# Partition Function Zeros of the Square Lattice Potts Model

Chi-Ning Chen and Chin-Kun Hu
*Institute of Physics, Academia Sinica, Nankang, Taipei 11529, Taiwan*

F. Y. Wu
*Department of Physics, Northeastern University, Boston, Massachusetts 02115*
(Received 13 February 1995)

We have evaluated numerically the zeros of the partition function of the $q$-state Potts model on the square lattice with reduced interactions $K$. On the basis of our numerical results, we conjecture that, both for finite planar self-dual lattices and for lattices with free or periodic boundary conditions in the thermodynamic limit, the zeros in the $\mathrm{Re}(x) > 0$ region of the complex $x = (e^K - 1)/\sqrt{q}$ plane are located on the unit circle $|x| = 1$.

PACS numbers: 05.50.+q, 75.10.–b

In 1952 Yang and Lee [1] introduced the concept of considering the zeros of the grand partition function of statistical mechanical systems, a consideration that has since opened new avenues to the study of phase transitions. While Yang and Lee considered the zeros in the complex fugacity plane, or equivalently the complex magnetic field plane in the case of spin systems, Fisher [2] in 1964 called attention to the relevance of the zeros of the canonical partition function in the complex temperature plane. Using the square lattice Ising model as an example, he showed that the partition function zeros are distributed on circles in the thermodynamic limit, and that the logarithmic singularity of the two-dimensional model arises as a consequence of the zero distribution. Since the consideration of zeros in the temperature plane is conceptually simpler, there have been numerous studies of the temperature zeros of spin systems. For example, the Ising partition function zeros have further been considered for the triangular [3], kagomé [4], and the simple cubic [5] lattices. Similarly, partition function zeros have been examined numerically for the square lattice Potts model [6,7], the three-state triangular Potts model [8,9], and the $Z_n$ models [10,11]. Specifically, the distribution of zeros of the three-state Potts model appears to follow a simple geometric locus in the ferromagnetic region [6,12], and the loci for the four-state Potts model appear to include a unit circle [7]. The partition function zeros have also been analyzed for lattices of $m \times \infty$ strips using a transfer matrix formalism [13]. However, except in the case of the triangular Potts model with pure three-spin interactions [9], there appears to have been no definite statement on the zero distributions, which is supported by numerical or exact results.

In this paper we follow up on the consideration of the partition function zeros of the $q$-state Potts model on the square lattice [6,7,12,13], and make a conjecture on their distribution. We first determine numerically the zeros in the complex temperature plane for small lattices under a special self-dual boundary condition. On the basis of our numerical results, we conjecture that, for *finite* planar self-dual lattices as well as for lattices with free or periodic boundary conditions in the thermodynamic limit, the zeros in the ferromagnetic regime are located on a unit circle. Unlike the Yang-Lee zeros of the Ising model for which the zeros are on a unit circle but with a density distribution which crosses the positive real axis only for temperatures $T \le T_c$, where $T_c$ is the critical temperature, the zero distribution of the Potts partition function crosses the positive real axis for all $q > 1$. In fact, it is the density distribution near the positive real axis that determines the critical behavior of spin systems [2].

Consider the $q$-state Potts model on a lattice, or graph, $G$, of linear dimension $L$ and having $N$ vertices and $E$ edges. Let the nearest-neighbor interaction be $J\delta_{\mathrm{Kr}}(\sigma_i, \sigma_j)$, where $\sigma_i, \sigma_j = 1, ..., q$ denote the spin states at vertices $i$ and $j$ connected by an edge and $q$ is an integer. The partition function can be written as [14]

$$Z \equiv Z_G(q,K) = \sum_{G' \subseteq G} (e^K - 1)^{b(G')} q^{n(G')}, \qquad (1)$$

where $K = J/kT$, the summation is taken over all subgraphs $G' \subseteq G$, and $b(G')$ and $n(G')$ are, respectively, the numbers of edges and clusters, including isolated vertices, of $G'$.

