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The partition function zeros in the one-dimensional q-state Potts model

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Abstract. The zeros of the partition function in the one-dimensional q-state Potts model with arbitrary and continuous $q \geqslant 0$ have been studied using a transfer matrix. The location of zeros and the Yang–Lee edge singularity have been analysed, and two different regimes, corresponding to $q > 1$ and $q < 1$, have been observed. A duality relation has also been derived, which relates the zeros in the complex field plane to those in the complex temperature plane.

1. Introduction

In order to better understand a phase transition in a certain model, it appears to be useful to study the distribution and behaviour of zeros of the partition function of this model in the plane of the complex symmetry breaking field or complex temperature.

In 1952, Yang and Lee (1952) formulated a theorem stating that for the Ising model with positive interactions these zeros are located on the unit circle of the complex activity plane. They pointed out a direct connection between the function representing the density of these zeros with the thermodynamic functions describing the phase transition. Their work was followed by a number of generalizations of their theorem to other statistical models such as quantum and classical Heisenberg models, the classical n-component model, models with $s > \frac{1}{2}$, the spherical model, models with multispin interactions, etc (for a review see, for example, Kurtze 1979).

Another interesting aspect related to this subject arose when it was shown (Fisher 1978) that the singularity existing at the edge value of Yang–Lee zeros can be considered by itself as a new second-order phase transition, different from the original one belonging to the zero symmetry breaking field.

We would like to consider both of these aspects for a simple one-dimensional case of the Potts model. The Potts model, although simple in formulation, hides a whole series of statistical models obtained by the different choice of the number of states q, including the Ising model as a special case with $q = 2$. For the Potts model various numerical studies exist in the complex temperature plane, performed for particular values of q in two and three dimensions (Pearson 1982, Bonnier and Leroyer 1991).

The aim of the present paper is to use the possibility of an analytic approach by using a transfer matrix in one dimension, to perform a systematic study for arbitrary and continuous q. Zeros will be calculated not by solving the polynomial, but directly by analysing the transfer-matrix eigenvalues.

As will be shown, two distinct regimes arise, corresponding to $q > 1$ and $q < 1$. While in the first one the Ising-like behaviour can be recovered, the second one displays a completely different, rather exotic behaviour with zeros on the real axis.

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Another interesting feature specific for the 1D case is that for the Ising model the duality transformations between the field and temperature variables have been established (Suzuki 1967). We shall present the generalization of these duality properties to the Potts case with arbitrary q. This brings an interesting correspondence between the complex field and complex temperature planes.

At the beginning of the next section we present the model and point out the connection between the degeneracy of eigenvalues of the transfer matrix and the zeros of the partition function in the thermodynamic limit. The following three subsections are devoted to the detailed treatment of the model corresponding to $q > 1$, $q < 1$ and $q = 1$. The duality relation between the field and temperature variables is presented in the third section. The conclusion is given at the end.

2. Model

We consider the 1D nearest-neighbour ferromagnetic q-state Potts model in the complex symmetry breaking field described by the following reduced Hamiltonian:

$$\mathcal{H} = K \sum_{n=1}^{N} \left[\delta(i_n, i_{n+1}) - \frac{1}{q} \right] + h \sum_{n=1}^{N} \left[\delta(i_n, 0) - \frac{1}{q} \right] \tag{1}$$

where i_n denotes q-state Potts variable at site n, N is the total number of particles, K is the reduced nearest-neighbour interaction strength in units $J = k_B$, $h = H/k_B T$ is the reduced external field coupled to the Potts state 0, and T is the temperature.

