Ground state entropy of the Potts antiferromagnet on homeomorphic expansions of kagomé lattice strips

Robert Shrock and Yan Xu

C. N. Yang Institute for Theoretical Physics, Stony Brook University, Stony Brook, New York 11794, USA

We present exact calculations of the chromatic polynomial and resultant ground state entropy of the q-state Potts antiferromagnet on lattice strips that are homeomorphic expansions of a strip of the kagomé lattice. The dependence of the ground state entropy on the form of homeomorphic expansion is elucidated.

I. INTRODUCTION

Nonzero ground state entropy (per lattice site), $S_0 \neq 0$, is an important subject in statistical mechanics, as an exception to the third law of thermodynamics and a phenomenon involving large disorder even at zero temperature. Since $S_0 = k_B \ln W$, where $W = \lim_{n\to\infty} W_{\text{tot}}^{1/n}$ and n denotes the number of lattice sites, $S_0 \neq 0$ is equivalent to $W > 1$, i.e., a total ground state degeneracy W_{tot} that grows exponentially rapidly as a function of n. One physical example is provided by H_2O ice, for which the residual entropy per site (at 1 atm pressure) is $S_0 = (0.41 \pm 0.03)k_B$, or equivalently, $W = 1.51 \pm 0.05$ [1] (a recent theoretical study is [2], which gets $W = 1.50738 \pm 0.00016$). In ice, the ground state entropy occurs without frustration; that is, each of the ground state configurations of the hydrogen atoms on the hydrogen bonds between water molecules minimizes the internal energy of the crystal. This is in contrast to systems where nonzero ground state entropy is associated with frustration, including the Ising antiferromagnet on the triangular lattice and spin glasses.

A model that exhibits ground state entropy without frustration and hence provides a useful framework in which to study this phenomenon is the q-state Potts antiferromagnet (PAF) [3–5] on a given lattice Λ or, more generally, a graph G, for sufficiently large q. An interesting question concerns how this ground state entropy, or equivalently, the ground state degeneracy per site, W, depends on properties of the graph. One can study this using such methods as Monte Carlo simulations, calculations of rigorous upper and lower bounds, and large-q series. One can also gain considerable insight from exact solutions for W on $n \to \infty$ limits of certain families of graphs.

A particular question is how W changes when one inserts new vertices on certain bonds of the graph. In mathematical graph theory, this insertion process is called a homeomorphic expansion of the graph (and the opposite process, removing degree-2 vertices from bonds of a graph, is called a homeomorphic reduction). It is useful to answer this question in simple cases such as lattice strips, since one can get exact explicit analytic results for these cases [6,7]. In this paper we shall continue this line of study, extending the results of earlier work that one of us did with Tsai [6,7]. We shall calculate exact expressions for the chromatic polynomial and resultant ground state degeneracy per site of the q-state Potts antiferromagnet on lattice strips that are homeomorphic expansions of a strip graph of the kagomé lattice. Our results and their comparison with analogous exact calculations for the kagomé strips without

homeomorphic expansion in [8–10] and with homeomorphic expansions of square-lattice ladder graphs in [7] add to our understanding of the effect of homeomorphic expansions on the per-site ground state degeneracy and entropy of the Potts antiferromagnet.

II. GENERALITIES AND CONNECTION WITH CHROMATIC POLYNOMIALS

Let us consider a graph $G = (V,E)$, defined by its vertex (site) set V and its edge (bond) set E. The number of vertices of G is denoted $n(G) = |V| \equiv n$, as above, and the number of edges of G is denoted $e(G) = |E|$. We use the symbol $\{G\}$ for the limit $\lim_{n(G)\to\infty} G$ of a given family of graphs, such as the infinite-length limit of a strip graph. The q-state Potts model partition function at a temperature $T = 1/(k_B\beta)$ on the graph G is $Z(G,q,T) = \sum_{\{\sigma_i\}} e^{-\beta\mathcal{H}}$, with Hamiltonian $\mathcal{H} = -J \sum_{e_{ij}} \delta_{\sigma_i\sigma_j}$, where J is the spin-spin interaction constant, i and j denote vertices on G, e_{ij} is the edge connecting them, and σ_i are classical spins taking on values in the set $\{1,\ldots,q\}$. For the Potts antiferromagnet, $J < 0$ so that, as $T \to 0, \beta J = -\infty$; hence, in this limit, the only contributions to the partition function are from spin configurations in which adjacent spins have different values. The resultant $T = 0$ PAF partition function is therefore precisely the chromatic polynomial $P(G,q)$ of the graph G:

$$Z(G,q,T=0)_{\text{PAF}} = P(G,q), \tag{2.1}$$

where $P(G,q)$ counts the number of ways of assigning q colors to the vertices of G subject to the condition that no two adjacent vertices have the same color (reviews include [11–13]). This is called a proper q-coloring of (the vertices of) G. Thus,

