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Partition function zeros of the one-dimensional Potts model: the recursive method

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Abstract

The Yang–Lee, Fisher and Potts zeros of the one-dimensional Q-state Potts model are studied using the theory of dynamical systems. An exact recurrence relation for the partition function is derived. It is shown that zeros of the partition function may be associated with neutral fixed points of the recurrence relation. Further, a general equation for zeros of the partition function is found and a classification of the Yang–Lee, Fisher and Potts zeros is given. It is shown that the Fisher zeros in a nonzero magnetic field are located on several lines in the complex temperature plane and that the number of these lines depends on the value of the magnetic field. Analytical expressions for the densities of the Yang–Lee, Fisher and Potts zeros are derived. It is shown that densities of all types of zeros of the partition function are singular at the edge singularity points with the same critical exponent $\sigma = -\frac{1}{2}$.

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1. Introduction

It is well established that the thermodynamic properties of a physical system can be derived from a knowledge of the partition function. Since the discovery of statistical mechanics it has been a central theme to understand how the analytic partition function for a finite-size system acquires a singularity in the thermodynamic limit if the system undergoes a phase transition. The answer to this question was given in 1952 by Lee and Yang in their famous papers [1]. They considered the partition function of the Ising model as a polynomial in activity ($\exp(-2H/kT)$, where H is a magnetic field) and studied the distribution of zeros of the partition function in the complex activity plane. It was shown that phase transitions occur in the systems where a continuous distribution of zeros of the partition function cuts the real axis in the thermodynamic limit. The circle theorem, which states that zeros of the partition function of the ferromagnetic Ising model lie on the unit circle in the complex activity plane (*Yang–Lee zeros*) was also proved. Later, Fisher [2] initiated a study of zeros of the partition function in the complex temperature plane (*Fisher zeros*). Fisher showed that complex temperature zeros of the partition function of the Ising model in zero magnetic field on a square lattice lie on two circles $|v \pm 1| = \sqrt{2}$, where $v = \tanh(J/2kT)$. Since that time zeros of the partition function have been studied for the Ising and Potts [3] models on various regular lattices, most notably in recent years [4–8]. Zeros of the partition function were also studied for spin models defined on hierarchical [9] and recursive [10] lattices, random graphs [11] and aperiodic systems [12], spin glasses [13], percolation and self-organized criticality models [14].

Recently, Alves and Hansmann [15] studied the helix–coil (order–disorder) transition in the model of polyalanine with long-range interactions (the all-atom model) by calculating zeros of the partition function. Using the microcanonical algorithm [16], they showed that the distribution of the Yang–Lee and Fisher zeros of the all-atom model differs from the predictions of the Zimm–Bragg theory [17]. Moreover, the distribution of Yang–Lee and Fisher zeros of the all-atom model supports recent claims that the polyalanine exhibits a true phase transition [18]. Although their results were not precise enough to determine the order of the phase transition due to the complexity of the simulated model, they demonstrated that the transition may be described by a set of critical exponents. Applying the finite-size scaling analysis to zeros of the partition function they found new estimates for the critical exponents α, β, γ and $d\nu$. Based on their study of zeros of the partition function Alves and Hansmann [15] concluded that the helix–coil transition in a polyalanine is not accurately described by the Zimm–Bragg model and that a more detailed, all-atom model of polyalanine should be used [15].

It is noteworthy that the classical one-dimensional Potts model was employed in [19] for the solvent influence on the helix–coil transition in polypeptides. Also, it has been shown that a multisite interaction Potts model may be used for studying helix–coil transitions in polypeptides [20]. It is outside the scope of this paper to investigate the properties of biological macromolecules, but we believe that the study of general properties of zeros of the partition functions for different one-dimensional systems may serve as a new independent method for investigating the properties of macromolecules as was done in [15].

In 1994, Glumac and Uzelac [21] using the transfer matrix method studied the Yang–Lee zeros of the one-dimensional ferromagnetic Potts model for non-integer values of $Q \geqslant 0$. They showed that for $0 < Q < 1$ the Yang–Lee zeros are located on a real interval and for low temperatures these are located partially on the real axis and in complex conjugate pairs on the activity plane. Later on, Monroe [22] numerically studied the Yang–Lee zeros of the Potts model for some particular values of Q. Then, Kim and Creswick [23] showed that for $Q > 1$ the Yang–Lee zeros lie on a circle with radius R, where $R < 1$ for $1 < Q < 2$, $R > 1$ for $Q > 2$ and $R = 1$ for $Q = 2$. Only recently has the full picture of Yang–Lee zeros of the ferromagnetic Potts model for $0 < Q < 1$ been found [10].

In this paper, the dynamical systems theory is used to study the Yang–Lee, Fisher and Potts zeros[3] of the partition function for the one-dimensional Q-state Potts model. In section 2, a recurrence relation for the partition function is derived. It is shown that zeros of the partition function may be associated with neutral fixed points of the recurrence relation. A general equation for zeros of the partition function is derived. Formulae for the free energy and the density of zeros of the partition function are found. In sections 3 and 4 the method developed in

[3] Zeros of the partition function are considered as a function of complex Q.

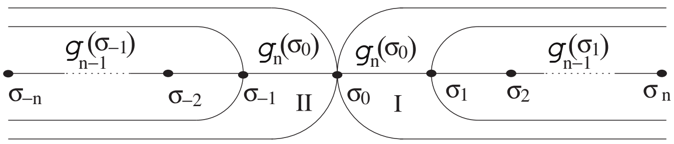

Figure 1. The procedure for derivation of the recurrence relation for the partition function.

section 2 is used to study the Yang–Lee and Potts zeros of ferromagnetic and antiferromagnetic Potts models. A classification of Yang–Lee and Potts zeros is given. In section 5, the Fisher zeros in a nonzero magnetic field are investigated. It is shown that the Fisher zeros in a nonzero magnetic field are located on several lines in the complex temperature plane and the density of Fisher zeros is singular at the edge singularity points with the same critical exponent as that of both the Yang–Lee and Potts zeros, $\sigma = -\frac{1}{2}$.

