Density of the Fisher zeros for the three-state and four-state Potts models

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(Received 2 March 2004; revised manuscript received 28 April 2004; published 8 July 2004)

The numbers of states up to $L=12$ for the three-state Potts model and up to $L=10$ for the four-state Potts model on $L\times L$ square lattice with self-dual boundary condition are enumerated using the microcanonical transfer matrix exploiting the permutation symmetry of the model. From these numbers of states, the densities of the Fisher zeros $g(\theta)$ of the partition function in the complex $u=(1+(Q-1)e^{-\beta J})/\sqrt{Q}$ plane are determined for the zeros on the unit circle $u_0=e^{i\theta}$. For small θ the density of zeros obeys the finite-size scaling, allowing us to estimate the order parameter and the thermal exponent.

DOI: 10.1103/PhysRevE.70.016110 PACS number(s): 05.50.+q, 05.70.−a, 64.60.Cn, 75.10.Hk

I. INTRODUCTION

The Q-state Potts model [1] in two dimensions exhibits a rich variety of critical behavior and is very fertile ground for the analytical and numerical investigation of first- and second-order phase transitions. With the exception of the two-state Potts (Ising) model, exact solutions for arbitrary Q are not known. The Potts model on a lattice G with N_s sites and N_b bonds is defined by the Hamiltonian

$$\mathcal{H}_Q=-J\sum_{\langle i,j\rangle}\delta(\sigma_i,\sigma_j), \tag{1}$$

where J is the coupling constant [$J>0$ ($J<0$) for (anti)ferromagnetic coupling], $\langle i,j\rangle$ indicates a sum over nearest-neighbor pairs, and $\sigma_i=1,2,\ldots,Q$. If we define the number of states $\Omega_Q(E)$ with a given energy E which is a positive integer $0\leqslant E\leqslant N_b$, the partition function (PF) of the model $Z=\sum_{\{\sigma_n\}}e^{-\beta\mathcal{H}}$, a sum over Q^{N_s} possible spin configurations, can be written as

$$Z_Q(y)=y^{-N_b}\sum_{E=0}^{N_b}\Omega_Q(E)y^E, \tag{2}$$

where $y=e^{-\beta J}$ and $\sum_{E=0}^{N_b}\Omega_Q(E)=Q^{N_s}$.

By introducing the concept of the zeros of the PF in the *complex* magnetic-field plane (Yang-Lee zeros), Yang and Lee [2] proposed a mechanism for the occurrence of phase transitions in the thermodynamic limit and yielded an insight into the unsolved problem of the ferromagnetic (FM) Ising model in magnetic field at arbitrary temperature [3]. Fisher [4] found that the PF zeros in the complex y plane (Fisher zeros) are also important in understanding phase transitions, and showed that for the square lattice Ising model in the absence of magnetic field the Fisher zeros in the complex y plane lie on two circles [the FM circle $y_{\rm FM}=-1+\sqrt{2}e^{i\theta}$ and the antiferromagnetic (AFM) circle $y_{\rm AFM}=1+\sqrt{2}e^{i\theta}$] in the thermodynamic limit. Recently it has been shown that for self-dual boundary condition near the FM critical point $y_c=1/(1+\sqrt{Q})$ the zeros of the Q-state Potts model on a finite square lattice in the absence of an external magnetic field lie on the circle with center $-1/(Q-1)$ and radius $\sqrt{Q}/(Q-1)$ in the complex y plane, while the AFM circle of the Ising model completely disappears for $Q>2$ [5,6].

If the density of zeros is found, the free energy, the equation of state, and all other thermodynamic functions can be obtained. However, very little is known about the actual form of the density of zeros. Recently Lu and Wu [7] found the density of the Fisher zeros for the square lattice Ising model with a Brascamp-Kunz boundary condition in the thermodynamic limit. They also determined the Fisher zeros of the square lattice Ising model with self-dual boundary condition, and calculated their densities for infinite strips [8]. Creswick and Kim [9] obtained the density of the Yang-Lee zeros for the square lattice Ising model by evaluating the exact PF on finite lattices. Furthermore, using Monte Carlo data, Janke and Kenna [10] investigated the properties of the density of zeros for the square lattice ten-state Potts model, the three-dimensional Ising and three-state Potts models, the square lattice XY model, and lattice gauge theories.

