Finite-size scaling of partition function zeros and first-order phase transition for infinitely long Ising cylinder

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The critical properties of an infinitely long Ising strip with finite width \( L \) joined periodically or antiperiodically are investigated by analyzing the distribution of partition function zeros. For periodic boundary condition, the leading finite-size scaling of partition function zeros and its corrections are given. For antiperiodic boundary condition, the critical point of 2D Ising transition is one of the loci of the zeros, and the associated non-analyticity is identified as a first-order phase transition. The exact amount of the latent heat released by the transition is \( 4/L \).

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The geometry of the system has been known to play a crucial role in many aspects of critical behavior: The way of taking the thermodynamic limit may affect the occurrence of a phase transition, and critical exponents depend on spatial dimensionality non-trivially. These result in more stringent test on the universality by including universal critical amplitudes and amplitude relations obtained from the finite-size effects\[1][2]. Boundary condition is an important factor in determining the finite-size scalings. In particular, aperiodic boundary conditions may introduce interfaces to the systems and lead to a profound change in the scaling behavior\[3][4]. In this letter, we report the appearance of a new first-order transition induced by the interface of a 2D semi-infinite Ising system. We consider the simplest system, an infinitely long Ising cylinder defined on a square \( L_x \times L_y \) lattice with infinite \( L_x \rightarrow \infty \) and finite \( L_y = L \). To have the system with cylindrical geometry, we impose periodic or antiperiodic condition on the infinitely extended boundary rows, \((m,1)\) and \((m,L)\) with \(-\infty < m < \infty\). The condition on the couplings of the boundary spin variables \( \sigma_{m,L} \) along the \( y \)-axis is \( \sigma_{m,L+1} = \sigma_{m,1} \) for periodically joined circumference (PJC, hereafter), and the condition becomes \( \sigma_{m,L+1} = -\sigma_{m,1} \) for antiperiodically joined circumference (AJC, hereafter). The free energy of the system with AJC contains the additional contribution from the interfacial tension in comparison with that of the system with PJC\[5][6]. To understand the differences in thermodynamic properties between the two boundary conditions, we analyze the distribution and the density of partition function zeros. Our results reveal some intriguing properties for the system with AJC of finite \( L \).

We already have a complete picture about the partition function zeros of the zero-field square Ising model in the thermodynamic limit\[7][8]. Fisher first showed that the partition function zeros, referred as Fisher zeros, all lie on the unit circle, \(|z|=1\), in the complex plane of \( z = \sinh (2\beta) \) with the zero on the positive real axis, \( z_c = 1 \), corresponding to the critical point of Ising transition\[7]. Then, Lu and Wu obtained the density associated with the zeros on the unit circle analytically\[8]. Based on these results, we study the finite-size scalings of Fisher zeros for infinitely long Ising cylinders. For the system with PJC, portions of the zeros, including the critical point, are always absent from the unit circle for finite \( L \), and the scaling behavior is given in the exact form. However, for the system with AJC, regardless the \( L \) value, the zeros distribution always contain the critical point. Then, by analyzing the cumulative distribution of Fisher zeros around the critical point we show that the singular property of the critical point can be classified into two types: One is the first-order transition for a finite circumference, and the other is the second-order transition for an infinite circumference. The latter corresponds to the Ising ferromagnetic phase transition, and the former is a new phase caused by the fluctuation of interface from AJC. Thus, in taking the thermodynamic limit \( L \rightarrow \infty \) from an infinitely long Ising cylinder of finite \( L \), we encounter different situations for two different boundary conditions: (i) For the case of PJC, only the second-order phase transition appears in the limit \( L \rightarrow \infty \), and there is no phase transition in the intermediate stage \( 0 < L < \infty \). (ii) For the case of AJC, we first have the first-order phase transition which becomes weaker as \( L \) increases and eventually reduces to a second-order phase transition in the limit \( L \rightarrow \infty \). This picture is further verified by measuring the latent heat per site released in the first-order transition as \( 4/L \).