Introducing the variable

$$x = (e^K - 1)/\sqrt{q}\,, \qquad (2)$$

we rewrite (1) as a polynomial in $x$,

$$Z \equiv P_G(q,x) = \sum_{b=0}^{E} c_b(q) x^b, \qquad (3)$$

where

$$c_b(q) = q^{b/2} {\sum_{G' \subseteq G}}' q^{n(G')}, \qquad (4)$$

and the prime denotes that the summation is taken over all $G' \subseteq G$ for fixed $b(G') = b$. Then, for planar $G$, the polynomial $P_G$ possesses the duality relation [15]

$$P_G(q,x) = q^{N-1-E/2} x^E P_D(q, x^{-1})\,, \qquad (5)$$

  

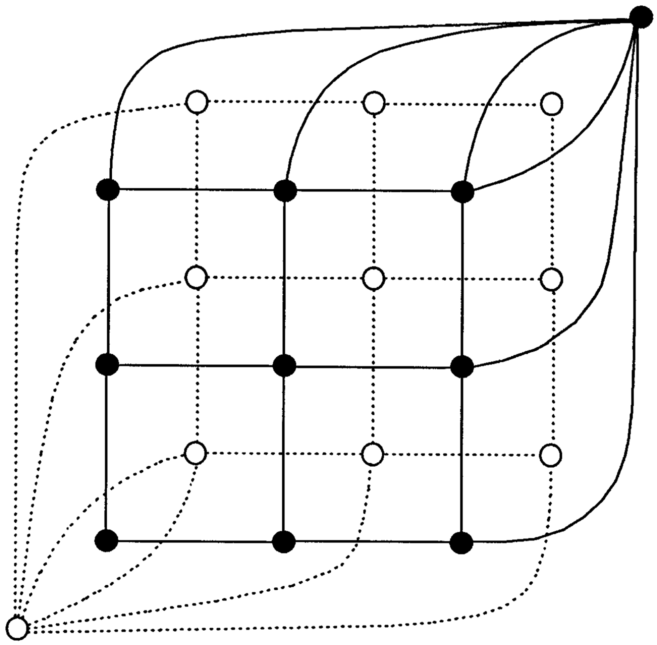

FIG. 1. An $L \times L$ self-dual lattice in solid lines and solid circles with $L = 3$. The dual lattice is denoted by dotted lines and open circles.

where $D$ is the graph dual to $G$. In the case of the square lattice for which $D$ is identical to $G$ in the thermodynamic limit regardless of boundary conditions, (5) implies that the system is critical at

$$x_c = 1\,. \tag{6}$$

To take full advantage of the duality relation (5), we consider a planar self-dual square lattice $G$, which is an $L \times L$ square lattice with $N = L^2 + 1, E = 2L^2$, and the special boundary condition shown in Fig. 1. While this lattice is planar and self-dual for any finite $L$, there is no difference between this lattice and square lattices with other boundary conditions in the thermodynamic limit.

We have used a fast algorithm proposed recently by two of us [16] to generate the partition function $P_G(q,x)$ for $L = 2$, 3, 4, 5, 6, and 7 [17]. The planar self-dual property (5) now implies the reciprocal relation

$$c_b(q) = c_{E-b}(q)\,, \tag{7}$$

and, as a result, the roots occur in pairs of $x_i$ and $x_i^{-1}$. We then computed the zeros of $P_G(q,x)$ in the complex $x$ plane and tracked their movement as $q$ increases from 1. At $q = 1$, all roots are found to be located at $x = -1$. As $q$ increases, some roots begin to spread into an arc of