In this paper, by enumerating the exact number of states for the three-state and four-state Potts models on $L\times L$ square lattices with self-dual boundary condition ($N_s=L^2+1$ and $N_b=2L^2$), we investigate the density of the Fisher zeros whose properties are not known. The self-dual boundary condition used in this paper is defined in Fig. 1 [6,8]. The microcanonical transfer matrix exploiting the permutation symmetry of the model [6,11] is used to enumerate the exact number of states up to $L=12$ for $Q=3$ ($3^{145}=1.523\times10^{69}$ configurations) and up to $L=10$ for $Q=4$ ($4^{101}=6.428\times10^{60}$ configurations). For example, Table I shows the number of states $\Omega_{Q=3}(E)$ of the three-state Potts model on 12×12 square lattice with self-dual boundary condition. $\Omega_3(0)=3$ is the number of the FM ground states whereas $\Omega_3(288)=1.080\times10^{26}$ is the number of the AFM ground states. The largest number of states is $\Omega_3(192)=7.606\times10^{67}$. Figure 2 shows the entropy $S(E)=\ln\Omega_3(E)$ of the three-state Potts model for $L=12$.

II. DENSITY OF ZEROS FOR THE THREE-STATE POTTS MODEL

For self-dual boundary condition, some of the Fisher zeros of the Potts model lie on the unit circle in the complex

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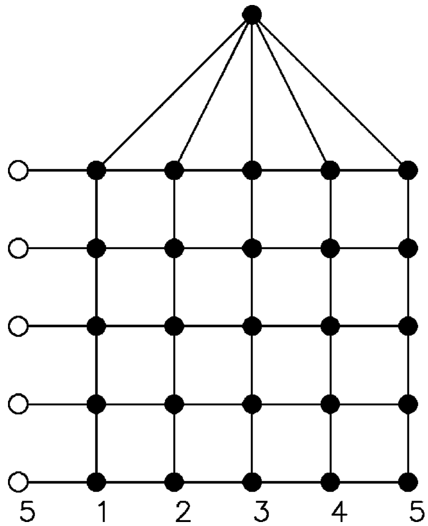

FIG. 1. 5×5 square lattice with self-dual boundary condition.

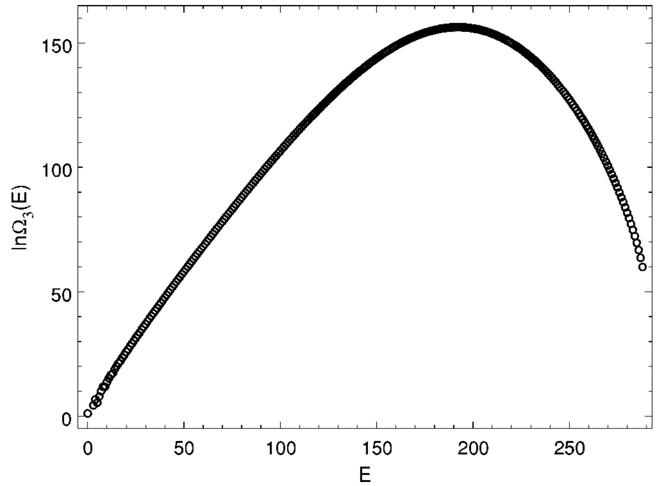

FIG. 2. The entropy $S(E)=\ln\,\Omega_3(E)$ for the 12×12 three-state Potts model with self-dual boundary condition. The corresponding values for $\Omega_3(1)=\Omega_3(2)=0$ are omitted in the figure.

