Ground-state entropy of the Potts antiferromagnet with next-nearest-neighbor spin-spin couplings on strips of the square lattice

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We present exact calculations of the zero-temperature partition function (chromatic polynomial) and $W(q)$, the exponent of the ground-state entropy, for the q-state Potts antiferromagnet with next-nearest-neighbor spin-spin couplings on square lattice strips, of width $L_y=3$ and $L_y=4$ vertices and arbitrarily great length L_x vertices, with both free and periodic boundary conditions. The resultant values of W for a range of physical q values are compared with each other and with the values for the full two-dimensional lattice. These results give insight into the effect of such nonnearest-neighbor couplings on the ground-state entropy. We show that the $q=2$ (Ising) and $q=4$ Potts antiferromagnets have zero-temperature critical points on the $L_x\to\infty$ limits of the strips that we study. With the generalization of q from $\mathbb{Z}_+$ to $\mathbb{C}$, we determine the analytic structure of $W(q)$ in the q plane for the various cases.

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I. INTRODUCTION

The q-state Potts antiferromagnet with the usual nearest-neighbor spin-spin couplings [1,2] exhibits nonzero ground-state entropy, $S_0>0$ (without frustration) for sufficiently large q on a given lattice Λ. This is equivalent to a ground-state degeneracy per site $W>1$, since $S_0=k_B \ln W$. Such nonzero ground-state entropy is important as an exception to the third law of thermodynamics [3,4]. A physical example of nonzero ground-state entropy is ice [5–7]. In this q state, Potts antiferromagnet at $T=0$, the value of each spin must be different than the values of all of the other spins to which it is coupled. There is a close connection with graph theory here, since the zero-temperature partition function of the above-mentioned q-state Potts antiferromagnet on a lattice Λ or, more generally, a graph G, satisfies

$$Z(G,q,T=0)_{PAF}=P(G,q), \tag{1.1}$$

where $P(G,q)$ is the chromatic polynomial expressing the number of ways of coloring the vertices of the graph G with q colors such that no two adjacent vertices have the same color (for reviews, see Refs. [8–11]). The minimum number of colors for which this coloring is possible, i.e., the minimum integer value of q for which $P(G,q)$ is nonzero, is denoted the chromatic number of G, $\chi(G)$.

From Eq. (1.1), it follows that[1]

$$W(\{G\},q)=\lim_{n\to\infty} P(G,q)^{1/n}, \tag{1.2}$$

where $n=v(G)$ is the number of vertices of G and $\{G\}=\lim_{n\to\infty} G$.

Since $P(G,q)$ is a polynomial, one can generalize q from $\mathbb{Z}_+$ to $\mathbb{C}$. The zeros of $P(G,q)$ in the complex q plane are called chromatic zeros; a subset of these may form an accumulation set in the $n\to\infty$ limit, denoted $\mathcal{B}$, which is the continuous locus of points where $W(\{G\},q)$ is nonanalytic. The maximal region in the complex q plane to which one can analytically continue the function $W(\{G\},q)$ from physical values where there is nonzero ground-state entropy, is denoted R_1. The maximal value of q where $\mathcal{B}$ intersects the (positive) real axis is labeled $q_c(\{G\})$. This value is important since $W(\{G\},q)$ is a real analytic solution for real q down to $q_c(\{G\})$. For regions other than R_1, one can only determine the magnitude $|W(\{G\},q)|$ unambiguously [12]. In addition to Refs. [8–12], some previous works on chromatic polynomials include Refs. [13–45].

In previous works we have carried out comparative studies of W for different lattices and have explored the effects of different lattice properties such as coordination numbers [12,26,29–31,34,35,39–42] and [45]. In general it was found that as one increased the lattice coordination number, the ground-state entropy of the q-state Potts antiferromagnet (if nonzero for the given value of q) decreased. This can be understood as a consequence of the fact that as one increases the lattice coordination number, one is increasing the constraints on the coloring of a given vertex subject to the constraint that other vertices of the lattice adjacent to this one (i.e., connected with a bond or edge of the lattice) have different colors. Another way in which to explore this effect is to consider non-nearest-neighbor spin-spin couplings. Again, in general, these increase the constraints on the values that any given spin can take on, and hence decrease the ground-state entropy. We wish to make this more quantitative and shall do so here using exact solutions for the chromatic polynomials and rigorous bounds. A natural starting point for

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[1]At certain special points q_s (typically $q_s=0,1,\ldots,\chi(G)$), one has the noncommutativity of limits $\lim_{q\to q_s}\lim_{n\to\infty}P(G,q)^{1/n} \neq \lim_{n\to\infty}\lim_{q\to q_s}P(G,q)^{1/n}$, and hence it is necessary to specify the order of the limits in the definition of $W(\{G\},q_s)$ [12]. We use the first order of limits here; this has the advantage of removing certain isolated discontinuities in W.

studies of such nonnearest-neighbor spin-spin couplings is to consider the model on a given lattice and add next-nearest-neighbor (*nnn*) spin-spin couplings. Equivalently, we can redefine the lattice itself by considering it as a graph G with vertices at the usual lattice sites but with bonds (= edges in graph theory nomenclature) consisting not only of the usual bonds joining these lattice sites but also bonds joining next-nearest-neighbor lattice sites. We then consider the nearest-neighbor Potts antiferromagnet on this redefined lattice.

Perhaps the simplest case that one could consider is the q-state Potts antiferromagnet in one dimension; the lattice here is just the line T_n or circle C_n for the case of free and periodic boundary conditions, respectively (denoted FBC_x and PBC_x). One has $P(T_n,q)=q(q-1)^{n-1}$ so $W=q-1$ and R_1 is the entire q plane. For the circle, $P(C_n,q)=(q-1)^n+(q-1)(-1)^n$. In this case, if $|q-1|>1$, then $W=q-1$, while if $|q-1|\leqslant 1$, then $|W|=1$, so that $q_c=2$. Hence for either FBC_x or PBC_x there is nonzero ground-state entropy $S_0=k_B\ln(q-1)$ for $q>2$. The addition of next-nearest neighbor bonds converts T_n or C_n to a open or cyclic strip of triangles, respectively, with each pair sharing an edge. We denote these strips $\mathrm{tri}(L_y=2)$, N_t, BC_x, where $\mathrm{BC}_x=\mathrm{FBC}_x$ or PBC_x. In the cyclic case, the degree Δ (number of neighboring vertices) of each vertex is changed from 2 to 4, and this is also true of the internal vertices in the open case. The chromatic numbers in these cases are (i) $\chi=2$ for the line T_n, (ii) $\chi=2(3)$ for C_n with n even (odd), (iii) $\chi=3$ for the open triangular strip, and (iv) $\chi=3(4)$ for the cyclic triangular strip with the number of triangles N_t even (odd). For the Potts antiferromagnet with *nnn* spin-spin couplings on the line (equivalently, on the open triangular strip) with n vertices,

$$P[\mathrm{sq}_d(L_y=1),\mathrm{FBC}_y,\mathrm{FBC}_x,q]=P[\mathrm{tri}(L_y=2),\mathrm{FBC}_y,\mathrm{FBC}_x,q]=q(q-1)(q-2)^{n-2} \tag{1.3}$$

and hence $W=q-2$ and R_1 is the full q plane.

For the Potts antiferromagnet with *nnn* spin-spin couplings on the circuit, the equivalence is with the cyclic triangular strip:

$$P[\mathrm{sq}_d(L_y=1),\mathrm{FBC}_y,\mathrm{PBC}_x,q]=P[\mathrm{tri}(L_y=2),\mathrm{FBC}_y,\mathrm{PBC}_x,q]. \tag{1.4}$$

If the strip length involves an even number of triangles $N_t=n=2m$, then [35,38]

$$P[\mathrm{tri}(L_y=2),N_t=2m,\mathrm{FBC}_y,\mathrm{PBC}_x,q]=q^2-3q+1+(q-2)^{2m}+(q-1)[(\lambda_{t2,3})^m+(\lambda_{t2,4})^m] \tag{1.5}$$

while for odd $N_t=n=2m+1$ [45]

$$P[\mathrm{tri}(L_y=2),N_t=2m+1,\mathrm{FBC}_y,\mathrm{PBC}_x,q]=-(q^2-3q+1)+(q-2)[(q-2)^2]^m+\frac{1}{2}(q-1)(q-3)\left[[(\lambda_{t2,3})^m+(\lambda_{t2,4})^m]+\frac{[(\lambda_{t2,3})^m-(\lambda_{t2,4})^m]}{\lambda_{t2,3}-\lambda_{t2,4}}\right], \tag{1.6}$$

where

$$\lambda_{t2,(3,4)}=\frac{1}{2}[5-2q\pm\sqrt{9-4q}]. \tag{1.7}$$

In both cases, $q_c=3$ and $W=q-2$ for $q\geqslant 3$ (and more generally, for q in the region R_1 given in [35]). Thus, the addition of next-nearest-neighbor couplings increases the value of q beyond which there is nonzero ground-state entropy from 2 to 3 and decreases the value of the resultant entropy from $S_0=k_B\ln(q-1)$ to $S_0=k_B\ln(q-2)$ for $q\geqslant 3$.

We proceed to consider the Potts antiferromagnet on the square lattice, and again add next-nearest-neighbor couplings, or equivalently redefine the lattice so that the bonds consists not just of the usual horizontal and vertical bonds, but also of bonds connecting the diagonally opposite vertices of each square. Following our earlier notation [25], we shall denote this lattice as sq_d, where the d refers to the addition of these diagonal bonds. For the square (sq) and sq_d lattices, the chromatic numbers are

$$\chi(\mathrm{sq})=2, \quad \chi(\mathrm{sq}_d)=4. \tag{1.8}$$

No exact solution is known for $W(q)$ on the sq_d lattice. In the absence of such an exact solution, Tsai and one of us (R.S.) have carried out Monte Carlo measurements of $W(\mathrm{sq}_d,q)$ and have derived a rigorous lower bound [25]

$$W(\mathrm{sq}_d,q)\geqslant\frac{(q-2)(q-3)}{q-1}\ \text{for} \quad q\geqslant\chi(\mathrm{sq}_d). \tag{1.9}$$

This lower bound was compared with the actual value of $W(\mathrm{sq}_d,q)$, as determined by the Monte Carlo measurements for $5\leqslant q\leqslant 10$ [25,24] and was found to lie very close it (cf. Table III of Ref. [25]). For example, for $q=6$ and $q=8$, the ratio of the lower bound divided by the actual value was 0.981 and 0.995, and it increased monotonically toward unity as q increased. Since it is possible to obtain exact analytic solutions for W on infinite-length, finite-width strips of two-dimensional (2D) lattices [13,12,29–31] and [34,35,39–41,45], one has an alternate way to investigate $W(\mathrm{sq}_d,q)$, namely, to calculate W exactly on strips of the sq_d lattice, with various boundary conditions. It has, indeed, been found [31] that for the square and triangular lattices, the values of W for such infinite-length strips of even rather modest widths are close to the corresponding values for the 2D thermodynamic limit, for moderate values of q. In the present paper we report exact calculations of $P(q)$, $W(q)$, and $\mathcal{B}$ on strips of the sq_d lattice with various boundary conditions. The longitudinal and transverse directions on the strip are taken to be $\hat{x}$ and $\hat{y}$, respectively. In Fig. 1 we show some illustrative strips of the sq_d lattice.

