Exact results for the zeros of the partition function of the Potts model on finite lattices

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Abstract

The Yang-Lee zeros of the $Q$-state Potts model are investigated in 1, 2 and 3 dimensions. Analytical results derived from the transfer matrix for the one-dimensional model reveal a systematic behavior of the locus of zeros as a function of $Q$. For $1 < Q < 2$ the zeros in the complex $x = \exp(\beta H_q)$ plane lie inside the unit circle, while for $Q > 2$ they lie outside the unit circle for finite temperature. In the special case $Q = 2$ the zeros lie exactly on the unit circle as proved by Lee and Yang. In two and three dimensions the zeros are calculated numerically and behave in the same way. Results are also presented for the critical line of the Potts model in an external field as determined from the zeros of the partition function in the complex temperature plane.

I. INTRODUCTION

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

The $Q$-state Potts model on a lattice $G$ in an external magnetic field $H_q$ is defined by the Hamiltonian

\begin{equation}
H_Q = J \sum_{\langle i,j \rangle} [1 - \delta(\sigma_i, \sigma_j)] - H_q \sum_k \delta(\sigma_k, q),
\end{equation}

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where $J$ is the coupling constant, $\langle i, j \rangle$ indicates a sum over nearest-neighbor pairs, $\sigma_i = 1, ..., Q$, and $q$ is a fixed integer between 1 and $Q$. The partition function of the model can be written as

$$Z_Q(x, y) = \sum_{M=0}^{N_s} \sum_{E=0}^{N_b} \Omega_Q(M, E)x^M y^E,$$  \hspace{1cm} (2)

where $x = e^{\beta H_q}$, $y = a^{-1} = e^{-\beta J}$, $E$ and $M$ are positive integers $0 \leq E \leq N_b$ and $0 \leq M \leq N_s$, respectively, $N_b$ and $N_s$ are the number of bonds and the number of sites on the lattice $G$, and $\Omega_Q(M, E)$ is the number of states with fixed $E$ and fixed $M$. From Eq. (2) it is clear that $Z_Q(x, y)$ is simply a polynomial in $x$ and $y$.

By introducing the concept of the zeros of the partition function in the complex magnetic-field plane (Yang-Lee zeros), Yang and Lee [7] proposed a mechanism for the occurrence of phase transitions in the thermodynamic limit and yielded a new insight into the unsolved problem of the two-dimensional Ising model in an arbitrary nonzero external magnetic field. It has been shown [7,8] that the distribution of the zeros of a model determines its critical behavior. Lee and Yang [7] also formulated the celebrated circle theorem which states that the Yang-Lee zeros of the Ising ferromagnet lie on the unit circle. While we lack the circle theorem of Lee and Yang to tell us the location of the zeros for $Q \neq 2$, something can be said about their general behavior as a function of temperature. At zero temperature ($y = 0$) from Eq. (2) the partition function is

$$Z_Q(x, 0) = \sum_{M=0}^{N_s} \Omega_Q(M, 0)x^M = (Q - 1) + x^{N_s}. \hspace{1cm} (3)$$

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

$$x_k = (Q - 1)^{1/N_s} \exp[i(2k - 1)\pi/N_s], \hspace{1cm} (4)$$

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. (2) becomes

$$Z_Q(x, 1) = \sum_{M=0}^{N_s} \sum_{E=0}^{N_b} \Omega_Q(M, E)x^M. \hspace{1cm} (5)$$

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

$$Z_Q(x, 1) = (Q - 1 + x)^{N_s}, \hspace{1cm} (6)$$

and its zeros are $N_s$-degenerate at $x = 1 - Q$, independent of lattice size.