$u=[1+(Q-1)y]/\sqrt{Q}$ plane. The zeros on the unit circle map into themselves under the duality transformation $u\to u^{-1}$. The self-duality condition $u^2=1$ determines the FM critical point $u_c=1$. Figure 3 shows the Fisher zeros in the complex u plane of the three-state Potts model on 12×12 square lattice. The figure shows only Fisher zeros on the unit disk $|u|\leqslant1$. The Fisher zeros with $|u|>1$ are obtained from those with $|u|<1$ by the duality transformation. The number of the zeros on the unit circle is 108, corresponding to 37.5% of the total of 288 zeros.

In the thermodynamic limit, the singular part of the free energy per site f_s can be written as

$$-\beta f_s=\int g(\theta)\ln(u-e^{i\theta})d\theta, \tag{3}$$

for the Fisher zeros on the unit circle ($u_0=e^{i\theta}$). The singular part of the energy per site is expressed as

$$e=\left(u-\frac{1}{\sqrt{Q}}\right)\int\frac{g(\theta)}{u-e^{i\theta}}d\theta, \tag{4}$$

and the latent heat is given by $\Delta e=(1-1/\sqrt{Q})2\pi g(0)$. For a finite-size system of size L, the singular part of the energy has the scaling form

$$e(t,L)=L^{-d+y_t}e(tL^{y_t}), \tag{5}$$

where y_t is the thermal exponent. In the critical region the singular part of the energy is a homogeneous function of the reduced temperature $u-u_c$ from which it follows that $g(\theta)$ must also be a homogeneous function for small θ of the form [9]

$$g(\theta,L)=L^{-d+y_t}g(\theta L^{y_t}). \tag{6}$$

If we let $\theta\to0$ and $L\to\infty$ keeping $\theta L^{y_t}=c$ fixed, then we have $g(\theta)\sim|\theta|^{(d-y_t)/y_t}$. This in turn implies that, for the mod-

TABLE I. The number of states $\Omega_{Q=3}(E)$ of the three-state Potts model for 12×12 square lattice with self-dual boundary condition.

E	$\Omega_{Q=3}(E)$
0	3
1	0
2	0
3	72
4	864
⋮	⋮
191	75225032927945592268009997855136811220062209360886072940230851457056
192	76060009304567600770980455752976522583135268602898164403429820493138
193	75704158671121305700548484295610849932031623011574915929856848371432
⋮	⋮
286	103861176439350537132456079800
287	44425389731774410245408596 64
288	108015898289079928962063078

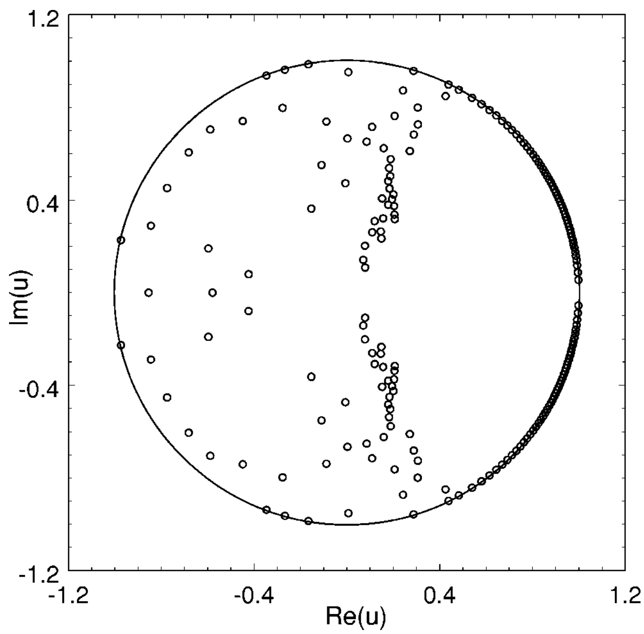

FIG. 3. Fisher zeros in the complex u plane for the 12×12 three-state Potts model with self-dual boundary condition. The figure shows only Fisher zeros on the unit disk $|u|\leqslant 1$. The Fisher zeros with $|u|>1$ are obtained from those with $|u|<1$ by the duality transformation.

els with second-order phase transitions ($Q\leqslant 4$) [1], $g(\theta)$ vanishes as $|\theta|^{\kappa}$ as θ goes to zero where $\kappa=(d-y_t)/y_t$. That is, for small θ

$$g(\theta)\sim|\theta|^{1-\alpha}, \tag{7}$$

where we have used $\alpha=2-d/y_t$. Equation (7) agrees with Fisher's result for the Ising model [4]. On the other hand, for the models with first-order phase transitions ($Q>4$), the density of zeros on the positive real axis is finite

$$\lim_{\theta\to 0} g(\theta)\sim \text{const (latent heat)},$$

where we have used $y_t=d$.

