Yang-Lee Zeros of the Q-State Potts Model in the Complex Magnetic Field Plane

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The microcanonical transfer matrix is used to study the distribution of Yang-Lee zeros of the Q-state Potts model in the complex magnetic field ($x = e^{\beta h}$) plane for the first time. Finite size scaling suggests that at (and below) the critical temperature the zeros lie close to, but not on, the unit circle with the two exceptions of the critical point $x = 1$ ($h = 0$) itself and the zeros in the limit $T = 0$. [S0031-9007(98)07026-4]

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The Q-state Potts model [1,2] in two dimensions is very fertile ground for the analytical and numerical investigation of first- and second-order phase transitions. With the exception of the $Q = 2$ Potts (Ising) model in the absence of a magnetic field [3], exact solutions for arbitrary Q are not known. However, some exact results have been established for the Q-state Potts model. For $Q = 2$, 3, and 4 there is a second-order phase transition, while for $Q > 4$ the transition is first order [4]. From the duality relation the critical temperature is known to be $k_B T_c / J = 1/\ln(1 + \sqrt{Q})$ [1]. For $Q = 3$ and 4 the critical exponents [5] are known, while for $Q > 4$ the latent heat [4], spontaneous magnetization [6], and correlation length [7] at T_c are also known.

By introducing the concept of the zeros in the *complex* magnetic field plane of the grand partition function (Yang-Lee zeros), Yang and Lee [8] proposed a mechanism for the occurrence of phase transitions in the thermodynamic limit and gained a new insight into the unsolved problem of the Ising model in an arbitrary nonzero external magnetic field. They have shown that the distribution of the zeros of a model determines its critical behavior. Lee and Yang [9] also formulated the celebrated circle theorem which states that the zeros of the grand partition function of the Ising ferromagnet in the complex magnetic field plane lie on the unit circle. In the 1960s, Fisher [10] initiated the study of the partition function zeros in the complex temperature plane (Fisher zeros) for the square lattice Ising model, and since that time this problem has attracted continuous interest. In particular, the Fisher zeros of the Q-state Potts model in the absence of a magnetic field have been studied extensively [11–14]. By numerical methods it has been shown [12] that for self-dual boundary conditions the Fisher zeros of the Q-state Potts model on a finite square lattice are located on the unit circle in the complex p plane for $\mathrm{Re}(p) > 0$, where $p = (y^{-1} - 1)/\sqrt{Q}$ and $y = e^{-\beta}$. The study of the Yang-Lee zeros of the Ising model has a long history, and some results have been reported in one [9], two [9,15], three [16], and four [17] dimensions. However, except for the one-dimensional Potts model [18], the Yang-Lee zeros of the $Q > 2$ Potts models have never been studied. In this paper we discuss the Yang-Lee zeros of the Q-state Potts model in two dimensions.

We use an *exact* numerical technique for the evaluation of grand partition functions, the microcanonical transfer matrix (μTM) [14,15,19]. The bond energy for the Q-state Potts model is (in dimensionless units)

$$E = \sum_{\langle i,j \rangle} [1 - \delta(\sigma_i, \sigma_j)], \tag{1}$$

where $\langle i, j \rangle$ indicates a sum over nearest-neighbor pairs, $\sigma_i = 0, \ldots, Q - 1$, and E is a positive integer $0 \le E \le N_b$, where N_b is the number of bonds on the lattice. We study the grand partition function of the Potts model in an external field which couples to the order parameter

$$M_q = \sum_k \delta(\sigma_k, q), \tag{2}$$

where q is a fixed integer between 0 and $Q - 1$. Note that $0 \le M_q \le N_s$ is also an integer and N_s is the number of sites on the lattice. By μTM it is possible to obtain *exact* integer values for the number of states with fixed energy E and fixed order parameter M, $\Omega_Q(M, E)$. The grand partition function in a magnetic field h is then a polynomial given by

$$Z_Q(x, y) = \sum_{M=0}^{N_s} \sum_{E=0}^{N_b} \Omega_Q(M, E) x^M y^E, \tag{3}$$

where $x = e^{\beta h}$ and $y = e^{-\beta}$. We have calculated the grand partition function of the Q-state Potts model on finite $L \times L$ square lattices with self-dual boundary conditions [12] and cylindrical boundary conditions for $3 \le Q \le 8$.