2. Zeros of the partition function of the Potts model

The Hamiltonian of the one-dimensional Q-state Potts model in a magnetic field is defined as follows:

$$\mathcal{H} = -\tilde{J}\sum_{\langle ij\rangle}\delta(\sigma_i,\sigma_j) - \tilde{H}\sum_i \delta(\sigma_i, 0) \tag{1}$$

where δ is the Kronecker delta function, σ_i denotes the Potts variable at site i and takes the values $0, 1, 2, \ldots, Q-1$. The first sum on the rhs of (1) goes over all edges and the second one over all sites on the lattice. For $\tilde{J} > 0$ the model is ferromagnetic and for $\tilde{J} < 0$ is antiferromagnetic. Note that due to the symmetry, the Hamiltonian (1) is the same if the external field $\tilde{H}$ is applied to any spin state, namely, if $\delta(\sigma_i, 0)$ in (1) is replaced by $\delta(\sigma_i, \alpha)$ for any $\alpha = 1, 2, \ldots, Q-1$. For $Q = 2$ the Potts model corresponds to the Ising model and in order to keep the analogy with the Ising model we designate $\tilde{H}$ as a magnetic field. We may assume the cyclic boundary condition $\sigma_n = \sigma_{-n}$ and that the number of sites is $2n+1$ without loss of generality. Cutting the lattice at the central site σ_0 will separate it into two branches I and II with equal statistical weights $g_n(\sigma_0)$ (figure 1)

$$g_n(\sigma_0) = \sum_{\sigma_1=0}^{Q-1}\sum_{\sigma_2=0}^{Q-1}\cdots\sum_{\sigma_n=0}^{Q-1}\prod_{i=1}^{n}\exp[J\delta(\sigma_{i-1},\sigma_i) + h\delta(\sigma_i, 0)]. \tag{2}$$

Cutting the branch I (II) at the site σ_1 (σ_{-1}), the recurrence relation for $g_n(\sigma)$ may be found as

$$g_n(\sigma_0) = \sum_{\sigma_1=0}^{Q-1}\exp[J\delta(\sigma_0,\sigma_1) + h\delta(\sigma_1, 0)]g_{n-1}(\sigma_1) \tag{3}$$

where $J = \tilde{J}/kT$ and $h = \tilde{H}/kT$. The partition function may be written in the form

$$\mathcal{Z} = \sum_{\sigma}\mathrm{e}^{-\mathcal{H}/kT} = \sum_{\sigma_0=0}^{Q-1}\exp[h\delta(\sigma_0, 0)]g_n^2(\sigma_0). \tag{4}$$

Introducing the notation

$$x_n = \frac{g_n(\sigma\neq 0)}{g_n(\sigma = 0)} \tag{5}$$

and using (3), the recurrence relation for x_n may be found as

$$x_n = f(x_{n-1}) \qquad f(x) = \frac{\mu + (z + Q - 2)x}{z\mu + (Q - 1)x} \tag{6}$$

where $\mu = \mathrm{e}^h$, and $z = \mathrm{e}^J$. x_n does not have a direct physical meaning, but the thermodynamic functions, such as the magnetization, the specific heat, etc, may be expressed in terms of x_n. For example, the magnetization for our model in the thermodynamic limit has the form

$$m = (N\mathcal{Z})^{-1} \sum_{\{\sigma\}} \delta(\sigma, 0)\, \mathrm{e}^{-\mathcal{H}/kT} = \frac{\mu}{\mu + (Q - 1)x^2} \tag{7}$$

where x is an attracting fixed point of the mapping (6). It will be shown below how the thermodynamic properties of the model may be defined from the dynamics of the recurrence relation (6).

The mapping (6) is a Möbius transformation, i.e. a rational map of the form

$$R(x) = \frac{ax + b}{cx + d} \qquad ad - bc \neq 0$$

where

$$R(\infty) = a/c \qquad R(-d/c) = \infty$$

if $c \neq 0$, while $R(\infty) = \infty$ when $c = 0$. The dynamics of such maps is well studied [24]. The mapping (6) has only two fixed points which are solutions to the equation $f(x) = x$. According to the theory of complex dynamical systems, fixed points are classified as follows: a fixed point x^* is attracting if $|\lambda| < 1$, repelling if $|\lambda| > 1$, and neutral if $|\lambda| = 1$, where $\lambda = \frac{\mathrm{d}}{\mathrm{d}x} f(x)|_{x=x^*} \equiv f'(x^*)$ is called the eigenvalue of x^*. It is easy to show that either both fixed points of the mapping (6) are neutral, or that one of them is attracting while the other is repelling. The correspondence between thermodynamical properties of the model and the dynamics of the mapping (6) is the following: if for a given temperature and magnetic field (z and μ) the mapping (6) has an attracting fixed point, then the system is in a stable paramagnetic state and its thermodynamical functions are defined by this fixed point (see, for example, (7)). The other fixed point is repelling and does not correspond to any phase. On the other hand, if the iterations of (6) do not converge to a fixed point, i.e. the mapping (6) has neutral fixed points only, the system undergoes a phase transition. Therefore, the existence of neutral fixed points of (6) corresponds to a phase transition in the model. It was mentioned in the introduction that zeros of the partition function correspond to phase transitions in the model. Thus, for our model zeros of the partition function are associated with neutral fixed points of the corresponding mapping. These may be found from the conditions of existence of neutral fixed points of the mapping (6). These conditions are the following:

$$\begin{cases} f(x) = x \\ f'(x) = \mathrm{e}^{\mathrm{i}\phi} \qquad \phi \in [0, 2\pi]. \end{cases} \tag{8}$$

Excluding x from the system (8) after some algebra the equation of phase transitions may be found as

$$z^2\mu^2 - 2[(z - 1)(z + Q - 1)\cos\phi + 1 - Q]\mu + (z + Q - 2)^2 = 0 \tag{9}$$

where $\phi \in [0, 2\pi]$. Solutions to this equation for different values of ϕ correspond to zeros of the partition function. Hence, the free energy of the model may be written in the form

$$F \sim \int_0^{2\pi} \ln(z^2\mu^2 + 2(Q - 1)\mu + (z + Q - 2)^2 - 2\mu(z - 1)(z + Q - 1)\cos\phi)\,\mathrm{d}\phi. \tag{10}$$