The partition function of a plane square \( L_x \times L_y \) Ising lattice with periodic or aperiodic boundary conditions can be expressed as the sum of four terms\[4][9], but the sum reduces to one term in the limit of \( L_x \) (or \( L_y \)) \( \rightarrow \infty \). In this limit, the system becomes an infinitely long Ising strip with finite width \( L \), and the corresponding free energy of the
system per site per $k_B T$ is

$$f_L = -\frac{1}{2} \ln (4z) - \frac{1}{2L} \sum_p \int_0^{2\pi} \frac{d\phi}{2\pi} \ln \left[ z + \frac{1}{z} - \Phi_p(\phi) \right],$$

(1)

for the case of isotropic ferromagnetic couplings. Here the possible $p$-values in the sum are half integers ranging from 1/2 to $L - 1/2$ for PJC and integers ranging from 0 to $L - 1$ for AJC, and the function $\Phi_p(\phi)$ is given as

$$\Phi_p(\phi) = \cos \phi + \cos \left( \frac{2\pi p}{L} \right).$$

(2)

Then, the loci of the Fisher zeros can be obtained as the union of the solutions of the condition

$$z + \frac{1}{z} - \Phi_p(\phi) = 0$$

(3)

with $0 \leq \phi \leq 2\pi$ for all allowed $p$-values. The solutions of Eq. (3) are expressed as

$$z = \exp (\pm i\theta),$$

(4)

for $0 \leq \theta \leq \pi$, where $\theta$ are the elements belonging to the union of the sets of $\theta_p$ for all allowed $p$-values with

$$\cos \theta_p = \frac{\Phi_p(\phi)}{2}.$$

(5)

For the function $\Phi_p(\phi)$ of Eq. (2), the value of $\theta_p$ for a given $p$-mode is in the range between $\theta_{p,\text{min}} = \cos^{-1} \left( \cos^2 \left( \frac{\pi p}{L} \right) \right)$ and $\theta_{p,\text{max}} = \pi - \cos^{-1} \left[ \sin^2 \left( \frac{\pi p}{L} \right) \right]$. An example of the curve of $\theta_p(\phi)$ obtained from Eq. (5) for various $p$-modes with $L = 6$ is shown in Fig. 1.

For PJC, by including all allowed $p$-modes we obtain the range of $\theta$ as $\theta_{p=1/2,\text{min}}$ and $\theta_{p=1/2,\text{max}}$ for even $L$, and $\theta_{\text{min}} = \theta_{p=1/2,\text{min}}$ and $\theta_{\text{max}} = \pi$ for odd $L$. Thus, as shown in Fig. 2(a) for $L = 5$ and 2(c) for $L = 6$, the zeros distribution can be summarized as the followings: (i) The zeros are absent from two arcs of the unit circle for even $L$ and from an arc for odd $L$, and the zeros do not contain the critical point for both even and odd finite $L$. (ii) By denoting the nearest zero to the critical point as $z_1(L)$, we obtain the opening angle between $z_1(L)$ and the critical point as $\theta_{\text{min}}$. To obtain the finite-size scaling behavior of $z_1(L)$, we expand $\sin \theta_{\text{min}}$ and $\cos \theta_{\text{min}}$ as a power series of $1/L$ to obtain

$$\text{Im } z_1(L) = \sum_{k=0}^{\infty} C_{2k+1}(\pi/2L)^{2k+1},$$

(6)

with the coefficients $C_1 = \sqrt{2}$, $C_3 = -5\sqrt{2}/12$, $C_5 = 49\sqrt{2}/480$, and etc.; and

$$|\text{Re } z_1(L) - z_c| = \sum_{k=1}^{\infty} C_{2k}^R \left( \frac{\pi}{2L} \right)^{2k},$$