Figure 1 shows the Yang-Lee zeros for the three-state Potts model in the complex x plane at the critical temperature $y_c = 1/(1 + \sqrt{3}) = 0.366, \ldots$ for $L = 4$ and $L = 10$ with cylindrical boundary conditions. Note that, unlike the Ising model, the zeros of the three-state Potts model lie close to, but not on, the unit circle. The zero farthest from the unit circle is in the neighborhood of $\arg(x) = \pi$, while the zero closest to the positive real axis lies closest to the unit circle. Note that the zeros for $L = 10$ lie on a locus interior to that for $L = 4$. We

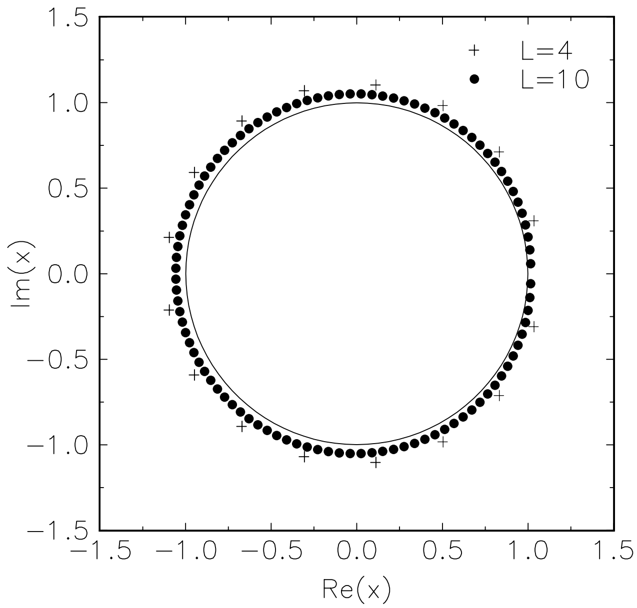

FIG. 1. Zeros of the three-state Potts model in the complex x plane at $y = y_c$ for $L = 4$ and $L = 10$ with cylindrical boundary conditions.

observe similar behavior for larger values of Q. We expect that in the thermodynamic limit the locus of zeros cuts the real x axis at the point $x = 1$, corresponding to $h = 0$. Table I shows the distance from the origin and the imaginary part of the first two zeros of the three-state Potts model for $3 \le L \le 12$. By using the Bulirsch-Stoer (BST) algorithm [20], we extrapolated our results for finite lattices to infinite size. The error bars are twice the difference between the $(n - 1, 1)$ and $(n - 1, 2)$ approximants. As one can see, these zeros converge to the critical point, $x = 1$, as described by Yang and Lee [8,9].

While we lack the circle theorem of Lee and Yang to tell us the location of the zeros, something can be said about their general behavior as a function of temperature. At zero temperature ($y = 0$) from Eq. (3), the grand partition function is

$$Z_Q(x,0) = \sum_M \Omega_Q(M,0)x^M = (Q - 1) + x^{N_s}. \tag{4}$$

Therefore, the Yang-Lee zeros at $T = 0$ are given by

$$x_k = (Q - 1)^{1/N_s} \exp[i(2k - 1)\pi/N_s], \tag{5}$$

where $k = 1, ..., N_s$. The zeros at $T = 0$ are uniformly distributed on the circle with radius $(Q - 1)^{1/N_s}$ which approaches unity in the thermodynamic limit, independent of Q. At infinite temperature ($y = 1$), Eq. (3) becomes

$$Z_Q(x,1) = \sum_{M=0}^{N_s} \sum_{E=0}^{N_b} \Omega_Q(M,E)x^M. \tag{6}$$

Because $\sum_E \Omega_Q(M,E)$ is simply $\binom{N_s}{M}(Q - 1)^{N_s - M}$, at $T = \infty$, the grand partition function is given by

$$Z_Q(x,1) = (Q - 1 + x)^{N_s}, \tag{7}$$

and its zeros are N_s degenerate at $x = 1 - Q$, independent of lattice size. Figure 2 shows the zeros for the three-state Potts model at several temperatures with cylindrical boundary conditions. At $y = 0.5y_c$ the zeros are uniformly distributed close to the unit circle. As the temperature is increased the edge singularity moves away from the real axis and the zeros detach from the unit circle. Finally, as y approaches unity, the zeros converge on the point $x = -2$.

