Exact $T=0$ partition functions for Potts antiferromagnets on sections of the simple cubic lattice

Jesús Salas[1,*] and Robert Shrock[2,†]
[1]Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, Zaragoza 50009, Spain
[2]C. N. Yang Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11794-3840

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We present exact solutions for the zero-temperature partition function of the q-state Potts antiferromagnet (equivalently, the chromatic polynomial P) on tube sections of the simple cubic lattice of fixed transverse size $L_x \times L_y$ and arbitrarily great length L_z, for sizes $L_x \times L_y = 2\times 3$ and 2×4 and boundary conditions (a) ($\mathrm{FBC}_x, \mathrm{FBC}_y, \mathrm{FBC}_z$) and (b) ($\mathrm{PBC}_x, \mathrm{PBC}_y, \mathrm{FBC}_z$), where FBC (PBC) denote free (periodic) boundary conditions. In the limit of infinite length, $L_z \to \infty$, we calculate the resultant ground-state degeneracy per site W (=exponent of the ground-state entropy). Generalizing q from $\mathbb{Z}_+$ to $\mathbb{C}$, we determine the analytic structure of W and the related singular locus $\mathcal{B}$ which is the continuous accumulation set of zeros of the chromatic polynomial. For the $L_z \to \infty$ limit of a given family of lattice sections, W is analytic for real q down to a value q_c. We determine the values of q_c for the lattice sections considered and address the question of the value of q_c for a d-dimensional Cartesian lattice. Analogous results are presented for a tube of arbitrarily great length whose transverse cross section is formed from the complete bipartite graph $K_{m,m}$.

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I. INTRODUCTION

The q-state Potts antiferromagnet [1,2] exhibits nonzero ground-state entropy, $S_0>0$ (without frustration) for sufficiently large q on a given lattice Λ or, more generally, on a graph G. 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]. One physical example is provided by ice, for which the residual molar entropy is $S_0 = 0.82 \pm 0.05$ cal/(K mol), i.e., $S_0/R = 0.41 \pm 0.03$, where $R = N_{Avog.} k_B$ [5]. Indeed, residual entropy at low temperatures has been observed in a number of molecular crystals, including nitrous oxide, NO and $FClO_3$ (a comprehensive review is given in Ref. [6]). In these physical examples, the entropy occurs without frustration, i.e., the configurational energy can be minimized, just as in the Potts antiferromagnet for sufficiently large q.

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 graph $G = (V,E)$ satisfies

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

where G is defined by its set of vertices V and edges E and $P(G,q)$ is the chromatic polynomial expressing the number of ways of coloring the vertices of G with q colors such that no two adjacent vertices have the same color (for reviews, see [7–10]). The minimum number of colors necessary for such a coloring of G is called the chromatic number $\chi(G)$. Thus

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

where $n = |V|$ is the number of vertices of G and we denote the formal infinite-length limit of strip graphs of type G as $\{G\} = \lim_{n\to\infty} G$. At certain special points q_s [typically $q_s = 0,1,\ldots,\chi(G)$], one has the noncommutativity of limits [11]

$$\lim_{q\to q_s} \lim_{n\to\infty} P(G,q)^{1/n} \neq \lim_{n\to\infty} \lim_{q\to q_s} P(G,q)^{1/n} \tag{1.3}$$

and hence it is necessary to specify the order of the limits in the definition of $W(\{G\},q_s)$. Denoting W_{qn} and W_{nq} as the functions defined by the different order of limits on the left and right-hand sides of Eq. (1.3), we take $W \equiv W_{qn}$ here; this has the advantage of removing certain isolated discontinuities that are present in W_{nq}. Using the expression for $P(G,q)$, 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. For some families of graphs $\mathcal{B}$ may be null, and W may also be nonanalytic at certain discrete points. 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 ground-state degeneracy per site $W(\{G\})$ is an analytic function of real q from large values down to the value q_c, which is the maximal value where $\mathcal{B}$ intersects the (positive) real axis. For some families of graphs, $\mathcal{B}$ does not cross or intersect the real q axis; in these cases, no q_c is defined. However, even in cases where no such intersection occurs, $\mathcal{B}$ often includes complex-conjugate arcs with end points close to the positive real axis, and hence, in these cases, it can be useful to define a quantity $(q_c)_{\mathrm{eff}}$ equal to the real part of the end points. We shall use this definition here.

In this work we present exact solutions for chromatic polynomials $P(G,q)$ for sections of the simple cubic (sc) lattice with fixed transverse size $L_x \times L_y$ and arbitrarily great

*Email address: jesus@melkweg.unizar.es
†Email address: robert.shrock@sunysb.edu

length L_z, for cross sections $L_x \times L_y = 3\times 2$ and 4×2. These calculations are carried out for the cases (a) $(\mathrm{FBC}_x, \mathrm{FBC}_y, \mathrm{FBC}_z)$ (rectangular solid) and (b) $(\mathrm{PBC}_x, \mathrm{FBC}_y, \mathrm{FBC}_z)$ (homeomorphic to an annular cylindrical solid), where FBC_i and PBC_i denote free and periodic boundary conditions in the ith direction, respectively. We shall use the notation $(L_i)_\mathrm{F}$ and $(L_i)_\mathrm{P}$ to denote free and periodic boundary conditions in the ith direction, so that, for example, the $3\times 2 \times L_z$ sections of the simple cubic lattice with the boundary conditions of type (a) and (b) are denoted $3_\mathrm{F}\times 2_\mathrm{F} \times (L_z)_\mathrm{F}$ and $3_\mathrm{P}\times 2_\mathrm{F} \times (L_z)_\mathrm{F}$, respectively. For each family of graphs, taking the infinite-length limit $L_z \to \infty$, we calculate $W(\{G\},q)$, $\mathcal{B}$, and hence q_c.