Formula (10) may also be derived from the transfer matrix method [21, 26] using two non-degenerate eigenvalues of the transfer matrix [26]

$$\lambda^*_{1,2} = \tfrac{1}{2}\big[z\mu + z + Q - 2 \pm \sqrt{(z\mu - z - Q + 2)^2 + 4(Q-1)\mu}\big] \tag{11}$$

and the following mathematical identity for any pair of scalars C, D:

$$C^N + D^N = \prod_n [C + \exp(2\pi \mathrm{i} n/N) D]$$

where the product is from $n = 1, 2, \ldots, N$ if N is odd; and from $n = 1/2, 3/2, \ldots, N - 1/2$ for N is even (see [27]). Moreover, one can easily show that the eigenvalues of fixed points of (6) are related to the eigenvalues of the transfer matrix (11) as follows:

$$\lambda_{1,2} = \frac{4\mu(z-1)(z+Q-1)}{\left(\lambda^*_{1,2}\right)^2}.$$

Hence, the condition of a phase transition $|\lambda_1| = |\lambda_2|$ (λ_1 and λ_2 are the eigenvalues of neutral fixed points) corresponds exactly to the $\left|\lambda^*_1\right| = \left|\lambda^*_2\right|$ condition for the eigenvalues of the transfer matrix (11). It means that the phase transition point based on the dynamical systems approach coincides exactly with the phase transition point based on free energy considerations. This correspondence seems to be general for spin models defined on recursive lattices [10, 28].

The density of zeros of the partition function may be found by differentiating both sides of equation (9) with respect to ϕ and ξ and has the form

$$g(\xi) = \frac{B\partial_\xi A - A\partial_\xi B}{2\pi B[-(A-B)(A+B)]^{\frac{1}{2}}} \tag{12}$$

where $\partial_\xi = \frac{\partial}{\partial\xi}$,

$$A = z^2\mu^2 + 2(Q-1)\mu + (z+Q-2)^2 \qquad B = 2\mu(z-1)(z+Q-1)$$

and $\xi = \mu, z$ or Q depending on whether the Yang–Lee, Fisher or Potts zeros are considered. It is interesting to note that in our case the numerator of (12) always contains the multiplier $(A+B)$. Hence, the density $g(\xi)$ is singular only when $A - B = 0$.[4] From (12) it follows that $g(\xi)$ has a singular behaviour $g(\xi) \sim |\xi - \xi^*|^\sigma$, where ξ^* is a solution to the equation $A - B = 0$. We will see that $\sigma = -\frac{1}{2}$ for all types of zeros of the partition function. Also, note that the equation $A - B = 0$ corresponds to the phase transitions equation (9) for $\phi = 0$. It defines the edge singularity points [10, 25]. In the subsequent sections we will apply equations (9) and (12) to the study of the Yang–Lee, Potts and Fisher zeros.

3. The Yang–Lee zeros

According to the results of the previous section the Yang–Lee zeros of the Q-state Potts model may be found by solving equation (9) with respect to μ. Equation (9) is a quadratic equation of μ with real coefficients. Note that solutions to equation (9) lie either on the real axis or in complex conjugate pairs on a circle with radius $R = |z + Q - 2|/z$ and have the form

$$\mu_{1,2} = E\left[2\cos^2\frac{\phi}{2} - F \pm 2\sqrt{\cos^2\frac{\phi}{2}\left(\cos^2\frac{\phi}{2} - F\right)}\right] \tag{13}$$

where

$$E = \frac{(z-1)(z+Q-1)}{z^2} \qquad \text{and} \qquad F = \frac{z(z+Q-2)}{(z-1)(z+Q-1)}.$$

[4] Solutions to the equation $B = 0$ should be neglected since these do not correspond to zeros of the partition function.

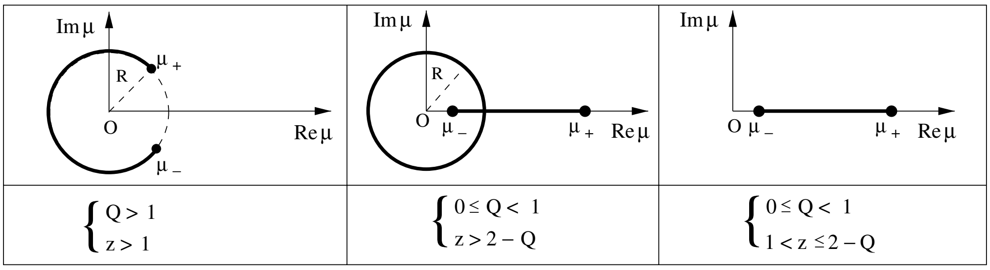

Figure 2. A schematic presentation of the Yang–Lee zeros of 1D ferromagnetic Potts model. Here $R = \frac{z+Q-2}{z}$ and $\mu_\pm$ are defined in (15).

A detailed study of (9) with respect to μ has already been performed [10]. Here, we will present only the main results for the Yang–Lee zeros of both ferromagnetic and antiferromagnetic Potts models.

For the ferromagnetic Potts model ($z > 1$) one can find that for $Q > 1$ all solutions (13) are complex conjugate and lie on an arc of circle with radius $R = (z + Q - 2)/z$. Writing μ in the exponential form $\mu = R\,\mathrm{e}^{\mathrm{i}\theta}$ the angular distribution of the Yang–Lee zeros may be found in the form

$$\cos\frac{\theta}{2} = \sqrt{F^{-1}}\cos\frac{\phi}{2}. \tag{14}$$

From (14) one can see a gap in the distribution of Yang–Lee zeros, i.e. there are no solutions to equation (9) in the interval $-\theta_0 < \theta < \theta_0$, where $\theta_0 = 2\arccos\sqrt{F^{-1}}$. This is the well-known gap in the distribution of Yang–Lee zeros of ferromagnetic models above the critical temperature (formally $T_\mathrm{c} = 0$ for the one-dimensional case) first studied by Kortman, Griffiths and Fisher [25]. The endpoints of the gap are called Yang–Lee edge singularity points. From (9) and (14) it follows that the Yang–Lee edge singularity points correspond to $\phi = 0$. Hence, according to (12) the density of Yang–Lee zeros is singular in the Yang–Lee edge singularity points. Substituting $\phi = 0$ into (13) the formula for Yang–Lee edge singularity points we have

$$\mu_\pm = \frac{1}{z^2}\left\{\sqrt{(z-1)(z+Q-1)} \pm \sqrt{1-Q}\right\}^2. \tag{15}$$

Substituting $\xi = \mu \equiv R\mathrm{e}^{\mathrm{i}\theta}$ in (12) after some algebra, the density of Yang–Lee zeros for $Q > 1$ may be found in the form

$$g(\theta) = \frac{1}{2\pi}\frac{\left|\sin\frac{\theta}{2}\right|}{\sqrt{\sin^2\frac{\theta}{2} - \sin^2\frac{\theta_0}{2}}}. \tag{16}$$

From equation (16) it follows that the density $g(\theta)$ diverges in the Yang–Lee edge singularity points $\mu_\pm$ with the critical exponent $\sigma = -\frac{1}{2}$, i.e. $g(\theta) \propto |\theta - \theta_0|^{-\frac{1}{2}}$ when $\phi \to 0$ or $\theta \to \theta_0$.