For finite systems the density of zeros (per site) at $\overline{\theta_k}=(\theta_k+\theta_{k+1})/2$ is defined as

$$g(\overline{\theta_k})=\frac{1}{N_s}\frac{1}{\theta_{k+1}-\theta_k}, \tag{8}$$

where θ_k $(k=1,2,3,\ldots)$ is the argument of the kth zero on the unit circle of $Z(u)$. Figure 4 shows the densities of zeros for $L=9$ and 12, respectively. It should be noted that the overall forms of the density of zeros for $L=9$ and 12 are almost identical. We expect that these densities of zeros approach a smooth limiting curve in the thermodynamic limit. Between $\theta/\pi=0.1$ and 0.4 the density of zeros decreases as θ increases. This fact implies that the density of zeros may vanish around $\theta/\pi=0.42$. A similar behavior is also observed for the density of zeros of the Ising model [7]. As shown in Fig. 3, around $\theta/\pi=0.42$, a branch of zeros lying off the unit circle begins to appear. This branch is directed to the point $u=0$ that is connected to the AFM critical point

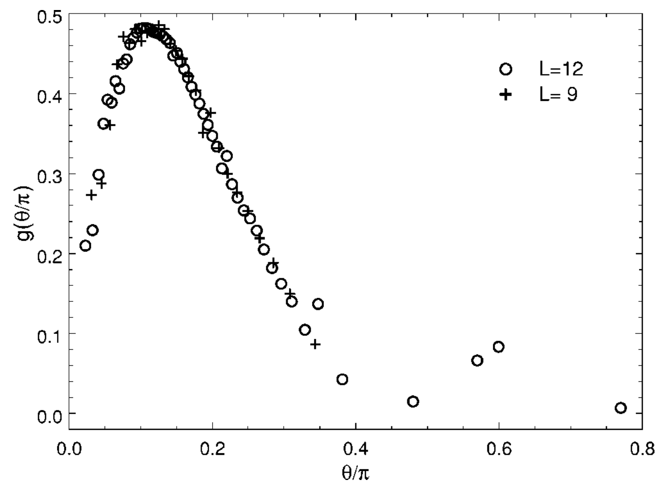

FIG. 4. Density of the Fisher zeros in the complex u plane of the three-state Potts model for $L=9$ and 12.

$u_c^{\mathrm{AFM}}=\infty$ by the duality transformation. It is reasonable to conjecture that, at the point where the zeros related to the FM critical point and the zeros related to the AFM critical point intersect, the density of zeros vanishes.

Figure 5 shows the scaled density of zeros versus the scaled argument, according to Eq. (6), for $L=9-12$. In the critical region, i.e., for small $L^{y_t}\theta$ the values of the scaled density of zeros are almost identical, independent of the lattice size, indicating that the form (6) is valid. If we set $\theta=0$ in Eq. (6), we have

$$g(0,L)=L^{-d+y_t}g(0). \tag{9}$$

The third column of Table II shows the density of zeros at $\overline{\theta_1}$ for $3\leqslant L\leqslant 12$. By using the BST algorithm [12], we extrapolated our results for finite lattices to infinite size and, for $\omega=\frac{4}{5}$ (the parameter of the BST algorithm), obtained $g(0)=0.000(4)$, which is an expected result for a second-order phase transition. The chosen value of $\omega=\frac{4}{5}$ for the three-state Potts model corresponds to the correction exponent $d-y_t$. For other models, different values of ω should be chosen