**II. YANG-LEE ZEROS IN ONE DIMENSION**

For the one-dimensional Potts model in an external field the eigenvalues of the transfer matrix were found by Glumac and Uzelac [9]. The two dominant eigenvalues are $\lambda_\pm = \frac{1}{2}$.
\( (A \pm iB)/2a, \) where \( A = a(1 + x) + Q - 2, \) \( B = -i\sqrt{[a(1 - x) + Q - 2]^2 + 4(Q - 1)x}, \) and \( \lambda_0 = (a - 1)/a \) is \( (Q - 2) \)-fold degenerate.

We will assume that \( |\lambda_\pm| > \lambda_0 \) and verify this assumption a posteriori. The partition function is

\[
Z_N = \lambda_+^N + \lambda_-^N + (Q - 2)\lambda_0^N, \tag{7}
\]

but, by the above approximation, for large \( N \) we have

\[
Z_N \simeq \lambda_+^N + \lambda_-^N. \tag{8}
\]

If we define \( A = 2C \cos \psi \) and \( B = 2C \sin \psi, \) where \( C = \sqrt{(a - 1)(Q + a - 1)x}, \) then \( \lambda_\pm = (C/a) \exp(\pm i\psi), \) and the partition function is

\[
Z_N = 2 \left( \frac{C}{a} \right)^N \cos N\psi. \tag{9}
\]

The zeros of the partition function are then given by

\[
\psi = \psi_k = \frac{2k + 1}{2N} \pi, \quad k = 0, 1, 2, \ldots, N - 1. \tag{10}
\]

The location of these zeros in the complex \( x \) plane is determined by the solution of

\[
A = 2C \cos \psi_k. \tag{11}
\]

This equation is quadratic in \( z = \sqrt{x} \) with roots

\[
z_k = \frac{1}{a} \left[ \sqrt{(a - 1)(Q + a - 1)} \cos \psi_k \pm i\sqrt{(a - 1)(Q + a - 1) \sin^2 \psi_k + Q - 1} \right]. \tag{12}
\]

It is easily verified that

\[
|z_k|^2 = |x_k| = \frac{Q + a - 2}{a}, \tag{13}
\]

and we see that all the zeros lie on a circle in the complex \( x \) plane. The argument of \( x_k \) is given by

\[
\cos \frac{\theta_k}{2} = \sqrt{\frac{(a - 1)(Q + a - 1)}{a(Q + a - 2)}} \cos \psi_k. \tag{14}
\]

Before we analyze these results we must verify that in fact \( |\lambda_\pm| > \lambda_0 \) in the region of these zeros. We find

\[
\frac{|\lambda_\pm|}{\lambda_0} = \sqrt{\frac{(Q + a - 1)(Q + a - 2)}{a(a - 1)}}, \tag{15}
\]

which is indeed greater than unity for \( Q > 1. \)
If we return to Eq. (13) we can discern a remarkably systematic behavior of the Yang-Lee zeros with $Q$. For $1 < Q < 2$, $|x_k| < 1$ and the zeros lie inside the unit circle. As $a \to \infty$, the zeros approach the unit circle from within, as we observed in Eq. (4), and for $a = 1$, $\cos(\theta_k/2) = 0$, so $\theta_k = \pi$ and all the zeros lie at $1 - Q$, as predicted in Eq. (6). For $Q > 2$, $|x_k| > 1$ and the zeros lie outside the unit circle and approach the unit circle as $a \to \infty$ from outside. In the special case $Q = 2$ we of course find that $|x_k| = 1$, as proved by Lee and Yang [7]. The edge singularity in the thermodynamic limit is given by

$$\theta_0 = 2 \cos^{-1} \left( \frac{(a - 1)(Q + a - 1)}{a(Q + a - 2)} \right) > 0,$$

from which we conclude that no transition occurs for any $T > 0$.

Finally, we can use these exact results to study finite size effects on the distribution of zeros. For finite $N$ we must find the zeros of the full partition function as given in Eq. (7). We find that finite size effects are very small in one dimension, but the largest deviation from the limiting locus occurs for $\arg(x) = \pi$.