For $Q < 1$ the Yang–Lee edge singularity points $\mu_\pm$ are real and the density of Yang–Lee zeros has the form

$$g(\mu) = \frac{1}{2\pi\mu}\frac{|\mu - \sqrt{\mu_+\mu_-}|}{\sqrt{(\mu_+ - \mu)(\mu - \mu_-)}}. \tag{17}$$

$g(\mu)$ diverges in the points $\mu_\pm$, i.e. $g(\mu) \propto |\mu - \mu_\pm|^\sigma$, with the critical exponent $\sigma = -\frac{1}{2}$. The summary of results for the Yang–Lee zeros of the ferromagnetic Potts model is given in figure 2.

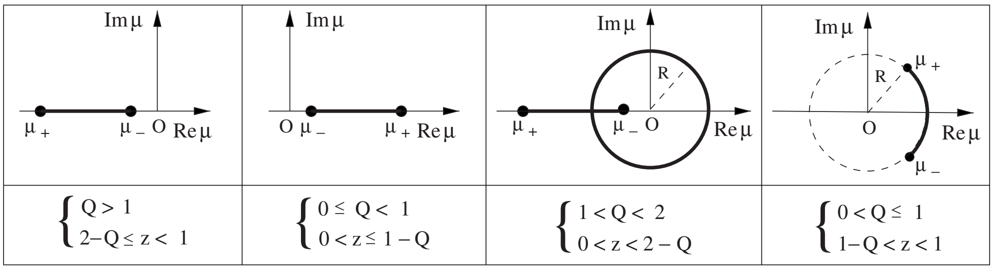

Figure 3. A schematic presentation of the Yang–Lee zeros of 1D antiferromagnetic Potts model. Here $R = \frac{2-Q-z}{z}$ and $\mu_\pm$ are defined in (15).

The Yang–Lee zeros of the antiferromagnetic Potts model ($z < 1$) may be studied in the same manner and the results are given in figure 3. For complex $\mu_\pm$ the angular distribution of Yang–Lee zeros has the form

$$\sin\frac{\theta}{2} = \sqrt{F^{-1}}\cos\frac{\phi}{2}. \tag{18}$$

In contrast to the ferromagnetic case, now the Yang–Lee zeros lie in the interval $-\theta^* < \theta < \theta^*$, where $\theta^* = 2\arcsin\sqrt{F^{-1}}$. The density of Yang–Lee zeros in this case has the form

$$g(\theta) = \frac{1}{2\pi}\frac{\cos\frac{\theta}{2}}{\sqrt{\sin^2\frac{\theta^*}{2} - \sin^2\frac{\theta}{2}}}. \tag{19}$$

For real values of $\mu_\pm$ the density of Potts zeros has the same form as for the ferromagnetic case (17). Actually, formula (17) is the most general from which formulae (16) and (19) may be derived (see also section 4). Note, that here also the density of Yang–Lee zeros diverges at the Yang–Lee edge singularity points with the same index $\sigma = -\frac{1}{2}$.

4. The Potts zeros

Recently, much attention has been given to the study of zeros of the partition function in the complex Q plane for the Potts model on regular lattices and finite graphs [29]. The partition function of the Potts model ($H = 0$) on a finite graph G, $\mathcal{Z}_G(Q, v)$, may be considered as a polynomial in the number Q of Potts states and the temperature-like variable $v = \exp(\tilde{J}/kT) - 1$. At zero temperature the partition function of the antiferromagnetic Potts model ($v = -1$) corresponds to the chromatic polynomial $P_G(Q)$, which is closely related to the Q-colouring problem. By definition, for graph G and positive Q, $P_G(Q)$ is the number of ways in which the vertices of G can be assigned 'colours' from the set $1, 2, \ldots, Q$ in such a way that adjacent vertices always receive different colours. The original hope was that study of the real or complex zeros of $P_G(Q)$ might lead to an analytic proof of the four-colour conjecture, which states that $P_G(4) > 0$ for all loopless planar graphs. To date this hope has not been realized, although combinatoric proofs of the four-colour theorem have been found [30]. Even so, the Potts zeros and zeros of $P_G(Q)$ are interesting in their own right and have been extensively studied in recent years [29–31].

In this section the Potts zeros of ferromagnetic and antiferromagnetic one-dimensional Potts models are studied. It was shown in section 2 that zeros of the partition function correspond to solutions of equation (9), which is a polynomial in Q. Hence, the Potts zeros

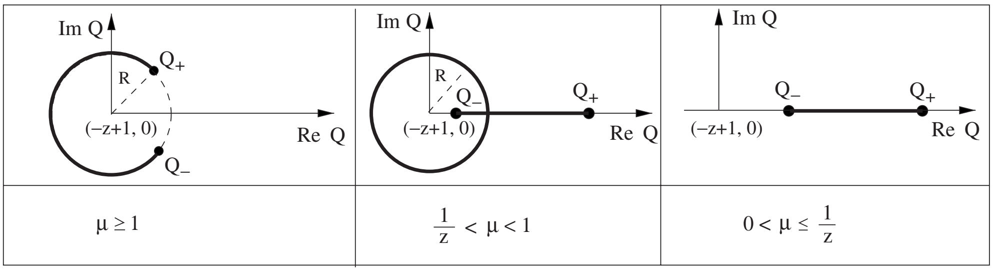

Figure 4. A schematic presentation of the Potts zeros of 1D ferromagnetic Potts model. Here $R = z\mu - 1$ and $Q_\pm$ are defined in (22).