We also present corresponding results for a tube of arbitrarily great length whose transverse cross section is formed from the complete bipartite graph $K_{m,m}$, for the cases $m = 2$ and 3. Here the complete graph K_n is defined as the graph consisting of n vertices such that each vertex is connected by edges (bonds) to every other vertex, and the complete bipartite graph $K_{m,n}$ is defined as the join $K_m + K_n$, where the join of two graphs G and H, denoted $G+H$ is the graph obtained by joining each of the vertices of G to each of the vertices of H. Although the complete bipartite graphs are not regular lattices as studied in statistical mechanics, they are useful since they allow us to obtain exact results for cases of high effective coordination number.

There are several motivations for this work. We have mentioned the basic importance of nonzero ground-state entropy in statistical mechanics and physical examples of this phenomenon. From the point of view of rigorous statistical mechanics, exact analytic solutions are always valuable since they complement results from approximate series expansions and numerical methods. We have defined the point q_c above in terms of the function $W(\{G\},q)$. This point has another important physical significance: for the $n\to\infty$ limit of a given family of graphs, $\{G\}$, the q-state Potts antiferromagnet has no finite-temperature phase transition but is disordered for all $T \geq 0$ if $q > q_c(\{G\})$, and has a zero-temperature critical point for $q = q_c(\{G\})$ [12]. For the Potts model on the (infinite) square lattice, via a mapping to a vertex model, it has been concluded that $q=3$ [15]. However, the value of q_c is not known for any lattice of dimension three or higher. One of the main motivations for our study is the insight that one gains concerning the dependence of q_c on the coordination number $\Delta = 2d$ of a d-dimensional Cartesian lattice $\mathbb{E}^d$ for the case $d=3$. Furthermore, although infinite-length sections of higher-dimensional lattices with fixed finite $(d-1)$-dimensional volume transverse to the direction in which the length goes to infinity are quasi-one-dimensional systems and hence (for finite-range spin-spin interactions) do not have finite-temperature phase transitions, their zero-temperature critical points are of interest. Finally, in addition to the physics motivations, the present results are of interest in mathematical graph theory. Some related earlier work is in Refs. [13–50].

Our exact calculations of q_c for the infinite-length limits of tube sections of the simple cubic lattice yield information relevant to estimates of q_c for the infinite cubic lattice. The point here is that as the area of the transverse cross section of the tube increases to infinity, the corresponding sequence of exact q_c or $(q_c)_\mathrm{eff}$ values is expected to converge to a limit. For the tube sections considered here, which have free longitudinal boundary conditions, this limit is a lower bound for the true q_c of the infinite simple cubic lattice. The reason that one can only say that it is a lower bound is that for these families with free longitudinal boundary conditions the respective limiting curve $\mathcal{B}$ exhibits a complex-conjugate pair of prongs that protrude to the right. It is possible that, as the area of the transverse cross section goes to infinity, the endpoints of these prongs will extend over and meet on the real axis, thereby defining a point q_c that could lie to the right of the limit of the q_c points for each of the tubes with finite transverse cross section. In this case, $\lim_{L_x, L_y \to\infty} q_c(\mathrm{sc}, (L_x)_{BCx} \times (L_y)_{BCy} \times \infty_\mathrm{F})$ is not equal to, but instead less than, the value $q_c(\mathrm{sc})$ for the infinite simple cubic lattice. Indeed, for finite-width, infinite-length strips of the triangular lattice with free longitudinal (z) boundary conditions and periodic transverse (y) boundary conditions, $\lim_{L_y\to\infty} q_c((L_y)_\mathrm{P} \times \infty_\mathrm{F}) \simeq 3.819\,67\ldots$ while $q_c = 4$ for the infinite triangular lattice [23]. This occurs because of the above-mentioned phenomenon in which the endpoints of the complex-conjugate pair of prongs protruding to the right on the limiting curve $\mathcal{B}$ move inward toward the real axis and, as $L_y \to \infty$, finally touch each other, thereby defining the true $q_c = 4$ about 5% greater than the above limit at ~ 3.82. The presence of these types of prongs protruding to the right on the limiting curves was also observed for a variety of infinite-length, finite-width two-dimensional (2D) lattice strips with free longitudinal boundary conditions (for both free and periodic transverse boundary conditions) [30,31,45–47,50]. Calculations for $L_\mathrm{P}\times\infty_\mathrm{F}$ (i.e., cylindrical) strips of the square lattice have been carried out in [31,46,47,50] with widths L extending up to 13 [50], with $q_c(\mathrm{sq}, 13_\mathrm{P}\times\infty_\mathrm{F}) \simeq 2.916$. This value is within about 3% of the value for the infinite square lattice, $q_c(\mathrm{sq}) = 3$. As the width increases, the end points of the prongs do move in toward the real axis. These calculations for $L_\mathrm{P}\times\infty_\mathrm{F}$ strips of the square lattice are consistent with either of the two possibilities, that $\lim_{L\to\infty} q_c(\mathrm{sq}, L_\mathrm{P}\times\infty_\mathrm{F})$ is equal to, or slightly less than, $q_c(\mathrm{sq})$.

