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Universal relations in the finite-size correction terms of two-dimensional Ising models

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Quite recently, Izmailian and Hu [Phys. Rev. Lett. **86**, 5160 (2001)] studied the finite-size correction terms for the free energy per spin and the inverse correlation length of the critical two-dimensional Ising model. They obtained the universal amplitude ratio for the coefficients of two series. In this study we give a simple derivation of this universal relation; we do *not* use an explicit form of series expansion. Moreover, we show that the Izmailian and Hu's relation is reduced to a simple and exact relation between the free energy and the correlation length. This equation holds at any temperature and has the same form as the finite-size scaling.

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Universality and scaling are two basic concepts in the study of phase transitions and critical phenomena [1,2]. The critical properties are universal to a large extent depending on a few parameters, such as the space dimensionality and the symmetry of the order parameter. Critical exponents, critical amplitude ratios, and scaling functions are examples of universal quantities [3,4]. Finite-size scaling [5,6] has been increasingly important, partly due to the progress in the theoretical understanding of finite-size effects, and partly due to the application to the analysis of simulational results. Recently, more attention has been paid to the universality of finite-size scaling functions [7] for both percolation models [8] and Ising models [9]. In two dimensions the relevance of the finite-size properties to the conformal field theory is another source of interest [10].

Quite recently, Izmailian and Hu [11] studied the finite-size correction terms for the free energy per spin and the inverse correlation length of critical two-dimensional (2D) Ising models [12–14]. They obtained the universal amplitude ratio for the coefficients of two series. Let us denote the free energy per spin and the inverse correlation length for $N\times\infty$ lattice as f_N and ξ_N^{-1}, respectively. Then, Izmailian and Hu [11] obtained analytic expressions for the finite-size correction coefficients a_k and b_k defined by

$$N(f_N-f_\infty)=\sum_{k=1}^{\infty}\frac{a_k}{N^{2k-1}}, \qquad (1)$$

$$\xi_N^{-1}=\sum_{k=1}^{\infty}\frac{b_k}{N^{2k-1}}, \qquad (2)$$

at the criticality for the square (sq), honeycomb (hc), and plane-triangular (pt) lattices. Here, f_∞ denotes the value of f_N as $N\to\infty$. They found that

$$\frac{b_k}{a_k}=\frac{2^{2k}-1}{2^{2k-1}-1} \qquad (3)$$

for all of these lattices, that is, the amplitude ratio b_k/a_k is universal. They also obtained similar expansions for the critical ground state energy $E^{(0)}$ and the first energy gap ($E^{(1)}-E^{(0)}$) of the one-dimensional (1D) quantum XY model with uniform field [15] at the critical field, and found that the amplitude ratios of two coefficients have the same values as Eq. (3).

The lowest-order correction terms a_1 and b_1 are related to the central charge c and the magnetic scaling field x_H in the conformal field theory by $a_1=c\pi/6$ and $b_1=2\pi x_H$, respectively. The finite-size correction terms of 2D systems have also received current interest. The finite-size corrections to scaling of correlation lengths and free energies of the critical 2D Ising and three-state Potts models were numerically studied by de Quieroz [16]. The finite-size corrections to the energy and specific heat of the critical 2D Ising model were also analyzed by Salas [17]. Moreover, Salas and Sokal studied several universal amplitude ratios for the critical 2D Ising model [18].

In this Rapid Communication we will give a simple derivation of the universal amplitude ratio, Eq. (3). Instead of using an explicit form of expansion in $1/N$, which is available only at the criticality, we show a finite-size-scaling–like relation which holds at an arbitrary temperature. The universal amplitude ratio can be readily derived from this relation.