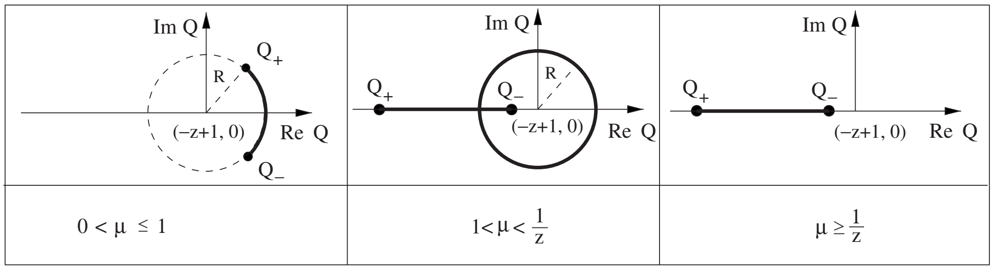

Figure 5. A schematic presentation of the Potts zeros of 1D antiferromagnetic Potts model. Here $R = 1 - z\mu$ and $Q_\pm$ are defined in (22).

may be found as solutions to (9) with respect to the parameter Q. It is convenient to rewrite (9) using the variable $P = Q + z - 1$ as

$$P^2 - 2P[1 - \mu + \mu(z-1)\cos\phi] + (1 - z\mu)^2 = 0. \tag{20}$$

Equation (20) is a quadratic equation in P with real coefficients. Solutions of (20) lie either on the real axis or on the circle with radius $R = |1 - z\mu|$ in the complex plane P, and have the form

$$P_{1,2} = 1 - \mu + \mu(z-1)\cos\phi \pm 2\cos\frac{\phi}{2}\sqrt{\mu(z-1)\left(1 - \mu - \mu(z-1)\sin^2\frac{\phi}{2}\right)}. \tag{21}$$

Since the analysis of (21) is standard, we will skip the details and give the results in figures 4 and 5 for ferromagnetic and antiferromagnetic Potts models, respectively. In analogy with the Yang–Lee zeros, the Potts edge singularity points are defined as solutions to equation (20) for $\phi = 0$, and have the form

$$Q_\pm = P_\pm - z + 1 = 1 - z + \left(\sqrt{1-\mu} \pm \sqrt{\mu(z-1)}\right)^2. \tag{22}$$

The general formula of the density of Potts zeros has the form

$$g(P) = \frac{1}{2\pi P}\frac{|P - \sqrt{P_+P_-}|}{\sqrt{(P_+ - P)(P - P_-)}}. \tag{23}$$

From (23) it follows that the density of Potts zeros is singular at the Potts edge singularity points. For complex values of $Q_\pm$, (23) may be written in the form

$$g(\theta) = \frac{1}{2\pi}\frac{\left|\sin\frac{\theta}{2}\right|}{\sqrt{\sin^2\frac{\theta}{2} - \sin^2\frac{\theta_0}{2}}} \tag{24}$$

for the ferromagnetic model, where $|\theta| > \theta_0$ and $\theta_0 = 2\arccos(\mu(z-1)/(\mu z-1))^{-\frac{1}{2}}$. For the antiferromagnetic model, $g(\theta)$ has the form

$$g(\theta) = \frac{1}{2\pi}\frac{\cos\frac{\theta}{2}}{\sqrt{\sin^2\frac{\theta_0}{2} - \sin^2\frac{\theta}{2}}} \tag{25}$$

where $|\theta| < \theta_0$ and $\theta_0 = 2\arcsin(\mu(1-z)/(1-\mu z))^{-\frac{1}{2}}$. Different formulae for the density of Potts zeros occur because the square root function in (23) is not a unique function in the complex plane P, i.e. one branch of the square root function in (23) corresponds to the ferromagnetic model and the other to the antiferromagnetic.

It is noteworthy that the density of Potts zeros diverges at the Potts edge singularity points with the same critical exponent $\sigma = -\frac{1}{2}$ as for the Yang–Lee zeros.

5. The Fisher zeros

In this section the Fisher zeros in a nonzero magnetic field are studied. Usually, the Fisher zeros are considered as zeros of the partition function with respect to a temperature-dependent parameter. In our case z is such a parameter. Formally, the magnetic field in the Hamiltonian (1) may be presented in the form $\tilde{H} = H\tilde{J}$, where H is the renormalized magnetic field. Later we will refer to H as a magnetic field. Then, μ may be written as z^H and equation (9) has the form

$$P_\phi(z, H, Q) = 0 \tag{26}$$

where

$$P_\phi(z, H, Q) = z^{2H+2} - 2\cos\phi z^{H+2} - 2(Q-2)\cos\phi z^{H+1} + 2(Q-1)z^H + (z+Q-2)^2.$$

$P_\phi(z, H, Q)$ is obviously a polynomial for integer values of H and (26) may be solved numerically. For non-integer values of H equation (26) becomes a transcendental equation and the Fisher zeros may be found by numerically checking the condition of existence of neutral fixed points of the mapping (6).

The density of Fisher zeros may be found from (12) by substituting $\xi = z$ and has the form

$$g(z) = \frac{1}{2\pi}\frac{HG_1(z, H, Q) - zG_2(z, H, Q)}{(z-1)z(z+Q-1)\sqrt{-P_0(z, H, Q)}} \tag{27}$$

where

$$G_1(z, H, Q) = (z-1)(z+Q-1)(z^{H+1} - z - Q + 2)$$
$$G_2(z, H, Q) = (z^H - 1)(2(z+Q-1) - Qz) + Q^2.$$

From (27) it follows that the density of Fisher zeros is singular in the Fisher edge singularity points, which are defined as solutions to equation (26) for $\phi = 0$.