III. YANG-LEE ZEROS IN TWO AND THREE DIMENSIONS

We have calculated exact integer values for $\Omega_Q(M, E)$ on $L \times L$ square lattice for $3 \leq L \leq 8$ and $3^3$ simple-cubic lattice ($Q = 3$) using the restricted microcanonical transfer matrix [10]. For square lattices up to $L = 12$ ($Q = 3$) the zeros are calculated using a semi-canonical variation of the transfer matrix. Fig. 1a shows the Yang-Lee zeros for the two-dimensional three-state Potts model in the complex $x$ plane at the critical temperature $y_c = 1/(1 + \sqrt{3}) = 0.366...$ for $L = 4$ and $L = 10$ with cylindrical boundary conditions. Note that just as in the one-dimensional 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. The behavior of the zeros with the size of the lattice also follows that of the one-dimensional model; the zeros for $L = 10$ lie on a locus interior to that for $L = 4$, and we find similar behavior for larger values of $Q$. In the thermodynamic limit the locus of zeros cuts the real $x$ axis at the point $x = 1$ [11] corresponding to $H_q = 0$, as described by Yang and Lee [9]. Fig. 1b shows the zeros for the two-dimensional three-state Potts model at several temperatures with cylindrical boundary conditions. At $y = 0.5y_c$ the zeros are nearly uniformly distributed in argument and 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 $x = -2$. As predicted by Eqs. (4) and (6), for periodic boundary conditions [12] and self-dual boundary conditions [11] we observe the same behaviors as those in Fig. 1 for cylindrical boundary conditions.

The exact nature of the locus of zeros for the $Q$-state Potts model in two dimensions is unknown, with the exception of $Q = 2$. It is clear that the Yang-Lee zeros of the two-dimensional $Q$-state Potts model do not lie on the unit circle for $Q > 2$ for any value of $y$ and any finite value of $L$. 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 the zeros should lie on the unit circle in this limit. In Fig. 2 we show values for \( |x(\pi)| \) extrapolated to infinite size using the Bulirsch-Stoer (BST) algorithm \([13]\) for \( 3 \leq Q \leq 8 \) at \( y = 0.5y_c \) and \( y = y_c \). The error bars are twice the difference between the \((n - 1, 1)\) and \((n - 1, 2)\) approximants. 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 \( x = 1 \). While the numerical evidence presented here suggests that the locus of zeros for the three-state model is not the unit circle, and the exact result in one-dimension provides an example where the locus varies continuously with \( Q \), the nature of the locus remains an open and fascinating question.

Fig. 3 shows the BST estimate of the modulus of the locus of zeros as a function of angle for the two-dimensional three-state Potts model at \( y = 0.5y_c \) and \( y = y_c \). To calculate the extrapolated values for each angle, \( \theta \), we selected the zero whose arguments were closest to \( \theta \) for lattices of size \( 3 \leq L \leq 12 \) for \( \theta = 0.0, 0.5, ..., 2.5 \) and \( \pi \). 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 \( \theta \) there may be no zero close to \( \theta \) for the smaller lattices. In Fig. 3 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 shows the Yang-Lee zeros for the three-dimensional three-state Potts model at several temperatures on the \( 3^3 \) simple-cubic lattices with periodic boundary conditions in \( x \) and \( y \) directions and free boundary conditions in \( z \) direction. The behaviors in Fig. 4 for the three-dimensional model are the same as those in Fig. 1b for the two-dimensional model.