Let us start with comparing the free energy per spin and the inverse correlation length for size N and $N/2$. Assuming the expansion, Eq. (1), we have the expression for the difference of f_N and $f_{N/2}$ as

$$f_{N/2}-f_N=\sum_{k=1}^{\infty}\frac{a_k}{N^{2k}}\{2^{2k}-1\}. \qquad (4)$$

In a similar way, using Eq. (2), we have

$$\xi_{N/2}^{-1}-\xi_N^{-1}=\sum_{k=1}^{\infty}\frac{b_k}{N^{2k-1}}\{2^{2k-1}-1\}. \qquad (5)$$

From Eqs. (4) and (5), we get the following statement: If the relation

$$f_{N/2}-f_N=\frac{1}{N}(\xi_{N/2}^{-1}-\xi_N^{-1}) \qquad (6)$$

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is satisfied, we have the relation of two coefficients, Eq. (3). If we can show Eq. (6) directly, explicit expressions for the coefficients a_k and b_k are not necessary. Equation (6) is compatible to the finite-size scaling [2,6] of the singular part of the free energy for $N\times\infty$ systems, $f_N \propto (1/N)\xi_N^{-1} (N\to\infty)$; namely, Eq. (6) should hold asymptotically at the critical point. In fact, as we show in the following, Eq. (6) holds *exactly* at *any* temperature for several models that belong to the 2D Ising universality class.

First, we deal with the 2D Ising model defined by the Hamiltonian

$$\beta\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j, \tag{7}$$

where the Ising variable s_i takes ± 1, $\beta=(k_B T)^{-1}$, and the summation is taken over the nearest-neighbor pairs of sites for $N\times\infty$ lattices. Using a transfer matrix method [19,20], we can calculate the free energy per spin, f_N, and the inverse correlation length, ξ_N^{-1}, through the relations

$$f_N = \frac{1}{\zeta N}\ln\Lambda_0, \tag{8}$$

$$\xi_N^{-1} = \frac{1}{\zeta}\ln(\Lambda_0/\Lambda_1), \tag{9}$$

where Λ_0 and Λ_1 are the largest and the second largest eigenvalues of the transfer matrix. Here, a geometric factor ζ is 1, $2/\sqrt{3}$ and $1/\sqrt{3}$ for sq, hc, and pt lattices, respectively. Exact expressions for eigenvalues Λ_0 and Λ_1 are available for sq [12,19,20], hc [14], and pt [13] lattices.

Let us consider the Onsager solution for the sq lattice with periodic boundary conditions [12]. The two leading eigenvalues of the transfer matrix are given by

$$\Lambda_0 = (2\sinh 2J)^{N/2}\exp\left(\frac{1}{2}\sum_{r=0}^{N-1}\gamma_{2r+1}\right), \tag{10}$$

$$\Lambda_1 = (2\sinh 2J)^{N/2}\exp\left(\frac{1}{2}\sum_{r=0}^{N-1}\gamma_{2r}\right). \tag{11}$$

Here, γ_r is implicitly given by

$$\cosh\gamma_r = \frac{\cosh^2 2J}{\sinh 2J} - \cos\frac{r\pi}{N}. \tag{12}$$

Then, we get the free energy per spin f_N, Eq. (8), and the inverse correlation length ξ_N^{-1}, Eq. (9), as

$$f_N = \frac{1}{2}\ln(2\sinh 2J) + \frac{1}{2N}\sum_{r=0}^{N-1}\gamma_{2r+1}, \tag{13}$$

$$\xi_N^{-1} = \frac{1}{2}\sum_{r=0}^{N-1}(\gamma_{2r+1}-\gamma_{2r}). \tag{14}$$

To express $f_{N/2}$ and $\xi_{N/2}$, we replace N by $N/2$ and γ_r by γ_r' in Eqs. (13) and (14), respectively. Here γ_r' is the value for size $N/2$, and is related to γ_r through the relation

$$\cosh\gamma_r' = \frac{\cosh^2 2J}{\sinh 2J} - \cos\frac{r\pi}{N/2} = \cosh\gamma_{2r}, \tag{15}$$

that is,

$$\gamma_r' = \gamma_{2r}. \tag{16}$$

Equation (16) is the basic relation for our argument. Using relation (16), we have

$$f_{N/2} - f_N = \frac{1}{2N}\{2(\gamma_2+\gamma_6+\cdots+\gamma_{2N-2}) - (\gamma_1+\gamma_3+\cdots+\gamma_{2N-1})\}. \tag{17}$$

Similarly, we have

$$\begin{aligned}\xi_{N/2}^{-1} - \xi_N^{-1} &= \frac{1}{2}\{(\gamma_2+\gamma_6+\cdots+\gamma_{2N-2}-\gamma_0-\gamma_4-\cdots \\ &\quad -\gamma_{2N-4}) - (\gamma_1+\gamma_3+\cdots+\gamma_{2N-1}-\gamma_0-\gamma_2 \\ &\quad -\cdots-\gamma_{2N-2})\} \\ &= \frac{1}{2}\{2(\gamma_2+\gamma_6+\cdots+\gamma_{2N-2}) - (\gamma_1+\gamma_3+\cdots \\ &\quad +\gamma_{2N-1})\}.\end{aligned} \tag{18}$$

Comparing Eqs. (17) and (18), we arrive at the desired relation, Eq. (6). This implies that the ratio for the finite-size correction coefficients b_k/a_k is given by Eq. (3).