$$W(\{G\},q) = \lim_{n\to\infty} P(G,q)^{1/n}. \tag{2.2}$$

The determination of $W(\{G\},q)$ is thus equivalent to the determination of $S_0(\{G\},q)$, and we shall generally give results in terms of $W(\{G\},q)$. The minimal integer value of q for which one can carry out a proper q-coloring of G is the chromatic number, $\chi(G)$. In general, for certain special values of q, denoted q_s, one has the following noncommutativity of limits [14]:

$$\lim_{n\to\infty} \lim_{q\to q_s} P(G,q)^{1/n} \neq \lim_{q\to q_s} \lim_{n\to\infty} P(G,q)^{1/n}, \tag{2.3}$$

and hence it is necessary to specify which order of limits one takes in defining $W(\{G\},q)$. Here, by $W(\{G\},q)$ we mean the

function obtained by setting q to the given value first and then taking $n \to \infty$. For the families of graphs considered here, the set $\{q_s\} = \{0,1,2\}$. The noncommutativity (2.3) will not be important for our discussion, since we will restrict our calculations of $W(\{G\},q)$ to $q \geqslant 3$. For lattice strips that are m-fold repetitions of some basic subgraph, one can take a limit $n \to \infty$ by taking the limit $m \to \infty$.

The family of homeomorphically expanded graphs of the kagomé lattice strip that we consider are denoted $[H_k(\text{kag})]_{m,\text{BC}}$, where H, kag, and BC stand for homeomorphic expansion, kagomé, and longitudinal boundary conditions, free (f) or cyclic (c). A member of this family is defined as follows. We start with a minimal-width kagomé strip graph, a portion of which is shown in Fig. 1(f) of Ref. [8], comprised of m subgraphs, each of which consists of a hexagon with its two adjoining triangles. We then insert k vertices on each longitudinal edge of a hexagon in this original kagomé strip graph. Thus, the graph $[H_k(\text{kag})]_{m,\text{BC}}$ is a strip of m subgraphs each of which consists of two triangles and a p-gon with

$$p = 6 + 2k. \qquad (2.4)$$

The graph $[H_1(\text{kag})]_{m,\text{BC}}$ involves subgraphs with two triangles and an octagon, and so forth for higher values of k. The kagomé strip itself is the case $k = 0$. The chromatic number of the free and cyclic kagomé strips is $\chi = 3$, and this remains true for the homeomorphic expansions $[H_k(\text{kag})]_{m,\text{BC}}$:

$$\chi([H_k(\text{kag})]_{m,f}) = \chi([H_k(\text{kag})]_{m,c}) = 3. \qquad (2.5)$$

We shall sometimes use the abbreviations $kag_{k,m,\text{BC}} \equiv [H_k(\text{kag})]_{m,\text{BC}}$ with $\text{BC} = f$ or $\text{BC} = c$ and, for the family as a whole, suppressing the m index, $kag_{k,\text{BC}} \equiv [H_k(\text{kag})]_{\text{BC}}$.

For the relevant range, $q \geqslant 3$, of interest here, the $W(\{G\},q)$ functions computed via the infinite-length limits of the $[H_k(\text{kag})]_{m,\text{BC}}$ strips with free and cyclic (and Möbius) longitudinal boundary conditions are all the same. Since the calculation is easiest if one uses strip graphs with free longitudinal boundary conditions, we shall do this. It is also of interest to calculate the chromatic polynomials for the corresponding strip graphs with cyclic boundary conditions and we will do this. The $m \to \infty$ limits for these families of homeomorphically expanded kagomé strips will be denoted $\{[H_k(\text{kag})]_{\text{BC}}\}$ and, for the W function, which is independent of the boundary conditions, $W(\{H_k(\text{kag})\},q)$.

As noted above, our exact results for the infinite-length homeomorphically expanded kagomé strip graphs complement other methods of studying W functions on lattices, such as rigorous bounds, large-q series, and Monte Carlo measurements [15–18]. Other homeomorphic expansions of this kagomé strip graph are also of interest, e.g., expansions in which additional vertices are added to edges of the triangles, but here we shall restrict ourselves to studying the specific homeomorphic expansion defined above. In passing, we mention that chromatic polynomials of homeomorphic expansions of other types of graphs have been studied in, e.g., Refs. [6,12,19–24].