For self-dual boundary conditions [12] we observe the same behaviors as those in Figs. 1 and 2 for cylindrical boundary conditions. $N_s = L^2$ and $N_b = 2L^2 - L$ for cylindrical boundary conditions, while $N_s = L^2 + 1$ and $N_b = 2L^2$ for self-dual boundary conditions [12]. One of the main differences between two boundary conditions

TABLE I. The distance from the origin and the imaginary part of the first two zeros of the three-state Potts model. Abs(x_1) and Im(x_1) are the modulus and the imaginary part of the first zero, x_2 is the second zero, and the last row is the BST extrapolation to infinite size.

L	Abs(x_1)	Im(x_1)	Abs(x_2)	Im(x_2)
3	1.133269811535	0.525147232092	1.154497346584	1.064547354702
4	1.080426920767	0.309148097981	1.095611066859	0.711951325609
5	1.054600270108	0.205103734779	1.065723514328	0.488677034595
6	1.039822577595	0.146911393618	1.048300166208	0.353845470678
7	1.030488924546	0.110897277587	1.037169667607	0.268016265956
8	1.024179322221	0.086960474252	1.029587245456	0.210307724775
9	1.019696144103	0.070189130073	1.024169532034	0.169679308232
10	1.016386584326	0.057951942531	1.020153066105	0.139981471036
11	1.013868175716	0.048731329669	1.017086499226	0.117596130069
12	1.011903888317	0.041599753769	1.014688183571	0.100288119772
∞	1.0000(1)	0.00002(7)	1.0000(3)	0.000(1)

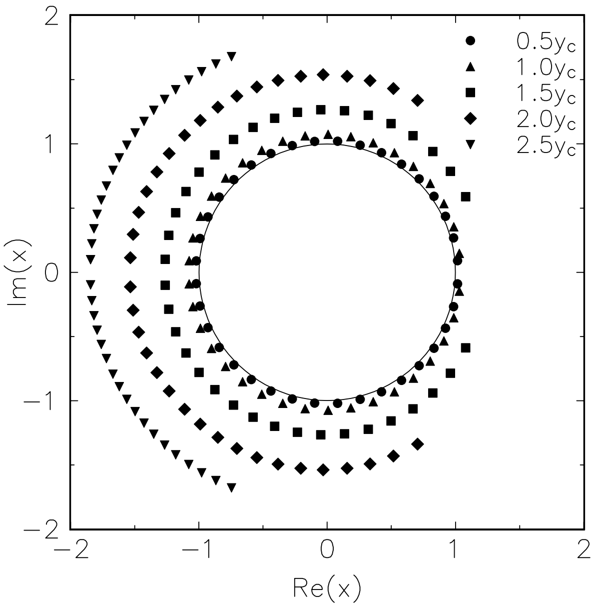

FIG. 2. Zeros of the three-state Potts model in the complex x plane for several values of y ($L = 6$ and cylindrical boundary conditions).

is the number of zeros, which is equal to N_s. Figure 3 shows the Yang-Lee zeros of the three-state Potts model at $y = y_c$ for $L = 7$ with self-dual and cylindrical boundary conditions. The difference in the number of zeros between two boundary conditions results in the difference in the locations of zeros near $x = -1$. However, as x approaches 1, the zeros for the two different boundary conditions are nearly identical. We observe that the effect of the boundary condition on the location of the Yang-Lee zeros near the critical point of the Potts model is very small, and in the rest of this paper we will consider only cylindrical boundary conditions.

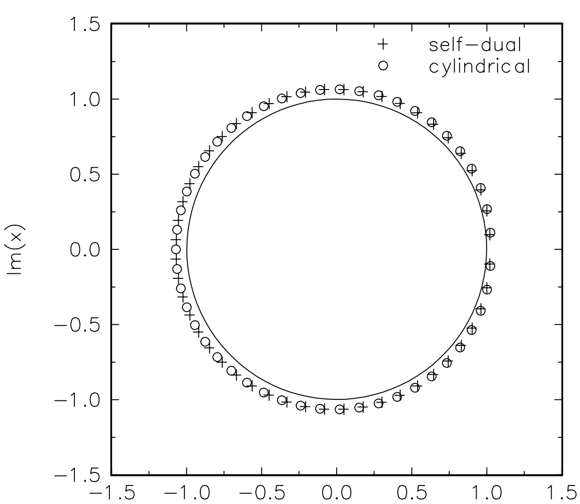

FIG. 3. Zeros of the three-state Potts model in the complex x plane at $y = y_c$ for $L = 7$ with self-dual boundary conditions (plus symbols) and cylindrical boundary conditions (open circles).