(7)

with the coefficients $C_2^R = 1$, $C_4^R = -1/3$, $C_6^R = 2/45$, and etc.. From the finite-size scaling theory of the zeros distributions, the leading finite-size scaling behavior of the imaginary part of a Fisher zero labelled by $j$ is given as

$$\text{Im } z_j(L) \sim L^{-1/\nu},$$

(8)

where $\nu$ is the correlation-length exponent; and the leading scaling behavior of the real part of the lowest zero ($j = 1$) can be written as

$$|\text{Re } z_1(L) - z_c| \sim L^{-\zeta_{\text{zero}}},$$

(9)

where $\zeta_{\text{zero}}$ is another critical exponent which is closely related to the shift exponent $\lambda$ characterizing the shift of the specific-heat peak from the critical point. Then, from Eqs. (6) and (7) we have $\nu = 1$ and $\zeta_{\text{zero}} = 2$. The two values are the same as the results obtained by Janke and Kenna for a finite rectangular lattice with the Brascamp-Kunz boundary condition but different from those obtained by other boundary conditions.

For AJC, we obtain the range of $\theta$ as $0 \leq \theta \leq \theta_{\text{max}}$, with $\theta_{\text{max}} = \pi$ for even $L$ and $\theta_{\text{max}} = \pi - \cos^{-1} \left[ \cos^2 \left( \frac{\pi p}{2L} \right) \right]$ for odd $L$. Thus, as shown in Fig. 2(b) for $L = 5$ and 2(d) for $L = 6$, the zeros distribution is absent from an arc of
the unit circle for odd \( L \) and fills the unit circle completely for even \( L \). Moreover, the critical point is one of the loci of the zeros for both even and odd \( L \). Then, a question naturally arises: What is the non-analytic property associated with the zero at the critical point? This can not be the second-order phase transition which occurs only in the limit \( L \to \infty \). To determine the nature of the non-analyticity, we study the functional form of the cumulative distribution of the zeros.

The cumulative distribution of zeros, \( G_L(\theta) \), is defined as the total number of Fisher zeros in the interval \([0, \theta]\) of the unit circle. By expressing in terms of the zeros density \( g_L(\theta) \), we have

\[
G_L(\theta) = \int_0^\theta g_L(x)dx.
\]

Here we always take the normalization as \( G_L(\pi) = 1/2 \) for any width \( L \). It has been shown that the zeros density \( g_\infty(\theta) \) near the critical point, \( \theta_c = 0 \), behaves as \( g_\infty(\theta) \approx a_2\theta^{1-\alpha} \) in a second-order phase transition for which the specific heat diverges as \( c \sim |T - T_c|^{-\alpha} \). Thence, the corresponding cumulative distribution of zeros is \( G_\infty(\theta) \approx b_2\theta^{2-\alpha} \). In 2D Ising transition for which we have \( \alpha = 0 \), the density \( g_\infty(\theta) \) was shown to vanish linearly as \( g_\infty(\theta) \approx |\theta|/2\pi \) near the critical point, and the corresponding \( G_\infty(\theta) \) obtained by the integration of \( g_\infty(\theta) \) given by Ref. [3] are shown as a solid line in Fig. 3. For the first-order transition, the asymptotic behavior of \( g_\infty(\theta) \) to the critical point was shown to take the form, \( g_\infty(\theta) \approx g_\infty(0) + a_1\theta^n + ... \), with \( g_\infty(0) \) proportional to the latent heat. Correspondingly, the behavior of \( G_\infty(\theta) \) is

\[
G_\infty(\theta) \approx g_\infty(0)\theta + b_1\theta^{n+1} + ....
\]