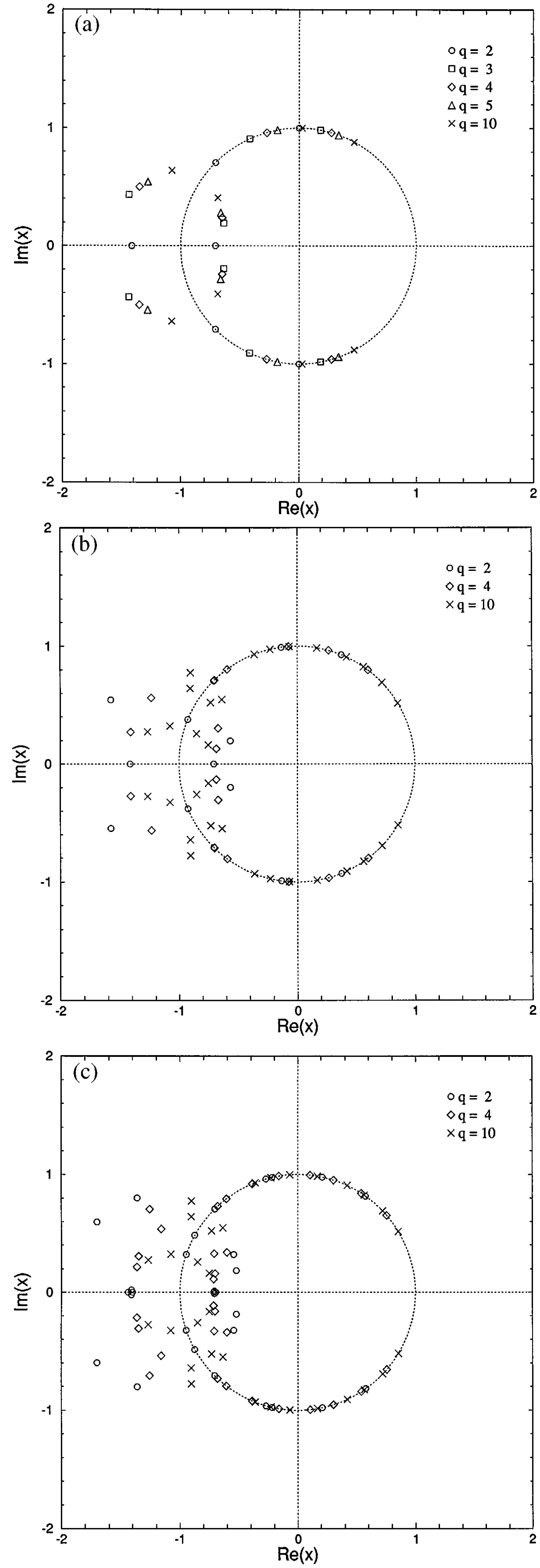


FIG. 2. The distribution of zeros of $P_G(q,x)$ for the $L \times L$ self-dual square lattice of Fig. 1 in the complex $x$ plane for (a) $L = 2$, (b) $L = 3$, and (c) $L = 4$.

the unit circle

$$|x| = 1, \tag{8}$$

with the arc centered about $x = -1$. As $q$ continues to increase, more and more roots appear on a larger arc and all zeros on the circle move on the circle toward the positive real axis, while others wander within the $\mathrm{Re}(x) < 0$ half plane. When $q$ reaches a certain critical value $q_c(L)$ which depends on $L$, all zeros are located at the unit circle $|x| = 1$. This implies that all roots of the Potts partition function are located on the unit circle in the limit of infinite $q$ and any finite $L$. We have established this latter result rigorously [18]. Typical results for $L = 2, 3, 4$ are shown in Fig. 3 (results for $L = 5, 6, 7$ are similar and not shown because they involve many more data points). For all practical purposes and within numerical errors, many roots are located precisely on the circle. We also find that, in all cases, zeros which are located off the unit circle are always confined in the $\mathrm{Re}(x) < 0$ half plane for integral $q$.

