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Exact Potts Model Partition Functions for Strips of the Honeycomb Lattice

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Abstract We present exact calculations of the Potts model partition function $Z(G,q,v)$ for arbitrary q and temperature-like variable v on strip graphs G of the honeycomb lattice for a variety of transverse widths equal to L_y vertices and for arbitrarily great length, with free longitudinal boundary conditions and free and periodic transverse boundary conditions. These partition functions have the form $Z(G,q,v)=\sum_{j=1}^{N_{Z,G,\lambda}} c_{Z,G,j}(\lambda_{Z,G,j})^m$, where m denotes the number of repeated subgraphs in the longitudinal direction. We give general formulas for $N_{Z,G,j}$ for arbitrary L_y. We also present plots of zeros of the partition function in the q plane for various values of v and in the v plane for various values of q. Plots of specific heat for infinite-length strips are also presented, and, in particular, the behavior of the Potts antiferromagnet at $q=(3+\sqrt{5}\,)/2$ is investigated.

Keywords Potts model · Honeycomb lattice · Exact solutions · Transfer matrix

1 Introduction

In this paper we present some theorems on structural properties of Potts model partition functions on strips of the honeycomb (*hc*) lattice of arbitrary width equal to L_y vertices and arbitrarily great length. We also report exact calculations of these partition functions for a number of honeycomb-lattice strips of various widths and arbitrarily great lengths. Using these results, we consider the limit of infinite length.

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We briefly define the Potts model and relevant notation. Consider a graph $G = (V, E)$, defined by its vertex set V and edge set E. Denote the number of vertices and edges as $|V| \equiv n$ and $|E|$, respectively. On the graph G, at temperature T, the (zero-field) Potts model is defined by the partition function $Z(G, q, v) = \sum_{\{\sigma_n\}} e^{-\beta\mathcal{H}}$ with the Hamiltonian $\mathcal{H} = -J \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j}$ where $\sigma_i = 1, \dots, q$ are the spin variables on each vertex (site) $i \in V$; $\beta = (k_B T)^{-1}$; $\langle ij \rangle \in E$ denotes pairs of adjacent vertices, and J is the spin-spin interaction constant. We use the notation $K = \beta J$, $a = e^K$, and $v = e^K - 1$. The physical ranges are thus (i) $a \ge 1$, i.e., $v \ge 0$ corresponding to $\infty \ge T \ge 0$ for the Potts ferromagnet with $J > 0$, and (ii) $0 \le a \le 1$, i.e., $-1 \le v \le 0$, corresponding to $0 \le T \le \infty$ for the Potts antiferromagnet with $J < 0$. A spanning subgraph of G is $G' = (V, E')$ with $E' \subseteq E$. Then $Z(G, q, v)$ can be defined for arbitrary q and v by the cluster representation [1]

$$Z(G, q, v) = \sum_{G' \subseteq G} q^{k(G')} v^{|E'|}, \tag{1.1}$$

where $k(G')$ denotes the number of connected components of G'. For the Potts antiferromagnet, since $v < 0$, this representation does not, in general, yield a Gibbs measure unless $q \in \mathbb{Z}_+$. ($Z(G, q, v)$ is equivalent to the Whitney rank polynomial and the Tutte polynomial, which have expansions in terms of spanning subgraph contributions analogous to (1.1); see, e.g., [2].) We define a (reduced) free energy per site $f = -\beta F$, where F is the free energy, via $f(\{G\}, q, v) = \lim_{n\to\infty} \ln[Z(G, q, v)^{1/n}]$, where the symbol $\{G\}$ denotes $\lim_{n\to\infty} G$ for a given family of graphs G.

There is a particular motivation for carrying out exact calculations of the Potts model partition function $Z(G, q, v)$ for arbitrary q and v, because this allows one to investigate more deeply a unique feature of the model, which is qualitatively different from the behavior on either the square or triangular lattice. This is the property that with increasing q, the critical temperature of the Potts antiferromagnet on the honeycomb lattice decreases to zero at a non-integral value,

$$q = q_c(hc) = 4\cos^2\left(\frac{\pi}{5}\right) = \frac{3 + \sqrt{5}}{2} \simeq 2.618 \tag{1.2}$$

(see (4.1) below). This result is only formal, however, since for $q \notin \mathbb{Z}_+$, the Potts model (with either sign of J) is only defined via the cluster representation [1], and in the antiferromagnet case, with $v < 0$, this formula can yield a negative, and hence unphysical, result for the partition function [3, 4]. Clearly, one cannot investigate this formal zero-temperature criticality of the Potts antiferromagnet for $q = q_c(hc)$ on the honeycomb lattice using the Hamiltonian formulation, which requires $q \in \mathbb{Z}_+$. Our exact calculations of the Potts model partition function for arbitrary q as well as arbitrary temperature thus provide a unique way to gain insight into the properties of the Potts antiferromagnet with $q = q_c(hc)$. In contrast, the analogous values of q at which the Potts antiferromagnet is critical at $T = 0$ on the square and triangular lattices are both integers: $q_c(sq) = 3$ and $q_c(tri) = 4$ [5, 6], so this subtlety does not arise for these lattices. For q equal to a Tutte-Beraha number, relations between the Potts model and a staggered RSOS model have been studied in [7, 8], focusing on the square lattice.