For the system of an infinitely long Ising cylinder, the value of \( G_L(\theta) \) is proportional to the sum of the lengths of the curves \( \theta_p(\phi) \), as shown in Fig. 1, over all possible \( p \)-values up to a given \( \theta \) value with \( 0 \leq \phi \leq 2\pi \). Because of the symmetry, \( \theta_p(\phi) = \theta_p(-\phi) \), we may restrict the \( \phi \)-values to the interval \([0, \pi]\). Then, by using the normalization condition \( G_L(\pi) = 1/2 \) we write

\[
G_L(\theta) = \frac{1}{2l_{tot}} \sum_p l_p(\theta),
\]

where \( l_p(\theta) \) is the length of the curve \( \theta_p(\phi) \) up to a given \( \theta \) value,

\[
l_p(\theta) = \int_0^{\phi(\theta)} \sqrt{1 + (d\theta_p(\phi)/d\phi)^2} \, d\phi,
\]

and \( l_{tot} \) is the sum of the lengths of all the curves,

\[
l_{tot} = \sum_p l_p(\theta_{p,\text{max}}).
\]

Our numerical result gives \( l_{tot} = 1.085(2) \pi L \). Note that the value of \( l_{tot} \) is linearly proportional to the width \( L \) and independent of boundary conditions. The numerical results of \( G_L(\theta) \) for both PJC and AJC with \( L = 20 \) are shown as circles in Fig. 3. There are two remarks on Fig. 3 worthy to be mentioned: (i) The differences in \( G_L(\theta) \) between AJC and PJC for \( L = 6 \) and 20 are shown in the up-left corner of Fig. 3, and it indicates the difference vanishes very quickly as \( L \) increases. (ii) By comparing with \( G_\infty(\theta) \) shown by the solid line, we know \( G_L(\theta) \) converges to \( G_\infty(\theta) \) very quickly as \( L \) increases.

For the system with AJC, the critical point is one of the zeros for both even and odd \( L \), and the cumulative distribution of zeros in the interval \( 0 \leq \theta \leq \theta_{p=1,\text{min}} \) is contributed solely by the zero mode \( p = 0 \). In this interval of \( \theta \), we have \( G_L(\theta) = l_{p=0}(\theta)/2l_{tot} \). By completing the integration of Eq. (13) for \( p = 0 \), we have

\[
G_L(\theta) \approx \left( \frac{\sqrt{3}}{2l_{tot}} \right) \left( \theta + \frac{1}{36}\theta^3 + ... \right) .
\]

This result yield \( g_L(0) = 0.254(0) / L \). Thus, by comparing Eq. (15) with Eq. (11) we may conclude the following properties for the system with AJC: (i) The system exhibits a first-order transition for finite \( L \). (ii) The transition temperature always locates at the critical point \( \beta_c \) of 2D Ising transition independent of the value of \( L \). (iii) The latent heat released by the transition is inversely proportional to the width \( L \).
To obtain the exact amount of the latent heat released in the transition, we can measure the discontinuity of the internal energy at the transition point. The dimensionless internal energy density \( \epsilon_L \) is defined as \( \epsilon_L = \partial f_L / \partial \beta \). By rewriting the free energy density of Eq. (1) as

\[
f_L = -\frac{1}{4} \ln (4z) - \frac{1}{2L} \sum_p \left[ -\ln F(p, \beta) + I(p, \beta) \right],
\]

(16)

with

\[
I(p, \beta) = \int_0^{2\pi} \frac{d\phi}{2\pi} \ln \left[ 1 - F(p, \beta) \cos \phi \right],
\]

(17)

\[
F(p, \beta) = z \left( z^2 + 1 - \cos \frac{2\pi p}{L} \right)^{-1},
\]

(18)

we may obtain \( \epsilon_L \) by first completing the integration of Eq. (17) and then performing the derivatives with respect to \( \beta \). However, to avoid any ill-defined result we have to be very cautious of continuity for the integrand. For concreteness, we proceed first with the derivative and then the integration. By using the technique of contour integration, we have

\[
\frac{\partial I}{\partial \beta} = \left( 1 - \frac{1}{\sqrt{1 - F^2(p, \beta)}} \right) \frac{\partial}{\partial \beta} \ln F(p, \beta), \quad \text{for } 1 - F^2(p, \beta) > 0.
\]

(19)