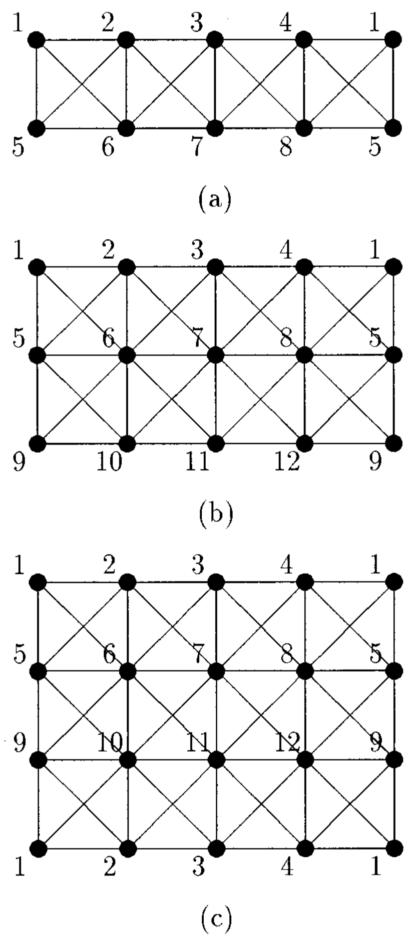

FIG. 1. Illustrative strip graphs of the sq_d lattice: (*a,b*) $L_y=2,3$ $(\mathrm{FBC}_y,\mathrm{PBC}_x)$ (cyclic); (c) $L_y=3$, $(\mathrm{PBC}_y,\mathrm{PBC}_x)$ (toroidal boundary conditions).

An important property is that with the two added diagonal bonds, each square of the sq_d lattice constitutes a complete graph on four vertices. [Here, the complete graph on r vertices K_r is defined as the graph each of whose vertices is connected to all of the other $r-1$ vertices by bonds (=edges); it has chromatic number $\chi(K_r)=r$.] Compared with the square lattice, for a given q coloring of the sq_d lattice, the addition of these bonds clearly increases the constraints on the coloring of each vertex and therefore decreases $P(G,q)$. As we proved earlier [26], if a lattice Λ' can be obtained from another Λ, by connecting disjoint vertices of Λ with bonds, then $W(\Lambda',q)\le W(\Lambda,q)$ for q colorings of the two lattices. An example of the application of this theorem was given in Ref. [26]: for q colorings of the square, triangular (tri), and honeycomb (*hc*) lattices, $W(\mathrm{tri},q)<W(\mathrm{sq},q)\le W(\mathrm{hc},q)$. [$W(\mathrm{sq},q)$ is strictly less than $W(hc,q)$ except at the value $q=2$, where $W(\mathrm{sq},2)=W(\mathrm{hc},2)=1$.] In the present context, we note the inequality for q colorings of these lattices:

$$W(\mathrm{sq}_d,q)<W(\mathrm{tri},q)<W(\mathrm{sq},q)\le W(\mathrm{hc},q) \qquad (1.10)$$

(for q values where such colorings are possible).

We use the symbols (FBC_y) and (PBC_y) for free and periodic transverse boundary conditions and, as above, FBC_x, PBC_x, and TPBC_x for free, periodic, and twisted periodic longitudinal boundary conditions. The term ‘‘twisted’’ means that the longitudinal ends of the strip are identified with reversed orientation. These strip graphs can be embedded on surfaces with the following topologies: (i) $(\mathrm{FBC}_y,\mathrm{FBC}_x)$: open strip, (ii) $(\mathrm{PBC}_y,\mathrm{FBC}_x)$: cylindrical, (iii) $(\mathrm{FBC}_y,\mathrm{PBC}_x)$: cylindrical (denoted cyclic here), (iv) $(\mathrm{FBC}_y,\mathrm{TPBC}_x)$: Möbius; (v) $(\mathrm{PBC}_y,\mathrm{PBC}_x)$: torus, and (vi) $(\mathrm{PBC}_y,\mathrm{TPBC}_x)$: Klein bottle.[2]

The labeling of the strips generally follows our earlier labeling conventions. Thus for a strip with free transverse and longitudinal boundary conditions. $(\mathrm{FBC}_y,\mathrm{FBC}_x)$, the length of the strip is taken to be $m+1$ squares or equivalently edges, with $L_x=m+2$, and the width is L_y vertices. This strip thus has $n=L_xL_y$ vertices and $e=4L_xL_y-3(L_x+L_y)+2$ edges. For cyclic strips, the width is defined in the same manner and the length is L_x vertices or equivalently edges. For strips with periodic transverse boundary conditions, including $(\mathrm{PBC}_y,\mathrm{FBC}_x)$ and $(\mathrm{PBC}_y,\mathrm{PBC}_x)$, a width of $L_y=3$ means that the cross section involves L_y vertices. For $L_x=m\ge 3$ to avoid certain degenerate cases, the sq_d strips with either cyclic or torus boundary conditions have $n=L_xL_y$ vertices. With the same restriction, the cyclic strips have $e=L_x(4L_y-3)$ edges and the torus strips have $e=4L_xL_y$ edges.

Let us next comment on the planarity or nonplanarity of the strips of the sq_d lattice with various boundary conditions. We shall concentrate here on nondegenerate cases where the strips are proper graphs without multiple edges. Consider first the strips with $(\mathrm{FBC}_y,\mathrm{FBC}_x)$ boundary conditions. For $L_y=2$ and arbitrary L_x, it is easy to show that these are planar by taking the second diagonal bond for each square and drawing it external to the strip; by redefining the labeling of the x and y axes, it follows that this strip with $(\mathrm{FBC}_y,\mathrm{FBC}_x)$ boundary conditions, $L_x=2$, and arbitrary L_y is also planar. For other cases we shall make use of two theorems from graph theory. The first of these states that if G is a planar graph with n vertices and e edges with $n\ge 3$, then $e\le 3(n-2)$ [e.g., Corollary 11.1(c) in Ref. [10]] and the second states that if G is a planar graph with $n\ge 4$, then G has at least four vertices of degree $\Delta\le 5$ [e.g., Corollary 11.1(e) in [10]]. Now

$$3(n-2)-e=-L_xL_y+3(L_x+L_y)-8 \quad \text{for} \quad \mathrm{sq}_d, \quad (\mathrm{FBC}_y,\mathrm{FBC}_x) \qquad (1.11)$$

so that for sufficiently great L_x and/or L_y, $3(n-2)-e$ is negative and hence the strip is nonplanar, by the first theorem. For example, $3(n-2)-e<0$ if $L_y=4$ and $L_x\ge 5$ or *vice versa*, i.e., $L_x=4$ and $L_y\ge 5$; and similarly, if $L_x=L_y\ge 5$. Considering next the strips of the sq_d lattice that are cyclic, i.e., have $(\mathrm{FBC}_y,\mathrm{PBC}_x)$ boundary conditions, we have

$$3(n-2)-e=-L_xL_y+3L_x-6 \quad \text{for} \quad \mathrm{sq}_d, \quad (\mathrm{FBC}_y,\mathrm{PBC}_x). \qquad (1.12)$$

[2]These BC's can all be implemented in a manner that is uniform in the length L_x; the case (vii) $(\mathrm{TPBC}_y,\mathrm{TPBC}_x)$ with the topology of the projective plane requires different identifications as L_x varies and will not be considered here.

Hence, $3(n-2)-e<0$ for all L_x if $L_y \geq 3$, so that these strips are nonplanar. For the strips with $(\mathrm{PBC}_y, \mathrm{PBC}_x)$, i.e., torus boundary conditions, we have

$$3(n-2)-e=-(L_x L_y+6) \quad \text{for} \quad \mathrm{sq}_d, \quad (\mathrm{PBC}_y, \mathrm{PBC}_x) \tag{1.13}$$

so that these strips are also nonplanar. This can be seen alternatively by observing that each vertex on the torus strips has degree $\Delta=8$ and applying the second theorem cited above. The second theorem also shows that the sq_d strip with Klein bottle boundary conditions is nonplanar.

A generic form for chromatic polynomials for recursively defined families of graphs, of which strip graphs G_s are special cases, is

$$P[(G_s)_m, q]=\sum_{j=1}^{N_{G_s,\lambda}} C_{G_s,j}(q)[\lambda_{G_s,j}(q)]^m, \tag{1.14}$$

where $c_{G_s,j}(q)$ and the $N_{G_s,\lambda}$ terms $\lambda_{G_s,j}(q)$ depend on the type of strip graph G_s, as indicated, but are independent of m.

II. STRIPS WITH $(\mathrm{FBC}_y, \mathrm{FBC}_x)$

A. $L_y=2$

The chromatic polynomial for the strip of the sq_d lattice with $L_y=1$ and free transverse and longitudinal boundary conditions was given above in Eq. (1.3). For the $L_y=2$ case the chromatic polynomial is

$$P[\mathrm{sq}_d(L_y=2)_m, FBC_y, FBC_x, q] = q(q-1)[(q-2)(q-3)]^{m+1}. \tag{2.1}$$

In the $m \to \infty$ limit,

$$W[\mathrm{sq}_d(L_y=2), \mathrm{FBC}_y, \mathrm{FBC}_x, q]=[(q-2)(q-3)]^{1/2}. \tag{2.2}$$

with $\mathcal{B}=\emptyset$.

B. $L_y=3$

For the $L_y=3$ strip, we use the same generating function method as we have before [29,30,35]. In general, for the family of strip graphs G_s, the generating function $\Gamma(G_s, q, x)$ is a rational function of the form

$$\Gamma(G_s, q, x)=\frac{\mathcal{N}(G_s, q, x)}{\mathcal{D}(G_s, q, x)} \tag{2.3}$$

with

$$\mathcal{N}(G_s, q, x)=\sum_{j=0}^{d_{\mathcal{N}}} A_{G_s,j}(q) x^j \tag{2.4}$$

and

$$\mathcal{D}(G_s, q, x)=1+\sum_{j=1}^{d_{\mathcal{D}}} b_{G_s,j}(q) x^j, \tag{2.5}$$

where the $A_{G_s,i}$ and $b_{G_s,i}$ are polynomials in q (with no common factors) and

$$d_{\mathcal{N}}=\deg_x(\mathcal{N}) \tag{2.6}$$

and

$$d_{\mathcal{D}}=\deg_x(\mathcal{D}). \tag{2.7}$$

This generating function yields the chromatic polynomials via the Taylor-series expansion in the auxiliary variable x:

$$\Gamma(G_s, q, x)=\sum_{m=0}^{\infty} P[(G_s)_m, q] x^m, \tag{2.8}$$

where we follow the notational convention in Ref. [29], according to which a strip is considered to be comprised of m repetitions of a basic subgraph unit H connected to an initial subgraph I; here we take $I=H$ so that a strip with a given value of m has $m+1$ columns of K_4's and $m+2$ vertices in the longitudinal direction. The denominator can be written in factorized form as

$$\mathcal{D}_{G_s}=\prod_{j=1}^{d_{\mathcal{D}}}(1-\lambda_{G_s,j} x). \tag{2.9}$$

These are the $\lambda_{G_s,j}$'s in Eq. (1.14); the coefficients are determined by Eqs. (2.14) or (2.19) in Ref. [30].