It is interesting that the exact calculations of the singular loci $\mathcal{B}$ for infinite-length, finite-width strips of various lattices with periodic longitudinal boundary conditions [51] (and either free or periodic transverse boundary conditions) yielded loci without such complex-conjugate prongs (or line segments on the real axis) [11,36,46,40,49,45]. For these families of strips it was found that $\mathcal{B}$ always crossed the positive real axis at $q=0$ and at a maximal point, so q_c is always defined; furthermore, $L_\mathrm{F}\times\infty_\mathrm{P}$, the value of q_c is a monotonically nondecreasing function of the width. For $L_\mathrm{P}\times\infty_\mathrm{P}$ strips, although q_c is not a nondecreasing function of the width, it is, for a given width, closer to the value for the infinite 2D lattice if one uses periodic, rather than free transverse boundary conditions, as one would expect since the former minimize finite-size effects.

Some definitions from graph theory will be useful here. The degree of a vertex in a graph $G=(V,E)$ is the number of edges to which it is attached. A graph G defined to be Δ regular if each of its vertices has the same degree, Δ. This is, in particular, true of an infinite regular lattice, where this degree is the coordination number. Even if some vertices have different degrees from others, one can define an effective coordination number,

$$\Delta_{\rm eff}=\lim_{|V|\to\infty}\frac{2|E|}{|V|}. \tag{1.4}$$

For example, for a strip of the square lattice of size of the type $(L_x)_{\rm F}\times(L_y)_{\rm F}$, in the limit in which the length $L_x\to\infty$ with fixed finite width L_y

$$\Delta_{\rm eff}({\rm sq},(L_x)_{\rm F}\times(L_y)_{\rm F};L_x\to\infty)=4-\frac{2}{L_y}. \tag{1.5}$$

For the same strip, but with periodic transverse boundary conditions, if $L_y\geqslant 3$ to avoid double edges, we have

$$\Delta_{\rm eff}({\rm sq},(L_x)_{\rm F}\times(L_y)_{\rm P};L_x\to\infty)=4. \tag{1.6}$$

For the $(L_x)_{\rm F}\times(L_y)_{\rm F}\times(L_z)_{\rm F}$ section of the simple cubic lattice with free boundary conditions in all three directions, the interior vertices have degree 6, the vertices on the surface away from the corners have degree 4, and the corner vertices have degree 3. For the minimal case $2_{\rm F}\times 2_{\rm F}\times(L_z)_{\rm F}$, there are no interior vertices in the 3D sense, so that

$$\Delta_{\rm eff}({\rm sc},2_{\rm F}\times 2_{\rm F}\times(L_z)_{\rm F};L_z\to\infty)=4. \tag{1.7}$$

For the next case $(L_x)_F\times 2_F\times(L_z)_{\rm F}$ with $L_x\geqslant 3$ there are also no interior vertices in the 3D sense; in this case

$$\Delta_{\rm eff}({\rm sc},(L_x)_{\rm F}\times 2_{\rm F}\times(L_z)_{\rm F};{\rm FBC}_x,{\rm FBC}_y,{\rm FBC}_z;L_z\to\infty)$$
$$=5-\frac{2}{L_x}. \tag{1.8}$$

For the $L_z\to\infty$ limit of the $L_x\times L_y\times L_z$ section with $L_x\geqslant 3$, $L_y\geqslant 3$, we have

$$\Delta_{\rm eff}({\rm sc},(L_x)_{\rm F}\times(L_y)_{\rm F}\times(L_z)_{\rm F};\;\; L_z\to\infty)=6-2\frac{(L_x+L_y)}{L_xL_y}. \tag{1.9}$$

We shall also use the corresponding formulas when periodic rather than free boundary conditions are imposed in one of the transverse directions. Of course, in the usual thermodynamic limit of the Cartesian lattice $\mathbb{E}^d$, with $L_i\to\infty$, $i=1,\ldots,d$ and $\lim_{L_i\to\infty}L_i/L_j$ equal to a finite nonzero constant, the effective degree is $\Delta_{\rm eff}(\mathbb{E}^d)=2d$ independent of boundary conditions. In this case, although free boundary conditions in one or more directions entail vertices of lower degree than $2d$, these vertices occupy a vanishing fraction of the total vertices in the thermodynamic limit. Concerning the chromatic number, for the sections of 3D lattices considered here, we have

$$\chi({\rm sc},(L_x)_{\rm F}\times(L_y)_{\rm F}\times(L_z)_{\rm F})=2, \tag{1.10}$$

i.e., these graphs are bipartite. For the sections of the simple cubic lattice with periodic boundary conditions in one of the transverse direction, taking this to be the x direction with no loss of generality,

$$\chi({\rm sc},(L_x)_{\rm P}\times(L_y)_{\rm F}\times(L_z)_{\rm F})=\begin{cases}2 & \text{if } L_x \text{ is even}\\ 3 & \text{if } L_x \text{ is odd.}\end{cases} \tag{1.11}$$

For an infinite regular lattice having coordination number Δ, a rigorous upper bound on q_c was derived in [13] using the Dobrushin theorem:

$$q_c\leqslant 2\Delta. \tag{1.12}$$

Aside from the general property that, for cases where there is a q_c, this point satisfies $q_c\geqslant 2$, we are not aware of a published lower bound on q_c.