III. CALCULATIONAL METHOD

The chromatic polynomial $P(G,q)$ can be calculated in several ways. One is via the deletion-contraction relation. For a graph G, let us denote $G - e$ as the graph obtained by deleting the edge e and G/e as the graph obtained by deleting the edge e and identifying the two vertices that were connected by this edge of G. The latter operation is called a contraction of G on e. Then the chromatic polynomial satisfies the deletion-contraction relation

$$P(G,q) = P(G - e,q) - P(G/e,q). \qquad (3.1)$$

$P(G,q)$ can also be determined via the cluster formula [25]

$$P(G,q) = \sum_{G' \subseteq G} q^{\kappa(G')}(-1)^{e(G')}, \qquad (3.2)$$

where G' is a spanning subgraph, $G' = (V,E')$ with $E' \subseteq E$, and $\kappa(G')$ denotes the number of connected components in G'.

The numbers of vertices and edges on the $[H_k(\text{kag})]_{m,f}$ and $[H_k(\text{kag})]_{m,c}$ graphs are

$$n([H_k(\text{kag})]_{m,c}) = n([H_k(\text{kag})]_{m,f}) - 3 = (5 + 2k)m, \quad (3.3)$$

and

$$e([H_k(\text{kag})]_{m,c}) = e([H_k(\text{kag})]_{m,f}) - 2 = (8 + 2k)m. \quad (3.4)$$

(For the cyclic strip with $m = 1$ some of these are double edges; this does not affect the chromatic polynomial.) The graph $[H_k(\text{kag})]_{m,c}$ has vertices with degrees 3, 4, and, for $k \geqslant 1$, also 2. For reference, the infinite two-dimensional (2D) kagomé lattice has vertices of uniform degree 4. Defining, as in Ref. [17], an effective vertex degree,

$$\Delta_{\text{eff}} \equiv \lim_{n \to \infty} \frac{2e(G)}{n(G)}, \qquad (3.5)$$

we have

$$\Delta_{\text{eff}} = \frac{4(4 + k)}{5 + 2k} \quad \text{for } \{H_k(\text{kag})\}. \qquad (3.6)$$

Because $\chi([H_k(\text{kag})]_{m,f}) = 3$, it follows that $P([H_k(\text{kag})]_{m,\text{BC}},q) = 0$ for $q = 0$, 1, 2 for free or cyclic BC. Since $P([H_k(\text{kag})]_{m,\text{BC}},q)$ is a polynomial, this implies that

$$P([H_k(\text{kag})]_{m,\text{BC}},q) \quad \text{contains the factor} \quad q(q-1)(q-2).$$
$$(3.7)$$

IV. STRIPS WITH FREE LONGITUDINAL BOUNDARY CONDITIONS

For the family $[H_k(\text{kag})]_f$ of strip graphs $[H_k(\text{kag})]_{m,f}$, it is convenient to use a generating function formalism, as before [6,8,21]. For arbitrary k, this generating function is

$$\Gamma([H_k(\text{kag})]_f,q,x) = \sum_{m=0}^{\infty} P([H_k(\text{kag})]_{m+1,f},q)x^m. \quad (4.1)$$

The generating function is a rational function in x and q of the form

$$\Gamma([H_k(\text{kag})]_f,q,x) = \frac{a_{k,0} + a_{k,1}x}{1 + b_{k,1}x + b_{k,2}x^2}. \qquad (4.2)$$

We write the denominator as

$$1 + b_{k,1}x + b_{k,2}x^2 = \prod_{j=1}^{2}(1 - \lambda_{\text{kag}_k,0,j}\,x). \quad (4.3)$$

By means of an iterative use of the deletion-contraction relation and induction on the homeomorphic expansion parameter k, we have calculated $\Gamma([H_k(\text{kag})]_f,q,x)$ and hence $P([H_k(\text{kag})]_{m,f},q)$ for arbitrary k and q. Recall that the chromatic polynomial of the circuit graph C_n is $P(C_n,q) = (q-1)^n + (q-1)(-1)^n$. Since this has a factor $q(q-1)$, it is convenient to define

$$D_n = \frac{P(C_n,q)}{q(q-1)} = \sum_{s=0}^{n-2}(-1)^s\binom{n-1}{s}q^{n-2-s}, \quad (4.4)$$

so that $D_2 = 1$, $D_3 = q - 2$, $D_4 = q^2 - 3q + 3$, etc. (Where it appears, we shall write D_3 simply as $q - 2$.) We find [with $p = 6 + 2k$ as given in Eq. (2.4)]

$$a_{k,0} = q(q-1)(q-2)^2 D_p, \quad (4.5)$$

$$a_{k,1} = -q(q-1)^{5+2k}(q-2)^3, \quad (4.6)$$

$$b_{k,1} = -(q-2)(D_p - D_{p-1} + 1), \quad (4.7)$$

and

$$b_{k,2} = (q-1)^{3+2k}(q-2)^3. \quad (4.8)$$

It is readily checked that for the special case $k = 0$, these results reduce to the generating function for the kagomé strip given in Ref. [8].