**IV. FISHER ZEROS IN AN EXTERNAL FIELD**

Fisher \([14]\) emphasized that the partition function zeros in the complex temperature plane (Fisher zeros) are also very useful in understanding phase transitions. In particular, using the Fisher zeros both the ferromagnetic phase and the antiferromagnetic phase can be considered at the same time. From the exact solutions \([2]\) of the square lattice Ising model it has been shown \([14]\) that in the absence of an external magnetic field the Fisher zeros lie on two circles in the thermodynamic limit. Recently the locus of the Fisher zeros of the \( Q \)-state Potts model in the absence of an external magnetic field has been studied extensively \([15,16]\). It has been shown \([16]\) that for self-dual boundary conditions near the ferromagnetic critical point \( y_c = 1/(1 + \sqrt{Q}) \) the Fisher zeros of the Potts model on a finite square lattice lie on the circle with center \(-1/(Q - 1)\) and radius \( \sqrt{Q}/(Q - 1) \) in the complex \( y \) plane, while the antiferromagnetic circle of the Ising model completely disappears for \( Q > 2 \). However, the properties of the Fisher zeros for \( Q > 2 \) in an external field are not known.

In the limit \( H_q \to -\infty \) (\( x \to 0 \)) the partition function of the \( Q \)-state Potts model becomes
\[ Z_Q = \sum_{E=0}^{N_b} \Omega_Q(M = 0, E)y^E, \quad (17) \]

where \( \Omega_Q(M = 0, E) \) is the same as the number of states \( \Omega_{Q-1}(E) \) of the \((Q-1)\)-state Potts model in the absence of an external magnetic field. As \( x \) decreases from 1 to 0, the \( Q \)-state Potts model is transformed into the \((Q-1)\)-state Potts model in zero external field \[17\]. For an external field \( H_q < 0 \), one of the Potts states is suppressed relative to the others. The symmetry of the Hamiltonian is that of the \((Q-1)\)-state Potts model in zero external field, so that we expect to see cross-over from the \( Q \)-state critical point to the \((Q-1)\)-state critical point as \(-H_q\) is increased.

We have studied the field dependence of the critical point for \( 0 \leq x \leq 1 \) through the Fisher zero closest to the real axis, \( y_1(x, L) \), for the two-dimensional three-state Potts model. For a given applied field \( y_1 \) approaches the critical point \( y_c(x) \) in the limit \( L \to \infty \), and the thermal exponent \( y_t(L) \) defined as \[10,15\]

\[ y_t(L) = -\ln\left\{ \frac{\text{Im}[y_1(L+1)]/\text{Im}[y_1(L)]}{\ln[(L+1)/L]} \right\} \quad (18) \]

will approach the critical exponent \( y_t(x) \). Table I shows values for \( y_c(x) \) extrapolated from calculations of \( y_1(x, L) \) on \( L \times L \) lattices for \( 3 \leq L \leq 8 \) using the BST algorithm. The critical points for \( x = 1 \) (three-state) and \( x = 0 \) (two-state) Potts models are known exactly and are included in Table I for comparison. Note that the imaginary parts of \( y_c(BST) \) are all consistent with zero. We have also calculated the thermal exponent, \( y_t \), applying the BST algorithm to the values given by Eq. (18), and these results are also presented in Table I. For \( x = 1 \) we find \( y_t \) very close to the known value \( y_t = 6/5 \) for the three-state model, but for \( x \) as large as 0.5 we obtain \( y_t = 1 \), the value of the thermal exponent for the two-state (Ising) model.

Fig. 5 shows the critical line of the two-dimensional three-state Potts ferromagnet for \( H_q < 0 \). In Fig. 5 the upper line is the critical temperature of the two-state model, \( T_c(Q = 2) = 1/\ln(1 + \sqrt{2}) \), and the lower line is the critical temperature for the three-state model, \( T_c(Q = 3) = 1/\ln(1 + \sqrt{3}) \). The critical line for small \(-H_q\) is given by \( T - T_c(Q = 3) \sim (-H_q)^{y_t/y_h} \), where \( y_t = 6/5 \) and \( y_h = 28/15 \) for the three-state Potts model.

V. CONCLUSION

Following the work of Glumac and Uzelac \[3\] we have studied the locus of Yang-Lee zeros in the complex \( x \) plane for the \( Q \)-state Potts model in one-dimension and find that for \( Q > 1 \) the zeros lie on a circle whose radius varies continuously with temperature and \( Q \). For \( 1 < Q < 2 \) and any finite temperature, the zeros lie inside the unit circle, while for \( Q > 2 \) they lie outside the unit circle. In the special case \( Q = 2 \) (Ising model) the zeros lie exactly on the unit circle, as first proved by Lee and Yang \[7\].