In our work we consider free and cylindrical strip graphs G of the honeycomb lattice of width L_y vertices and of arbitrarily great length L_x vertices. Here, free boundary conditions (sometimes denoted FF), mean free in both the transverse, y direction and the longitudinal, x direction (the latter being the one that we let vary for a fixed width), while cylindrical boundary conditions (sometimes denoted PF) mean periodic in the transverse direction and free in the longitudinal direction. We represent the strip of the honeycomb lattice in the form of bricks oriented horizontally. For the honeycomb lattice with cylindrical boundary conditions, the number of vertices in the transverse direction, L_y, must be an even number, and the smallest value without degeneracy (multiple edges) is $L_y = 4$. Exact partition functions for arbitrary q and v have previously been presented for strips of the honeycomb lattice with free boundary conditions for width $L_y = 2$ in [9]. As part of our work, we calculate zeros of the partition function in the q plane for fixed v and in the v plane for fixed q. In the limit of infinite strip length, $L_x \to \infty$, there is a merging of such zeros to form continuous loci of points where the free energy is nonanalytic, which we denote generically as $\mathcal{B}$. For the limit $L_x \to \infty$ of a given family of strip graphs, this locus is determined as the solution to an algebraic equation and is hence an algebraic curve.

2 General Structural Theorems

2.1 Preliminaries

Here we give several general theorems that describe the structure of the partition function for the honeycomb-lattice strips under consideration. Let m denote the number of bricks in the longitudinal direction for such a strip. Then the length L_x is $2m + 1$ for odd L_x and $2m + 2$ for even L_x. For this type of strip graph, $Z(G, q, v)$ has the form

$$Z(G,q,v) = \sum_{j=1}^{N_{Z,G,\lambda}} c_{G,j}(\lambda_{Z,G,j})^m, \tag{2.1}$$

where the coefficients $c_{G,j}$ and corresponding terms $\lambda_{G,j}$, as well as the total number $N_{Z,G,\lambda}$ of these terms, depend on the type of strip (width and boundary conditions) but not on its length. In the special case $v = -1$, the numbers $N_{Z,G,\lambda}$ will be denoted $N_{P,G,\lambda}$. We define $N_{Z,hc,BC_y\ BC_x,L_y,\lambda}$ as the total number of λ's for the honeycomb-lattice strip with the transverse and longitudinal boundary conditions BC_y and BC_x of width L_y. Henceforth, where no confusion will result, we shall suppress the λ subscript. The explicit labels are N_{Z,hc,FF,L_y} and N_{Z,hc,PF,L_y} for the strips of the honeycomb lattices with free and cylindrical boundary conditions.

2.2 Case of Free Boundary Conditions

Theorem 2.1 *For arbitrary L_y,*

$$N_{Z,hc,FF,L_y} = \begin{cases} C_{L_y} & \textit{for odd } L_y, \\ \frac{1}{2}[C_{L_y} + \binom{L_y}{L_y/2}] & \textit{for even } L_y. \end{cases} \tag{2.2}$$

Proof A honeycomb-lattice strip with free boundary conditions is symmetric under reflection about the longitudinal axis if and only if L_y is even. Therefore, for odd L_y, the total number of λ's in the Potts model partition function, N_{Z,hc,FF,L_y}, is the same as the number for the triangular lattice strips N_{Z,tri,FF,L_y}, namely, the number of non-crossing partitions of the set $\{1, 2, \ldots, L_y\}$. This is the Catalan number [10, 11], $C_L = (L+1)^{-1}\binom{2L}{L}$. For even L_x, the reflection symmetry reduces N_{Z,hc,FF,L_y} to the number for the square lattice strips N_{Z,sq,FF,L_y}, which was given in Theorem 5 of [12]. □

Table 1 Numbers of λ's for the Potts model partition function and chromatic polynomials for the strips of the honeycomb lattices having free boundary conditions and various widths L_y

L_y	N_{Z,hc,FF,L_y}	N_{P,hc,FF,L_y}
2	2	1
3	5	3
4	10	5
5	42	19
6	76	25
7	429	145
8	750	194
9	4862	1230
10	8524	1590
11	58786	11139
12	104468	14681

We list the first few values of N_{Z,hc,FF,L_y} in Table 1. The next theorem concerns the number of λ's N_{P,hc,FF,L_y} in the chromatic polynomial for the free *hc* strip.

Theorem 2.2 *For arbitrary* L_y,

$$N_{P,hc,FF,L_y} = \begin{cases} \sum_{i=0}^{(L_y-1)/2} M_{L_y-1-i} \binom{(L_y-1)/2}{i} & \text{for odd } L_y, \\ \sum_{i=0}^{L_y/2-1} N_{P,sq,FF,L_y-i} \binom{L_y/2-1}{i} & \\ \quad - \frac{1}{2} \sum_{i=1}^{L_y/2-2} PL(L_y/2-1,i) N_{P,FP,[(L_y+1-i)/2]} & \text{for even } L_y, \end{cases} \tag{2.3}$$

where M_L is the Motzkin number, N_{P,sq,FF,L_y} is the number of λ's for the square lattice with free boundary conditions given in Theorem 2 *of* [12], *N_{P,FP,L_y} is the total number of λ's for the square, triangular, or honeycomb lattices with cyclic boundary conditions given in* (5.2) *of* [11], *and $PL(j,k)$ is the number given by the subtraction of the elements of Losanitsch's triangle from the corresponding elements of Pascal's triangle.*

Proof Consider odd strips widths L_y first; for these, there is no reflection symmetry. For each transverse slice containing L_y vertices of the honeycomb lattice with free boundary conditions, there are $(L_y-1)/2$ edges. Compared with the calculation of partitions for strips of the square lattice, the same numbers of edges are removed, such that the end vertices of each of these missing edges are allowed to have the same color. Firstly, all of the possible partitions for the triangular-lattice strip with free boundary conditions $N_{P,tri,FF,L_y} = M_{L_y-1}$ [10] are valid for the honeycomb lattice. Among $(L_y-1)/2$ missing edges, if one pair of end vertices has the same color, the number of partitions is given by N_{P,tri,FF,L_y-1}. As an example, for the $L_y=3$ slice of the honeycomb-lattice strip, there is an edge connecting vertices 1 and 2 and no edge connecting vertices 2 and 3. It follows that the set of partitions is comprised of $\{1, \delta_{1,3}, \delta_{2,3}\}$ in the shorthand notation used in [12, 13]. Similarly, if two pairs of end vertices of missing edges separately have the same color, there are $\binom{(L_y-1)/2}{2}$ choices for the locations of missing edges and the number of partitions for each choice is N_{P,tri,FF,L_y-2}. By including all the possible missing edges with the same color on their end vertices, the first line in (2.3) is established for the honeycomb lattice with odd L_y.