The analytic solution for thermodynamic properties of this model is straightforward using a transfer matrix. The partition function is then written as

$$Z_N = \mathrm{Tr}\, \mathbf{T}^N \tag{2}$$

where the elements of the transfer matrix $\mathbf{T}$ are given by

$$\mathbf{T}(i, j) = \exp K \left[\delta(i, j) - \frac{1}{q} \right] \exp h \left[\delta(j, 0) - \frac{1}{q} \right] . \tag{3}$$

Originally of order q, $\mathbf{T}$ is reduced by invariance to permutations leaving the Potts state 0 unchanged to the 2×2 sub-matrix

$$\begin{bmatrix} yz & \sqrt{q-1} \\ z\sqrt{q-1} & y+q-2 \end{bmatrix} \tag{4}$$

and $(q - 2)$ identical diagonal elements proportional to $y - 1$, where $y = \exp(K)$ and $z = \exp(h)$. The expressions for the eigenvalues λ_i are

$$\lambda_{0,1} = \tfrac{1}{2} \left\{ [y(1+z) + q - 2] \pm \sqrt{[y(1-z) + q - 2]^2 + (q-1)4z} \right\} e^{-(K+h)/q} \tag{5}$$

$$\lambda_2 = \cdots = \lambda_{q-1} = (y - 1) e^{-(K+h)/q} . \tag{6}$$

These expressions also extend to non-integer q. The same eigenvalues are obtained when performing the analogous calculation within the continuous-q formalism (Blöte and Nightingale 1982), which produces a transfer matrix of the form

$$q \begin{bmatrix} v+u+qvu & 1 & 0 \\ v+vu & 1+u & 0 \\ vu & 0 & u \end{bmatrix} e^{-(K+h)/q} \tag{7}$$

where $v = (z - 1)/q$ and $u = (y - 1)/q$. Consequently, in the following, q will be treated as a real parameter.

We are interested in zeros of the partition function, i.e. the solution of the equation $Z_N = 0$ within this transfer-matrix approach. Close to the thermodynamic limit the dominant contribution comes from the largest eigenvalues, and one can distinguish two cases.

In the first case the largest eigenvalue is a singlet. The partition function is given by

$$Z_N = \lambda_{\max}^N \left[1 + 0\left((\lambda_i/\lambda_{\max})^N\right)\right] \qquad |\lambda_i| < \lambda_{\max} \tag{8}$$

which reduces the solution to the equation $\lambda_{\max} = 0$.

A qualitatively different case arises when the two largest eigenvalues are complex, but with equal absolute values. Then, one has

$$Z_N = |\lambda_{\max}|^N \left[\mathrm{e}^{\mathrm{i}N\varphi_0} + \mathrm{e}^{\mathrm{i}N\varphi_1} + 0\left((\lambda_i/\lambda_{\max})^N\right)\right] \qquad |\lambda_i| < |\lambda_{\max}| \tag{9}$$

where φ_0 and φ_1 denote the different phases of λ_0 and λ_1. The zeros are then obtained for $\cos(N\varphi) = 0$, i.e. when $\varphi = (\varphi_0 - \varphi_1)/2 = \pi(2n+1)/(2N)$ for $n = 0, 1, \ldots, N-1$.

Another important situation occurs when the two largest eigenvalues become degenerate, i.e. when the expression under the square root in (5) vanishes. The expression (5) can be rewritten in a more transparent notation as

$$\lambda_{0,1} = \tfrac{1}{2}y\left[t_+t_- + z \pm \sqrt{\left(z - t_+^2\right)\left(z - t_-^2\right)}\right]\mathrm{e}^{-(K+h)/q} \tag{10}$$

where we defined new variables

$$t_\pm = \frac{1}{y}\left\{\sqrt{(y-1)(y+q-1)} \pm \sqrt{1-q}\right\} \tag{11}$$

depending only on temperature and q. The degeneracy is achieved for the two values of the field

$$z_\pm = t_\pm^2\,. \tag{12}$$

By analogy with the Ising case, we shall call the points $z_\pm$ the Yang–Lee edges. It will be shown later that they do actually represent the edges of the partition function zeros. Also, it will be shown that this degeneracy is related to a second-order phase transition, the Yang–Lee edge singularity, and that the corresponding critical exponents are equal to those for the Ising case.

We shall distinguish two regimes corresponding to $q > 1$ and $q < 1$.