For $L_y=3$, we find $d_{\mathcal{D}}=2$, $d_{\mathcal{N}}=1$, and

$$\Gamma[\mathrm{sq}_d(L_y=3), \mathrm{FBC}_y, \mathrm{FBC}_x, q, x] =\frac{q(q-1)(q-2)(q-3)^2[(q-2)-(q-1)(q-3)x]}{1-(q-3)(q^2-6q+11)x+(q-2)(q-3)^3x^2}. \tag{2.10}$$

The denominator can be written as

$$\mathcal{D}_{\mathrm{sq}_d 3o}=(1-\lambda_{\mathrm{sq}_d 3o,1} x)(1-\lambda_{\mathrm{sq}_d 3o,2} x), \tag{2.11}$$

where

$$\lambda_{\mathrm{sq}_d 3o,(1,2)}=\frac{1}{2}(q-3)[q^2-6q+11 \pm(q^4-12q^3+54q^2-112q+97)^{1/2}] \tag{2.12}$$

and the shorthand sq$d3o$ denotes the strip of the sq_d lattice with $L_y=3$ and open (o) boundary conditions. From this, using the general formulas in Ref. [30], one can write the chromatic polynomial in the form of Eq. (1.14) (with $N_\lambda=2$). In the $m \to \infty$ limit.

$$W[\mathrm{sq}_d(L_y=3), \mathrm{FBC}_y, \mathrm{FBC}_x, q]=(\lambda_{\mathrm{sq}_d 3o,1})^{1/3}. \tag{2.13}$$

The nonanalytic locus $\mathcal{B}$ is shown in Fig. 2 and is comprised of an arc stretching between endpoints at $q \simeq 1.95+1.43i$ and $4.05+0.396i$, together with the complex conjugate arc. In agreement with the general discussion given before [29,30,41], these four points are the branch points of the square root in Eq. (2.12). $\mathcal{B}$ does not intersect the real q axis,

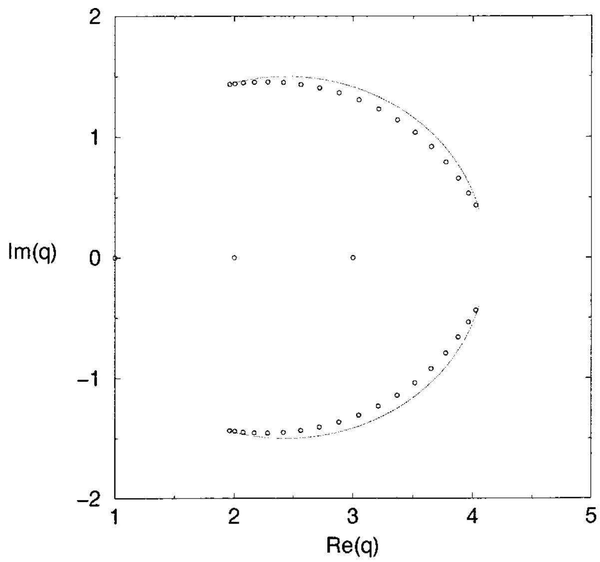

FIG. 2. Locus $\mathcal{B}$ for W for the $3\times\infty$ strip of the sq_d lattice with free transverse and longitudinal boundary conditions. Chromatic zeros are shown for the case $L_x=20$ (i.e., $n=60$).

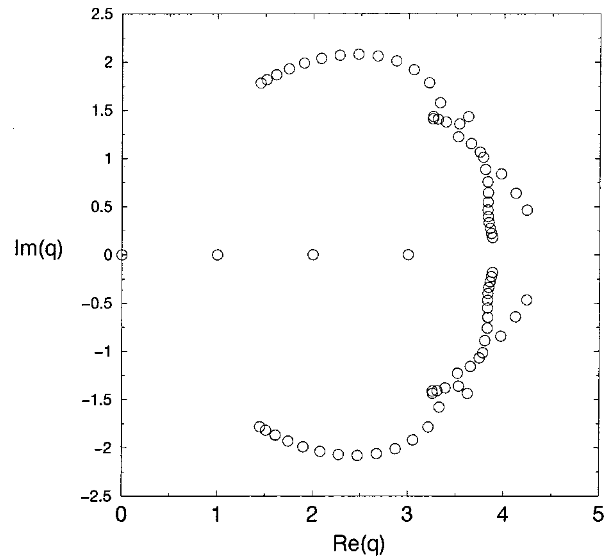

FIG. 3. Chromatic zeros for the $4\times L_x$ strip of the sq_d lattice with free boundary conditions and $L_x=20$ (i.e., $n=80$).

so that no q_c is defined. The region R_1 is the entire q plane, with the exception of the arcs lying on $\mathcal{B}$.

C. $L_y=4$

Here we find $d_{\mathcal{D}}=4$, $d_{\mathcal{N}}=3$. Again using the shorthand notation sq_d4o to denote this open strip of the sq_d lattice with $L_y=4$ we have

$$b_{\mathrm{sq}_d4o,1}=-q^4+13q^3-68q^2+171q-176, \tag{2.14}$$

$$b_{\mathrm{sq}_d4o,2}=(q-3)\times(2q^5-33q^4+219q^3-729q^2+1214q-803), \tag{2.15}$$

$$b_{\mathrm{sq}_d4o,3}=(q-3)^3(q^5-17q^4+118q^3-420q^2+770q-586), \tag{2.16}$$

$$b_{\mathrm{sq}_d4o,4}=-(q-2)(q-3)^6(q-4). \tag{2.17}$$

For the functions $A_{\mathrm{sq}_d4,o,j}$ in the numerator $\mathcal{N}$, it is convenient to extract a common factor and thus define

$$A_{\mathrm{sq}_d4o,j}=q(q-1)(q-2)(q-3)^3\overline{A}_{\mathrm{sq}_d4o,j}. \tag{2.18}$$

Then

$$\overline{A}_{\mathrm{sq}_d4o,0}=(q-2)^2, \tag{2.19}$$

$$\overline{A}_{\mathrm{sq}_d4o,1}=-(2q^4-21q^3+78q^2-113q+47), \tag{2.20}$$

$$\overline{A}_{\mathrm{sq}_d4o,2}=-(q-3)(q^5-14q^4+77q^3-204q^2+245q-91), \tag{2.21}$$

and

$$\overline{A}_{\mathrm{sq}_d4o,3}=(q-1)^2(q-3)^3(q-4). \tag{2.22}$$

Let us write the denominator as

$$\mathcal{D}_{\mathrm{sq}_d4o}=\prod_{j=1}^{4}(1-\lambda_{\mathrm{sq}_d4o,j}x). \tag{2.23}$$

Then

$$W=(\lambda_{\mathrm{sq}_d4o,j,\max})^{1/4} \quad \text{for} \quad q\in R_1, \tag{2.24}$$

where $\lambda_{\mathrm{sq}_d4o,j,\max}$ is the $\lambda_{\mathrm{sq}_d4o,j}$ in Eq. (2.23) with maximal magnitude in this region.

Chromatic zeros are shown in Fig. 3 for $L_x=20$, i.e., $n=80$. For this great a length, these chromatic zeros give a reasonably good approximation to the asymptotic locus $\mathcal{B}$. As is evident from this figure, $\mathcal{B}$ does not cross the real q axis, so that no q_c is defined.

III. STRIPS WITH $[\mathrm{FBC}_y,(T)\mathrm{PBC}_x]$

A. $L_y=2$

The chromatic polynomial for the $L_y=1$ cyclic strip of the sq_d lattice was given above in Eqs. (1.5) and (1.6). Here we consider the $L_y=2$ strip of the sq_d lattice with $(\mathrm{FBC}_y,\mathrm{PBC}_x)$, i.e., cyclic, boundary conditions. For a given value of L_x, this cyclic strip graph is identical to the corresponding strip with Möbius boundary conditions $(\mathrm{FBC}_y,(T)\mathrm{PBC}_x)$:

$$G(\mathrm{sq}_d,L_y=2,L_x,\mathrm{FBC}_y,\mathrm{PBC}_x) =G(\mathrm{sq}_d,L_y=2,L_x,\mathrm{FBC}_y,T\mathrm{PBC}_x). \tag{3.1}$$

This can be proved by calculating the adjacency matrices for the cyclic and Möbius strips, which are identical. [Here the adjacency matrix of an n-vertex graph is the $n\times n$ matrix A with A_{ij} equal to the number of bonds (edges) that connect the ith and jth vertices. The adjacency matrix fully defines the graph.] Because of the identity of the $L_y=2$ cyclic and Möbius strips, we shall refer to them both with the designation $\mathrm{sq}_d(L_y=2)_m$, FBC_y, $(T)\mathrm{PBC}_x$. For the general cyclic-strip of the sq_d strip, with $L_x \geq 4$ to avoid degenerate cases, the chromatic number is given by

$$\chi(\mathrm{sq}_d, L_y, L_x, \mathrm{FBC}_y, \mathrm{PBC}_x) = \begin{cases} 4 & \text{if } L_x \text{ is even} \\ 5 & \text{if } L_x \text{ is odd} \end{cases}. \tag{3.2}$$

For the present $L_y=2$ cyclic/Möbius strips, the degenerate cases are as follows: for $L_x=2$, the strip reduces to K_4 while for $L_x=3$ it reduces to K_6, with $\chi(K_p)=p$.

The chromatic polynomial for the cyclic strip of the sq_d lattice with $L_y=2$ and $L_x \equiv m$ is [20]

$$P[\mathrm{sq}_d\{(L_y=2),\mathrm{FBC}_y,(T)\mathrm{PBC}_x\}_m,q] = \frac{1}{2}q(q-3)2^m + [(q-2)(q-3)]^m + (q-1)[2(3-q)]^m. \tag{3.3}$$

We determine the boundary $\mathcal{B}$ to be the union of a circle centered at $q=2$ with radius 2 and a circle centered at $q=3$ with radius 1:

$$\mathcal{B}:\{|q-2|=2\} \cup \{|q-3|=1\}. \tag{3.4}$$

These two circles osculate (i.e., intersect with equal tangents) at q_c, where

$$q_c[\mathrm{sq}_d(L_y=2),\mathrm{FBC}_y,(T)\mathrm{PBC}_x]=4. \tag{3.5}$$

In the terminology of algebraic geometry, this point q_c is thus a tacnode.