For the honeycomb lattice with even L_y, reflection symmetry must be taken into account. We thus consider partitions with the transverse slice composed of edges connecting vertices 1 and 2, vertices 3 and 4, …, vertices L_y-1 and L_y. That is, there are $L_y/2$ edges in each slice and $L_y/2-1$ missing edges. Naively, one would expect that the number of partitions is $\sum_{i=0}^{L_y/2-1} N_{P,sq,FF,L_y-i}\binom{L_y/2-1}{i}$ by the above argument. However, this would actually involve an overcounting, because certain partitions with the same color on end vertices of missing edge(s) are equivalent under the reflection symmetry. For example, the $L_y=6$ strip of the honeycomb lattice has two missing edges, i.e., there is no edge between vertices 2 and 3, and between vertices 4 and 5. There are $N_{P,sq,FF,5}=7$ partitions if vertices 2 and 3 have the same color, and separately seven partitions if vertices 4 and 5 have the same color. Five partitions for the first case $\delta_{2,3}$, $\delta_{2,3}\delta_{1,6}$, $\delta_{2,3,5}$, $\delta_{2,3}\delta_{1,4,6}$ and $\delta_{2,3,5}\delta_{1,6}$ are equivalent under reflection to the following partitions for the second case: $\delta_{4,5}$, $\delta_{4,5}\delta_{1,6}$, $\delta_{2,4,5}$, $\delta_{4,5}\delta_{1,3,6}$, and $\delta_{2,4,5}\delta_{1,6}$. In general, the double-counted partitions are those symmetric partitions in N_{P,sq,FF,L_y-i} such that i pairs of end vertices of missing edges have the same color. This number of symmetric partitions is $\frac{1}{2}N_{P,FP,[(L_y+1-i)/2]}$, given as Theorem 1 in [12]. The double counting occurs when two choices of i missing edges are reflection-symmetric to each other. This number of asymmetric choices of missing edges is given by $PL(j,k)$. □

We list the first few values of N_{P,hc,FF,L_y} for the honeycomb lattice with free boundary conditions in Table 1.

2.3 Case of Cylindrical Boundary Conditions

For the honeycomb lattice with cylindrical boundary condition, only strips with even L_y can be defined. The number of λ's can be reduced from the number of non-crossing partitions $N_{Z,tri,FF,L_y}=C_{L_y}$ with length-two rotational symmetry, and this first reduction will be denoted as N'_{Z,hc,PF,L_y}. This number can be further reduced with reflection symmetry, and this further-reduced number will be denoted as N_{Z,hc,PF,L_y}. We list the first few relevant numbers in the Potts model partition function for the strips of the honeycomb lattices with cylindrical boundary conditions in Table 2.

Lemma 2.1 *For arbitrary even L_y,*

$$\frac{L_y}{2}N'_{Z,hc,PF,L_y}-N_{Z,tri,FF,L_y}=\sum_{\text{even}\, d|L_y;\ 1\le d<L_y}\phi\left(\frac{L_y}{d}\right)\binom{2d}{d}, \tag{2.4}$$

where $d|L_y$ means that d divides L_y, and $\phi(n)$ is the Euler totient function, equal to the number of positive integers not exceeding the positive integer n and relatively prime to n.

Table 2 Numbers of λ's in the Potts model partition function for the strips of the honeycomb lattices having cylindrical boundary conditions and various even L_y

L_y	N_{Z,tri,FF,L_y}	N'_{Z,hc,PF,L_y}	N_{Z,hc,PF,L_y}	$2N_{Z,hc,PF,L_y}-N'_{Z,hc,PF,L_y}$	$\frac{L_y}{2}N'_{Z,hc,PF,L_y}-N_{Z,tri,FF,L_y}$
2	2	2	2	2	0
4	14	10	8	6	6
6	132	48	34	20	12
8	1430	378	224	70	82
10	16796	3364	1808	252	24
12	208012	34848	17886	924	1076

Lemma 2.2 *For arbitrary even L_y,*

$$2N_{Z,hc,PF,L_y} - N'_{Z,hc,PF,L_y} = N_{Z,FP,\frac{L_y}{2}}, \tag{2.5}$$

where $N_{Z,FP,L_y} = \binom{2L_y}{L_y}$ is the total number of λ's for the square or triangular or honeycomb lattices with cyclic boundary conditions, given in (5.6) *of* [11].

For brevity, we omit the proofs of these lemmas and our other new theorems; they are given in the cond-mat version of this paper [14]. The exact formula for N_{Z,hc,PF,L_y} follows from Lemmas 2.1 and 2.2:

Theorem 2.3 *For arbitrary even L_y,*

$$N_{Z,hc,PF,L_y} = \frac{1}{2}\binom{L_y}{L_y/2} + \frac{1}{L_y}\left[C_{L_y} + \sum_{\text{even}\, d|L_y;\ 1\le d<L_y} \phi\left(\frac{L_y}{d}\right)\binom{2d}{d}\right]. \tag{2.6}$$

We list the first few relevant numbers in the chromatic polynomial for the strips of the honeycomb lattices with cylindrical boundary conditions in Table 3. Analogously to Lemmas 2.1 and 2.2, we state the following conjectures

Conjecture 2.1 *For arbitrary even L_y,*

$$\frac{L_y}{2} N'_{P,hc,PF,L_y} - n_P(hc, L_y, 0) = \sum_{\text{even}\, d|L_y;\ 1\le d<L_y} \phi\left(\frac{L_y}{d}\right) N_{P,hc,FP,d}, \tag{2.7}$$

where $n_P(hc, L_y, 0)$ is the number of λ's for the cyclic strips of the honeycomb lattice with level $d = 0$, and N_{P,hc,FP,L_y} is the total number of λ's for these strips given in [9].