2.1. $q > 1$

In this region, the behaviour of zeros can be presented as a simple generalization of the Ising case.

By using the notation $z = \mathrm{e}^{h'}\mathrm{e}^{\mathrm{i}h''}$, where we decomposed the symmetry breaking field into its real (h') and imaginary (h'') parts, the positions of the Yang–Lee edges (h'_0, $\pm h''_0$) are given by

$$\mathrm{e}^{h'_0} = t_+t_- = \frac{y+q-2}{y} \tag{13}$$

$$\cos(\pm h''_0) = 1 - 2\frac{q-1}{y(y+q-2)}\,. \tag{14}$$

In the temperature range $0 \leqslant K \leqslant \infty$ they lie in the interval

$$\begin{aligned} &0 \leqslant h'_0 \leqslant \ln(q-1) \qquad -\pi \leqslant h''_0 \leqslant \pi \quad \text{for} \quad q \geqslant 2 \\ &\ln(q-1) \leqslant h'_0 \leqslant 0 \qquad -\pi \leqslant h''_0 \leqslant \pi \quad \text{for} \quad 1 < q < 2\,. \end{aligned} \tag{15}$$

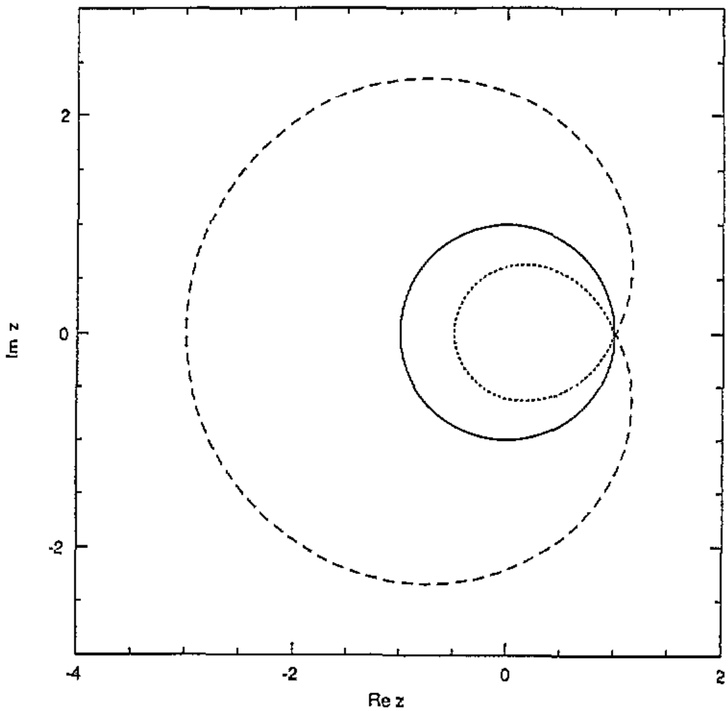

Figure 1. Positions of YL edges (the endpoints of zeros of the partition function) in the complex z-plane for different values of temperature. Values for $q = 1.5$ are denoted by a dotted curve, those for $q = 2.0$ by a full curve, and for $q = 4.0$ by a broken curve.

We observe that, unlike the Ising case, the real field component is different from zero, so that, with varying temperature, $z_\pm$ move along a certain contour in the complex z-plane instead of the unit circle (figure 1).

This difference can be ruled out by replacing the variable z with the reduced-field variable $\tilde{z}$ defined by

$$\tilde{z} = \frac{z}{t_+ t_-} \tag{16}$$

so that the Yang–Lee edges will again fall on the unit circle for all $q > 1$.