Substituting the results for $b_{k,1}$ and $b_{k,2}$ in Eq. (4.3) and solving for $\lambda_{\text{kag}_k,0,j}$, we find

$$\lambda_{\text{kag}_k,0,j} = \tfrac{1}{2}(q-2)(D_p - D_{p-1} + 1 \pm \sqrt{R_{kkd0}}), \quad (4.9)$$

where $p = 6 + 2k$ as given in Eq. (2.4), $j = 1,2$ correspond to the $\pm$ signs, and

$$R_{kkd0} = (D_p - D_{p-1} + 1)^2 - 4(q-1)^{3+2k}(q-2). \quad (4.10)$$

Using the general methods of [6] for expressing the chromatic polynomial in terms of the coefficients in the generating function, we find that $P([H_k(\text{kag})]_{m,f},q)$ is given by

$$P([H_k(\text{kag})]_{m,f},q) = \frac{(a_{k,0}\lambda_{\text{kag}_k,0,1} + a_{k,1})}{(\lambda_{\text{kag}_k,0,1} - \lambda_{\text{kag}_k,0,2})}(\lambda_{\text{kag}_k,0,1})^{m-1}$$
$$+ \frac{(a_{k,0}\lambda_{\text{kag}_k,0,2} + a_{k,1})}{(\lambda_{\text{kag}_k,0,2} - \lambda_{\text{kag}_k,0,1})}(\lambda_{\text{kag}_k,0,2})^{m-1}. \quad (4.11)$$

(Note that this is symmetric under the interchange $\lambda_{\text{kag}_k,0,1} \leftrightarrow \lambda_{\text{kag}_k,0,2}$.) For the relevant range of q, $\lambda_{\text{kag}_k,0,1} > \lambda_{\text{kag}_k,0,2}$. Therefore, in the limit $m \to \infty$, the ground state degeneracy per vertex of this family of lattice strips is

$$W(\{H_k(\text{kag})\},q) = (\lambda_{\text{kag}_k,0,1})^{\frac{1}{5+2k}}, \quad (4.12)$$

where the $\lambda_{\text{kag}_k,0,j}$ for $j = 1,2$ were given in Eq. (4.9). This and Eq. (4.11) are the main results of the present paper.

From the analytic result (4.12), there follow two monotonicity properties: (i) for a given k, $W(\{H_k(\text{kag})\},q)$ is a monotonically increasing function of q in the range $q \geqslant$

$\chi = 3$; and (ii) for a given $q \geqslant 3$, $W(\{H_k(\text{kag})\},q)$ is a monotonically increasing function of k for $k \geqslant 0$. The fact that $W(\{G\},q)$ is an increasing function of q for $q \geqslant \chi(G)$ is quite general and is a consequence of the greater freedom in performing proper q-colorings of G for larger q. Property (ii) can be understood as a result of the fact that a proper q-coloring of a graph G involves a constraint on the coloring of adjacent vertices of G, and this, in turn, gives rise to a constraint from circuits in G. Since the minimum length of a circuit is the girth, increasing the girth tends to reduce the severity of this latter constraint. (Here, the girth of a graph G is defined as the number of edges that one traverses in a minimum-length circuit on G.) Although the girth of $[H_k(\text{kag})]_{m,\text{BC}}$ (ignoring the double edges that occur for $m = 1$ with cyclic BC) is equal to 3, independent of k, the girth of the polygons with $p = 6 + 2k$ sides in the strip does increase with k. Hence, for a fixed $q \geqslant \chi(G) = 3$, this increase in the girth of the p-gons increases the possibilities for proper q-colorings, and this, in turn, increases the W function. These monotonicity properties are reflected in the large-q Taylor series expansions of the W functions. As $q \to \infty$, the leading terms of the large-q series expansions of $q^{-1}W(\{H_k(\text{kag})\},q)$ are of the form $q^{-1}W(\{H_k(\text{kag})\},q) = 1 - \alpha_k/q + \cdots$, where $\cdots$ represents higher order terms in $1/q$, and the coefficients for $k = 0$, 1, 2 are $\alpha_0 = 8/5$, $\alpha_1 = 10/7$, and $\alpha_2 = 4/3$, so that $\alpha_0 > \alpha_1 > \alpha_2$, and so forth for higher k.

In Table I we list values of $W(\{\text{kag}\},q) \equiv W(\{H_0(\text{kag})\},q)$, $W(\{H_1(\text{kag})\},q)$, and $W(\{H_2(\text{kag})\},q)$ for $3 \leqslant q \leqslant 10$. The two general monotonicity properties stated above are evident in the table. As is also evident, $W(\{H_k(\text{kag})\})$ is an approximately linear function of q for values of q moderately above the chromatic number, $\chi = 3$.