Compared with Lemma 2.1, the number of non-crossing partitions $N_{Z,tri,FF,L_y} = C_{L_y}$ is now replaced by the corresponding number $n_P(hc, L_y, 0)$ for the honeycomb strip in the chromatic polynomial, and the number $\binom{2d}{d} = N_{Z,hc,FP,d}$ is replaced by $N_{P,hc,FP,d}$.

Table 3 Numbers of λ's for the chromatic polynomial for the strips of the honeycomb lattices having cylindrical boundary conditions and various even L_y

L_y	$n_P(hc, L_y, 0)$	N'_{P,hc,PF,L_y}	N_{P,hc,PF,L_y}	$2N_{P,hc,PF,L_y} - N'_{P,hc,PF,L_y}$	$\frac{L_y}{2}N'_{P,hc,PF,L_y} - n_P(hc, L_y, 0)$
2	1	1	1	1	0
4	6	5	4	3	4
6	43	17	12	7	8
8	352	99	62	25	44
10	3114	626	346	66	16
12	29004	4907	2576	245	438

Conjecture 2.2 *For arbitrary even L_y,*

$$2N_{P,hc,PF,L_y} - N'_{P,hc,PF,L_y} = \begin{cases} \frac{1}{2} N_{P,hc,FP,\frac{L_y}{2}} & \text{for odd } L_y/2 > 1, \\ \frac{1}{2}[N_{P,hc,FP,\frac{L_y}{2}} + N_{P,hc,FP,\frac{L_y-2}{2}}] & \text{for even } L_y/2. \end{cases} \tag{2.8}$$

Conjectures 2.1 and 2.2 imply an exact formula for N_{P,hc,PF,L_y}.

3 Partition Functions for Honeycomb Strips with Free and Cylindrical Boundary Conditions

The Potts model partition function for a strip of the honeycomb lattice of width L_y and length L_x vertices with free boundary conditions is given by

$$Z(L_y \times L_x, FF, q, v) = \mathbf{w}^{\mathrm{T}} \cdot \mathsf{T}^m \cdot \mathbf{u}_{\mathrm{id}}, \tag{3.1}$$

where $\mathsf{T} = \mathsf{V} \cdot \mathsf{H}_2 \cdot \mathsf{V} \cdot \mathsf{H}_1$ is the transfer matrix. H_1 and H_2 are matrices corresponding respectively to adding two kinds of transverse bonds in a slice, and V corresponding to adding longitudinal bonds in each slice. The number m is related to L_x as defined above and the vector w is given by

$$\mathbf{w}^{\mathrm{T}} = \begin{cases} \mathbf{w}^{\mathrm{T}}_{\mathrm{odd}} = \mathbf{v}^{\mathrm{T}} \cdot \mathsf{H}_1 & \text{for odd } L_x, \\ \mathbf{w}^{\mathrm{T}}_{\mathrm{even}} = \mathbf{v}^{\mathrm{T}} \cdot \mathsf{H}_2 \cdot \mathsf{V} \cdot \mathsf{H}_1 & \text{for even } L_x. \end{cases} \tag{3.2}$$

Hereafter we shall follow the notation and the computational methods of [12, 13]. The matrices T, V, H_1 and H_2 act on the space of connectivities of sites on the first slice, whose basis elements $\mathbf{v}_{\mathcal{P}}$ are indexed by partitions $\mathcal{P}$ of the vertex set $\{1, \ldots, L_y\}$. In particular, $\mathbf{u}_{\mathrm{id}} = \mathbf{v}_{\{\{1\},\{2\},\ldots,\{L_y\}\}}$. We denote the set of basis elements for a given strip as $\mathbf{P} = \{\mathbf{v}_{\mathcal{P}}\}$.

Strips of the honeycomb lattice with free boundary conditions are well-defined for widths $L_y \geq 2$. The partition function $Z(G, q, v)$ was calculated, for arbitrary q, v, and m, for the strip with $L_y = 2$ and free boundary conditions in [9], using a systematic iterative application of the deletion-contraction theorem. The explicit results for $L_y = 2, 3$ and free boundary conditions in the present transfer matrix formalism are given in the cond-mat version of this paper. For $4 \leq L_y \leq 7$, the expressions for $\mathsf{T}(L_y)$, $\mathbf{w}(L_y)$ and $\mathbf{u}_{\mathrm{id}}(L_y)$ are too lengthy to include there, but are available from the authors.

For the honeycomb lattice with cylindrical boundary conditions, the width must be even (and larger than two in order to avoid the degenerate situation of vertical edges forming emanating from and returning to a given vertex). The Potts model partition function $Z(G, q, v)$ for a honeycomb-lattice strip with cylindrical boundary conditions can be written in the same form as in (3.1). Here either H_1 or H_2 should include the bond connecting the boundary sites in the transverse direction. The dimension of the transfer matrix can be reduced by the two symmetries discussed in Sect. 2, namely the length-two translation symmetry along the transverse direction and reflection symmetry. This number is N_{Z,hc,PF,L_y} and is given in terms of L_y by (2.6) (see Table 2 for some numerical values). We consider the basis in the translation-invariant and reflection-invariant subspace to construct the transfer matrix and the corresponding vectors. We have calculated the transfer matrix $\mathsf{T}(L_y)$ and the vectors $\mathbf{w}(L_y)$ and $\mathbf{u}_{\mathrm{id}}(L_y)$ for $L_y = 4$ and $L_y = 6$. The explicit results for $L_y = 4$ are given in the cond-mat version of this paper; the results for $L_y = 6$ are too lengthy to present there, but are available from the authors.