We have noted that in the infinite-length limit of given family of lattice strip graphs, $\mathcal{B}$ does not necessarily intersect or cross the real q axis, and if there is no such crossing, then there is no q_c. It has been found that for a graph consisting of a strip of a regular lattice, a sufficient condition for $\mathcal{B}$ to cross the (positive) real q axis is that there be periodic boundary conditions in the longitudinal direction, i.e., the direction in which the length goes to infinity as $n\to\infty$ [11–41].

An interesting question is how q_c depends on the lattice coordination number, equivalent to the vertex degree for an infinite lattice. For families of $L_x\times L_y$ lattice strip graphs with periodic longitudinal (L_x) boundary conditions, whose $L_x\to\infty$ limits are guaranteed to have a q_c, it is found that the value of q_c is a nondecreasing function of the effective vertex degree $\Delta_{\rm eff}$. Thus, for the family of cyclic strips of the square lattice with free transverse boundary conditions, besides the $1_F\times\infty_F$ case with $\Delta=2$ and $q_c=2$, one finds the following results: (i) $2_F\times\infty_F(\Delta=3)$ yields $q_c=2$ [11], (ii) $3_F\times\infty_F(\Delta_{\rm eff}=10/3)$ yields $q_c\simeq 2.3365$ [36], (iii) $3_F\times\infty_F(\Delta_{\rm eff}=7/2)$ yields $q_c\simeq 2.4928$ [46]. When one makes both the longitudinal and transverse boundary conditions periodic, the vertex degree is fixed. In this case, q_c does not necessarily increase with increasing width L_y. For example, for strips of the square lattice with toroidal boundary conditions and hence $\Delta=4$, the $3_P\times\infty_P$ strip yields $q_c=3$ [40] while the $4_P\times\infty_P$ strips yields the smaller value $q_c\simeq 2.78$ [49].

When one considers strips without periodic longitudinal boundary conditions, there may or may not be a q_c. We have found that for strips with free transverse and longitudinal boundary conditions, q_c or $(q_c)_{\rm eff}$, where the latter can be defined, is a monotonically increasing function of L_y, and since in these families of lattice strips, $\Delta_{\rm eff}$ is a monotonically increasing function of L_y, this means that $(q_c)_{\rm eff}$ is also a monotonically increasing function of $\Delta_{\rm eff}$. Thus, for $1_F\times\infty_F$ with $\Delta_{\rm eff}=2$ and $2_F\times\infty_F$ with $\Delta_{\rm eff}=3$, $\mathcal{B}=\emptyset$ and there is no $(q_c)_{\rm eff}$, while $3_F\times\infty_F$ with $\Delta_{\rm eff}=10/3$ yields $q_c=2$ [30], $4_F\times\infty_F$ with $\Delta_{\rm eff}=7/2$ yields $q_c\simeq 2.3014$ [30],

$5_F\times\infty_F$ with $\Delta_{\rm eff}=3.60$ yields $q_c\simeq 2.428$ [46,47], etc. up to $8_F\times\infty_F$ with $\Delta_{\rm eff}=3.75$, which yields arc endpoints at $q \simeq 2.6603\pm 0.0013i$ and hence $(q_c)_{\rm eff}=2.6603$ [47].

In contrast, for strips with free longitudinal and periodic transverse boundary conditions, $\Delta_{\rm eff}$ is fixed, e.g., equal to 4 for strips of the square lattice. Insofar as one expects q_c or $(q_c)_{\rm eff}$ to depend on $\Delta_{\rm eff}$, it is not clear, *a priori*, how these quantities should behave as functions of L_y. Indeed, one finds that q_c or $(q_c)_{\rm eff}$ have no monotonic dependence on L_y. For example, for $3_P\times\infty_F$, $\mathcal{B}=\emptyset$, $4_P\times\infty_F$ yields $q_c \simeq 2.3517$ [31], $5_P\times\infty_F$ yields $q_c\simeq 2.6917$ [46,47], but $6_P\times\infty_F$ yields $q_c\simeq 2.6132$ [46,47]. For $7_P\times\infty_F$, $\mathcal{B}$ has arc endpoints near the real axis at $q\simeq 2.7515\pm 0.0025i$, so $(q_c)_{\rm eff}\simeq 2.7515$ [47]. For the cases $(L_y)_P\times\infty$ up to $L=11$, it is found empirically that q_c or $(q_c)_{\rm eff}$ is monotonically increasing separately for the even-L_y and odd-L_y sequences [50].

Since q_c has thermodynamic significance as the value of q above which the Potts antiferromagnet has no finite-temperature phase transition and is disordered even at $T=0$, the value of q_c for a lattice with dimensionality $d\geqslant 2$ should be independent of the boundary conditions used to take the thermodynamic limit. (Strictly speaking, this is not true for $d=1$, since no q_c is defined for the infinite-length limit of the line graph, while $q_c=2$ for the infinite-length limit of the circuit graph, but this may be considered to be an exception due to the special nature of this graph.) For the infinite 2D lattices where q_c is known exactly, it is also a monotonically increasing function of the lattice coordination number. Specifically, as noted above, on the square lattice ($\Delta=4$), one has $q_c=3$ [16]. For the kagomé lattice, again with $\Delta=4$, one finds $q_c=3$ [17], and on the triangular lattice with $\Delta=6$, one has $q_c=4$ [23].