Let us first study the Fisher zeros for the Ising model ($Q = 2$). For $Q = 2$ equation (26) has the form

$$z^{2H+2} - 2\cos\phi z^{H+2} + 4\cos^2\frac{\phi}{2}z^H + z^2 = 0. \tag{28}$$

This equation is symmetric under the $H \to -H$ transformation because of the $Z(2)$ symmetry of the Ising model. Since all coefficients of (28) are real, its solutions will be either real or complex conjugate. For integer values of H the Fisher zeros have the form shown in figure 6. From figure 6 and (28) one can see that the Fisher zeros are located on lines ending at the Fisher edge singularity points and the number of lines equals the value of the magnetic field

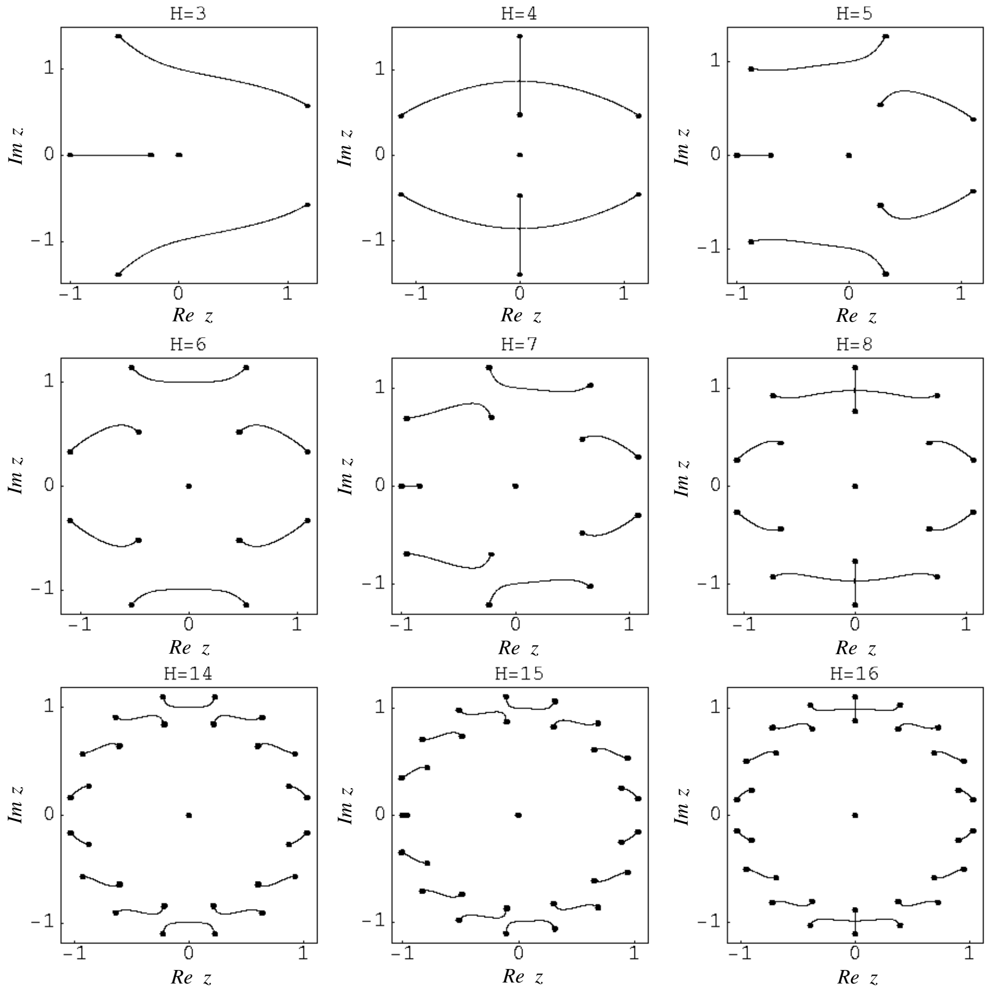

Figure 6. The Fisher zeros of 1D Ising model for different values of a magnetic field. The big dots at the ends of the lines show Fisher edge singularity points.

$|H| + 1$. Fisher edge singularity points are divided into pairs and every pair corresponds to a line. Note that $z = 0$ is a twice degenerate Fisher edge singularity point with the critical exponent $\sigma = -\frac{1}{2}$. Formally, two degenerate $z = 0$ edge singularity points are considered here as forming a 'line'. One can see that for odd values of $|H|$ there are negative Fisher zeros and for $|H| = 4n, n \in N$, the Fisher zeros are partially located on the imaginary axis. Since $P_\phi(z, H, Q)$ is an analytic function of H the lines of Fisher zeros for non-integer values of H are continuous deformations of Fisher zeros in the field $[|H|]$ or $[|H|] + 1$, where $[|H|]$ is the integer part of $|H|$, i.e. the minimal integer less than $|H|$. The location of Fisher zeros for non-integer H may be found numerically from the condition of existence of neutral fixed points of the mapping (6). As an illustration the Fisher zeros for non-integer values of $0 < H < 2$ are given in figure 7.

The Fisher zeros for $Q \neq 2$ Potts model may be studied in the same way as for the Ising model. It is impossible to give all possible configurations of Fisher zeros for any H and Q. Here we give only the summary of the main properties. First of all, there is no $H \to -H$ symmetry for $Q \neq 2$ and the Fisher zeros are different for positive and negative values of H.