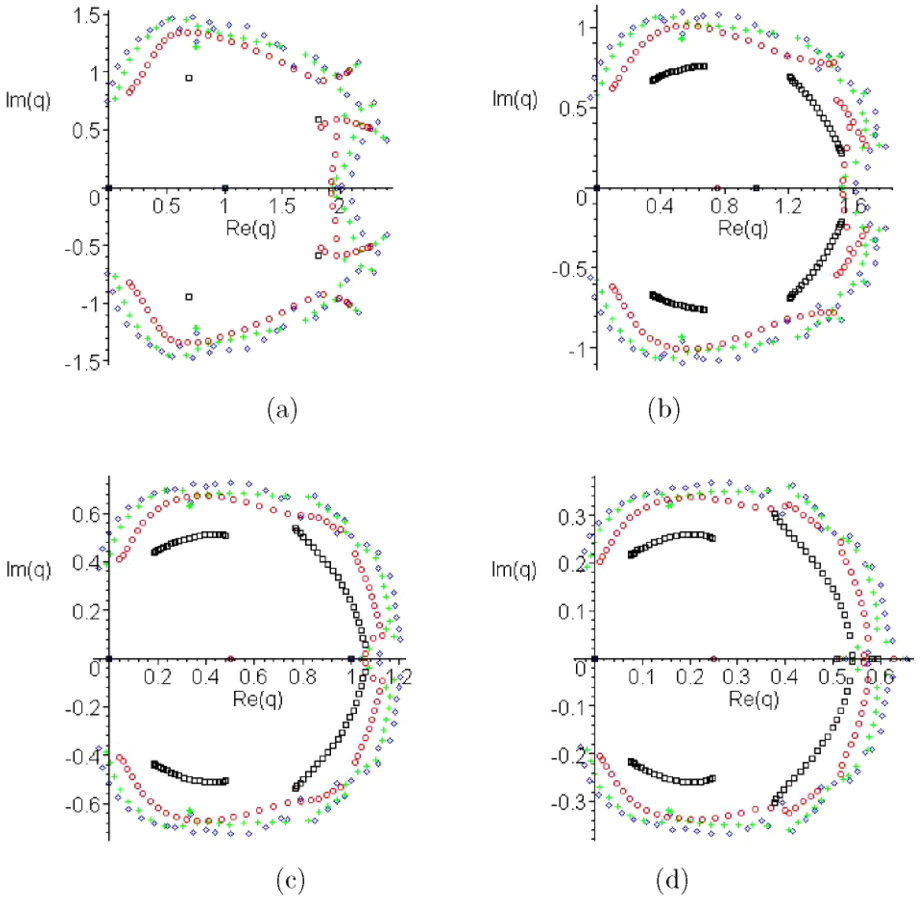

Fig. 1 Partition-function zeros in the q plane for the Potts antiferromagnet with (**a**) $v=-1.0$, (**b**) $v=-0.75$, (**c**) $v=-0.5$, and (**d**) $v=-0.25$ on strips with free boundary conditions and several widths L_y: 2 ($\square$, *black*), 3 ($\circ$, *red*), 4 ($+$, *green*), and 5 ($\Diamond$, *blue*), where the colors refer to the online paper

4 Partition Function Zeros

First we present results for zeros in the q-plane for the partition function of the Potts antiferromagnet on strips of the honeycomb lattice with free and cylindrical boundary conditions, for various values of the temperature-like variable v. Figure 1 shows these zeros for strips of widths $2 \le L \le 5$ and free boundary conditions, while Fig. 2 shows the zeros for widths $L_y = 4, 6$ and cylindrical boundary conditions. In the limit $L_x \to \infty$ the zeros merge to form sets of curves which, together, comprise the locus $\mathcal{B}$. Our results are consistent with the inference that for $v=-1$, i.e., for the zero-temperature Potts antiferromagnet, as $L_y \to \infty$, the maximal point at which the locus $\mathcal{B}$ crosses the real axis is at $q_c(hc)$, as given in (1.2). For this $v=-1$ case, $Z(G,q,v) = P(G,q)$, the chromatic polynomial, and the relation of our present results to our previous work is discussed in [14].

Next, we present results for zeros in the v-plane for the partition function of the Potts antiferromagnet on strips of the honeycomb lattice with free and cylindrical boundary conditions, for various values of q. Figure 3 shows these zeros for strips of widths $2 \le L \le 5$