These exact results are all consistent with the inference that the value of q_c increases as a function of the coordination number for the thermodynamic limit of a regular lattice or, more generally, for infinite-length strips or tubes of regular lattices with prescribed boundary conditions in the transverse directions. A plausibility argument for this is as follows. For $q>q_c$, the zero-temperature Potts antiferromagnet has nonzero ground-state entropy per site, $S=k_B\ln W>0$, i.e., ground-state degeneracy per site $W>1$. This entropy reflects the fact that the number of ways of carrying out a proper coloring of the lattice or lattice strip increases exponentially with the number of vertices. Roughly speaking, the constraint that no two adjacent vertices can be assigned the same color is more restrictive the greater the number of neighboring vertices there are, i.e., the greater $\Delta_{\rm eff}$ is. Therefore, as one increases $\Delta_{\rm eff}$ for a fixed q, W decreases. This is borne out by exact and numerical calculations of W (for 2D lattices, see, e.g., Fig. 5 of [11] or Fig. 6 of [29]). In the context of d-dimensional Cartesian lattices, this means that q_c should increase as a function of d. Such a monotonicity relation is valuable to have since the value of q_c is not known exactly for lattices with dimension $d\geqslant 3$.

It is useful to define a ratio of the actual value of q_c to the upper bound in Eq. (1.12), namely,

$$R_{q_c}=\frac{q_c}{2\Delta}. \tag{1.13}$$

Evidently, $R_{q_c}=0.5$ for the infinite-length limit of the circuit graph and $R_{q_c}=0.375$ for the infinite square lattice. Similarly, for other exactly known cases, the actual value of q_c is considerably less than the rigorous upper bound (1.12). This suggests that it may be possible to improve the upper bound (1.12).

A generic form for chromatic polynomials for a strip graph of type G_s, or, more generally, a recursive family of graphs composed of m repetitions of a basic subgraph, is [22]

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

where $c_{G_s,j}(q)$ and the $N_{G_s,\lambda}$ terms (eigenvalues) $\lambda_{G_s,j}(q)$ depend on the type of strip graph G_s including the boundary conditions but are independent of m. Here, $N_\lambda\leqslant\dim(T)$, where $\dim(T)$ is the dimension of the transfer matrix in the Fortuin-Kasteleyn representation, and the difference, $N_{0a}=\dim(T)-N_\lambda$, is the number of zero amplitudes (coefficients). The coefficients $c_{G_s,j}$ can be regarded as the multiplicities of the eigenvalues $\lambda_{G_s,j}$ (for some real positive q values, these coefficients can be zero or negative, so that this interpretation presumes a sufficiently large real positive q, followed by analytic continuation to other values of q).

II. TUBES OF THE SIMPLE CUBIC LATTICE WITH FREE TRANSVERSE BOUNDARY CONDITIONS

The computations of the transfer matrix and the chromatic polynomials were performed following the methods described in Sec. III of Ref. [47]. The idea is to construct the partition function by building the lattice layer by layer. In all the computations we have chosen the Fortuin-Kasteleyn representation of the transfer matrix. Thus, our basis will be the connectivities of the top layer, whose basis elements $\mathbf{v}_{\mathcal{P}}$ are indexed by partitions $\mathcal{P}$ of the single-layer vertex set V^0. We shall abbreviate δ functions $\delta(\sigma_1,\sigma_3)$ as $\delta_{1,3}$. Moreover, we shall also abbreviate partitions $\mathcal{P}$ by writing instead the corresponding product $\mathbf{v}_{\mathcal{P}}$ of δ functions: e.g., in place of $\mathcal{P}=\{\{1,3\},\{2,4\},\{5\}\}$ we shall write simply $\mathcal{P}=\delta_{1,3}\delta_{2,4}$. The transfer matrix can be expressed as

$$\mathsf{T}=\mathsf{V}\,\mathsf{H} \tag{2.1}$$

where the matrices H and V are defined as

$$\mathsf{H}=\prod_{\langle xx'\rangle\in E^0}[I-J_{xx'}] \tag{2.2}$$

$$\mathsf{V}=\prod_{x\in V^0}[-I+D_x]. \tag{2.3}$$

In these formulas E^0 is the single-layer edge set, and $J_{x,x'}$ and D_x are, respectively, the ''join'' and ''detach'' operators whose action on the elements of the basis $\mathbf{v}_{\mathcal{P}}$ is as follows:

$$J_{xx'}\mathbf{v}_{\mathcal{P}}=\mathbf{v}_{\mathcal{P}\bullet xx'} \tag{2.4}$$

$$D_x\mathbf{v}_{\mathcal{P}}=\begin{cases}\mathbf{v}_{\mathcal{P}\backslash x} & \text{if } \{x\}\notin\mathcal{P}\\ q\mathbf{v}_{\mathcal{P}} & \text{if } \{x\}\in\mathcal{P},\end{cases} \tag{2.5}$$

where $\mathcal{P}\bullet xx'$ is the partition obtained from $\mathcal{P}$ by amalgamating the blocks containing x and x' (if they were not already in the same block); and $\mathcal{P}\backslash x$ is the partition obtained from $\mathcal{P}$ by detaching x from its block (and thus making it what we term a ''singleton''). In Eq. (2.3) we have written the formulas for H and V in the zero-temperature Potts antiferromagnet limit; the general expressions can be found in [47].