It is of interest to compare these results for the ground state degeneracy and entropy on infinite-length limits of homeomorphic expansions of the kagomé strip with those obtained for homeomorphic expansions of the square-lattice ladder strip in Ref. [7]. The strip graphs considered in Ref. [7] were constructed by starting with a free or cyclic (or Möbius) square-ladder strip of m squares and adding $k - 2$ vertices to each longitudinal edge, with $k \geqslant 2$. Thus, the parameter $k - 2$ of Ref. [7] corresponds to the parameter k in our present notation, and the resultant strip is (with our present notational convention for k) $[H_k(\text{sq})]_{m,\text{BC}}$. This graph is thus a homopolygonal strip of p'-gons, where $p' = 2k + 4$. We denote the $m \to \infty$ limit of this strip as $\{[H_k(\text{sq})]_{\text{BC}}\}$. For $\{[H_k(\text{sq})]_c\}$, $q_c = 2$ (independent of k) and, for $q \geqslant q_c$, W is the same for the free and cyclic (and Möbius) longitudinal boundary conditions; $W(\{[H_k(\text{sq})]_f\},q) = W(\{[H_k(\text{sq})]_c\},q) \equiv W(\{H_k(\text{sq})\},q)$. Converting the result of Ref. [7] to our present notation by the replacement $k - 2 \to k$, one has

$$W(\{H_k(\text{sq})\},q) = (D_{2k+4})^{\frac{1}{2k+2}}. \quad (4.13)$$

In general, for even $p' = 2k + 4$, (i) $D_{p'} = 1$ if $q = 2$ and hence $W(\{H_k(\text{sq})\},2) = 1$; (ii) $D_{p'}$ is a monotonically increasing function of q, and hence so is $W(\{H_k(\text{sq})\},q)$; (iii) for a given $q > 2$, $W(\{H_k(\text{sq})\},q)$ is a monotonically increasing function of k. This monotonic increase as a function of the homeomorphic expansion parameter k is understandable in a manner analogous to that explained above, with the

TABLE I. Values of $W(\{kag\},q) \equiv W(\{H_0(kag)\},q)$, $W(\{H_1(kag)\},q)$, and $W(\{H_2(kag)\},q)$ for $3 \leqslant q \leqslant 10$. For comparison, we also show $W(\{sq\},q) \equiv W(\{H_0(sq)\},q)$, $W(\{H_1(sq)\},q)$, and $W(\{H_2(sq)\},q)$ for the square-lattice ladder strips. To save space, we omit the argument q in these W functions below. See text for further details.

q	$W(\{kag\})$	$W(\{H_1(kag)\})$	$W(\{H_2(kag)\})$	$W(\{sq\})$	$W(\{H_1(sq)\})$	$W(\{H_2(sq)\})$
3	1.409	1.550	1.639	1.732	1.821	1.872
4	2.410	2.564	2.655	2.646	2.795	2.860
5	3.410	3.569	3.660	3.606	3.784	3.854
6	4.410	4.571	4.663	4.583	4.778	4.850
7	5.409	5.571	5.664	5.568	5.773	5.848
8	6.408	6.572	6.665	6.557	6.770	6.846
9	7.407	7.572	7.665	7.550	7.768	7.844
10	8.407	8.572	8.665	8.544	8.766	8.843

difference that whereas the girth of the $[H_k(kag)]_{m,BC}$ strip is 3, independent of k, the girth of $[H_k(sq)]_{m,BC}$ is p'.

The comparison of the exact analytic result (4.13) for $W(\{H_k(sq)\},q)$ from Ref. [7] for homeomorphic expansions of the square-lattice ladder strip with our result (4.12) for homeomorphic expansions of the kagomé strip yields another inequality, namely, that for $q \geqslant 3$ (so that one can perform a proper q-coloring of the $[H_k(kag)]_{m,BC}$ strip),

$$W(\{H_k(kag)\},q) < W(\{H_k(sq)\},q). \quad (4.14)$$

This inequality can be understood heuristically as follows. As before, it will suffice to use free longitudinal boundary conditions and hence the graphs $[H_k(sq)]_{m,f}$ and $[H_k(kag)]_{m,f}$ for the $m \to \infty$ limits that define the respective W functions. Roughly speaking, for a given k, the larger $q - \chi(G)$ is for a given graph G, the more freedom there is in performing proper q-colorings of this graph. Now, for any k, the chromatic number χ is larger (namely, 3) for $[H_k(kag)]_{m,f}$ than for $[H_k(sq)]_{m,f}$ (namely, 2). Hence, for q greater than the larger of the two chromatic numbers on these strips, $q - \chi(G)$ is larger for the homeomorphic expansion of the square strip than for the homeomorphic expansion of the kagomé strip. The resultant greater freedom in performing proper q-colorings of $[H_k(sq)]_{m,f}$ than of $[H_k(kag)]_{m,f}$ makes the inequality (4.14) understandable.