In order to find the zeros we start from the Yang–Lee edge positions and consider the structure of eigenvalues while fixing the real part of h to its Yang–Lee edge value h'_0. Equation (10) then gives

$$\lambda_{0,1} = y\mathrm{e}^{h'_0+\mathrm{i}h''/2}\left\{\cos\tfrac{1}{2}h'' \pm \sqrt{\cos^2\tfrac{1}{2}h'' - \cos^2\tfrac{1}{2}h''_0}\right\}\mathrm{e}^{-(K+h'_0+\mathrm{i}h'')/q}\,. \tag{17}$$

For $|h''| < |h''_0|$, the difference between λ_0 and λ_1 is real, there is no degeneracy and zeros are absent. For $|h''| \geqslant |h''_0|$ we obtain

$$|\lambda_0|^2 = |\lambda_1|^2 = \mathrm{e}^{h'_0}(y-1)(y+q-1)\mathrm{e}^{-2(K+h'_0)/q} > |\lambda_2|^2\,. \tag{18}$$

The eigenvalues λ_0 and λ_1 are equal in absolute values and larger than λ_2. This locates the zeros outside the interval $(-h''_0, h''_0)$, on the circle of radius $\mathrm{e}^{h'_0}$. Their positions on the circle follow from the condition on the phase difference $\varphi = (\varphi_0 - \varphi_1)/2$ between λ_0 and λ_1,

$$\tan\varphi = \frac{\sqrt{\cos^2\frac{1}{2}h_0'' - \cos^2\frac{1}{2}h''}}{\cos\frac{1}{2}h''}. \tag{19}$$

In the $\tilde{z}$-plane the zeros lie on the unit circle and are given by

$$\tilde{z}_\pm(n) = 2\cos^2\varphi_n\cos^2\tfrac{1}{2}h_0'' - 1 \pm 2\mathrm{i}\sqrt{\cos^2\varphi_n\cos^2\tfrac{1}{2}h_0''\left[1 - \cos^2\varphi_n\cos^2\tfrac{1}{2}h_0''\right]} \tag{20}$$

with $\varphi_n = \pi(2n+1)/(2N)$ and $n = 0, 1, \ldots, \mathcal{N}$ (where $\mathcal{N} = N/2 - 1$ for N even, and $\mathcal{N} = (N-1)/2$ for N odd).

By transition to the continuum in the standard way, we obtain the expression for the density of zeros $g(h_0', h'')$,

$$g(h_0', h'') = \begin{cases} \dfrac{1}{2\pi}\dfrac{\sin|\frac{1}{2}h''|}{\sqrt{\sin^2\frac{1}{2}h'' - \sin^2\frac{1}{2}h_0''}} & |h''| \geqslant h_0'' \\ 0 & -h_0'' < h'' < h_0'' . \end{cases} \tag{21}$$

Equation (21) shows the cumulation of zeros around $\pm h_0''$ and the divergence of their density. The corresponding critical exponent σ, defined by

$$g(h_0', h'' = \pm h_0'' \pm 0) \sim |h'' - h_0''|^\sigma \tag{22}$$

is equal to $-\frac{1}{2}$ for every $q > 1$.

One can also easily calculate the exponent of the correlation length given by

$$\xi = \frac{1}{\ln\lambda_0/\lambda_1} \simeq |T - T_c|^{-\nu}. \tag{23}$$

Expansion around YL edges gives $\nu = \frac{1}{2}$, independently of $q > 1$.

2.2. $0 \leqslant q < 1$

For $0 \leqslant q < 1$, the values for $t_\pm$ in (11) become real, which leads to a very unusual situation where points $z_\pm$ lie on the positive real z-axis for the entire range of temperatures.

Let us first examine (10) by constraining z to the real axis. The eigenvalues $\lambda_{0,1}$ are real and non-degenerate outside the interval (z_-, z_+), and complex-valued with the same magnitude for $z_- \leqslant z \leqslant z_+$. Inside the interval $z_- \leqslant z \leqslant z_+$, the third eigenvalue λ_2 is also to be taken into account. Namely, one can define points $z^*(K)$ on the real axis (figure 2)

$$z^* = \frac{y-1}{y+q-1} \tag{24}$$

where $|\lambda_0| = |\lambda_1| = |\lambda_2|$. For $z^* < z \leqslant z_+$, it holds that $|\lambda_0| = |\lambda_1| > |\lambda_2|$, while for $z_- \leqslant z < z^*$ one has $|\lambda_2| > |\lambda_0| = |\lambda_1|$.