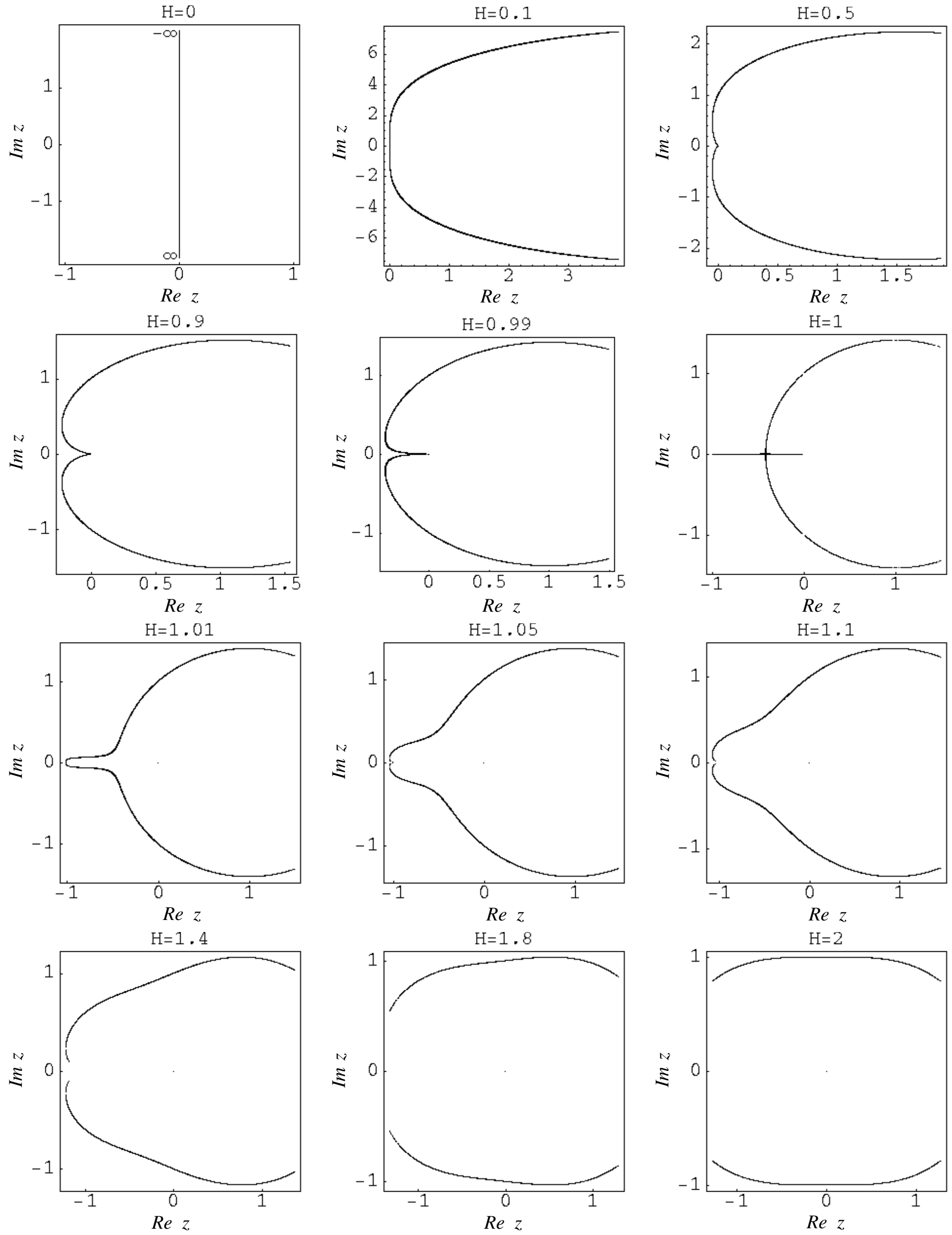

Figure 7. The Fisher zeros of the one-dimensional Ising model for non-integer values of a magnetic field $0 \leqslant H \leqslant 2$.

For $Q = 1$ the Fisher zeros are located on a closed curve and the density of Fisher zeros is not singular on this curve (figure 8).

For $Q \neq 1$ Fisher zeros are located on several lines (figure 8) and the density of Fisher zeros is singular at the endpoints of these lines with the edge singularity exponent $\sigma = -\frac{1}{2}$.

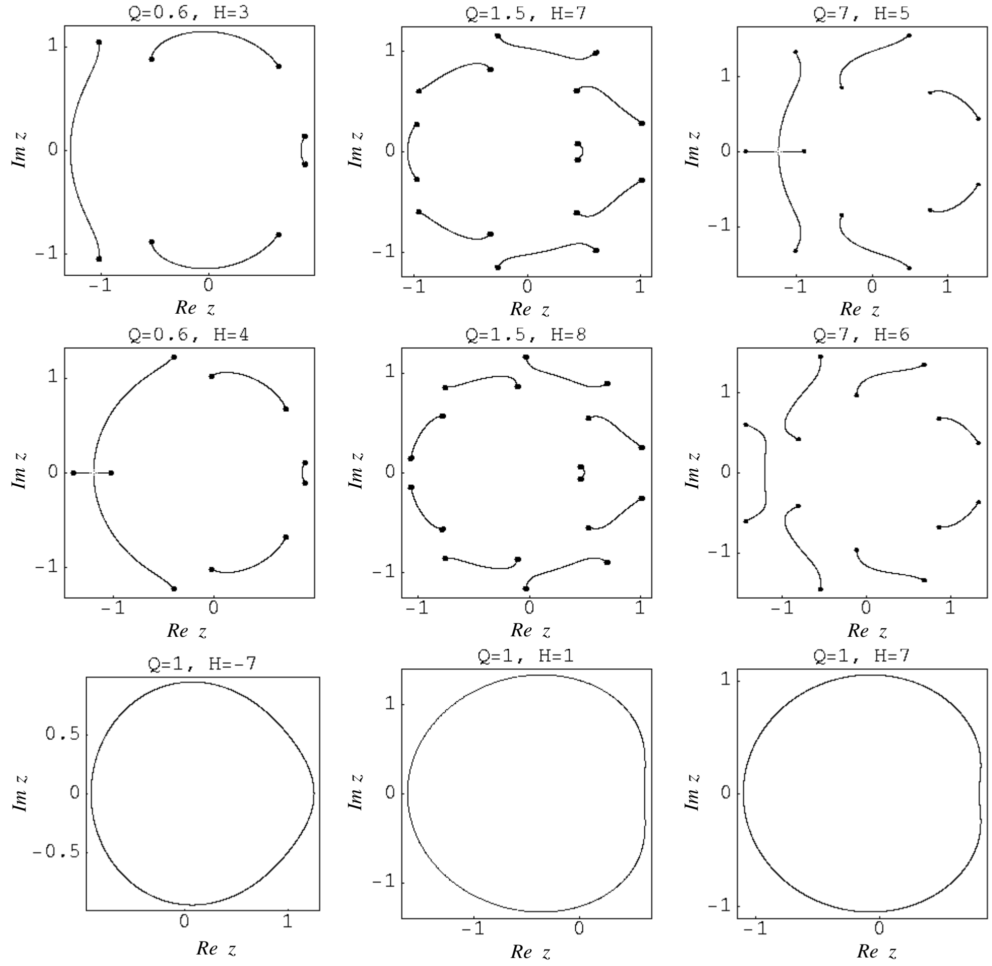

Figure 8. The Fisher zeros of the one-dimensional Ising model for some integer values of a magnetic field H and a Potts variable Q.