Finally, the partition function can be written as

$$Z(L_x\times L_y\times L_z;q)=\mathbf{u}^{\mathrm{T}}\cdot\mathsf{H}(\mathsf{VH})^{L_z-1}\cdot\mathbf{v}_{\mathrm{id}}, \tag{2.6}$$

where ''id'' denotes the partition in which each site $x\in V^0$ is a singleton, and $\mathbf{u}^{\mathrm{T}}$ is defined by

$$\mathbf{u}^{\mathrm{T}}\cdot\mathbf{v}_{\mathcal{P}}=q^{|\mathcal{P}|}. \tag{2.7}$$

In the zero-temperature limit the horizontal operator H is a projection. This implies that we can work in its image subspace by using the modified transfer matrix $\mathsf{T}'=\mathsf{HVH}$ in place of $\mathsf{T}=\mathsf{VH}$, and using the basis vectors

$$\mathbf{w}_{\mathcal{P}}=\mathsf{H}\,\mathbf{v}_{\mathcal{P}} \tag{2.8}$$

in place of $\mathbf{v}_{\mathcal{P}}$. Note that $\mathbf{w}_{\mathcal{P}}=0$ if $\mathcal{P}$ contains any pair of nearest neighbors in the same block. In the following subsections we will list the basis $\mathbf{P}=\{\mathbf{v}_{\mathcal{P}}\}$, although we performed the actual computations with the basis $\{\mathbf{w}_{\mathcal{P}}\}$.

The computation of the limiting curves $\mathcal{B}$ was performed with either the resultant or the direct-search methods (see Ref. [47] for details). The computation of the zeros of the chromatic polynomials was done using the package MPSOLVE designed by Bini and Fiorentino [52,53], whose performance is superior to that of MATHEMATICA for this particular task [47].

A. $2_F\times 2_F\times(L_z)_F$ section of the simple cubic lattice

Before proceeding to our new results, we note the identity

$$\mathrm{sc}(2_{\mathrm{F}}\times 2_{\mathrm{F}}\times(L_z)_{\mathrm{F}})=\mathrm{sq}(4_{\mathrm{P}}\times(L_z)_{\mathrm{F}}). \tag{2.9}$$

The left-hand side of this identity is evidently a tube of the simple cubic lattice with a minimal-size transverse cross section, viz., a single square; the right-hand side of the identity is a strip of the square lattice of width 4 squares, and periodic transverse boundary conditions. The chromatic polynomials for the family of graphs on the right-hand side of this identity were calculated in Sec. VII of [31] and, in the infinite-length limit, W and $\mathcal{B}$ were determined (see Fig. 3(a) of [31]). In Ref. [31], the longitudinal direction was taken as L_x, while we take it to be L_z here. In [30–32], a generating function formalism was developed and used; for a given strip graph G_s of length m, the chromatic polynomial $P((G_s)_m,q)$ is given as the coefficient of z^m, where z is the auxiliary expansion variable,

$$\Gamma(G_s,q,z)=\sum_{m=0}^{\infty}P((G_s)_m,q)z^m. \tag{2.10}$$

This generating function is a rational function of q and z. For the strip considered here, of length $L_z=m$ edges,

$$\Gamma(G_s,q,z)=\frac{a_0+a_1z}{1+b_1z+b_2z^2}. \tag{2.11}$$

where

$$a_0=q(q-1)(q^2-3q+3), \tag{2.12}$$

$$a_1=-q(q-1)(q^4-7q^3+16q^2-13q+5), \tag{2.13}$$

$$b_1=-q^4+8q^3-29q^2+55q-46, \tag{2.14}$$

$$b_2=q^6-12q^5+61q^4-169q^3+269q^2-231q+85. \tag{2.15}$$

(Here we have converted the numerator coefficients from [31] to be in accord with the labeling convention of Eq. (2.10); in the labeling convention of [31], the strip with length $m+1$ edges.) The chromatic polynomial can equivalently be written as in (2.6): in the basis $\mathbf{P}=\{1,\delta_{1,4}+\delta_{2,3}\}$ it is given by

$$Z(2_{\mathrm{F}}\times 2_{\mathrm{F}}\times(L_z)_{\mathrm{F}};q)=\begin{pmatrix}q(q-1)(q^2-3q+3)\\ 2q(q-1)^2\end{pmatrix}^{\mathrm{T}}\cdot T(2_{\mathrm{F}}\times 2_{\mathrm{F}})^{L_z-1}\cdot\begin{pmatrix}1\\0\end{pmatrix}. \tag{2.16}$$

The transfer matrix $T(2_{\mathrm{F}}\times 2_{\mathrm{F}})$ is equal to

$$T(2_{\mathrm{F}}\times 2_{\mathrm{F}})=\begin{pmatrix}41-51q+28q^2-8q^3+q^4 & 2(-12+14q-6q^2+q^3)\\ -5+2q & 5-4q+q^2\end{pmatrix}. \tag{2.17}$$

Note that in general, we should have considered an additional element in the basis, namely, the partition $\delta_{1,4}\delta_{3,2}$; however, its amplitude vanishes identically. This can be easily understood by noting that this particular graph (2.9) is planar and $\delta_{1,4}\delta_{3,2}$ is a crossing partition.