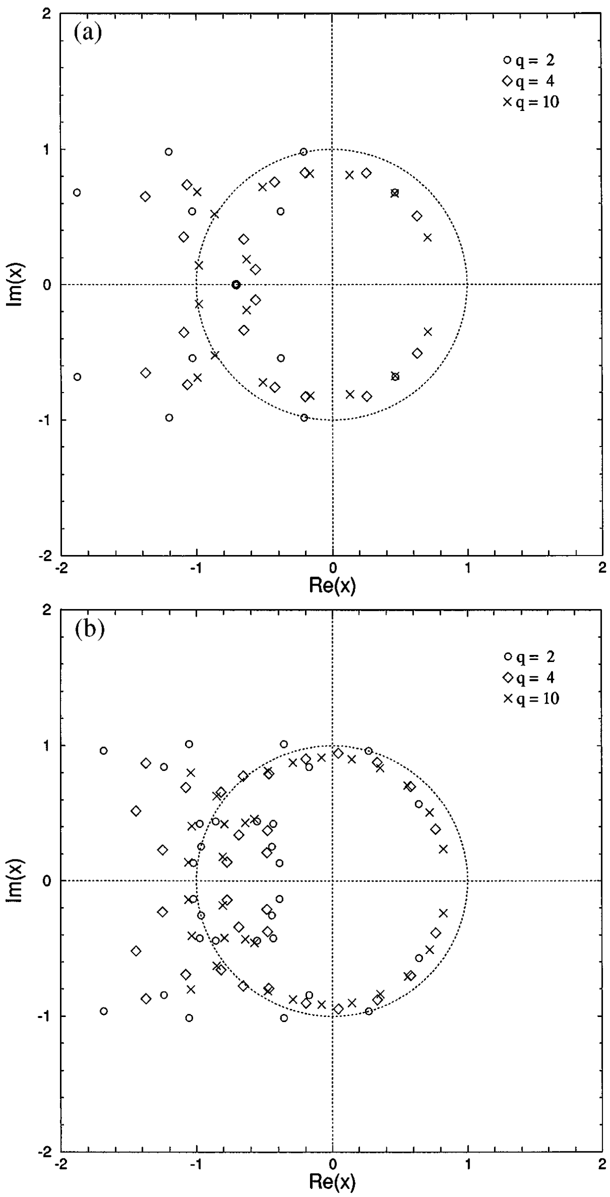


FIG. 3. The distribution of zeros of $P_G(q,x)$ for the $L \times L$ square lattice with periodic boundary conditions for (a) $L = 3$, and (b) $L = 4$.

It is significant that zeros do reside on the circle (8), as this is *not* a consequence of the duality relation (5). As a comparison, we have computed the partition function zeros for $L \times L$ lattices with periodic boundary conditions which are nonplanar. The results, shown in Fig. 4 for $L = 3, 4$, indicate that none of the zeros are on the unit circle, even though zeros do approach the circle as $L$ and $q$ increase. However, the distribution of zeros should be independent of the boundary condition in the thermodynamic limit. In addition, we have computed the zeros of the Potts partition function for square lattices under two other types of boundary conditions which are also planar and self-dual, and extended computations to different horizontal and vertical linear dimensions. In all cases we have arrived at the same conclusion: The Potts partition function zeros in the $\mathrm{Re}(x) > 0$ half plane all reside on the unit circle $|x| = 1$. These findings now lead us to make the following conjecture.

*Conjecture:* For finite planar self-dual lattices and for square lattice with free or periodic boundary conditions in the thermodynamic limit, the Potts partition function zeros in the $\mathrm{Re}(x) > 0$ half plane are located on the unit circle $|x| = 1$.

It is a curious fact that the self-dual feature of a planar lattice somehow forces many roots to locate on the circle, even for small lattices. Furthermore, our conjecture is consistent with a similar conjecture on the zero distribution of the Potts model with pure three-site interactions [9], which also possesses a duality relation similar to (5). The key appears to lie in the validity of the duality relation (5).

For $q = 2$, it is known [2] that, in the thermodynamic limit, zeros also lie on the circle

$$|x + \sqrt{2}| = 1. \tag{9}$$

Maillard and Rammal [6] have suggested on the basis of an inversion relation consideration that, for $q < 4$, the circle

$$\left| x + \frac{2}{\sqrt{q}} \right| = \sqrt{\frac{4}{q} - 1} \tag{10}$$

can be a good candidate as the generalization of (9). However, (10) does not appear to be in agreement with our numerical data. It should also be pointed out that our conjecture is consistent with prior numerical studies [6,7] as well as results of certain algebraic approximations for $m \times \infty$ strips [13].