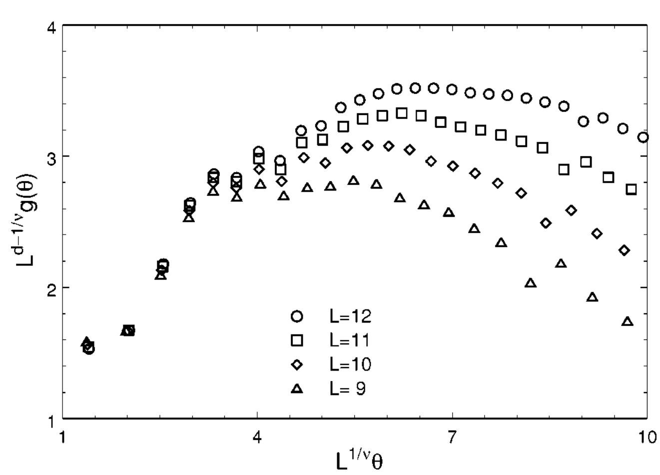

FIG. 5. The scaled density of zeros versus the scaled argument for the three-state Potts model with $L=9-12$.

TABLE II. The argument θ_1 of the first zero, the density of zeros $g(\overline{\theta_1})$ at $\overline{\theta_1}$, and the thermal exponent $y_t(L)$ for the three-state Potts model.

L	θ_1	$g(\overline{\theta_1})$	$y_t(L)$
3	0.265876	0.610828	1.580517
4	0.188912	0.541388	1.266530
5	0.146544	0.459651	1.157568
6	0.119459	0.394206	1.111652
7	0.100590	0.343757	1.091091
8	0.086680	0.304468	1.082282
9	0.076003	0.273274	1.079390
10	0.067554	0.248013	1.079618
11	0.060708	0.227183	1.081520
12	0.055051	0.209734	

depending on their universality classes. From Eq. (9) we obtain the thermal exponent

$$y_t(L) = d + \frac{\ln[g(0,L+1)/g(0,L)]}{\ln[(L+1)/L]} \tag{10}$$

for finite lattices. The fourth column of Table II shows $y_t(L)$ for several lattices. We again applied the BST algorithm and, for $\omega=1$, obtained $y_t=1.20(1)$ in excellent agreement with the exact value $y_t=\frac{6}{5}$.

III. DENSITY OF ZEROS FOR THE FOUR-STATE POTTS MODEL

The two-dimensional Potts model has a second-order phase transition for $Q\leqslant 4$ and a first-order transition for $Q>4$ [1]. The critical properties of the four-state Potts model have been studied extensively as the limiting case of a sequence ($Q\leqslant 4$) of models with continuous phase transitions. As is often the case, the limit of such a sequence $Q=4$ exhibits strong corrections to scaling [13]. The borderline case $Q=4$ is the most difficult.

The overall form of the density of zeros for $Q=4$ is qualitatively similar to that for $Q=3$. The third column of Table III shows the density of zeros at $\overline{\theta_1}$ for $3\leqslant L\leqslant 10$. The BST algorithm produces $g(0)=-0.003(7)$, for $\omega=\frac{1}{2}(=d-y_t)$, which is an expected result for the four-state model. The fourth column of Table III shows the values of the thermal exponent $y_t(L)$ by Eq. (10). Here, a simple power-law is assumed as a test. The extrapolated value is 1.366(3) for $\omega=1$, which is in disagreement with the exact value $y_t=\frac{3}{2}$. Figure 6(a) shows the scaled density of zeros versus the scaled argument, according to Eq. (6), for $L=7-10$. The values of the scaled density of zeros are divergent in the critical region, indicating that the form (6) is too simple to the four-state model.

The singular part of the energy for $Q=4$ has the scaling behavior with the logarithmic correction [13] as

TABLE III. The argument θ_1 of the first zero, the density of zeros $g(\overline{\theta_1})$, the thermal exponent $y_t(L)$ by Eq. (10), and the thermal exponent $y_t(L)^{\ln}$ with the logarithmic correction for the four-state Potts model.