For this family, $\mathcal{B}$ consists of two complex-conjugate arcs, a self-conjugate arc that crosses the real axis at $q\simeq 2.3026$ and a line segment on this axis extending from $q\simeq 2.2534$ to $q\simeq 2.3517$, which latter point is thus q_c. It should be noted also that although this graph is included here as the minimal-

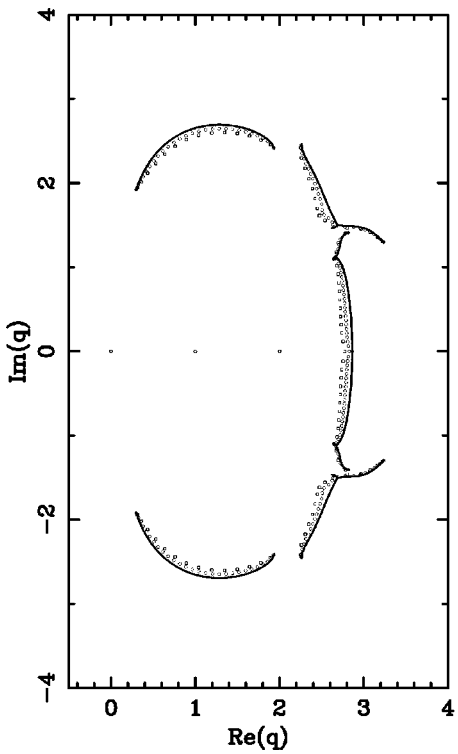

FIG. 1. Chromatic zeros for the $3_F\times 2_F\times (L_z)_F$ section of the simple cubic lattice, for (a) $L_z=15$, i.e., $n=90$ (□), (b) $L_z=30$, i.e., $n=180$ (○).

transverse-size member of a family of $L_x\times L_y\times L_z$ sections of the simple cubic lattice, it is degenerate in the sense that it is actually planar, in contrast to the others that we shall study here. There are eight endpoints in $\mathcal{B}$; two of them are given by the real values $q\simeq 2.3026$ and $q\simeq 2.3517$; the other six end points are the complex-conjugate pairs $q\simeq 0.7098 \pm 2.0427i$, $q\simeq 1.9923\pm 1.5942i$, and $q\simeq 2.9953\pm 1.4266i$.

B. $3_F\times 2_F\times (L_z)_F$ section of simple cubic lattice

The section of the simple cubic lattice with the next larger transverse cross section is the $3_F\times 2_F\times (L_z)_F$, or equivalently, $2_F\times 3_F\times (L_z)_F$, family. For this family, the dimension of the transfer matrix is 13. (In general the transfer matrix has dimension 15, but two basis elements, namely $\delta_{1,5}\delta_{2,6}\delta_{3,4}+\delta_{2,4}\delta_{3,5}\delta_{1,6}$ and $\delta_{1,3,5}\delta_{2,4,6}$, can be eliminated as they have zero amplitudes.) Since the entries in the transfer matrix are rather long, we relegate them to the MATHEMATICA file `transfer_sc.m` that is available with this paper in the LASL cond-mat archive. We have computed the chromatic zeros for $L_z=15$ and 30, i.e., $n=90$ and 180 vertices, respectively. These are shown in Fig. 1. This value of L_z is sufficiently large that these zeros give a reasonably accurate indication of the location of the asymptotic limiting curves comprising the locus $\mathcal{B}$. As is generally true, for the larger value of L_z, and hence n, the chromatic zeros move slightly outward, approaching the limiting curve $\mathcal{B}$ from smaller values of $|q|$.

The limiting curve $\mathcal{B}$ consists of two complex-conjugate arcs, a self-conjugate arc that crosses the real q axis at $q \simeq 2.8645$, and a horizontal real segment from $q\simeq 2.8566$ to $q\simeq 2.8723$. This latter value corresponds to the value of q_c for this family. This information is listed, together with that from other lattices, in Table I. There are 16 endpoints: two are the real values $q\simeq 2.8566$ and $q\simeq 2.8723$; the other 14 are the complex-conjugated pairs: $q\simeq 0.2943\pm 1.9150i$, $q\simeq 1.9371\pm 2.4040i$, $q\simeq 2.6374\pm 1.0937i$, $q\simeq 2.8250 \pm 1.4087i$, $q\simeq 2.6255\pm 1.4647i$, $q\simeq 3.2410\pm 1.2920i$, and $q\simeq 2.2645\pm 2.4605i$. Finally, there are four T points at $q \simeq 2.670\pm 1.117i$ and $q\simeq 2.689\pm 1.500i$.

TABLE I. Results for tube graphs of the simple cubic lattice. The table shows the relation between the degree (coordination number) Δ of a Δ-regular family or the effective degree $\Delta_{\rm eff}$, and q_c, if a q_c exists, for the infinite-length limit of the family. Boundary conditions are indicated with a subscript F for free, P for periodic, in a given direction. In column q_c, an asterisk indicates that $\mathcal{B}$ does not actually cross the real axis, so that, strictly speaking, no q_c is defined, but arcs on $\mathcal{B}$ end very close to the real axis, at the positions given. Similar results are listed for the tubes with $K_{m,m}$ cross sections.

G_s	Δ	$\Delta_{\rm eff}$	q_c	Ref.
sc, $2_F\times 2_F\times \infty_F$		4	2.3517	[31]
sc, $3_F\times 2_F\times \infty_F$		4.33	2.8723	Here
sc, $4_F\times 2_F\times \infty_F$		4.50	3.1498 ± 0.0021*	Here
sc, $2_P\times 2_P\times \infty_F$		4	2.3517	[31]
sc, $3_P\times 2_P\times \infty_F$		5	$3.3255\pm 0.0184i$*	Here
sc, $4_P\times 2_P\times \infty_F$		5	$3.3623\pm 0.0061i$*	Here
$K_{2,2}\times \infty_F$		4	2.3517	[31]
$K_{3,3}\times \infty_F$		5	$3.0452\pm 0.0082i$*	Here
$K_{4,4}\times \infty_F$		6	$3.6743\pm 0.0085i$*	Here