V. CYCLIC STRIP $[H_k(kag)]_{m,c}$

Using similar methods, we have calculated the chromatic polynomial for the homeomorphically expanded cyclic kagomé strip, $P([H_k(kag)]_{m,c},q)$. We find that (using the abbreviation $kag_k = [H_k(kag)]_c$ here)

$$P([H_k(kag)]_{m,c},q) = \sum_{d=0}^{2} c^{(d)} \sum_{j=1}^{n_P(kag_k,d)} \left(\lambda_{kag_k,d,j} \right)^m, \quad (5.1)$$

where $c^{(0)} = 1$, $c^{(1)} = q - 1$, and $c^{(2)} = q^2 - 3q + 1$, and

$$n_P(kag_k,0) = 2, \quad n_P(kag_k,1) = 3, \quad n_P(kag_k,2) = 1, \quad (5.2)$$

independent of k. Hence, the total number of λ terms that enter into Eq. (5.1) is

$$N_{P,[H_k(kag)]_c,\lambda} = 6, \quad (5.3)$$

independent of k. Our structural result (5.1) showing the role that the coefficients $c^{(d)}$ play for these homeomorphic expansions of a cyclic kagomé strip graph generalizes what had been established earlier, namely, that they occur for the corresponding homeomorphic expansions of a square-lattice strip graph [7] and for (nonhomeomorphically expanded) cyclic strips of the square [26,27], triangular [27], and honeycomb [28] strip graphs, with the maximal d corresponding to the width L_y. Although it is not needed here, we recall the general formula

$$c^{(d)} = \sum_{s=0}^{d} (-1)^s \binom{2d-s}{s} q^{d-s}. \quad (5.4)$$

We give the λ terms that enter into Eq. (5.1) next. As is true in general for these recursive strip graphs [29], the λ's that occur for the strip with free longitudinal boundary conditions, $\lambda_{kag_k,0,j}$ [given in Eq. (4.9)], are the same as the λ's with $d = 0$ in Eq. (5.1) for the cyclic strip. Note that

$$\lambda_{kag_k,0,1} \lambda_{kag_k,0,2} = b_{k,2} = (q-1)^{3+2k}(q-2)^3. \quad (5.5)$$

At $q = 0$,

$$(\lambda_{kag_k,0,j})_{q=0} = -2(p - 1 \pm \sqrt{p^2 - 2p - 1}). \quad (5.6)$$

For the λ's with $d = 1$, we find, first,

$$\lambda_{kag_k,1,1} = (-1)^k(q-1)^{1+k}(q-2)^2. \quad (5.7)$$

Let us define

$$S_{k,1} = q - 4 + (-1)^k(q-2)(D_{k+4} - 2D_{k+3} + D_{k+2}) \quad (5.8)$$

and

$$P_{k,1} = (-1)^k(q-1)^{1+k}(q-2)^3. \quad (5.9)$$

Then

$$\lambda_{kag_k,1,j} = \frac{1}{2}\left(S_{k,1} \pm \sqrt{S_{k,1}^2 - 4P_{k,1}}\right), \quad (5.10)$$

where $j = 2,3$ corresponds to the $\pm$ sign. Thus,

$$\lambda_{kag_k,1,2} \lambda_{kag_k,1,3} = P_{k,1}, \quad (5.11)$$

so that

$$\prod_{j=1}^{3} \lambda_{\mathrm{kag}_k,1,j} = (q-1)^{2(1+k)}(q-2)^5. \quad (5.12)$$

For the λ with $d = 2$, we calculate

$$\lambda_{\mathrm{kag}_k,2} = q - 4, \quad (5.13)$$

independent of k. It is easily checked that the $k = 0$ special case of these general results agrees with the calculation of the chromatic polynomial for the cyclic kagomé strip in [9].

VI. LOCUS $\mathcal{B}$

From Eq. (3.2), it follows that $P(G,q)$ can be written in terms of its zeros (called chromatic zeros) q_{zj}, $j = 1, \ldots, n$, as $P(G,q) = \prod_{j=1}^{n}(q - q_{zj})$. These zeros are a natural topic for study in the context of chromatic polynomials. For a strip graph such as the ones considered here, as $m \to \infty$, chromatic zeros merge to form an asymptotic accumulation set (locus) consisting of various curves. As in our earlier work, we denote this locus as $\mathcal{B}$. This locus is the solution to the equation of degeneracy in magnitude of the dominant λ's (i.e., the λ's with the largest absolute value in the complex q plane [30]).