This locus is shown in Fig. 4. The locus $\mathcal{B}$ separates the q plane into three regions: (i) the outermost region R_1, which is the exterior of the larger circle, $|q-2| \geq 2$ and which thus includes the real intervals $q \geq 4$ and $q \leq 0$, (ii) region R_2, which is the interior of the smaller circle, $|q-3| \leq 1$ and includes the real interval $2 \leq q \leq 4$, and (iii) region R_3, which is the interior of the larger circle $|q-2| \leq 2$ minus the smaller disk $|q-3|=1$ and includes the real interval $0 \leq q \leq 2$. Thus, $\mathcal{B}$ crosses the real q axis at $q=0,2,4$ and $q_c=4$. As is evident in Fig. 4, the chromatic zeros lie near to the asymptotic locus $\mathcal{B}$. In the various regions

$$W=[(q-2)(q-3)]^{1/2} \quad \text{for} \quad q \in R_1, \tag{3.6}$$

$$|W|=2^{1/2} \quad \text{for} \quad q \in R_2, \tag{3.7}$$

$$|W|=|2(q-3)|^{1/2} \quad \text{for} \quad q \in R_3 \tag{3.8}$$

(for q in regions other than R_1, only the magnitude $|W(q)|$ can be determined unambiguously).

We define the sum of the coefficients as

$$C(G)=\sum_{j=1}^{N_{\lambda_G}} c_{G,j}. \tag{3.9}$$

For sufficiently large positive integer q, the coefficient $c_{G,j}$ in Eq. (3.9) can be interpreted as the multiplicity of the corresponding eigenvalue $\lambda_{G,j}$ of the coloring matrix, i.e., the dimension of the corresponding invariant subspace in the full space of coloring configurations [15,24,38]. We recall that the coloring matrix can be defined as the matrix whose i,j element is 1 (0) if the coloring configurations on two adjacent transverse slices of the strip are compatible (incompatible). Thus, in the absence of zero eigenvalues of the coloring matrix, $C(G)$ is the dimension of the space of coloring configurations of such a transverse slice. For the cyclic strip graphs of the sq_d lattice, the transverse slice is the line graph L_n of length L_y vertices, so the space of coloring configurations of this transverse slice is

$$P(L_n,q)=P(T_n,q)=q(q-1)^{n-1}. \tag{3.10}$$

In case where the cyclic strip and the Möbius strip of the sq_d lattice are identical, the full coloring matrix automatically takes account of both contributions, so that for each individual strip, corresponding to a given permutation in the identification of vertices at the longitudinal boundary, one must divide by the symmetry factor. In the present case, $L_y=2$ and there are two permutations of the identifications of the boundary conditions that give identical strip graphs, so that this symmetry factor is 1/2! so that

$$C(\mathrm{sq}_d,L_y=2,\mathrm{FBC}_y,\mathrm{PBC}_x)=C(\mathrm{sq}_d,L_y=2,\mathrm{FBC}_y,T\mathrm{PBC}_x) = \frac{1}{2}q(q-1). \tag{3.11}$$

This agrees with the sum of the coefficients in the expression (3.3). A remark that will be relevant later is that if the coloring matrix has a zero eigenvalue of multiplicity c_{zero}, then, since this eigenvalue does not appear in Eq. (1.14), the sum of the coefficients that do appear in the chromatic polyno-

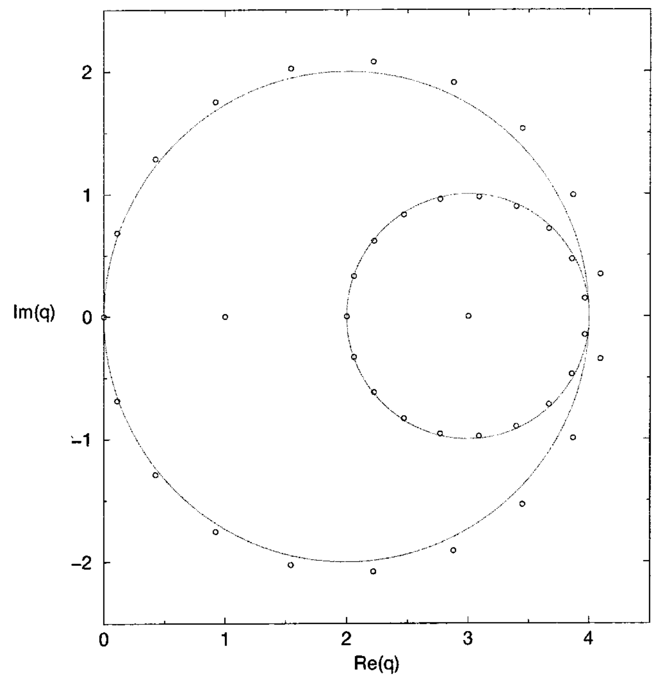

FIG. 4. Locus $\mathcal{B}$ for W for the $2\times\infty$ cyclic or Möbius strip of the sq_d lattice. Chromatic zeros are shown for the case $L_x=20$ (i.e., $n=40$).

mial (1.14) is equal to the full dimension of the space of coloring configurations minus $c_{\rm zero}$.

B. $L_y=3$

We have calculated the chromatic polynomial for the next wider cyclic strip, with $L_y=3$. For this strip the chromatic numbers χ are the same as for the $L_y=2\,{\rm sq}_d$ strip. We find $N_{{\rm sq}_d,L_y=3,cyc,\lambda}=16$ and

$$P[{\rm sq}_d\{(L_y=3),{\rm FBC}_y,{\rm PBC}_x\}_m,q]=\sum_{j=1}^{16} c_{{\rm sq}_d3c,j}(\lambda_{{\rm sq}_d3c,j})^m. \tag{3.12}$$

(The terms $\lambda_{{\rm sq}_d3c,j}$ are the same for cyclic and Möbius longitudinal boundary conditions.) With the $\lambda_{{\rm sq}_d3c,j}$'s ordered according to decreasing degrees of their coefficients for the cyclic strip, we find

$$\lambda_{{\rm sq}_d3c,1}=1, \tag{3.13}$$

$$\lambda_{{\rm sq}_d3c,2}=-2, \tag{3.14}$$

$$\lambda_{{\rm sq}_d3c,3}=-3, \tag{3.15}$$

$$\lambda_{{\rm sq}_d3c,4}=q-3, \tag{3.16}$$

$$\lambda_{{\rm sd}_d3c,5}=-(q-3), \tag{3.17}$$

and

$$\lambda_{{\rm sq}_d3c,(6,7)}=q-4\pm\sqrt{2q^2-14q+25}. \tag{3.18}$$

The terms $\lambda_{{\rm sq}_d3c,j}$, $j=8,9,10$ are the roots of the cubic equation

$$\xi^3-4(q-4)\xi^2+(q^2-10q+17)\xi+2(q-1)(q-3). \tag{3.19}$$

For $j=11$ we have

$$\lambda_{{\rm sq}_d3c,11}=-(q-3)^2. \tag{3.20}$$

The terms $\lambda_{{\rm sq}_d3c,j}$, $j=12$, 13 and 14 are the roots of the cubic equation

$$\xi^3+(2q^2-15q+30)\xi^2-(q-3)^2(q^2-5q+5)\times\xi-2(q-3)^4. \tag{3.21}$$

Finally,

$$\lambda_{{\rm sq}_d3c,(15,16)}=\lambda_{{\rm sq}_d3o,(1,2)}. \tag{3.22}$$

For the coefficients we calculate

$$c_{{\rm sq}_d3c,1}=\frac{1}{6}(q-1)(q-2)(q-3), \tag{3.23}$$

$$c_{{\rm sq}_d3c,2}=\frac{1}{3}(q-2)(q-4), \tag{3.24}$$

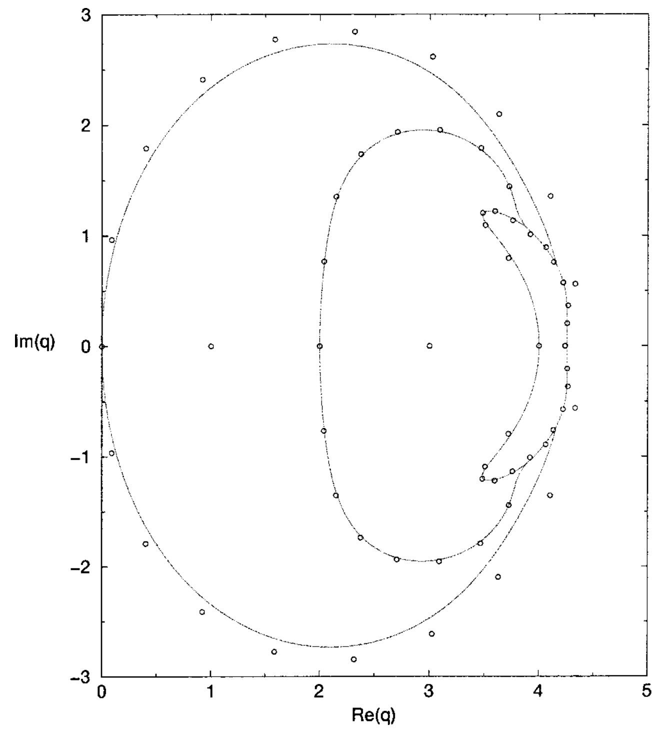

FIG. 5. Locus $\mathcal{B}$ for W for the $3\times\infty$ cyclic or Möbius strip of the ${\rm sq}_d$ lattice. Chromatic zeros are shown for the case $L_x=20$ (i.e., $n=60$).

$$c_{{\rm sq}_d3c,3}=\frac{1}{6}q(q-1)(q-5), \tag{3.25}$$

$$c_{{\rm sq}_d3c,j}=\frac{1}{2}q(q-3) \quad \text{for} \quad j=4,8,9,10, \tag{3.26}$$

$$c_{{\rm sq}_d3c,j}=\frac{1}{2}(q-1)(q-2) \quad \text{for} \quad j=5,6,7, \tag{3.27}$$

$$c_{{\rm sq}_d3c,j}=q-1 \quad \text{for} \quad j=11,12,13,14, \tag{3.28}$$

and

$$c_{{\rm sq}_d3c,j}=1 \quad \text{for} \quad j=15,16. \tag{3.29}$$

Summing the coefficients $c_{{\rm sq}_d3c,j}$, we find

$$C[{\rm sq}_d(L_y=3),{\rm FBC}_y,{\rm PBC}_x]=\frac{1}{6}q(q+1)(4q-7). \tag{3.30}$$

Since for $L_y=3$ the cyclic and Möbius strips of the ${\rm sq}_d$ lattice are distinct, the full sum of eigenvalue multiplicities is equal to Eq. (3.10) with $n=L_y=3$ (without dividing by any symmetry factor). The sum of the coefficients appearing in Eq. (3.12) is less than this quantity, $q(q-1)^2$, by the amount

$$c_{{\rm sq}_d3c,{\rm zero}}=\frac{1}{6}q(2q^2-9q+13), \tag{3.31}$$

which indicates that for this strip the coloring matrix has a zero eigenvalue with this multiplicity.