The reduced per-site free energy of the Potts model is now given by the expression

$$f = N^{-1} \sum_i \ln(1 - x/x_i) + \text{const}, \qquad (11)$$

where the summation is taken over all roots $x_i$ of the polynomial (3). Fisher [2] has pointed out that the critical behavior near the critical point $x_c$ is determined solely by the root distribution in the regime near the positive real axis. Thus, for $x$ near $x_c = 1$, we collect those zeros along an arc of the unit circle intersecting the positive real axis or, equivalently, the zeros $x_i = e^{i\theta_i}, \theta_i$ small. Let the zeros be distributed with a density $Ng(\theta)$. We can rewrite, in the thermodynamic limit, the singular part of (11) as

$$f_{\text{sing}} = \frac{1}{2\pi} \int_{-\Delta}^{\Delta} g(\theta) \ln(t + i\theta)\, d\theta\,, \qquad (12)$$

where $t = x_c - x$ and $\Delta$ is a small number. Note that we have $g(\theta) = g(-\theta)$ since $c_b(q)$ is real. Fisher [2] has shown that the density $g(\theta) = a|\theta|$ near $\theta = 0$, where $a$ is a constant, yields the logarithmic singularity of the Ising model. Along the same line, the small $\theta$ density distribution [2,19]

$$g(\theta) = \begin{cases} a|\theta|^{1-\alpha(q)}, & q \leq 4\,, \\ \epsilon(q), & q > 4\,, \end{cases} \qquad (13)$$

leads to the specific singularity $|t|^{-\alpha(q)}$ for $q \leq 4$ and a jump discontinuity of amount $\epsilon(q)$ in $U$ for $q > 4$. These are the known critical behaviors of the Potts model.

We thank J. M. Maillard for calling our attention to Ref. [6] and useful comments. Two of us (C. N. C. and C. K. H.) are supported by the National Science Council of the Republic of China (Taiwan) under Grants No. NSC 84-2112-M-001-013 Y, No. 84-0501-I-001-037-B12, and No. NSC 84-2112-M-001-048. The work by F. Y. W. is supported in part by the National Science Foundation through Grants No. DMR-9313648 and No. INT-920788261; he would also like to thank T. T. Tsong for the kind hospitality extended to him at the Academia Sinica where this work was completed.

[1] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952).
[2] M. E. Fisher, in *Lecture Notes in Theoretical Physics*, edited by W. E. Brittin (University of Colorado Press, Boulder, 1965), Vol. 7c.
[3] J. Stephenson, J. Phys. A **13**, 4513 (1987).
[4] R. Abe, T. Dotera, and T. Ogawa, Prog. Theor. Phys. **85**, 509 (1991).
[5] R. B. Pearson, Phys. Rev. B **26**, 6285 (1982).
[6] J. M. Maillard and R. Rammal, J. Phys. A **16**, 353 (1983).
[7] P. P. Martin, J. Phys. A **19**, 3267 (1986).
[8] P. P. Martin and J. M. Maillard, J. Phys. A **19**, L547 (1986).
[9] J. C. A. d'Auriac, J. M. Maillard, G. Rollet, and F. Y. Wu, Physica (Amsterdam) **206A**, 441 (1994).
[10] P. P. Martin, J. Phys. A **21**, 4415 (1988).
[11] B. Bonnier and Y. Leroyer, Phys. Rev. B **44**, 9700 (1991).
[12] P. P. Martin, in *Integrable Systems in Statistical Mechanics*, edited by G. M. d'Ariano, A. Montorsi, and M. G. Rasetti (World Scientific, Singapore, 1985).
[13] D. W. Wood, R. W. Turnbull, and J. K. Ball, J. Phys. A **20**, 3495 (1987).
[14] See, for example, F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).
[15] F. Y. Wu and Y. K. Wang, J. Math. Phys. (N.Y.) **17**, 439 (1976).
[16] C. N. Chen and C. K. Hu, Phys. Rev. B **43**, 11 519 (1991).
[17] The series for the partition function $P_G(q,x)$ for $L = 2, 3, ..., 7$ can be obtained from CNC at the e-mail address "chencn@phys.sinica.edu.tw".
[18] F. Y. Wu, G. Rollet, H. Y. Huang, J. M. Maillard, C.-K. Hu and C.-N. Chen, following Letter, Phys. Rev. Lett. **76**, 173 (1996).
[19] P. P. Martin, *Potts Models and Related Problems in Statistical Mechanics* (World Scientific, Singapore, 1991).