Numerical experiments show the following properties for integer values of H: for $0 < Q < 1$ there is an interval of real Fisher zeros only for even values of H; for $1 < Q < 2$, the Fisher zeros intersect the negative real semi-axis only for odd values of H; for $Q > 2$ there is an interval of real Fisher zeros only for odd values of H. The number of lines of Fisher zeros is defined as in the Ising model. In figure 8 we give some plots that illustrate these properties.

6. Discussion of the results

In this paper, the Yang–Lee, Fisher and Potts zeros of the one-dimensional Q-state Potts model are studied using the dynamical systems theory. A recurrence relation for the partition function is derived. It is shown that for this model zeros of the partition function may be associated with neutral fixed points of the corresponding recurrence relation. A general equation for zeros of the partition function is derived. It is shown that for $Q \neq 1$ the density of zeros of the partition function is singular in the edge singularity points with the critical exponent $\sigma = -\frac{1}{2}$ and the critical exponent σ *is the same for all types* of zeros of the partition function (the Yang–Lee, Fisher and Potts zeros).

In section 2 we showed that the recursive method used in this paper is equivalent to the transfer matrix method if one neglects the degenerated eigenvalues of the transfer matrix. Indeed, the transfer matrix of the one-dimensional Q-state Potts model for integer values of $Q > 2$ has Q eigenvalues, where $Q - 2$ eigenvalues are degenerated. For the $Q > 1$ case Glumac and Uzelac [21] showed that in the thermodynamical limit the Yang–Lee zeros may be found from the first two non-degenerate eigenvalues of the transfer matrix. For the $Q < 1$ case they considered the contribution of degenerated eigenvalues (λ_2 in their notation) also. This led to identities for low temperatures, and the full picture of Yang–Lee zeros for the $Q < 1$ case was not found (for more details see [21]). Using a recursive method, we found the Yang–Lee and Potts zeros for any value of Q analytically, and gave their full classification for both ferromagnetic and antiferromagnetic interactions. We proved that the degenerated eigenvalues of the transfer matrix do not affect the thermodynamic properties of the one-dimensional Q-state Potts model, and in the transfer matrix method their contribution to the partition function should be neglected.

It is noteworthy to discuss the properties of our model for the $Q = 1$ case. In this case our model shows a different behaviour for zeros of the partition function compared to the $Q \neq 1$ models. Indeed, for $Q = 1$ the Yang–Lee and Fisher zeros lie on closed curves and the density of zeros of the partition function is not singular on these curves. The reason for such behaviour is that for $Q = 1$ the recursive mapping (6) is a linear transformation

$$x_n = f(x_{n-1}) \qquad f(x) = \frac{1}{z} + \frac{z-1}{z\mu}x. \tag{29}$$

The derivative of (29) does not depend on x and has the form

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = \frac{z-1}{z\mu}. \tag{30}$$

The mapping (29) has only one fixed point $x^* = \mu(z\mu - z + 1)^{-1}$, which is either attracting, repelling or neutral. When the fixed point x^* is attracting, i.e. $|f'(x^*)| < 1$, the system is in a stable state, and the order parameter (7) $m = 1$. In the case when the fixed point x^* is repelling, i.e. $|f'(x^*)| > 1$, the system does not have an equilibrium state, since the mapping (29) does not have other attracting fixed points. The mapping (6) also does not have attracting periodical points. The periodical point of period n is defined as a solution to the equation $f^n(x) = x$, where $f^n = \underbrace{f \circ f \circ \cdots \circ f}_{n\ \text{times}}$ is a superposition function. According to the chain rule for the derivative of a superposition function and the fact that the derivative (30) does not depend on x, any periodical point of (29) is repelling when the fixed point x^* is repelling, i.e. $|f'(x^*)| > 1$. Thus, for $|f'(x^*)| > 1$ the system either crashes or remains always in a non-equilibrium state. The border of the stability region is defined by the condition that the only fixed point of the mapping (29) is a neutral fixed point. Hence, for the $Q = 1$ case, zeros of the partition function in the complex plane separate a region, where the system is in a stable state, from the region where the system either crashes or remains always in a non-equilibrium state. Such behaviour is different from the $Q \neq 1$ case, where zeros of the partition function separate different 'stable phases' of the system on the corresponding complex plane. Now it is clear why the Yang–Lee and Fisher zeros lie on closed curves for the $Q = 1$ case. Direct calculation of densities of the Yang–Lee and Fisher zeros shows that the Yang–Lee and Fisher zeros are uniformly distributed on closed curves and that their densities are not singular on these curves.

The relation between zeros of the partition function and the existence of neutral fixed points of the recursive mapping gives a numerical algorithm for studying zeros of the partition function. The algorithm is based on testing the condition of existence of neutral fixed points of the corresponding recurrence relation: if neutral fixed points exist, then the partition function is zero for given values of z, μ and Q. In section 5 we saw that this algorithm is very useful for studying the Fisher zeros in an arbitrary magnetic field. Moreover, it is the only method for studying the Fisher zeros for non-integer values of H, where H is the renormalized magnetic field, $H = \tilde{H}/\tilde{J}$. For integer values of H equation (26) is a polynomial, and the Fisher zeros may be found as solutions to that polynomial. The crucial point, why we consider integer and non-integer values of H, is that for integer values of H the number of Fisher edge singularity points equals exactly the order of the polynomial $P_0(z, H, Q)$ (26), and the number of lines on which the Fisher zeros lie may be found exactly (see section 5). $P_\phi(z, H, Q)$ (26) is an analytic function of H, hence, the lines of Fisher zeros for non-integer values of H are smooth deformations of the lines of Fisher zeros for the renormalized magnetic field, that is equal to one of the integers near H. Integer values of renormalized magnetic field H should not lead to a confusion, since, in this case, the magnetic field, which contributes to the Hamiltonian (1), is simply a multiple of the pair interaction constant $\tilde{J}$.

7. Conclusions

In conclusion we would like to note that the results given in this paper show that the thermodynamic properties of the one-dimensional Potts model are completely defined by the recurrence relation (6) or equivalently, by two non-degenerate eigenvalues of the corresponding transfer matrix (11) (see also [10]). Moreover, it is proved that the phase transition point based on the dynamical systems approach coincides exactly with the phase transition point based on free energy considerations. The dynamical systems approach used here gives a numerical method which may be used for studying other one-dimensional systems for which a one-dimensional recurrence relation may be derived.

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