The boundary $\mathcal{B}$ is shown in Fig. 5. This boundary separates the q plane into four regions. These include (i) the outermost region R_1, which contains the semi-infinite intervals $q > q_c$ and $q < 0$, where q_c is

$$q_c[\mathrm{sq}_d(L_y=3),\mathrm{FBC}_y,\mathrm{PBC}_x]=4.254654... \quad (3.32)$$

(a root of the equation $q^4-14q^3+72q^2-168q+162=0$), (ii) a narrow crescent-shaped region R_2 containing the real interval $4 \le q \le q_c$, (iii) the region R_3 containing the real interval $2 \le q \le 4$, and (iv) the region R_4 containing the real interval $0 \le q \le 2$. Associated with these regions are two complex-conjugate pairs of triple points, as is evident in Fig. 5. Note that q_c is not a tacnode for the ($L_x \to \infty$ limit of the) $L_y=3$ cyclic strip, in contrast to the situation for the corresponding $L_y=2$ cyclic strip.

In the various regions

$$W=(\lambda_{\mathrm{sq}_d 3c,15})^{1/3} \quad \text{for} \quad q \in R_1, \quad (3.33)$$

$$|W|=3^{1/3} \quad \text{for} \quad q \in R_2, \quad (3.34)$$

and

$$|W|=|\lambda_{\mathrm{sq}_d 3c,810m}|^{1/3} \quad \text{for} \quad q \in R_3, \quad (3.35)$$

where $\lambda_{\mathrm{sq}_d 3c,810m}$ denotes the root of the cubic (3.19) of maximal magnitude in R_3, and

$$|W|=|\lambda_{\mathrm{sq}_d 3c,1214m}|^{1/3} \quad \text{for} \quad q \in R_4, \quad (3.36)$$

where $\lambda_{\mathrm{sq}_d 3c,1214m}$ denotes the root of the cubic (3.21) of maximal magnitude in R_4.

IV. STRIPS WITH (PBC$_y$,FBC$_x$)

A. $L_y=3$

For the $L_y=3$, $L_x=m+2$ strip of K_4's forming squares, with (PBC$_y$,FBC$_x$) boundary conditions [for which $n=3(m+2)$] we find

$$P[\mathrm{sq}_d(L_y=3)_m,\mathrm{PBC}_y,\mathrm{FBC}_x,q] = q(q-1)(q-2)[(q-3)(q-4)(q-5)]^{m+1}, \quad (4.1)$$

where

$$W[\mathrm{sq}_d(L_y=3),\mathrm{PBC}_y,\mathrm{FBC}_x,q]=[(q-3)(q-4)(q-5)]^{1/3}. \quad (4.2)$$

The continuous nonanalytic locus $\mathcal{B}=\emptyset$; W has isolated branch point singularities where it vanishes at $q=3$, 4, and 5. Aside from these, R_1 is the full q plane.

B. $L_y=4$

For this case it is again convenient to give our results in terms of a generating function Γ [sq$_d(L_y=4)$,PBC$_y$,FBC$_x$,q,x]. We find $d_{\mathcal{D}}=3$, $d_{\mathcal{N}}=2$, and (using the abbreviation sq$_d$4cyl for this strip)

$$b_{\mathrm{sq}_d 4\mathrm{cyl},1}=-q^4+16q^3-104q^2+316q-372, \quad (4.3)$$

$$b_{\mathrm{sq}_d 4\mathrm{cyl},2}=(q-3)(5q^4-74q^3+422q^2-1100q+1109), \quad (4.4)$$

and

$$b_{\mathrm{sq}_d 4\mathrm{cyl},3}=-(q-2)(q-3)^2(2q^2-16q+33). \quad (4.5)$$

Defining

$$A_{\mathrm{sq}_d 4\mathrm{cyl},j}=q(q-1)(q-2)(q-3)\overline{A}_{\mathrm{sq}_d 4\mathrm{cyl},j} \quad (4.6)$$

we calculate

$$\overline{A}_{\mathrm{sq}_d 4\mathrm{cyl},0}=q^4-14q^3+79q^2-210q+220, \quad (4.7)$$

$$\overline{A}_{\mathrm{sq}_d 4\mathrm{cyl},1}=-(5q^5-79q^4+501q^3-1586q^2+2485q-1513) \quad (4.8)$$

and

$$\overline{A}_{\mathrm{sq}_d 4\mathrm{cyl},2}=(q-3)(q^2-3q+3)(2q^2-16q+33). \quad (4.9)$$

Writing

$$\mathcal{D}_{\mathrm{sq}_d 4\mathrm{cyl}}=\prod_{j=1}^{3}(1-\lambda_{\mathrm{sq}_d 4\mathrm{cyl},j}x) \quad (4.10)$$

we have

$$W=(\lambda_{\mathrm{sq}_d 4\mathrm{cyl},j,\max})^{1/4} \quad \text{for} \quad q \in R_1, \quad (4.11)$$

where $\lambda_{\mathrm{sq}_d 4\mathrm{cyl},j,\max}$ is the $\lambda_{\mathrm{sq}_d 4\mathrm{cyl},j}$ in Eq. (4.10) with maximal magnitude in this region.

Chromatic zeros for the $4 \times L_x$ strip of the sq$_d$ lattice with cylindrical boundary conditions are shown in Fig. 6 for $L_x=20$, i.e., $n=80$. Again, the length L_x is sufficiently great that these give a good idea of the location of the asymptotic curve $\mathcal{B}$. Since $\mathcal{B}$ does not cross the real q axis, there is no q_c for this case.

V. STRIP WITH $L_y=3$ AND [PBC$_y$,(T)PBC$_x$]

We consider here the sq$_d$ strip with $L_y=3$ and torus boundary conditions (PBC$_y$,PBC$_x$). By the same method as mentioned above, e.g., calculating the associated adjacency matrices and showing that they are the same, it follows that for a given L_x, this strip with torus boundary conditions is identical to the corresponding $L_y=3$ strip with Klein bottle boundary conditions (PBC$_y$,TPBC$_x$):

$$G(\mathrm{sq}_d,L_y=3,L_x,\mathrm{PBC}_y,\mathrm{PBC}_x) = G(\mathrm{sq}_d,L_y=3,L_x,\mathrm{PBC}_y,T\mathrm{PBC}_x). \quad (5.1)$$

Since there are 3 vertices on the vertical slice, and hence 3! permutations that yield identical graphs, it follows, as explained above, that the sum of the eigenvalue multiplicities for each individual strip contributes only 1/3! of this total:

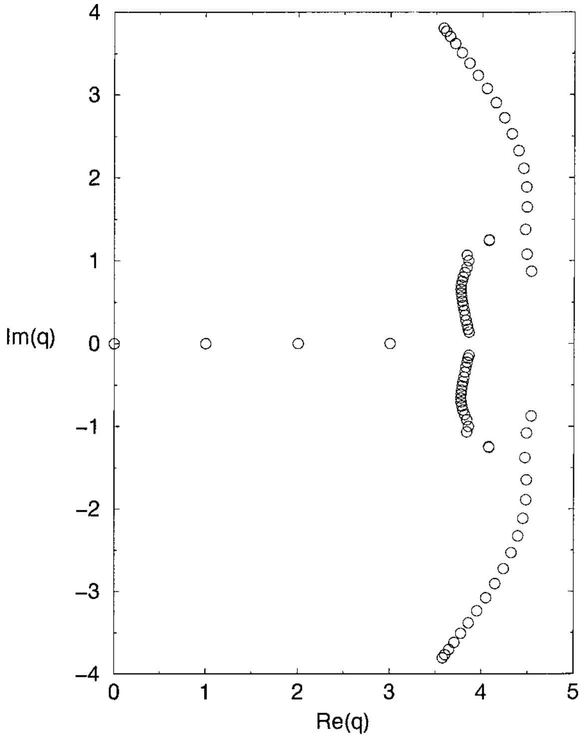

FIG. 6. Chromatic zeros for the $4\times L_x$ cylindrical strip of the sq_d lattice, i.e., with (PBC_y,FBC_x) boundary conditions with $L_x=20$ (i.e., $n=80$ vertices).

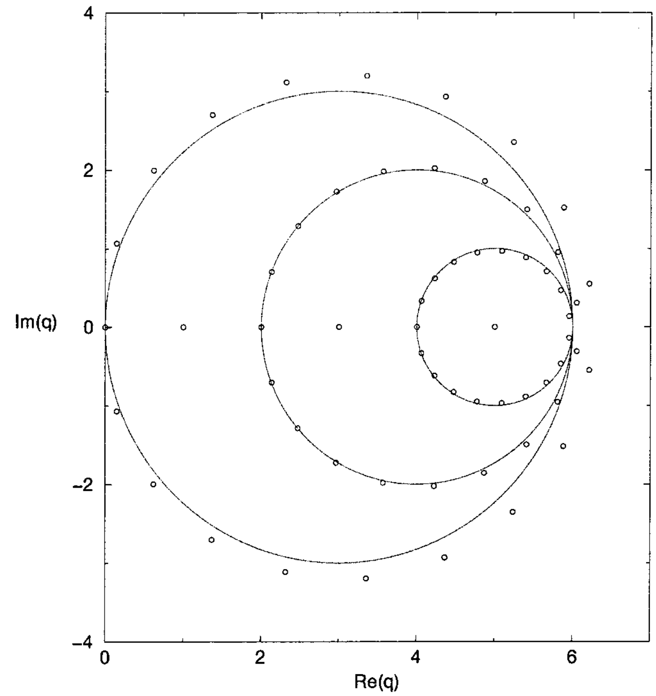

FIG. 7. Locus $\mathcal{B}$ for W for the $3\times\infty$ strip of the sq_d lattice with $[PBC_y,(T)PBC_x]$ = torus or Klein bottle boundary conditions. Chromatic zeros are shown for the case $L_x=20$ (i.e., $n=60$).

$$C[sq_d,L_y=3,PBC_y,(T)PBC_x] = \frac{1}{3!}P(C_3,q)=\frac{1}{6}q(q-1)(q-2). \tag{5.2}$$

These strips have the chromatic number

$$\chi[sq_d(L_y=3)_m,PBC_y,(T)PBC_x]=\begin{cases}6 & \text{for even } m\geq 4\\ 7 & \text{for odd } m\geq 7\end{cases}. \tag{5.3}$$

For $m=2$ and $m=3$, the $L_y=3$ sq_d torus strip degenerates to K_6 and K_9, respectively, with $\chi(K_p)=p$ as before; for $m=5$ this strip has $\chi=8$. The fact that the values of χ for the $L_y=3$ torus strip of the sq_d lattice in Eq. (5.3) and the special cases noted are larger than the value $\chi=4$ for the infinite 2D sq_d lattice can be ascribed in part to the constraints arising from the small girth of the triangular transverse cross section of these strips.