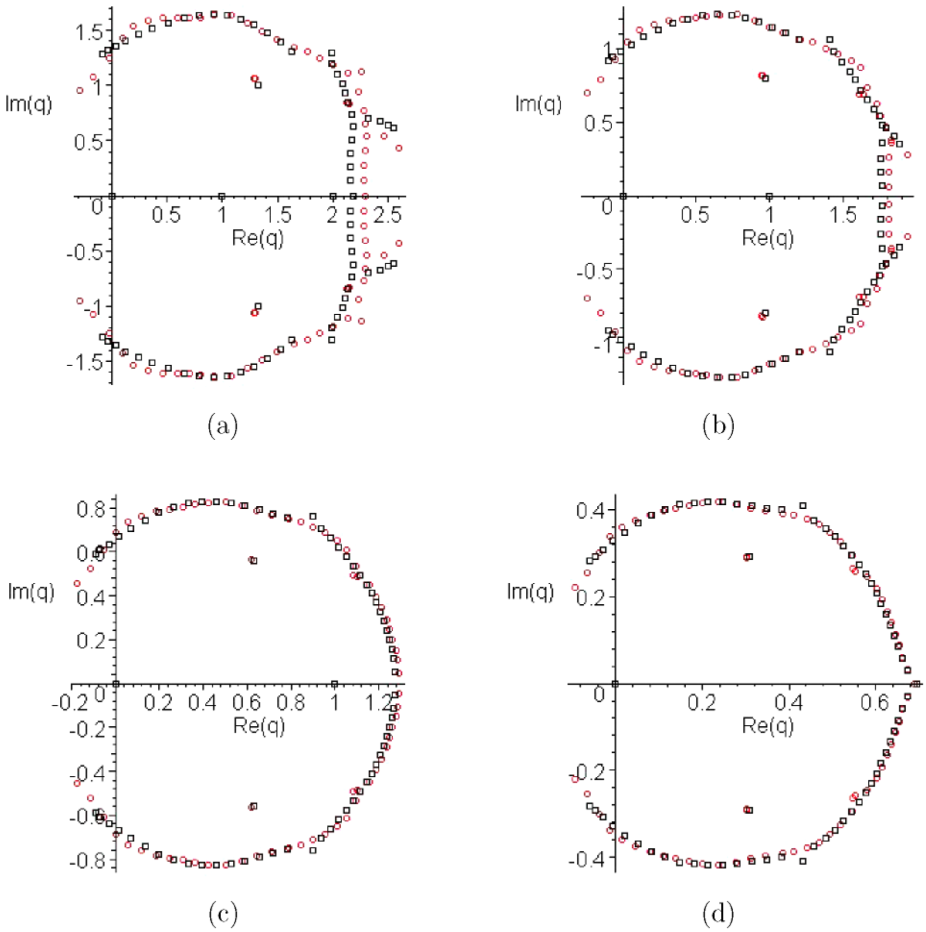

Fig. 2 Partition-function zeros for (**a**) $v = -1.0$, (**b**) $v = -0.75$, (**c**) $v = -0.5$, and (**d**) $v = -0.25$ on strips with cylindrical boundary conditions and several widths L_y: 4 (□, *black*), 6 (∘, *red*), where the colors refer to the online paper

and free boundary conditions. Figure 4 shows the zeros for widths $L_y = 4, 6$ and cylindrical boundary conditions. Again, in the limit $L_x \to \infty$ the zeros merge to form sets of curves which, together, comprise the locus $\mathcal{B}$. The criticality condition for the Potts model on the honeycomb lattice is [15, 16]

$$v^3 - 3qv - q^2 = 0. \tag{4.1}$$

For $q = 4\cos^2(\pi/r)$ with $r \in \mathbb{Z}_+$, the solutions to (4.1) have simple expressions in terms of trigonometric functions, namely

$$v_{hc1}(r) = -4\cos\left(\frac{\pi}{r}\right)\cos\left[\frac{\pi}{3}\left(\frac{1}{r} - 1\right)\right], \tag{4.2}$$

$$v_{hc2}(r) = -4\cos\left(\frac{\pi}{r}\right)\cos\left[\frac{\pi}{3}\left(\frac{1}{r} + 1\right)\right] \tag{4.3}$$

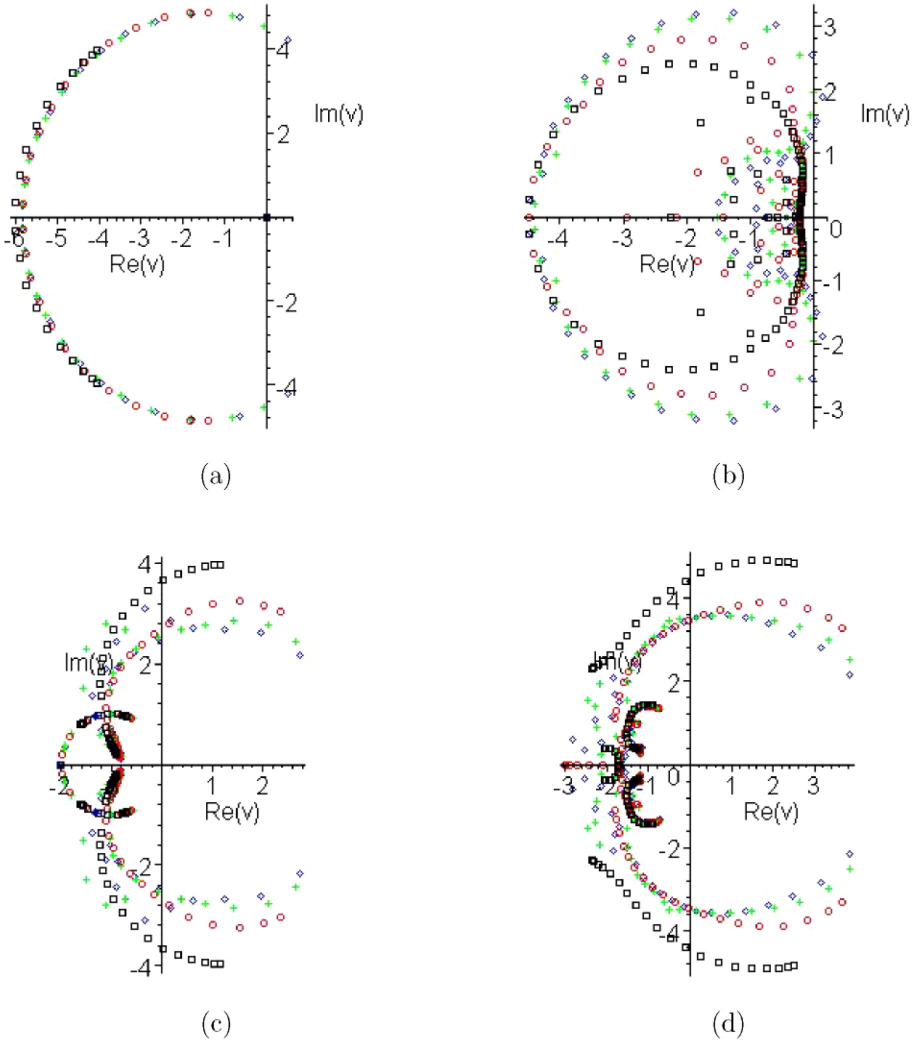

Fig. 3 Partition-function zeros, in the v plane, of (**a**) $Z(G,q,v)/q$ for $q=0$, and $Z(G,q,v)$ for (**b**) $q=0.999$, (**c**) $q=2$, and (**d**) $q=3$ on strips with free boundary conditions and several widths L_y: 2 ($\square$, *black*), 3 ($\circ$, *red*), 4 ($+$, *green*), and 5 ($\Diamond$, *blue*), where the colors refer to the online paper

and

$$v_{hc3}(r) = 4\cos\left(\frac{\pi}{r}\right)\cos\left(\frac{\pi}{3r}\right). \tag{4.4}$$