Next we consider the Ising model on the hc lattice. The two leading eigenvalues of the transfer matrix are given by [14]

$$\Lambda_0 = (2\sinh 2J)^N\exp\left(\sum_{r=0}^{N/2-1}\gamma_{2r+1}\right), \tag{19}$$

$$\Lambda_1 = (2\sinh 2J)^N\exp\left(\sum_{r=1}^{N/2-1}\gamma_{2r} + \frac{\gamma_0+\gamma_N}{2}\right). \tag{20}$$

In this case, γ_r is implicitly given by

$$\cosh\gamma_r = \cosh 2J\cosh 2J^* - \sin^2\frac{\pi r}{N} - \cos\frac{\pi r}{N}\left(\sinh^2 2J\sinh^2 2J^* - \sin^2\frac{\pi r}{N}\right)^{1/2}, \tag{21}$$

where J^* is defined by $(\cosh 2J-1)(\cosh 2J^*-1)=1$. For size $N/2$, we replace N by $N/2$ and γ_r by γ_r' in Eqs. (19) and (20). The relation of γ_r', the value for size $N/2$, and γ_r can be obtained by using Eq. (21); we have the same relation as

Eq. (16), $\gamma_r' = \gamma_{2r}$. Starting from Eqs. (8) and (9) together with Eqs. (19) and (20), with some algebra, we get

$$N\zeta(f_{N/2} - f_N) = \zeta(\xi_{N/2}^{-1} - \xi_N^{-1}) = 2(\gamma_2 + \gamma_6 + \cdots + \gamma_{N-2}) - (\gamma_1 + \gamma_3 + \cdots + \gamma_{N-1}). \tag{22}$$

Thus, we again obtain relation (6). In this way, we have shown that the amplitude ratio b_k/a_k is given by Eq. (3). For the pt lattice, we may use the star-triangle transformation [21] to show Eq. (6) from the result of the hc lattice without making an explicit calculation.

Some comments should be added here. We have shown the universality of the amplitude ratio, Eq. (3), without using the condition of the criticality. This means that the property of this universality holds not only at the critical point but also at any temperature in 2D Ising models. The ratio b_k/a_k takes the universal value for all the temperatures. However, we should note that the expression for the inverse correlation length, Eq. (9), is valid only for $T \geqslant T_c$. For $T < T_c$, Λ_0 and Λ_1 are degenerate in the thermodynamic limit, $N \to \infty$, which means the existence of the long-range order [19,20]. We should subtract the long-range order contribution from the correlation function when considering the correlation length. We may regard b_k as the correction amplitude for the right-hand side of Eq. (9) for $T < T_c$.

Izmailian and Hu [11] also studied another model which belongs to the 2D Ising universality class. The 1D quantum XY model with uniform field, whose Hamiltonian is given by

$$\mathcal{H} = -\frac{1}{4}\sum_{n=1}^{N} [(1+\gamma)\sigma_n^x\sigma_{n+1}^x + (1-\gamma)\sigma_n^y\sigma_{n+1}^y] - \frac{h}{2}\sum_{n=1}^{N}\sigma_n^z, \tag{23}$$

was exactly solved by Katsura [15]. Here, σ^x, σ^y and σ^z are the Pauli matrices. For $0 < \gamma \leqslant 1$, there is a critical magnetic field $h_c = 1$, and the phase transition of this model belongs to the 2D Ising universality class. For $\gamma = 1$ it is also called the 1D transverse Ising model. The Hamiltonian of Eq. (23) is diagonalized by a Jordan-Wigner transformation as

$$\mathcal{H} = -\sum_k \Lambda(k)\left(\eta_k^* \eta_k - \frac{1}{2}\right), \tag{24}$$

where η_k^*, η_k are fermionic creation and annihilation operators and

$$\Lambda(k) = \sqrt{(\cos k + h)^2 + (\gamma \sin k)^2}. \tag{25}$$

We should note that the choice of k depends on the boundary condition. The ground state energy $E^{(0)}$ and the first energy gap $\Delta E = E^{(1)} - E^{(0)}$ of the quantum spin model, respectively, correspond to the free energy and inverse correlation length for the Ising model; that is,

$$N f_N \Leftrightarrow -E_N^{(0)} \quad \text{and} \quad \xi_N^{-1} \Leftrightarrow \Delta E_N.$$

