitting results coincide with this prediction precisely. For $\rho = 1, 2$, the fitted values $-f_{\text{surf}}$ are $0.18173141698441877(3)$, $0.1817314169844188(1)$ respectively, and for $\rho = 4, 8, 16$, they are all $0.1817314169844188(2)$. The correction term $f_{\text{corn}} \ln S/S$ stems from the corners of the rectangle. According to Cardy and Peschel, the four corners, at $M = N$, give rise to the term $\frac{2}{\pi} \ln(N)/N^2$, where $c = 1/2$ is the central charge. Kleban and Vassileva extended the results to a rectangle with $M \neq N$ using CFT: The corner free energy is $c \ln(S)/(8S)$, which yields

$$f_{\text{corn}} = \frac{c}{8} \ln(2) = 0.0625.$$

In our fitting $f_{\text{corn}}$ are found to be $0.0625 + (2 \pm 3) \times 10^{-14}$, $0.0625 + (1 \pm 2) \times 10^{-12}, 0.0625 + (1 \pm 5) \times 10^{-12}, 0.0625 + (1 \pm 5) \times 10^{-12}, 0.0625 \pm 1 \times 10^{-11}$ for $\rho = 1, 2, 4, 8, 16$ respectively. All of them lead to the central charge $c = 0.5$ with the error less than $10^{-10}$. There is a $1/N^2$ correction for the infinitely long strip $[12, 18]$ with the coefficient $c \pi/24 \approx 0.0654498$. Kleban and Vassileva proved that, for a finite rectangle, the correction is proportional to $1/S = 1/(M \times N)$ with the coefficient

$$A'_1 = -\frac{c}{4} \ln[\eta(q) \eta(q')],$$

where $\eta(q) = q^{1/24} \prod_{n=1}^{\infty}(1 - q^n)$ with $q = e^{-2\pi \rho}, q' = e^{-2\pi / \rho}$. At the limit $\rho \to \infty$, $A'_1 \rho^{-1} \to c \pi/24$ which recovers the infinitely long strip result.

However, Kleban and Vassileva mentioned that, in their derivation, a possible geometry-independent additive constant was ignored $[18]$. In other words, the coefficient of $1/S$ should be

$$A_1 = A'_1 + F_0,$$

where $F_0$ is the constant which contributes $F_0/S = F_0/(\rho N^2)$ to the free energy density, which tends to 0 in the infinitely long strip limit. For $\rho = 1, 2, 4, 8, 16$, the values of $A'_1$ are $0.065918017562, 0.087578866954, 0.17555900232, 0.393633679243, 0.873910756056$ respectively. By comparing the fitted $A_1$ (see Tab. II) and the theoretical $A'_1$, we obtained this constant

$$F_0 = -0.0049488147(2).$$

The other parameters $A_2, \cdots, A_8$ are fitted and listed in Tab. II. For the infinitely long strip, $A_2 \rho^{-3/2}, A_3 \rho^{-2}$ and $A_4 \rho^{-5/2}$, at the limit $\rho \to \infty$, correspond to the coefficients of $N^{-3}, N^{-4}$ and $N^{-5}$ terms in the finite size free energy expansion respectively, which have been obtained as $-0.04616(2), 0.024(1), 0.69(6)$, by using numerical transfer matrix techniques $[22]$. Simple extrapolations of the fitted values of $A_2, A_3, A_4$ show that the magnitude of $A_2, A_3$ agree with the transfer matrix results, but $A_4$ does not. We have tried other forms of formula to fit the critical free energy data. For example, we added the terms $\ln S/S^{1/2}, \ln S/S^2$ in the fitting formula and found that the corresponding coefficients are extremely small (less than $10^{-7}$). We concluded that the logarithmic correction only appears in the corner term $\ln S$. We note here that, in the asymptotic expansion of the free energy for the Ising model with periodic boundary conditions $[8]$, with Braskamp-Kunz boundary conditions $[11]$ and with helical boundary conditions $[10]$, only integer powers of $S$ appear.

**Critical internal energy.** We fit the data of critical internal energy with the formula given by Eq. (2) with $k$ from 1 to 4. The bulk value $U_\infty$ is known to be $\sqrt{2} \approx 1.41421356237 \cdots$. Our fit of $U_\infty$ is 1.4142135624 for the five aspect ratios. The leading correction should be caused by the edges. In the exact result of Au-Yang and Fisher $[2]$ on the strip with two free edges, the edges’ correction is given by $-\frac{1}{2} \ln N/N$. We conjecture that, on the rectangle with four free edges, the edge correction is given by $-\frac{1}{2} (M \ln N + N \ln M)/(M N)$ with the coefficient $U_{\text{surf}}(\rho) = -\frac{1}{2} \approx -0.636619773 \cdots$. This conjecture is proved by the fitted $U_{\text{surf}}$ for all $\rho$ ($U_{\text{surf}} = -0.6366198\cdots$), which agree with the predicted value in the accuracy $10^{-7}$.