Let us consider first the temperature range with only one regime, $|\lambda_{0,1}| > |\lambda_2|$, i.e. where $K < K_0 = \ln[1 + (\sqrt{q} - q)/2]$. The zeros in this region can be calculated from the equation

$$\tan\varphi = \frac{\sqrt{(z_+ - z)(z - z_-)}}{t_+t_- + z} \tag{25}$$

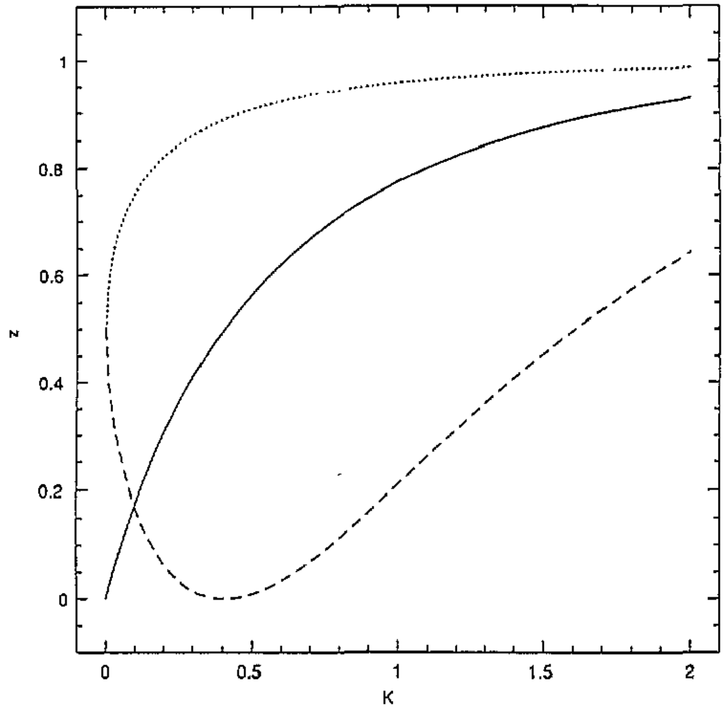

Figure 2. Positions of real values of z_+ (dotted curve), z_- (broken curve) and z^* (full curve) for $q = 0.5$ as a function of temperature.

which is an analogue of (19) for $q > 1$ models. It follows that, in this case, all zeros are located within the real interval (z_-, z_+). In the thermodynamic limit, the density of zeros obtained from the above equation is

$$g(h') = \frac{1}{2\pi}\frac{z - t_+t_-}{\sqrt{(z_+ - z)(z - z_-)}}\,. \tag{26}$$

It diverges in both points z_+ and z_- with the exponent $\frac{1}{2}$.

For temperatures corresponding to $K > K_0$, the two regimes bring a more complex behaviour. One part of the zeros lies within the real interval (z^*, z_+). The rest of the zeros should lie in the complex plane. Indeed, if we extend the real interval $(z_-,\ z^*)$ to complex values, one obtains $|\lambda_0| = |\lambda_2| > |\lambda_1|$, which leads to zeros of the partition function placed in complex-conjugate pairs in the z-plane.

In the thermodynamic limit, the zeros on the real z-axis only accumulate around the z_+ point, and the density of zeros diverges with the exponent $\frac{1}{2}$ (as for $q > 1$ models),

$$g(h' = h'_+ - 0) \sim \frac{1}{2\pi}\sqrt{\frac{t_+ - t_-}{t_+ + t_-}}\frac{1}{\sqrt{h'_+ - h'}} \sim |h'_+ - h'|^{\sigma}\,. \tag{27}$$

At the point $z = z^*$, the density $g(h')$ is finite.

By expanding the correlation length $\xi(h', T)$ around $z = z_+$, one obtains the singular behaviour of ξ in both variables (temperature and field) with the same exponent $\nu = \frac{1}{2}$.