A. Case of Free Longitudinal Boundary Conditions

For the $m \to \infty$ limit of the free strip $[H_k(\mathrm{kag})]_{m,f}$, the locus $\mathcal{B}$ involves a set of curves forming arcs. For the kagomé strip itself (i.e., the case $k = 0$), these were shown in Fig. 7 of Ref. [8], and we find a similar arc-like structure for $k \geqslant 1$. The arc endpoints occur at the zeros of the polynomial R_{kkd0} given in Eq. (4.10). For example, for the actual kagomé strip itself, this is a polynomial of degree 8, with zeros at

$$q_1, q_1^* = 0.41 \pm 0.955i, \quad q_2, q_2^* = 1.18 \pm 1.14i,$$
$$q_3, q_3^* = 1.80 \pm 1.19i, \quad q_4, q_4^* = 2.62 \pm 0.15i. \quad (6.1)$$

In this case, $\mathcal{B}$ consists of four arcs, forming two complex-conjugate pairs, namely, an arc connecting q_1 and q_2, an arc connecting q_3 and q_4, and the complex-conjugate arcs. For general k, R_{kkd0} is a polynomial in q of degree

$$\deg(R_{kkd0}) = 8 + 4k. \quad (6.2)$$

For this case of $m \to \infty$ limit of $[H_k(\mathrm{kag})]_{m,f}$ with general k, the locus $\mathcal{B}$ consists of $4 + 2k$ arcs consisting of $2 + k$ complex-conjugate pairs, with endpoints at the $8 + 4k$ zeros of R_{kkd0}.

B. Case of Cyclic Longitudinal Boundary Conditions

The analysis of the locus $\mathcal{B}$ is more complicated for the $m \to \infty$ limit of the cyclic $[H_k(\mathrm{kag})]_{m,c}$ strips because of the presence of more λ's, namely, six in all. Again, the locus is determined by the equality in magnitude of two dominant λ's. For the infinite-length limit of a given family of graphs $\{G\}$, the maximal point at which $\mathcal{B}$ crosses the real axis is denoted $q_c(\{G\})$. As our previous work showed, for families of graphs with free longitudinal boundary conditions, $\mathcal{B}$ does not necessarily cross the real axis. However, for families of

graphs with cyclic boundary conditions, $\mathcal{B}$ always crosses the real axis, so a q_c is defined. For the $m \to \infty$ limit of the $[H_k(\mathrm{kag})]_{m,c}$ graphs, considered here, denoted as $\{[H_k(\mathrm{kag})]_c\}$, q_c is determined by the equality of the dominant λ's

$$\left| \lambda_{\mathrm{kag}_k,0,1} \right| = \left| \lambda_{\mathrm{kag}_k,2} \right| = |q - 4|. \quad (6.3)$$

For the infinite-length limit of the cyclic kagomé strip, $\{\mathrm{kag}_c\}$ [9],

$$q_c(\{\mathrm{kag}_c\}) \simeq 2.62. \quad (6.4)$$

In the thermodynamic limit of the 2D kagomé lattice, previous work suggests that $q_c(\mathrm{kag},2D) = 3$ [3]. Hence, one sees that the q_c value for this kagomé strip is already within about 13% of the value for the infinite 2D lattice. For the $[H_k(\mathrm{kag})]_{m,c}$ graphs, as k increases, the effect of the p-gons with $p = 6 + 2k$ becomes greater, so one expects that q_c will decrease as k increases, since $q_c = 2$ for the $m \to \infty$ limit of the circuit graph C_m. Our exact results confirm this expectation. For example, for the infinite-length limits of the $[H_k(\mathrm{kag})]_{m,c}$ strips with $k = 1$, $k = 2$, and $k = 3$, we find