The term $B_1/S^{1/2}$ is in fact scaled as $1/N$. In the infinitely long strip limit, the coefficient before $1/N$ is known as $\frac{1}{\pi} (\ln 2 + \gamma - \frac{2}{\pi} - \ln \pi) \approx 0.683158 \cdots$. As we can see in Tab. III, $B_1/\sqrt{\rho}$ indeed approaches this limit as $\rho$ increases.

Following the convention in the critical free energy, we write the coefficient of $\ln(S)/S$ as $U_{\text{corn}}$. We found

$$U_{\text{corn}}(\rho) \approx -0.45025(3),$$

which is independent of aspect ratio $\rho$. Apparently, this contribution becomes zero in the limit of infinitely long strip, in which there is no corner. From this point, it is rational to call this term corner’s correction.
Onsager’s exact result \[5\], which reads

\[
\frac{U}{S} = -c_0 \ln \rho + c_{s_{surf}} + c_{corn} \rho, \quad \rho = 1, 2, 4, 8, 16
\]

for the critical free energy. We brought numerical evidence that the correction term \(c_{corn}\) stems from the corners of the rectangle is Indeed universal and is proportional to the central charge \(c\). We also found that the terms \(U_{surf}\) and \(c_{corn}\) are independent from the aspect ratio \(\rho\). In order to check whether or not the terms \(U_{corn}\) and \(c_{corn}\) are universal quantities, it is useful to extend our study to the Ising model on other types of lattices, e.g., the triangular, honeycomb, Kagome lattices. In such studies, the BP algorithm which is suitable for any planar network of Ising spins with arbitrary bond strengths \([13, 20]\) is still a powerful tool. In addition, we can enhance the accuracy of the internal energy and specific heat by using an extended BP algorithm to calculate the internal energy without the using of differentiation\[20\]. Moreover the finite size effects of the correlation can be investigated by using the site propagation algorithm \[23\]. As we have shown, the sharp corners induce remarkable effects in critical region not only on the free energy, but also on the internal energy and the specific heat. It is expected that the sharp corners can induce remarkable effects on other properties of finite size systems in critical regime, for example, thermal conductivity, electric conductivity, etc. All of these effects should be observable in experiments.

### Table I. The fitted parameters of Eq. \([3]\) for the critical free energy.

| parameter | \(\rho = 1\) | \(\rho = 2\) | \(\rho = 4\) | \(\rho = 8\) | \(\rho = 16\) |
|-----------|---------------|---------------|---------------|---------------|---------------|
| \(A_1\)   | 0.000999202833(3) | 0.0826300522(2) | 0.17020715502(4) | 0.388684864512(8) | 0.86896194132(2) |
| \(A_2\)   | 0.0883883476(2) | 0.059556310(1) | -0.1009034881(4) | -0.666287857(1) | -2.43248445(3) |
| \(A_3\)   | -0.0175362651(2) | 0.04067435(2) | 0.418424017(7) | 2.1854954(3) | 9.76558(1) |
| \(A_4\)   | -0.02405666(2) | -0.174428(2) | -1.2901339(9) | -8.155035(3) | -48.5563(3) |
| \(A_5\)   | 0.066893(8) | 0.4351(1) | 3.9657(8) | 33.676(6) | 277.21(5) |
| \(A_6\)   | -0.16558(2) | -1.147(4) | -13.85(5) | -161.7(5) | -1857(6) |
| \(A_7\)   | 0.3851(4) | 3.22(8) | 53(1) | 86(2) | 137(4) |
| \(A_8\)   | -0.703(3) | -7.6(8) | -17(2) | -387(4) | -8(1) |

### Table II. The fitted parameters of Eq. \([2]\) for the critical internal energy per spin.

| parameter | \(\rho = 1\) | \(\rho = 2\) | \(\rho = 4\) | \(\rho = 8\) | \(\rho = 16\) |
|-----------|---------------|---------------|---------------|---------------|---------------|
| \(U_{surf}\) | -0.63661981(1) | -0.63661983(3) | -0.63661985(4) | -0.63661987(5) | -0.63661988(5) |
| \(B_1\)   | -0.1213621(2) | -0.2586182(5) | -0.6453965(8) | -1.266482(1) | -2.151535(2) |
| \(U_{corn}\) | -0.450170(3) | -0.45018(1) | -0.45022(2) | -0.45028(4) | -0.45042(9) |
| \(B_2\)   | -0.98604(2) | -1.1278(9) | -1.7138(2) | -3.2016(4) | -6.4893(9) |
| \(B_3\)   | -0.2969(2) | -0.101(1) | 0.833(3) | 3.943(8) | 13.40(2) |
| \(B_4\)   | -0.040(2) | -0.41(1) | -2.40(4) | -11.2(2) | -47.7(7) |