L	θ_1	$g(\overline{\theta_1})$	$y_t(L)$	$y_t(L)^{\ln}$
3	0.289372	0.567991	1.507125	2.113488
4	0.201117	0.492904	1.254577	1.756218
5	0.153134	0.417372	1.179878	1.621322
6	0.122811	0.359406	1.156125	1.557673
7	0.101911	0.315566	1.151111	1.523886
8	0.086657	0.281748	1.153872	1.504702
9	0.075059	0.255023	1.159983	1.493392
10	0.065964	0.233422		

$$e \sim L^{-d+y_t}(\ln L)^{-3/4}. \tag{11}$$

Similarly, the scaling form of the density of zeros can be modified by replacing L^{-d+y_t} with $L^{-d+y_t}(\ln L)^{-3/4}$. Figure 6(b) shows the scaled density of zeros with the logarithmic correction versus the scaled argument. The divergence be-

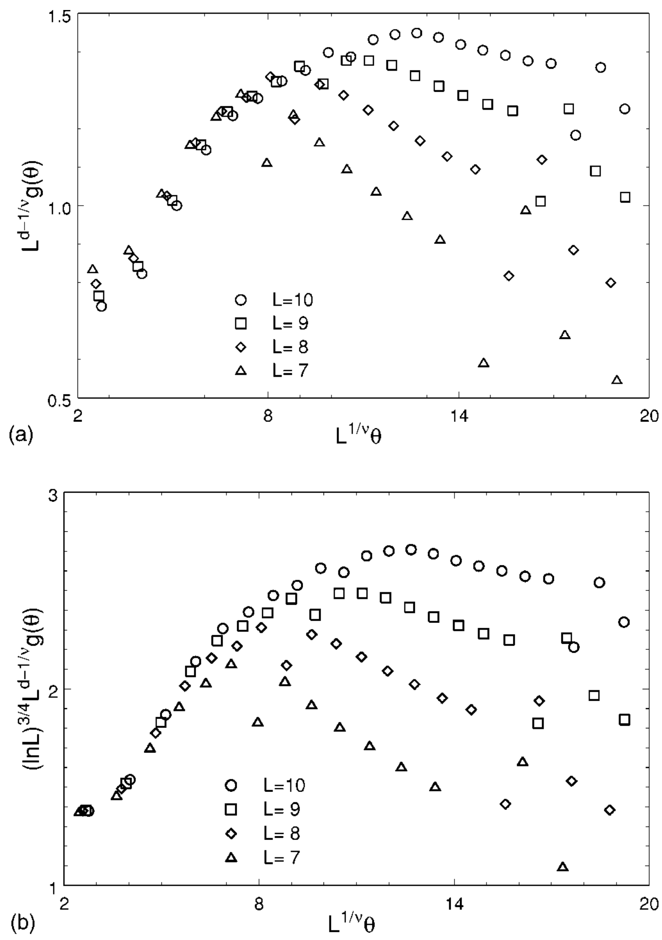

FIG. 6. The scaled density of zeros versus the scaled argument for the four-state Potts model ($L=7-10$) (a) without the logarithmic correction and (b) with the logarithmic correction.

tween the values of the scaled density of zeros is disappeared in the critical region. Now, with the logarithmic correction, we again evaluate the thermal exponents for finite sizes that are shown in the fifth column of Table III. The extrapolated value is 1.525(9) for $\omega = 1$, which is close to the exact value.

IV. CONCLUSION

We have enumerated the exact numbers of states up to $L=12$ for the three-state Potts model and up to $L=10$ for the four-state Potts model on $L\times L$ square lattice with self-dual boundary condition, using the microcanonical transfer matrix. If the number of states is known, the exact PF is obtained, and its zeros in the complex temperature plane are determined. For self-dual boundary condition, some of the Fisher zeros lie on the unit circle ($u_0 = e^{i\theta}$) in the complex $u=[1+(Q-1)y]/\sqrt{Q}$ plane. For these zeros, the density of the Fisher zeros $g(\theta)$ of the PF is calculated. For small θ the density of zeros obeys the finite-size scaling. This fact allows us to estimate the order parameter and the thermal exponent.

ACKNOWLEDGMENT

The author thanks Professor R. J. Creswick for valuable discussions.

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