We calculate the chromatic polynomial by iterated use of the deletion-contraction theorem, via a generating function approach [29,30]. From this we obtain the chromatic polynomial in the form (1.14) via the general formulas in Ref. [30] and obtain

$$\begin{aligned}P[sq_d(L_y=3)_m,PBC_y,(T)PBC_x,q] &= \frac{1}{6}q(q-1)(q-5)(-6)^m+\frac{1}{2}q(q-3)[6(q-5)]^m\\ &\quad +(q-1)[-3(q-4)(q-5)]^m\\ &\quad +[(q-3)(q-4)(q-5)]^m.\end{aligned} \tag{5.4}$$

Thus, $N_\lambda=4$ for this strip. The labeling of the coefficients c_j and terms λ_j in Eq. (5.4) is consecutive. Explicitly calculating the sum of the coefficients in the chromatic polynomial (5.4), one sees that the result agrees with Eq. (5.2). It is interesting that the coefficients that occur in Eq. (5.4) are the same as a subset of the coefficients that occur in the chromatic polynomial for the $L_y=3$ cyclic strip. We find that the degrees in x of the numerator and denominator of the generating function for this strip graphs are 2 and 4, so that all of the λ_j's in $d_{\mathcal{D}}=4$ contribute to P.

The nonanalytic locus (boundary) $\mathcal{B}$ is shown in Fig. 7 and consists of three circles that osculate at q_c, where

$$q_c[sq_d(L_y=3),PBC_y,(T)PBC_x]=6, \tag{5.5}$$

namely,

$$\mathcal{B}:\{|q-3|=3\}\cup\{|q-4|=2\}\cup\{|q-5|=1\}. \tag{5.6}$$

Thus, as was true for the $L_y=2$ cyclic strip, q_c is a tacnode. Evidently, $\mathcal{B}$ crosses the real axis at $q=0$, 2, and 4 as well as at q_c. This locus $\mathcal{B}$ divides the q plane into four regions: (i) the outermost region R_1, including the real intervals $q\geq 6$ and $q\leq 0$, (ii) region R_2, the interior of the smallest circle, $|q=5|=1$, containing the real interval $4\leq q\leq 6$, (iii) region R_3, the interior of the circle $|q-4|=2$ minus the disk $|q-5|=1$ comprising R_2 and including the real interval $2\leq q\leq 4$, and (iv) region R_4, the interior of the largest circle, $|q-3|=3$ minus the disk $|q-4|=2$ and including the real interval $0\leq q\leq 2$. We have

$$W=[(q-3)(q-4)(q-5)]^{1/3} \quad \text{for} \quad q\in R_1. \tag{5.7}$$

The fact that this coincides with the W calculated for the corresponding strip with (PBC_y,FBC_x) [see Eq. (4.2)] is a general result [35,39,41]. For the other regions we have

$$|W| = 6^{1/3} \quad \text{for} \quad q \in R_2, \tag{5.8}$$

$$|W| = |6(q-5)|^{1/3} \quad \text{for} \quad q \in R_3, \tag{5.9}$$

and

$$|W| = |3(q-4)(q-5)|^{1/3} \quad \text{for} \quad q \in R_4. \tag{5.10}$$

Evidently, for all of these strips, the locus $\mathcal{B}$ has support for $\mathrm{Re}(q) \geqslant 0$.

It is of interest to comment further on the q_c values for (the $L_x \to \infty$ limits of) these strips of the sq_d lattice. In our previous exact calculations of chromatic polynomials for various strip graphs of regular lattices and the resultant W functions for their $L_x \to \infty$ limits, it was found that if one uses free transverse boundary conditions and periodic longitudinal boundary conditions, the value of q_c for a given family is a nondecreasing function of L_y. Our results for the strips of the sq_d lattice exhibit the same behavior. Hence, our finding that $q_c \simeq 4.25$ for the ($L_x \to \infty$ limit of the) $L_y = 3$ cyclic/Möbius strip graph suggests that q_c for the infinite 2D sq_d lattice, which we denote $q_c(sq_d)$, is greater than 4.25. Note that we cannot use our finding that $q_c = 6$ for the $L_x \to \infty$ limit of the $L_y = 3$ torus/Klein bottle graph of the sq_d lattice to suggest that $q_c(sq_d)$ might be 6 because we have previously obtained exact solutions for W that show that q_c is not, in general, a nondecreasing function of L_y on strip graphs with periodic transverse boundary conditions [29,45]. For example, from exact results, we have found that for the $L_x \to \infty$ limit of strips of the triangular lattice with cylindrical boundary condition (PBC_y,FBC_x), $q_c = 4$ for $L_y = 4$ [29], while $q_c \simeq 3.28$ for $L_y = 5$ and $q_c \simeq 3.25$ for $L_y = 6$ [45]. For the square, triangular, and sq_d lattices, constructed, say, as the L_x, $L_y \to \infty$ limits of open rectangular sections, one has the chromatic numbers $\chi = 2$, 3, and 4, respectively. Now the Potts antiferromagnet has a zero-temperature critical point at $q = 3$ on the square lattice [6,17,18] and at $q = 4$ on the triangular lattice [19], respectively (which should be independent of boundary conditions used in taking the thermodynamic limit), corresponding to the values $q_c(\mathrm{sq}) = 3$ and $q_c(\mathrm{tri}) = 4$. These results are consistent with the possibility that $q_c(sq_d) = 5$, i.e., the possibility that the $q = 5$ Potts antiferromagnet has a $T = 0$ critical point on the sq_d lattice. However, there is not a 1-1 correspondence between chromatic number and q_c; for example, the Kagomé lattice (again constructed, say, as the limit of a finite section with free transverse and longitudinal boundary conditions) has $\chi = 3$ like the triangular lattice, but $q_c = 3$, in contrast to the $q_c = 4$ value for the triangular lattice. If, indeed, $q_c(sq_d) = 5$, this would also mean that q_c for an infinite-length, finite-width strip could be larger than q_c for the full infinite lattice since we have obtained $q_c = 6$ in Eq. (5.5) from our exact solution for the chromatic polynomial for the strip with torus boundary conditions above.

VI. RIGOROUS LOWER BOUNDS ON *W* AND APPROACH TO THE INFINITE-WIDTH LIMIT

Here we present rigorous lower bounds on W for strip graphs and show that these are very close to the actual values obtained from our exact solutions and hence serve as very good approximations to the actual W functions. Using our exact solutions and these approximations, we then determine how, for a given q, the values of W for the infinite-length, finite-width strips approach the value for the infinite 2D sq_d lattice as the strip width L_y gets large.

As discussed in Refs. [39] and [41], a general result for a given type of strip graph G_s is

$$\begin{aligned} &W[G_s(L_y), BC_y, FBC_x, q] \\ &\quad = W[G_s(L_y), BC_y, PBC_x, q] \\ &\quad \quad \text{for } q \geqslant q_c[G_s(L_y), BC_y, PBC_x], \end{aligned} \tag{6.1}$$

where $BC_y = FBC_y$ or PBC_y. Hence, for example, $W[sq_d(L_y=2), FBC_y, FBC_x, q] = W[sq_d(L_y=2), FBC_y, PBC_x, q]$ for $q \geqslant 4$ and

$$\begin{aligned} &W[sq_d(L_y=3), PBC_y, FBC_x, q] \\ &\quad = W[sq_d(L_y=3), PBC_y, PBC_x, q] \quad \text{for} \quad q \geqslant 6. \end{aligned} \tag{6.2}$$

We recall that, using coloring matrix methods [15], Tsai and one of us (R.S.) previously derived rigorous upper and lower bounds on W for various 2D lattices [24–26]. It was found that the lower bounds W_{lb} were actually very good approximations to the actual W values, as determined, e.g., by Monte Carlo simulations. This was also seen analytically from the property that the large-q Taylor series expansions of $q^{-1}W$ and $q^{-1}W_{lb}$ coincided to several orders beyond the first term, which is unity. The lower bound (1.9) was derived as part of this paper. As noted above, this bound agrees very well with the actual values of W, as determined via Monte Carlo measurements (see Table III of [25]).

Using the same methods, we can obtain a lower bound on W for the sq_d strips of interest here. Here we restrict to $q \geqslant 6$. For the case of free transverse boundary conditions and either free or periodic longitudinal boundary conditions we obtain the lower bound

$$W[sq_d(L_y), FBC_y, BC_x, q] \geqslant \frac{[(q-2)(q-3)]^{1-1/L_y}}{(q-1)^{1-2/L_y}}. \tag{6.3}$$

For the sq_d strips with periodic transverse boundary conditions and either free or periodic longitudinal boundary conditions, we obtain the lower bound

$$W[sq_d(L_y), PBC_y, BC_x, q] \geqslant A^{1/L_y}, \tag{6.4}$$

where

$$A = \frac{(q/2)(q-3)2^{L_y} + [(q-2)(q-3)]^{L_y} + (q-1)[2(3-q)]^{L_y}}{(q-1)^{L_y} + (q-1)(-1)^{L_y}}. \tag{6.5}$$

TABLE I. Values of W for infinite-length, finite-width strips of the sq_d lattice with free transverse boundary conditions, as functions of q, from evaluation of our exact solutions. For each pair of values of L_y and q, the upper entry is the value of W from the exact solution and the lower entry is the ratio R_{WF}.

q \ L_y	6	7	8	9	10
2	3.464	4.472	5.477	6.481	7.483
	1	1	1	1	1
3	3.083	4.066	5.055	6.047	7.0415
	1.006	1.003	1.002	1.001	1.001
4	2.909	3.878	4.857	5.842	6.831
	1.009	1.004	1.002	1.0015	1.001

Evidently, for large q, the lower bound (6.4) with Eq. (6.5) goes over to Eq. (1.9) for the infinite lattice.