In two and three dimensions we have used the microcanonical transfer matrix \[10\] to find the Yang-Lee zeros for finite lattices. The general trends observed in one dimension are repeated in two and three dimensions. In two dimensions with \( 3 \leq Q \leq 8 \) the zeros
lie outside the unit circle, and finite-size scaling suggests that the locus of zeros in the thermodynamic limit touches the unit circle only at the critical point, $x = 1$. In three dimensions with $Q = 3$ we have calculated the zeros on a single $3 \times 3 \times 3$ lattice, and there again the zeros lie outside the unit circle. While the exact form of the locus of zeros remains an open and important question, our results suggest a universal behavior which incorporates the Lee-Yang circle theorem. For $1 < Q < 2$ the locus of zeros lies within the unit circle while for $Q > 2$ it lies outside the unit circle and in each case touches the unit circle at the critical point $x = 1$.

We have also studied the Fisher (complex temperature) zeros of the two-dimensional three-state Potts model for lattices of size $3 \leq L \leq 8$ in the presence of an external field. The field reduces the symmetry of the Hamiltonian to that of the $(Q - 1)$-state model, and by studying the edge singularity we are able to determine the critical point and temperature exponent as a function of the field. Cross-over from the 3-state to the 2-state universality class is apparent. A more detailed analysis using larger lattices and allowing for confluent singularities is in progress.
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TABLES

TABLE I. The critical temperature $y_c$ and the critical exponent $y_t$ of the two-dimensional three-state Potts model for $0 \leq x \leq 1$.

| $x$  | $y_c$ (BST)          | $y_c$ (exact)          | $y_t$ (BST)  | $y_t$ (exact) |
|-----|----------------------|------------------------|--------------|---------------|
| 0   | $0.414(3) + 0.0002(4)i$ | $0.414213...$          | $1.001(2)$   | 1             |
| 0.001| $0.414(3) + 0.0002(4)i$ | $0.414213...$          | $1.001(2)$   | 1             |
| 0.05 | $0.413(5) + 0.0002(3)i$ | $0.414213...$          | $1.0009(6)$  | 1             |
| 0.5  | $0.400(2) + 0.0000(2)i$ | $0.400(2)$             | $0.982(21)$  | 1             |
| 1    | $0.366(2) + 0.0000(5)i$ | $0.366025...$          | $1.195(3)$   | 1             |


FIG. 1. Zeros of the two-dimensional three-state Potts model in the complex $x$ plane with cylindrical boundary conditions (a) at $y = y_c$ for $L = 4$ and $L = 10$ and (b) for several values of $y$ ($L = 6$).
FIG. 2. 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. 3. Modulus of the locus of zeros as a function of angle for the two-dimensional three-state Potts model at $y = 0.5y_c$, $y_c$, and $1.2y_c$ with cylindrical boundary conditions. The slight horizontal off-set for data for $y = y_c$ is for clarity only. However, the off-set of the edge singularity for $y = 1.2y_c$ from $\theta = 0$ is real.
FIG. 4. Zeros of the three-state Potts model in the complex $x$ plane on a $3 \times 3 \times 3$ simple-cubic lattice for $y = 0.1$, $y = y_c \approx 0.576624$ (Ref. [18]), and $y = 0.9$. 
FIG. 5. Critical temperatures of the two-dimensional three-state Potts ferromagnet as a function of the magnetic field. $H_q$ is in unit of $J$ and $T$ is in unit of $J/k_B$. The upper dotted line is the Ising transition temperature in the limit $H_q \to -\infty$, while the lower dotted line shows the critical temperature of the three-state Potts model for $H_q = 0$. 