2.3. $q = 1$

The model with $q = 1$ shows a different behaviour for zeros of the partition function compared to the $q \neq 1$ models. The positions of zeros are given by

$$z(n) = \frac{y-1}{y} \mathrm{e}^{\pi \mathrm{i}(2n+1)/N} \qquad n = 0, 1, \ldots, N-1 \tag{28}$$

i.e. they lie on the circle in the z-plane whose radius depends on temperature, but the distribution of zeros on the circle is temperature-independent and equidistant and leads to the constant value of the density of zeros in the thermodynamic limit,

$$g(h'') = \frac{1}{2\pi} \,. \tag{29}$$

3. Duality relation

It has already been pointed out for the Ising model (Suzuki 1967) that in one dimension there is a simple duality between field and temperature.

This duality can be generalized to the present problem (1) by using a transformation similar to the one used by Kramers and Wannier (1941) for the 2D Ising model,

$$\mathbf{S}\mathbf{T}(y, z)\mathbf{S}^{-1} = \alpha \mathbf{T}^{T}(y^{\mathrm{D}}, z^{\mathrm{D}}), \tag{30}$$

where y^{D} and z^{D} are the dual variables. In the present case the rows of the transformation matrix $\mathbf{S}$ are the eigenvectors of the operator $\mathbf{K}$ which performs the cyclic translation in the space of Potts states. The definitions of $\mathbf{K}$ and their eigenvectors $|K_n\rangle$ are

$$\mathbf{K}|i\rangle = |(i+1)_{\mathrm{mod}(q)}\rangle \qquad i = 0, 1, \ldots, q-1 \tag{31}$$

$$|K_n\rangle = \frac{1}{\sqrt{q}} \sum_{l=0}^{q-1} \omega^{-nl} \mathbf{K}^{l} |0\rangle \qquad \omega = \exp(2\pi \mathrm{i}/q) \tag{32}$$

$$\mathbf{K}|K_n\rangle = \omega^{n} |K_n\rangle \qquad n = 0, 1, \ldots, q-1 \,. \tag{33}$$

By performing the transformation (30) for arbitrary q, we obtain

$$y^{\mathrm{D}} = \frac{z+q-1}{z-1} \qquad z^{\mathrm{D}} = \frac{y+q-1}{y-1} \tag{34}$$

and

$$\alpha = \frac{(y-1)(z-1)}{q} \mathrm{e}^{(K^{\mathrm{D}}+h^{\mathrm{D}})/q} \mathrm{e}^{-(K+h)/q} \,. \tag{35}$$

Equation (30) establishes the connection between partition functions in dual and non-dual variables

$$\frac{Z_N(y^{\mathrm{D}}, z^{\mathrm{D}}, q)}{(z^{\mathrm{D}}-1)^N} \mathrm{e}^{N(K^{\mathrm{D}}+h^{\mathrm{D}})/q} = \frac{Z_N(y, z, q)}{(z-1)^N} \mathrm{e}^{N(K+h)/q} \tag{36}$$

or, symmetrically, in the y variable,

$$\frac{Z_N(y^{\mathrm{D}}, z^{\mathrm{D}}, q)}{(y^{\mathrm{D}}-1)^N} \mathrm{e}^{N(K^{\mathrm{D}}+h^{\mathrm{D}})/q} = \frac{Z_N(y, z, q)}{(y-1)^N} \mathrm{e}^{N(K+h)/q} \,. \tag{37}$$

Equation (37) connects the analytic properties of $Z_N(y, z, q)$ and $Z_N(y^{\mathrm{D}}, z^{\mathrm{D}}, q)$. In particular, the YL edges and the zeros of the partition function in the complex y-plane are the dual images of those in the complex z-plane obtained in sections 2.1 and 2.2. For