For the N quantum spin systems with the periodic boundary condition, we have [22,23]

$$E_N^{(0)} = -\frac{1}{2}\sum_{r=0}^{N-1} \gamma_{2r+1}, \tag{26}$$

$$\Delta E_N = -\frac{1}{2}\sum_{r=0}^{N-1} (\gamma_{2r} - \gamma_{2r+1}), \tag{27}$$

where we have used the notation $\gamma_r = \Lambda(r\pi/N)$. Let us consider the energy for size N and that for $N/2$ as in the classical 2D Ising model. For size $N/2$, we replace N by $N/2$ and γ_r by γ_r' in Eqs. (26) and (27). Here, γ_r' is again the value for $N/2$, and the relation of γ_r' and γ_r can be obtained by using Eq. (25). As a result, we have the same relation as Eq. (16), that is,

$$\gamma_r' = \gamma_{2r}. \tag{28}$$

Then, we obtain the expression for the difference between $E_N^{(0)}$ and $E_{N/2}^{(0)}$ as

$$E_{N/2}^{(0)} - E_N^{(0)} = -\frac{1}{2}\{2(\gamma_2 + \gamma_6 + \cdots + \gamma_{2N-2}) - (\gamma_1 + \gamma_3 + \cdots + \gamma_{2N-1})\}. \tag{29}$$

For the first energy gap, we can also calculate the difference between the values for N and $N/2$. Using Eq. (28), with some algebra, we finally have

$$\Delta E_{N/2} - \Delta E_N = \frac{1}{2}\{2(\gamma_2 + \gamma_6 + \cdots + \gamma_{2N-2}) - (\gamma_1 + \gamma_3 + \cdots + \gamma_{2N-1})\}. \tag{30}$$

From Eqs. (29) and (30), we have

$$-(E_{N/2}^{(0)} - E_N^{(0)}) = \Delta E_{N/2} - \Delta E_N, \tag{31}$$

which shows that the amplitude ratio of the finite-size correction coefficient for the ground state energy $(-E^{(0)})$, a_k, and that for the first energy gap ΔE, b_k, is given by Eq. (3).

The amplitude ratio b_k/a_k takes the same value as the classical case. And this is not only at the critical field $h_c = 1$ but also for all the magnetic fields. However, it should be mentioned that for low field, $h < h_c$, $E_N^{(1)}$ does not necessarily give the first excited energy level. We should interpret that b_k is the correction amplitude for the right-hand side of Eq. (27) for $h < h_c$.

To summarize, we have given a simple derivation of the universal amplitude ratio, Eq. (3). We have shown the relation of Eq. (6) and its quantum counterpart, Eq. (31). Although these equations have the same form as the finite-size scaling [2,6], they are exact and valid for an arbitrary temperature. One can perform an analytic calculation of each correction amplitude only at the criticality [11]. Our key relations are Eqs. (16) and (28), and we have not used the condition of the critical point.

Izmailain and Hu [11] used a perturbed conformal field theory to understand the correction terms. It is interesting to study directly the amplitude ratio by using the conformal field theory. The present study may give a hint for such a direction.

The finite-size properties depend on the boundary conditions. Recently, the effect of peculiar boundary conditions, such as the Möbius strip and the Klein bottle, was studied for the 2D Ising model [24,25]. The effect of boundary conditions on the finite-size correction terms is an interesting subject to study, which is now in progress.

In this study, we have started from the expansion of the free energy and the inverse correlation length in odd powers of $1/N$ in Eqs. (1) and (2). Away from the critical point, correction terms in even powers of $1/N$ may appear. Our argument is easily extended to such a case, and the main conclusion remains the same.

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