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

### Critical specific heat.

The data of the critical specific heat are fitted using the formula given by Eq. \([15]\) with \(k\) from 1 to 4. The leading term \(A_0 \ln N\) is known from Onsager’s exact result \([3]\), which reads \(A_0 = \frac{\gamma}{4} \ln (1 + \sqrt{2})^2 \approx 0.494538589\). Our fitting gives \(A_0 \approx 0.49453858\).

The other fitted parameters are shown in Tab. III. The coefficient \(c_0\) increases with the aspect ratio. For the strip case it is known that \(-c_0(\rho = \infty) = \frac{4}{N} \ln 2 + \gamma - 14(3)/21\pi \approx 0.3125538\). \(c_0\) approaches this limit as \(\rho \to \infty\) obviously, see Tab. III. However we have not obtained an analytical expression for the dependence of \(c_0\) on \(\rho\).

The term \((M \ln N + N \ln M)/S\) is the next order correction. Its coefficient \(c_{surf}\) is independent of \(\rho\), and its average value over \(\rho\) is \(c_{surf} = 0.524529(3)\). Note that this term is absent in the torus case \([7]\) and not mentioned in the long strip case \([7]\), but exists in the cylinder case with Brascamp-Kunz boundary conditions \([11, 12]\).

The corner term \(c_{corn}\) also seems independent of aspect ratio \(\rho\) and its average value is about

\[
c_{corn} = 0.368(1).
\]

We have also tried many other forms of 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.

### Conclusion.

Using the BP algorithm, we studied the Ising model on a rectangle of size \(M \times N\) with free boundaries. For five aspect ratios \(\rho = 1, 2, 4, 8, 16\), the critical free energy, internal energy and specific heat were calculated. We brought numerical evidence that the correction term \(c_{corn}\) stems from the corners of the rectangle is indeed universal and is proportional to the central charge \(c\). We also found that the terms \(U_{corn}\) and \(c_{corn}\) are independent from the aspect ratio \(\rho\). In order to check whether or not the terms \(U_{corn}\) and \(c_{corn}\) are universal quantities, it is useful to extend our study to the Ising model on other types of lattices, e.g., the triangular, honeycomb, Kagome lattices. In such studies, the BP algorithm which is suitable for any planar network of Ising spins with arbitrary bond strengths \([13, 20]\) is still a powerful tool. In addition, we can enhance the accuracy of the internal energy and specific heat by using an extended BP algorithm to calculate the internal energy without the using of differentiation\[20\]. Moreover the finite size effects of the correlation can be investigated by using the site propagation algorithm \[23\]. As we have shown, the sharp corners induce remarkable effects in critical region not only on the free energy, but also on the internal energy and the specific heat. It is expected that the sharp corners can induce remarkable effects on other properties of finite size systems in critical regime, for example, thermal conductivity, electric conductivity, etc. All of these effects should be observable in experiments.
| parameter | $\rho = 1$ | $\rho = 2$ | $\rho = 4$ | $\rho = 8$ | $\rho = 16$ |
|-----------|-----------|-----------|-----------|-----------|-----------|
| $c_0$     | $-0.57078599(3)$ | $-0.44276294(2)$ | $-0.37766115(2)$ | $-0.34510742(2)$ | $-0.32883055(2)$ |
| $c_{surf}$ | 0.524516(2) | 0.524533(2) | 0.524531(2) | 0.524530(3) | 0.524529(3) |
| $D_1$     | $-0.34928(3)$ | $-0.29524(1)$ | $-0.17826(1)$ | $-0.05986(2)$ | 0.03117(2) |
| $c_{corr}$| 0.3683(7) | 0.3704(3) | 0.3696(7) | 0.368(1) | 0.365(3) |
| $D_2$     | 1.144(5) | 1.293(2) | 1.914(5) | 3.42(1) | 6.67(3) |
| $D_3$     | 0.02(4) | $-0.13(2)$ | $-1.25(7)$ | $-4.8(2)$ | $-15.4(6)$ |
| $D_4$     | 0.8(3) | 0.7(2) | 3.6(8) | 16(3) | 7(1)0 |

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

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