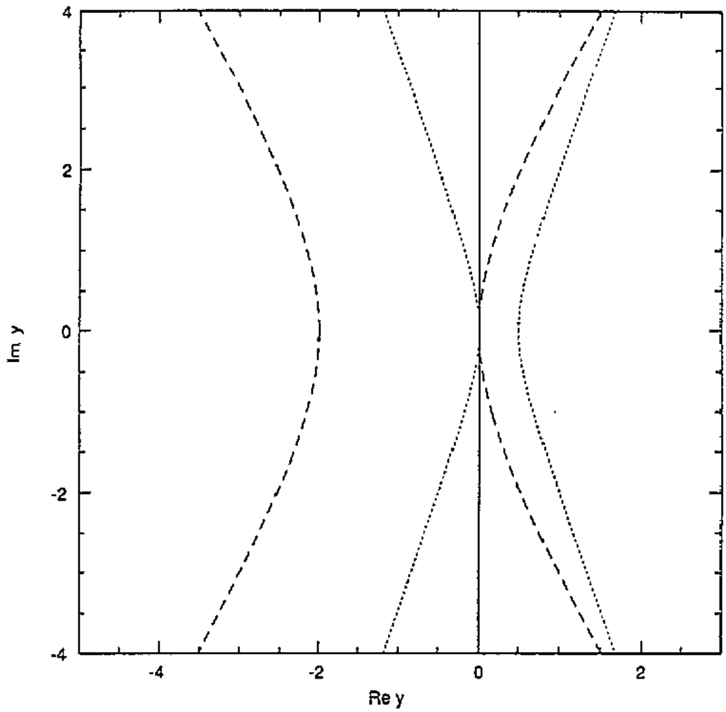

Figure 3. Positions of YL edges (the endpoints of zeros of the partition function) in the complex y-plane for different values of the field. Values for $q = 1.5$ are denoted by a dotted curve, those for $q = 2.0$ by a full curve, and for $q = 4.0$ by a broken curve.

example, the YL edges for all q, and the zeros of the partition function in the complex y-plane for $q > 1$, are given by

$$y_{\pm} = \frac{1}{z-1}\left[q - 2 \pm 2\sqrt{z(1-q)}\right] \tag{38}$$

$$y_{\pm}(n) = \frac{(q-2)(z\cos 2\varphi_n - 1) \mp 2\mathrm{i}\sqrt{z\cos^2\varphi_n\left[(z+q-1)(zq-z+1) - \cos^2\varphi_n zq^2\right]}}{1 - 2z\cos 2\varphi_n + z^2} \tag{39}$$

respectively.

In figure 3 one can compare the YL edge contours in the complex y-plane with the contours in the complex z-plane (figure 1) obtained for the same values of q.

4. Conclusion

An analytic study of the distribution of zeros using the transfer matrix was performed for the 1D Potts model with arbitrary and continuous $q \geqslant 0$. Two different regimes are observed corresponding to $q > 1$ and $q < 1$.

For $q > 1$ the behaviour is similar to that of the Ising model. The zeros lie on the circle in the complex z-plane, but the radius of that circle is not unity for $q \neq 2$, and varies with temperature. Points corresponding to the Yang–Lee edges can also be defined, but for the same reasons they move along a contour different from a circle when the temperature varies. By extracting the real field contribution, we recover the zeros on the unit circle, as in the Ising case.

For $q < 1$ we observe a pathological situation, where for all temperatures the zeros lie in part or completely (depending on temperature) on the real axis and cumulate around a point on the real axis. This would mean that we obtain the second-order phase transition at finite temperature and in the presence of a real field. The eigenvalues of the transfer matrix, which give the correlation length, are, however, not real. The situation could, in some aspects, be compared to the phase transition in the one-dimensional n-component model with $n < 1$ (Balian and Toulouse 1974). The phase transition at finite temperature was also considered for the 1D Potts model in the case of antiferromagnetic interaction and $0 < q < 2$ (Wu 1983).

The density of zeros can be defined in both regimes. Its divergence follows the same critical exponent $\frac{1}{2}$ for all q except $q = 1$. The $q = 1$ model is a particular case with no divergence of the density of zeros.

We have also established the duality relation between the zeros in the complex field plane with those in the complex temperature plane.

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