It is clear that the Yang-Lee zeros of the Q-state Potts model do not lie on the unit circle for $Q > 2$ for any value of y and any finite value of L. However, there is some cause to speculate that for $y \leq y_c$ the zeros *do* lie on the unit circle in the thermodynamic limit. Since the zero in the neighborhood of $\arg(x) = \pi$ is always the farthest from the unit circle, if this zero can be shown to approach $|x(\pi)| = 1$ in the limit $L \to \infty$, all of the zeros should lie on the unit circle in this limit. In Fig. 4 we show values for $|x(\pi)|$ extrapolated to infinite size using the BST algorithm [20] for $3 \leq Q \leq 8$ at $y = 0.5y_c$ and $y = y_c$. From these results it is clear that, while the locus of zeros lies *close* to the unit circle at $y = y_c$, it does not coincide with it, except at the critical point $x = 1$.

Figure 5 shows the BST estimate of the modulus of the locus of zeros as a function of angle for the three-state Potts model at $y = 0.5y_c$, $y = y_c$, and $y = 1.2y_c$. To calculate the extrapolated values for each angle θ we selected the zero whose arguments were closest to θ, for lattices of size $3 \leq L \leq 12$ for $\theta = 0.0, 0.5, \ldots, 2.5$, and π. The BST algorithm was then used to extrapolate these values for finite lattices to infinite size. The large variation in the size of the error bars is due to the fact that for a given θ there may be no zero *close* to θ for the smaller lattices. In Fig. 5 at $y = y_c$ the first four angles are shifted slightly from the original values ($\theta = 0.0$, 0.5, 1.0, and 1.5) to be distinguished from the results at $y = 0.5y_c$. For $y = 0.5y_c$ and $y = y_c$ the first zeros definitely lie on the point $r(\theta = 0) = 1$ in the thermodynamic limit. However, for $y = 1.2y_c$, the BST estimates of the modulus and angle of the first zero are 1.054(2) and 0.09(6). Therefore, at $y = 1.2y_c$, the locus of zeros does not cut the positive real axis in the thermodynamic limit, consistent with the absence of a physical singularity for $y > y_c$.

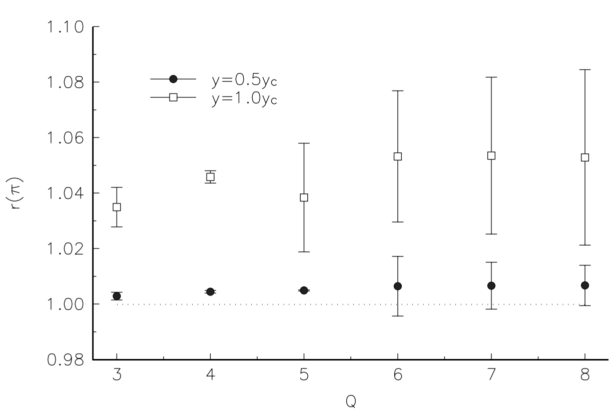

FIG. 4. Modulus of the zero at $\theta = \pi$ extrapolated to infinite size for $3 \leq Q \leq 8$ at $y = 0.5y_c$ and $y = y_c$ with cylindrical boundary conditions.

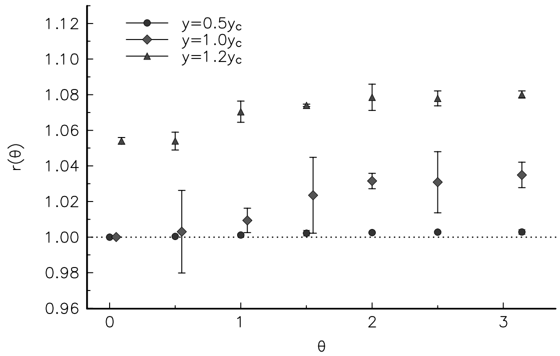

FIG. 5. Modulus of the locus of zeros as a function of angle for the three-state Potts model at $y = 0.5y_c$, y_c, and $1.2y_c$ with cylindrical boundary conditions. The slight horizontal offset for data for $y = y_c$ is for clarity only. However, the offset of the edge singularity for $y = 1.2y_c$ from $\theta = 0$ is real.

From these results, we come to the conclusion that, in fact, the locus of zeros in the thermodynamic limit *is not* the unit circle, although, due to the relatively small lattices studied here, we certainly do not offer this as a proof. Rather, we believe the nature of the locus of zeros remains an open and interesting question.

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