In Table I, we compare the values of W for $6 \leqslant q \leqslant 10$ from exact solutions for the $L_y = 2,3,4$ open strips with the respective lower bound (1.9). For each pair of values of L_y and q, the upper entry is the value of W from the exact solution and the lower entry is the ratio

$$R_{WF} = \frac{W[\mathrm{sq}_d(L_y),\mathrm{FBC}_y,\mathrm{BC}_x,q]}{W[\mathrm{sq}_d(L_y),\mathrm{FBC}_y,\mathrm{BC}_x,q]_{lb}}, \qquad (6.6)$$

where $W[\mathrm{sq}_d(L_y),\mathrm{FBC}_y,\mathrm{BC}_x,q]_{lb}$ is the lower bound (lb) given by the right-hand side of Eq. (6.3) and the numerator and denominator are independent of the boundary conditions in the longitudinal direction. The bound is identical to the exact expression for W for $L_y = 2$ and is very close for $L_y = 3$ and $L_y = 4$. Thus, just as was found in our earlier work with Tsai [24–26], the lower bound is not just a bound but also a very accurate approximation to the exact value of W, especially for moderate and large q. Having confirmed this again for the present type of strip graphs, we use this approximation to study the approach to the infinite-width limit, i.e., the full infinite 2D sq_d lattice. In Table II we show values of W for $6 \leqslant q \leqslant 10$ and widths $2 \leqslant L_y \leqslant 10$, as compared with the values for $L_y = \infty$, i.e., for the full 2D sq_d lattice. For each pair of values L_y and q, the upper entry is the value of W and the lower entry is the ratio of this value divided by the corresponding value of W for the 2D sq_d lattice. For $L_y = 2,3,4$, the values of W are from evaluations of the exact solutions, while for L_y from 5 to 10 they are from the approximation provided by Eq. (6.3) and for $L_y = \infty$ they are from the Monte Carlo measurements given in Ref. [25]. One sees that for a fixed L_y, the value of W on the infinite-length strip approaches that for the 2D lattice as q increases. Clearly, for fixed q, the value of W for the infinite-length strip approaches the value for the 2D lattice as L_y increases, and Table II provides a quantitative picture of this approach; for example, for $L_y = 10$ and a moderate value of q such as 7 or 8, the W values are within several percent of their 2D lattice values. We recall that this approach for this type of strip with free transverse boundary conditions was proved to be monotonic in Ref. [31].

We next study the approach of the values of W on strips of the sq_d lattice with periodic transverse boundary conditions to their values for the infinite 2D sq_d lattice. In Table III, we compare the values of W for $6 \leqslant q \leqslant 10$ from our exact solutions for the $L_y = 3,4$ cylindrical strips with the respective lower bound (6.4) with Eq. (6.5). For each pair of values of L_y and q, the upper entry is the value of W from the exact solution and the lower entry is the ratio

$$R_{WP} = \frac{W[\mathrm{sq}_d(L_y),\mathrm{PBC}_y,\mathrm{BC}_x,q]}{W[\mathrm{sq}_d(L_y),\mathrm{PBC}_y,\mathrm{BC}_x,q]_{lb}}, \qquad (6.7)$$

where $W[\mathrm{sq}_d(L_y),\mathrm{PBC}_y,\mathrm{BC}_x,q]_{lb}$ is the lower bound (lb) given by the right-hand side of Eq. (6.4) with Eq. (6.5) and the numerator and denominator are independent of the boundary conditions in the longitudinal direction. The bound is identical to the exact expression for W for $L_y = 3$ and is

TABLE II. Values of W for infinite-length, width L_y strips of the sq_d lattice with $(\mathrm{FBC}_y,\mathrm{BC}_x)$, as functions of q, compared with the corresponding values for the infinite 2D sq_d lattice. For each value of L_y and q, the upper entry is the value of W and the lower entry is the ratio of this value divided by $W(\mathrm{sq}_d,q)$ for the 2D sq_d lattice. For $L_y = 2,3,4$, the values of W are taken from the exact solutions; for $5 \leqslant L_y \leqslant 10$ the values are from Eq. (6.3).

q \ L_y	6	7	8	9	10
2	3.46	4.47	5.48	6.48	7.48
	1.42	1.33	1.27	1.23	1.20
3	3.08	4.07	5.055	6.05	7.04
	1.26	1.21	1.17	1.15	1.13
4	2.91	3.88	4.86	5.84	6.83
	1.19	1.15	1.13	1.11	1.10
5	2.78	3.75	4.73	5.71	6.70
	1.14	1.11	1.10	1.08	1.07
6	2.71	3.68	4.65	5.63	6.62
	1.11	1.09	1.08	1.07	1.06
7	2.665	3.625	4.60	5.58	6.56
	1.09	1.08	1.07	1.06	1.05
8	2.63	3.59	4.56	5.53	6.52
	1.075	1.07	1.06	1.05	1.04
9	2.60	3.56	4.53	5.50	6.48
	1.06	1.06	1.05	1.04	1.04
10	2.58	3.535	4.50	5.48	6.46
	1.06	1.05	1.04	1.04	1.04
∞	2.45	3.37	4.31	5.27	6.24
	1	1	1	1	1

TABLE III. Values of W for infinite-length, finite-width strips of the sq_d lattice with periodic transverse boundary conditions, as functions of q, from evaluation of our exact solutions. For each pair of values of L_y and q, the upper entry is the value of W from the exact solution and the lower entry is the ratio R_{WP}.

q \ L_y	6	7	8	9	10
3	1.817	2.8845	3.915	4.932	5.944
	1	1	1	1	1
4	2.629	3.5005	4.412	5.348	6.300
	1.024	1.014	1.009	1.006	1.004

TABLE IV. Values of W for infinite-length, width L_y strips of the sq$_d$ lattice with (PBC$_y$,BC$_x$), as functions of q, compared with the corresponding values for the infinite 2D sq$_d$ lattice. For each value of L_y and q, the upper entry is the value of W and the lower entry is the ratio of this value divided by $W(\mathrm{sq}_d,q)$ for the 2D sq$_d$ lattice. For $L_y=3,4$, the values of W are taken from the exact solutions; for $5\leqslant L_y \leqslant 10$ the values are from Eq. (6.4) with Eq. (6.5).

q \ L_y	6	7	8	9	10
3	1.82	2.88	3.91	4.93	5.94
	0.743	0.857	0.908	0.936	0.953
4	2.63	3.50	4.41	5.35	6.30
	1.07	1.04	1.02	1.015	1.01
5	2.32	3.29	4.26	5.23	6.21
	0.949	0.978	0.989	0.994	0.996
6	2.43	3.35	4.29	5.25	6.22
	0.994	0.994	0.996	0.997	0.998
7	2.39	3.33	4.28	5.25	6.22
	0.976	0.989	0.994	0.996	0.998
8	2.41	3.33	4.29	5.25	6.22
	0.984	0.991	0.995	0.997	0.998
9	2.40	3.33	4.29	5.25	6.22
	0.980	0.990	0.994	0.997	0.998
10	2.40	3.33	4.29	5.25	6.22
	0.982	0.990	0.995	0.997	0.998
∞	2.45	3.37	4.31	5.27	6.24
	1	1	1	1	1

TABLE V. Properties of P, W, and $\mathcal{B}$ for strip graphs G_s of the sq$_d$ lattice. The properties apply for a given strip of type G_s of size $L_y \times L_x$; some apply for arbitrary L_x, such as N_λ, while others apply for the infinite-length limit, such as the properties of the locus $\mathcal{B}$. For the boundary conditions in the y and x directions (BC$_y$,BC$_x$), F, P, and T denote free, periodic, and orientation-reversed (twisted) periodic, and the notation (T)P means that the results apply for either periodic or orientation-reversed periodic. The column denoted Eqs. describe the numbers and degrees of the algebraic equations giving the $\lambda_{G_s,j}$; for example {6(1), 2(2), 2(3)} means that there are six linear equations, two quadratic equations and two cubic equations. The column denoted BCR lists the points at which $\mathcal{B}$ crosses the real q axis; the largest of these is q_c for the given family G_s. The notation ''none'' in this column indicates that $\mathcal{B}$ does not cross the real q axis. The column labeled ''SN'' refers to whether $\mathcal{B}$ has support for negative Re(q), indicated as yes (y) or no (n).

L_y	BC$_y$	BC$_x$	N_λ	Eqs.	BCR	SN
1	F	F	1	{1(1)}	none	n
2	F	F	1	{1(1)}	none	n
3	F	F	2	{1(2)}	none	n
4	F	F	4	{1(4)}	none	n
1	F	(T)P	4	{2(1),1(2)}	0, 2, 3	n
2	F	(T)P	3	{3(1)}	0, 2, 4	n
3	F	(T)P	16	{6(1),2(2),2(3)}	0, 2, 4, 4.25	n
3	P	F	1	{1(1)}	none	n
4	P	F	3	{1(3)}	none	n
3	P	(T)P	4	{4(1)}	0, 2, 4, 6	n

very close for $L_y=4$. Hence, as was the case for the open strip of the sq$_d$ lattice, the lower bound is not just a bound but also a very accurate approximation to the exact value of W, especially for moderate and large q. Having established this, we use this approximation to study the approach to the infinite-width limit, i.e., the full infinite 2D sq$_d$ lattice. In Table IV we show values of W for $6\leqslant q \leqslant 10$ and widths $3 \leqslant L_y \leqslant 10$, as compared with the values for $L_y=\infty$, i.e., for the full 2D sq$_d$ lattice. For each pair of values L_y and q, the upper entry is the value of W for the infinite cylindrical or torus strip and the lower entry is the ratio of this value divided by the corresponding value of W for the 2D sq$_d$ lattice. For $L_y=3,4$, the values of W are from evaluations of the exact solutions, while for L_y from 5 to 10 they are from the approximation provided by bound (6.4) with (6.5) and for $L_y=\infty$ they are from the Monte Carlo measurements given in Ref. [25]. One sees that for a fixed L_y, the value of W on the infinite-length strip approaches that for the 2D lattice as q increases. Also, for fixed q, the value of W for the infinite-length strip approaches the value for the 2D lattice as L_y increases. In Ref. [31] it was shown that this approach is nonmonotonic for strips of the square and triangular lattice with periodic transverse boundary conditions and the same is true here. The approach of the values of W for the infinite-length finite-width strips to their respective values for the infinite sq$_d$ lattice is more rapid for the case of periodic transverse boundary conditions than free transverse boundary conditions. This is similar to what was found in Ref. [31] and is due to the fact that periodic transverse boundary conditions minimize finite-size artifacts. Quantitatively, for a moderate value of the width, such as $L_y=6$, and $q\sim 8$, W is already within a few parts per thousand of its infinite 2D lattice value.

One can also compare the results for W with those on the square and triangular lattices; this comparison shows the effect of the addition of a single diagonal bond to each square to go from the square to the triangular lattice, and then the addition of a second opposite diagonal bond to each square to go from the triangular to sq$_d$ lattice. This was done before in Refs. [12,24] and [25].