Note that the above equality holds only when the condition \( 1 - F^2(p, \beta) > 0 \) is met, and this condition ensures the continuity of the integrand. Then, we have

\[
\epsilon_L = -\frac{\sqrt{1 + z^2}}{8z} + \frac{1}{2L} \sum_p D_c(p, \beta),
\]

(20)

with

\[
D_c(p, \beta) = \frac{1}{\sqrt{1 - F^2(p, \beta)}} \frac{\partial}{\partial \beta} \ln F(p, \beta).
\]

(21)

For PJC, the functional values of \( F(p, \beta) \) satisfy the inequality \( 0 < F(p, \beta) < 1 \), and the internal energy of Eq. (20) is a continuous function of \( \beta \). For AJC, the functional values of \( F(p, \beta) \) also satisfy the condition \( 1 - F^2(p, \beta) > 0 \) with one exceptional point locating at \( p = 0 \) and \( \beta = \beta_c \), for which we have \( 1 - F^2(0, \beta_c) = 0 \). Thus, for AJC we may expect to have the mismatch of the left and right derivatives of the free energy at \( \beta_c \). The discontinuity \( \Delta_\epsilon \) defined as the differences between \( \epsilon_L(\beta_c - \varepsilon) \) and \( \epsilon_L(\beta_c + \varepsilon) \) exactly is the latent heat per site released by the transition. Since the zero mode of Eq. (21) is solely responsible for the discontinuity, we have

\[
\Delta_\epsilon = \frac{1}{2L} \lim_{\varepsilon \to 0} \left[ D_c(0, \beta_c - \varepsilon) - D_c(0, \beta_c + \varepsilon) \right].
\]

(22)

This yields \( \Delta_\epsilon = 4/L \). Thus, the latent heat scales as \( 1/L \), and this agrees with the result obtained from the analysis of the zeros.

In summary, we analyze the distribution of Fisher zeros in the complex sinh(2\( \eta \)) plane for an infinitely long Ising strip with finite width \( L \) joined periodically or antiperiodically. For periodically joined circumference, the the leading finite-size scaling behavior for the distribution of Fisher zeros give the exact values of the correlation-length and shift exponents, \( \nu \) and \( \lambda_{zero} \), as \( \nu = 1 \) and \( \lambda_{zero} = 2 \). For antiperiodically joined circumference, the system contains the interface, and the fluctuation of the interface renders the critical point of Ising transition to be non-analytic in thermodynamic quantities for any width \( L \). The nature of the non-analytic associated with the critical point is identified as the first-order phase transition for finite \( L \). Because of the existence of the interface, the system can not be identified as an effective one-dimensional system with short-range Hamiltonian, and the appearance of the first-order transition does not contradict with the Mermin-Wagner theorem. The latent heat released by the transition scales exactly as \( 1/L \) with the the exact amount \( 4/L \). Thus, as \( L \) increases, the strength of the first-order transition decreases, and eventually the system exhibits the second-order phase transition in the limit of \( L \to \infty \).
FIG. 1: The curves of $\theta_p$ versus $\phi/\pi$ for various $p$-modes with $L = 6$ and periodic (solid lines) and antiperiodic (dot lines) boundary conditions. The number on a curve is the $p$-value.

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FIG. 2: The distributions of Fisher zeros in the complex $z$ plane for infinitely long Ising strip with width $L = 5$ for (a) periodic and (b) antiperiodic boundary conditions and width $L = 6$ for (c) periodic and (d) antiperiodic boundary conditions. The opening angle is $\theta_{\text{min}} = \cos^{-1}\left[\cos^2(\pi/2L)\right]$.

FIG. 3: The cumulative distribution of Fisher zeros $G(\theta)$ as a function of $\theta$. The circles are the results for infinitely long Ising strip with width $L = 20$ for periodic and antiperiodic boundary conditions, and the solid line corresponds to the results from the integration of the zeros density given by Ref. [8]. The differences in $G_L(\theta)$ between the antiperiodic and the periodic boundary conditions for $L = 6$ (dot line) and 20 (solid line) are shown in the up-left corner.