We give a discussion of the connection of the accumulation sets of these zeros, which define the complex-temperature phase boundaries, the points at which they cross the real q axis, and the solutions of (4.1) in [14]. Here we focus on the case $r=5$, for which q is given by (1.2). The solutions of (4.1) for this case are

$$v_{hc3} = \frac{1}{2}\left[1+\sqrt{15+6\sqrt{5}}\right] \simeq 3.165, \tag{4.5}$$

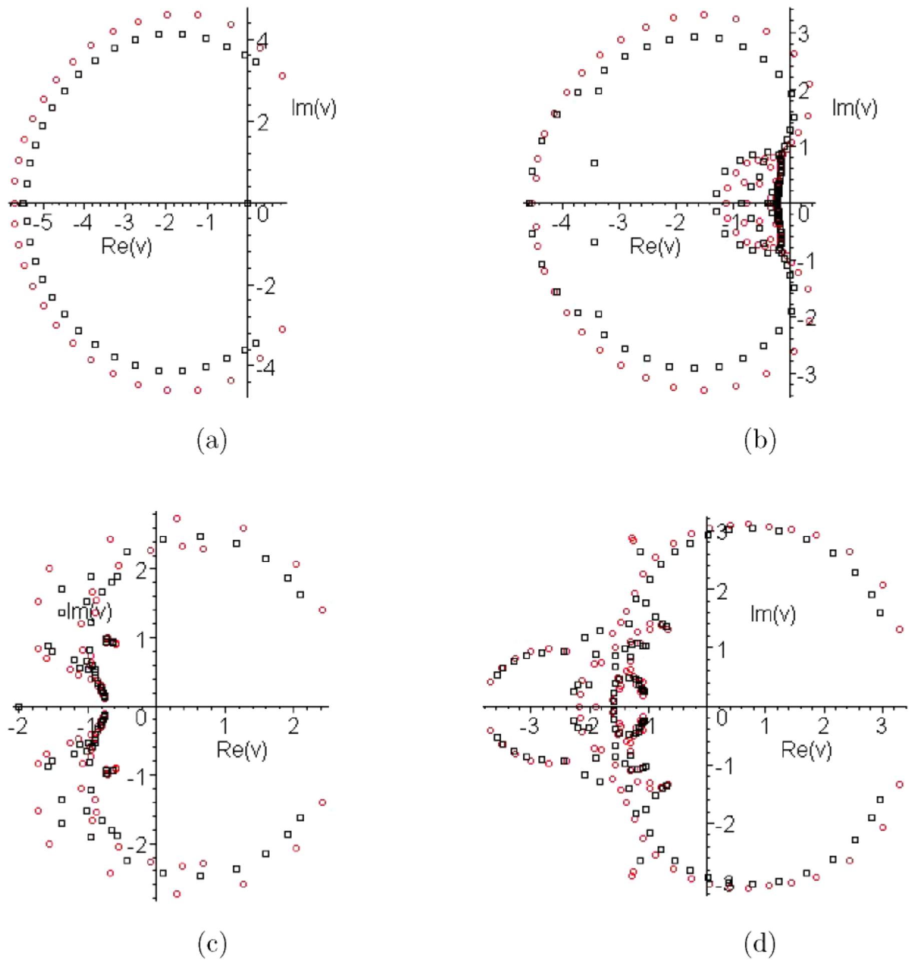

Fig. 4 Partition-function zeros, in the v plane, of (**a**) $Z(G,q,v)/q$ for $q=0$, and $Z(G,q,v)$ for (**b**) $q=0.999$, (**c**) $q=2$, and (**d**) $q=3$ on strips with cylindrical boundary conditions and several widths L_y: 4 ($\square$, *black*), 6 ($\circ$, *red*), where the colors refer to the online paper

$$v_{hc2}=-1, \tag{4.6}$$

$$v_{hc1}=\frac{1}{2}\left[1-\sqrt{15+6\sqrt{5}}\right]\simeq -2.165. \tag{4.7}$$

The first of these is the ferromagnetic critical point, while the second formally corresponds to the zero-temperature critical point for the Potts antiferromagnet. The third is a complex-temperature singular point. In Fig. 5 we plot zeros of the partition function in the v plane for $q=q_c(hc)$ and strips with free and cylindrical boundary conditions. From these zeros, one can infer that as $L_y\to\infty$, the rightmost complex-conjugate arc endpoints would move in and pinch the real axis at the ferromagnetic critical point $v_{hc3}\simeq 3.165$ given in (4.5). Our results are also consistent with crossings on $\mathcal{B}$ at the zero-temperature point $v=-1$ for the antiferromagnet. This is an important result, since it supports the conclusion that for $q=q_c(hc)$ the Potts antiferromagnet has a physical zero-temperature critical point. The zeros for free