VII. ZERO-TEMPERATURE CRITICAL POINTS

We summarize some of the results obtained in this paper in Table V. Note that the $L_y=1$ strips of the sq$_d$ lattice are equivalent to $L_y=2$ strips of the triangular lattice, as discussed above. At the value of q where the nonanalytic locus $\mathcal{B}$ crosses the positive real axis, the q-state Potts antiferromagnet has a zero-temperature critical point [41,44,45]. From the exact solutions for the chromatic polynomials and W functions, we thus conclude that the $q=2$ Potts (Ising) antiferromagnet has a $T=0$ critical point on the $L_x\to\infty$ limits of the cyclic/Möbius strips with $L_y=2$ and $L_y=3$ as well as the $L_y=3$ strip with torus (equivalently Klein bottle) boundary conditions. Note that this involves frustration owing to the nonbipartite nature of these graphs. As is generic for a $T=0$ critical point, the critical singularities are essential, rather than algebraic singularities, as we have verified from an explicit transfer-matrix calculation. The use of strip graphs with periodic or twisted periodic longitudinal boundary conditions is useful since the crossings of $\mathcal{B}$ on the real q axis signal the presence of $T=0$ critical points for the Potts antiferromagnet at these values of q. Just as was the case with the square and triangular strips, for which the Ising antiferromagnet also has a $T=0$ critical point [35,41,44,45], if one uses free longitudinal boundary conditions, $\mathcal{B}$ does not, in general, cross the positive real axis at $q=2$. This difference is associated with the noncommutativity in the definition of W, as discussed before [12,41,44,45]. We also find, for both the cyclic/Möbius strips and the torus/Klein bottle strips for which we have calculated exact solutions for W, in the nondegenerate cases $L_y \geqslant 2$, that the q-state Potts antiferromagnet has a $T=0$ critical point at $q=4$. Since the $L_x \to \infty$ limit of the cyclic/Möbius strips can be carried out with increasing even values of L_x, for which the chromatic number is 4, this zero-temperature critical point is unfrustrated for these strips. In contrast, for the $L_x \to \infty$ limit of the torus/Klein bottle strip, since min(χ)=6, it is frustrated. Finally, there is formally a similar critical point at $q=0$.

VIII. CONCLUSIONS

In this paper we have presented exact calculations of the zero-temperature partition function (chromatic polynomial) and $W(q)$, the exponent of the ground-state entropy, for the q-state Potts antiferromagnet with next-nearest-neighbor spin-spin couplings on strips of the square lattice strips (equivalently, the nearest-neighbor Potts model on strips of the sq$_d$ lattice) with width $L_y=3$ and $L_y=4$ vertices and arbitrarily great length L_x vertices. Both free and periodic boundary conditions are considered. In the $L_x \to \infty$ limit, the resultant W function was calculated. By comparing the values of the exact W functions thus obtained for strips with various widths and boundary conditions versus numerical measurements of W for the full 2D sq$_d$ lattice, we evaluated the effects of the next-neighbor spin-spin couplings. We showed that the $q=2$ (Ising) and $q=4$ Potts antiferromagnets have zero-temperature critical points on the $L_x \to \infty$ limits of the strips that we studied. With the generalization of q from $\mathbb{Z}_+$ to $\mathbb{C}$, we also determined the analytic structure of $W(q)$ in the q plane.

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APPENDIX

A. A reduction theorem

Consider a strip of a given width and length, made up of squares such that the four vertices of each square are connected to form a complete graph K_r (so that there are $r-4$ vertices outside of the strip) with some set of boundary conditions (BC). We shall denote this strip temporarily as $G_{\mathrm{sq},k_r,\mathrm{BC}}$. We first show that the chromatic polynomial for this graph can easily be expressed in terms of the chromatic polynomial for the corresponding graph with the vertices of each square forming a K_4, i.e., such that the two diagonally opposite vertices of each square are connected by an edge. For this purpose we use the intersection theorem from graph theory; this states that a graph G can be expressed as the union of two subgraphs $G=G_1 \cup G_2$ such that the intersection of these subgraphs is a complete graph, $G_1 \cap G_2 = K_j$ for some j, then $P(G,q)=P(G_1,q)P(G_2,q)/P(K_j,q)$. Applying this theorem to each square of the above strip, we have

$$P(G_{\mathrm{sq},K_r,\mathrm{BC}},q)=\left(\frac{q^{(r)}}{q^{(4)}}\right)^{N_4} P(G_{\mathrm{sq},K_4,\mathrm{BC}},q) = \left[\prod_{j=4}^{r-1}(q-j)\right]^{N_4} P(G_{\mathrm{sq},K_4,\mathrm{BC}},q) \quad \text{(A1)}$$

where N_4 denotes the number of squares on the strip and we use the standard notation from combinatorics for the ''falling factorial,''

$$q^{(s)} \equiv \prod_{j=0}^{s-1}(q-j). \quad \text{(A2)}$$

Our results in the text thus also apply to lattices comprised of squares such that the four vertices of each square form a K_r with $r>4$.

B. (K_r,K_s) Strips

We discuss here a strip of tK_r subgraphs, connected such that successive K_r subgraphs intersect on a K_s subgraph, with $1 \leqslant s \leqslant r-1$, with some longitudinal boundary conditions imposed. A member of this general family may be labeled as $(K_r,K_s,t,\mathrm{BC}_x)$. Two of the simplest longitudinal boundary conditions to impose are free and cyclic, which we shall denote as FBC$_x$ and PBC$_x$. The general $(K_r,\ K_s,\ t=m,\ \mathrm{FBC}_x)$ graph has $n=(r-s)m+s$ vertices.

One simple set of families is the cyclic strip $(K_r,\ K_1,\ t=m,\ \mathrm{PBC}_x)$. These may think of these graphs as being formed by starting with a circuit graph, C_m and gluing to each edge one edge of a complete graph K_r. For these we find

$$P[(K_r,K_1,m,\mathrm{PBC}_x),q]=\left(\frac{q^{(r)}}{q^{(2)}}\right)P(C_m,q) = \left[\prod_{j=2}^{r-1}(q-j)\right]^m P(C_m,q), \quad \text{(A3)}$$

where $P(C_m,q)$ is the chromatic polynomial for the circuit graph with m vertices, given in the introduction.

Another interesting family is the open strip $(K_r,K_s,m,\mathrm{FBC}_x)$. We calculate

$$P[(K_r,K_s,m,\mathrm{FBC}_x),q]=q^{(s)}\left(\frac{q^{(r)}}{q^{(s)}}\right)^m = q^{(s)}\left[\prod_{j=s}^{r-1}(q-j)\right]^m. \quad \text{(A4)}$$

Hence, in the $m \to \infty$ limit,

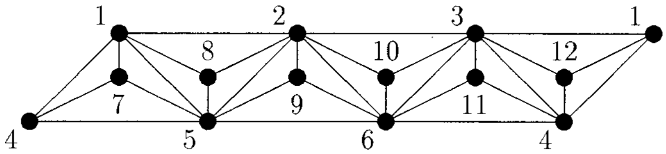

FIG. 8. Illustrative strip graph comprised of K_4 subgraphs intersecting on common edges (K_2's), of a type different than that shown in Fig. 1(a).

$$W=\left(\frac{q^{(r)}}{q^{(s)}}\right)^{1/(r-s)}=\left[\prod_{j=s}^{r-1}(q-j)\right]^{1/(r-s)} \tag{A5}$$

and $\mathcal{B}=\emptyset$.

Other cases are more complicated. For a strip of K_3's, i.e., triangles, in addition to free and periodic (cyclic) boundary conditions, one also has the possibility of twisted periodic boundary conditions, which form a Möbius strip. The chromatic polynomial for the $(K_3,K_2,t,\mathrm{PBC}_x)$ strip for even t was given in Ref. [35] (see also Ref. [38]); in this case, the strip can be regarded as being formed from a strip of m squares with a bond added to each square connecting the lower-left to upper-right vertex of the square, so that $t=2m$. The chromatic polynomial for the corresponding Möbius strip, $(K_3,K_2,t,T\mathrm{PBC}_x)$ with even t was also given in Ref. [35]. For the $t\to\infty$ limit, the W function and associated nonanalytic locus $\mathcal{B}$ were given in Ref. [35]. The chromatic polynomials for the corresponding strip with odd t, viz., $(K_3,K_2,t,\mathrm{PBC}_x)$ and $(K_3,K_2,t,T\mathrm{PBC}_x)$, were given in Ref. [45]; the $t\to\infty$ function W and locus $\mathcal{B}$ are the same for both the cyclic and Möbius strips as t increases through even or odd values.

In the text we have considered strips in which each square forms a K_4 subgraph. There are actually different classes of strips with t repeated K_4 subgraphs, in the notation introduced above. An illustration of these is given in Fig. 8.

As an example, we calculate

$$P[(K_4,K_2,t,\mathrm{BC}_x),q]=(q-3)^t P[(K_3,K_2,t,\mathrm{BC}_x),q], \tag{A6}$$

where $\mathrm{BC}_x=\mathrm{PBC}_x$ or $T\mathrm{PBC}_x$, respectively, and the $(K_3,K_2,t,\mathrm{PBC}_x)$ and $(K_3,K_2,t,T\mathrm{PBC}_x)$ strips are the cyclic and Möbius triangular-lattice strips mentioned above. Thus, explicitly, for even $t=2m$,

$$P[(K_4,K_2,t=2m,\mathrm{PBC}_x),q] =(q-3)^{2m}[(q^2-3q+1)+[(q-2)^2]^m +(q-1)[(\lambda_{t2,3})^m+(\lambda_{t2,4})^m]], \tag{A7}$$

$$P[(K_4,K_2,t=2m,TPBC_x),q] =(q-3)^{2m}\left[-1+[(q-2)^2]^m -(q-1)(q-3)\frac{[(\lambda_{t,2,3})^m-(\lambda_{t2,4})^m]}{\lambda_{t2,3}-\lambda_{t2,4}}\right], \tag{A8}$$

where $\lambda_{t2,j}$, $j=3,4$, were defined in Eqs. (1.7) above.

For the case of odd $t=2m+1$, we have

$$P[(K_4,K_2,t=2m+1,\mathrm{PBC}_x),q] =(q-3)^{2m+1}\Bigg[-(q^2-3q+1)+(q-2)[(q-2)^2]^m +\frac{1}{2}(q-1)(q-3)\Bigg\{[(\lambda_{t2,3})^m+(\lambda_{t2,4})^m] +\frac{[(\lambda_{t2,3})^m-(\lambda_{t2,4})^m]}{\lambda_{t2,3}-\lambda_{t2,4}}\Bigg\}\Bigg], \tag{A9}$$

$$P[(K_4,K_2,t=2m+1,T\mathrm{PBC}_x),q] =(q-3)^{2m+1}\Bigg\{1+(q-2)[(q-2)^2]^m+\frac{1}{2}(1-q) \times\Bigg[[(\lambda_{t2,3})^m+(\lambda_{t2,4})^m] +(9-4q)\frac{[(\lambda_{t2,3})^m-(\lambda_{t2,4})^m]}{\lambda_{t2,3}-\lambda_{t2,4}}\Bigg]\Bigg\}. \tag{A10}$$

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