$$q_c(\{[H_1(\mathrm{kag})]_c\}) \simeq 2.52, \quad (6.5)$$

$$q_c(\{[H_2(\mathrm{kag})]_c\}) \simeq 2.44, \quad (6.6)$$

$$q_c(\{[H_3(\mathrm{kag})]_c\}) \simeq 2.38. \quad (6.7)$$

The boundary $\mathcal{B}$ crosses the real q axis at $q = 0$, $q = 2$, and $q = q_c$. The degeneracy of λ magnitudes at q_c was given above in Eq. (6.3). At $q = 0$ there is a degeneracy in magnitude between $\lambda_{\mathrm{kag}_k,0,1}$ and the dominant $\lambda_{\mathrm{kag}_k,1,j}$, $j = 2,3$. At $q = 2$, there is a degeneracy in magnitude between this dominant $\lambda_{\mathrm{kag}_k,1,j}$ and $\lambda_{\mathrm{kag}_k,2}$, with both having magnitude equal to 2. There are thus three regions that include parts of the real axis. Region R_1 includes the two semi-infinite line segments $q > q_c$ and $q < 0$ and extends outward infinitely far from the origin. In region R_1, $\lambda_{\mathrm{kag}_k,0,1}$ is the dominant λ (i.e., the one with the largest magnitude). Region R_2 includes the interval $2 \leqslant q \leqslant q_c$. In region R_2, $\lambda_{\mathrm{kag}_k,2} = q - 4$ is the dominant λ. Region R_3 includes the real interval $0 \leqslant q \leqslant 2$, and in this region, the dominant term is the maximal-magnitude $\lambda_{\mathrm{kag}_k,1,j}$ for $j = 2,3$. Other complex-conjugate bubble phases are also present, as was found in Refs. [7,9]. Indeed, as is evident from Fig. 2 of Ref. [9], for the infinite-length strip of the cyclic kagomé lattice itself, the boundary $\mathcal{B}$ encloses two very small complex-conjugate phases centered at approximately $q \simeq 2.53 \pm 0.50i$.

VII. CONCLUSIONS

In conclusion, we have presented exact calculations of the chromatic polynomial and ground state degeneracy and entropy per site of the q-state Potts antiferromagnet on lattice strips that are homeomorphic expansions of a free or cyclic strip of the kagomé lattice. These results show how W and hence S_0 increase as functions of the homeomorphic expansion parameter k. We have also compared the values of W computed for the infinite-length limits of these homeomorphically expanded kagomé strips with corresponding calculations for kagomé strips without homeomorphic expansion given in Refs. [9,10] and for homeomorphic expansions of square-lattice ladder strips given in Ref. [7]. Our present results yield

further interesting insights into the effect of homeomorphic graph expansions on nonzero ground state entropy in the Potts antiferromagnet.

[1] L. Pauling, J. Am. Chem. Soc. **57**, 2680 (1935).

[2] B. A. Berg, C. Muguruma, and Y. Okamoto, Phys. Rev. B **75**, 092202 (2007).

[3] F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982).

[4] R. J. Baxter, *Exactly Solved Models* (Oxford University, Oxford, 1982).

[5] Y. Chow and F. Y. Wu, Phys. Rev. B **36**, 285 (1987).

[6] R. Shrock and S.-H. Tsai, Physica A **259**, 315 (1998).

[7] R. Shrock and S.-H. Tsai, J. Phys. A: Math. Gen. **32**, L195 (1999).

[8] M. Roček, R. Shrock, and S.-H. Tsai, Physica A **252**, 505 (1998).

[9] R. Shrock and S.-H. Tsai, Phys. Rev. E **60**, 3512 (1999).

[10] R. Shrock and S.-H. Tsai, Physica A **275**, 429 (2000).

[11] N. Biggs, *Algebraic Graph Theory* (Cambridge University, Cambridge, England, 1993).

[12] F. M. Dong, K. M. Koh, K. L. Teo, *Chromatic Polynomials and Chromaticity of Graphs* (World Scientific, Singapore, 2005).

[13] Workshop on Zeros of Graph Polynomials, Newton Institute for Mathematical Sciences, Cambridge University, 2008 (unpublished), [http://www.newton.ac.uk/programmes/CSM/seminars].

[14] R. Shrock and S.-H. Tsai, Phys. Rev. E **55**, 5165 (1997).

[15] N. L. Biggs, Bull. London Math. Soc. **9**, 54 (1977).

[16] R. Shrock and S.-H. Tsai, Phys. Rev. E **56**, 2733 (1997).

[17] R. Shrock and S.-H. Tsai, Phys. Rev. E **56**, 4111 (1997).

[18] R. Shrock and Y. Xu, Phys. Rev. E **81**, 031134 (2010).

[19] E. G. Whitehead and L. C. Zhao, J. Graph Theory **8**, 355 (1984).

[20] R. Shrock and S.-H. Tsai, J. Phys. A **31**, 9641 (1998).

[21] R. Shrock and S.-H. Tsai, Physica A **265**, 186 (1999).

[22] R. C. Read and E. G. Whitehead, Discrete Math. **204**, 337 (1999).

[23] A. Sokal, Combin. Probab. Comput. **13**, 221 (2004).

[24] Y. L. Peng, Discrete Math. **288**, 177 (2004).

[25] C. M. Fortuin and P. W. Kasteleyn, Physica **57**, 536 (1972).

[26] H. Saleur, Nucl. Phys. B **360**, 219 (1991).

[27] S.-C. Chang and R. Shrock, Physica A **296**, 131 (2001).

[28] S.-C. Chang and R. Shrock, Physica A **296**, 183 (2001).

[29] S.-C. Chang and R. Shrock, Physica A **316**, 335 (2002).

[30] S. Beraha, J. Kahane, and N. Weiss, J. Combin. Theory B **28**, 52 (1980).