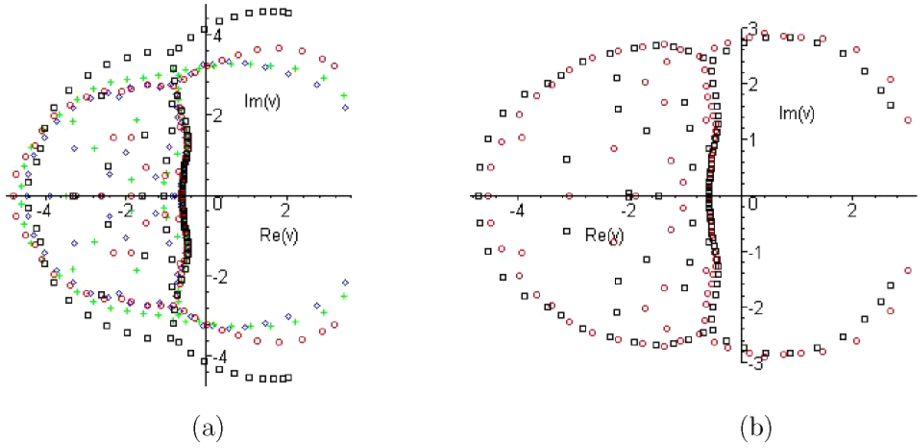

Fig. 5 Partition-function zeros, in the v plane for $q = q_c(hc) = (1/2)(3 + \sqrt{5})$ for (**a**) free boundary conditions with $L_y = 2$ (□, *black*), 3 (○, *red*), 4 (+, *green*), and 5 (◇, *blue*); (**b**) cylindrical boundary conditions and $L_y =$: 4 (□, *black*), 6 (○, *red*), where the colors refer to the online paper

boundary conditions exhibit this crossing at $v = -1$ more clearly than those for cylindrical boundary conditions. Our results also show clear crossings on $\mathcal{B}$ at the complex-temperature points $v \simeq -0.6$ and $v \simeq -4.4$ which are not roots of the criticality condition (4.1), and are consistent with a crossing at $v = v_{hc1}$ (where the latter is again more clearly suggested for free, rather than cylindrical, boundary conditions).

5 Internal Energy and Specific Heat

It is of interest to display some of the physical thermodynamic functions for the Potts model on the infinite-length limits of these strips. Having calculated the partition function, one obtains the free energy per site, $f(G, q, v)$ as $f(G, q, v) = n^{-1} \ln Z(G, q, v)$ for finite n. The internal energy per site, E, is

$$E(G, q, v) = -\frac{\partial f}{\partial \beta} = -J(v + 1)\frac{\partial f}{\partial v} \tag{5.1}$$

and the specific heat per site, C, is

$$C = \frac{\partial E}{\partial T} = k_B K^2 (v + 1)\left[\frac{\partial f}{\partial v} + (v + 1)\frac{\partial^2 f}{\partial v^2}\right]. \tag{5.2}$$

As the strip width $L_y \to \infty$, these approach the internal energy and specific heat for the infinite 2D honeycomb lattice. For convenience we define a dimensionless internal energy $E_r = -E/J = (v + 1)\partial f/\partial v$. Note that $\mathrm{sgn}(E_r)$ is (i) opposite to $\mathrm{sgn}(E)$ in the ferromagnetic case where $J > 0$ for which the physical region is $0 \le v \le \infty$ and (ii) the same as $\mathrm{sgn}(E)$ in the antiferromagnet case $J < 0$ for which the physical region is $-1 \le v \le 0$.

We have calculated the (reduced) internal energy E_r per site and the specific heat per site C on infinite-length honeycomb-lattice strips for three values of q in increasing order,

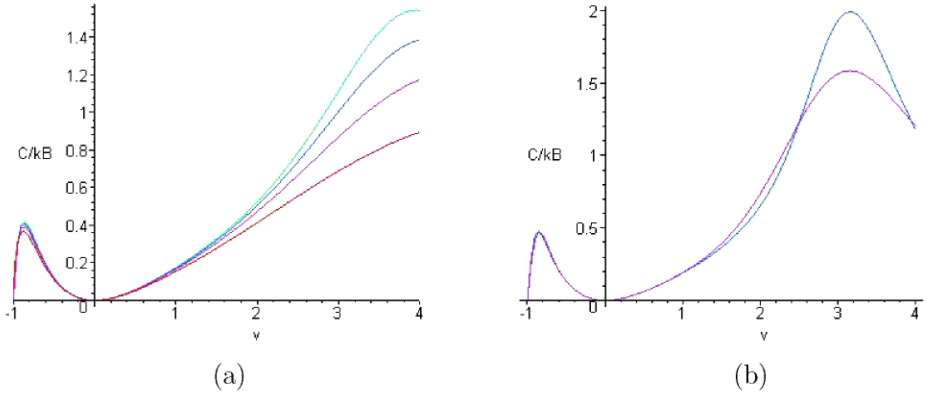

Fig. 6 Specific heat C/k_B as functions of the temperature-like variable v for the Potts model with $q=(3+\sqrt{5})/2$ on the honeycomb-lattice strips of width $2 \le L_y \le 5$ with free boundary conditions (**a**) and of width $L_y = 4, 6$ with cylindrical boundary conditions (**b**). The four curves shown for the case of free boundary conditions correspond to $L_y = 2, 3, 4, 5$ as one moves upward and the two curves for cylindrical boundary conditions correspond to $L_y = 4, 6$ as one moves upward

$q=2$, $q=q_c(hc)=(3+\sqrt{5})/2$, and $q=3$.[1] Here we concentrate on C for $q=q_c(hc)$. In the ferromagnetic case, the position where C has a maximum approaches the critical value for the infinite honeycomb lattice, $v_{hc3}=3.165$, as L_y increases. The heights of the maxima increase as L_y increases, in accordance with the fact that on 2D lattices, the specific heat diverges at the ferromagnetic critical point (with exponent $\alpha = 2/9$ for $q=q_c(hc)$. For the antiferromagnet case with $q=q_c(hc)$, the curves for C in Fig. 6 exhibit a maximum close to the zero-temperature value $v=-1$. This supports the inference of a zero-temperature critical point for this value of q, which also follows from our analysis of the zeros in the v plane. Together, these results are consistent with the conclusion that, at least as far as $\mathcal{B}$ and C are concerned, it is meaningful to regard the Potts antiferromagnet with $q=(3+\sqrt{5})/2$ as having a $T=0$ critical point.

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[1] The present paper is a shortened version of arXiv:cond-mat/0703014. Further results and references are given there.

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