C. $4_F\times 2_F\times (L_z)_F$ section of simple cubic lattice

The section of the simple cubic lattice with the next larger transverse cross section is the $4_F\times 2_F\times (L_z)_F$, or equivalently, $2_F\times 4_F\times (L_z)_F$ family. For this family, the dimension of the transfer matrix is 156. However, there are 20 basis elements that correspond to zero amplitudes, so the effective dimension of the transfer matrix is 136. This transfer matrix $T(4_F\times 2_F)$, as well as the vectors $\mathbf{v}$ and $\mathbf{u}_{\rm id}$ can be found in the MATHEMATICA file `transfer_sc.m`. We have computed the chromatic zeros for $L_z=20$ and 40, i.e., $n=160$ and 320 vertices, respectively. These are shown in Fig. 2.

The limiting curve $\mathcal{B}$ consists of eight complex-conjugate arcs; none of them crosses the real axis, so, strictly speaking, there is no value of q_c. However, we can define $(q_c)_{\rm eff} \approx 3.1498$. This value is larger than the corresponding value for the family $3_F\times 2_F\times L_F$ $q_c\approx 2.8723$ and larger than the value for the square lattice $q_c(sq)=3$. There are 11 pairs of complex-conjugate end points: $q\simeq 0.073\pm 1.747i$, $q\simeq 1.582 \pm 2.845i$, $q\simeq 1.684\pm 2.871i$, $q\simeq 2.379\pm 2.503i$, $q\simeq 2.513 \pm 1.569i$, $q\simeq 2.661\pm 1.816i$, $q\simeq 2.697\pm 1.889i$, $q\simeq 3.034 \pm 1.367i$, $q\simeq 3.035\pm 1.385i$, $q\simeq 3.150\pm 0.002i$, and $q \simeq 3.383\pm 1.157\,i$. Finally, there are three pairs of complex-

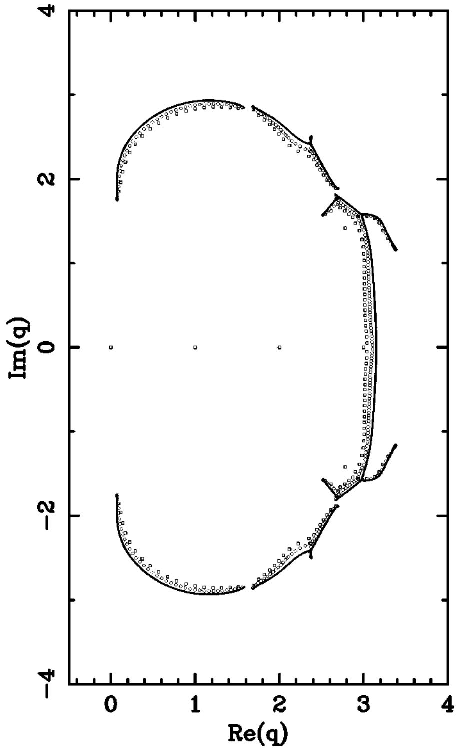

FIG. 2. Chromatic zeros for the $4_F \times 2_F \times (L_z)_F$ section of the simple cubic lattice, for (a) $L_z=20$, i.e., $n=160$ (□), (b) $L_z=40$, i.e., $n=320$ (○).

conjugate T points: $q \simeq 2.381 \pm 2.404i$, $q \simeq 2.695 \pm 1.793i$, and $q \simeq 2.972 \pm 1.578i$.

III. TUBES OF THE SIMPLE CUBIC LATTICE WITH TRANSVERSE PERIODIC BOUNDARY CONDITIONS

The method we have used to compute the chromatic polynomials and the transfer matrix is the same as in Sec. II. The only difference is that we enlarge the single-layer edge set E^0.

A. $2_P \times 2_P \times (L_z)_F$ section of simple cubic lattice

This family has (trivially) the same chromatic polynomials as the family $sc(2_F \times 2_F \times (L_z)_F$. (This is not true for the finite-temperature Potts model partition function, or equivalently, the Tutte polynomial; however we only deal with the chromatic polynomial here.) Thus, the transfer matrix and chromatic polynomials are given, respectively, by Eqs. (2.1) and (2.6).

B. $3_P \times 2_P \times (L_z)_F$ section of simple cubic lattice

In general, finite-size artifacts are minimized if one uses periodic boundary conditions in as many directions as possible. Hence, it is useful to calculate P and $\mathcal{B}$ for the same section of the simple cubic lattice as in the previous section, but with periodic boundary conditions imposed on the longer of the two transverse directions. This family is again bipartite. In this case, the dimension of the transfer matrix is 4.

In the basis $\mathbf{P}=\{1, \delta_{2,4}+\delta_{2,6}+\delta_{1,5}+\delta_{3,5}+\delta_{1,6}+\delta_{3,4}, \delta_{1,5}\delta_{2,6}+\delta_{2,4}\delta_{3,5}+\delta_{3,4}\delta_{1,5}+\delta_{3,4}\delta_{2,6}+\delta_{1,6}\delta_{3,5}+\delta_{1,6}\delta_{2,4}, \delta_{1,6}\delta_{3,4}+\delta_{1,5}\delta_{2,4}+\delta_{2,6}\delta_{3,5}\}$, the transfer matrix can be written as

$$T(3_P \times 2_P) = \begin{pmatrix} T_{11} & T_{12} & T_{13} & T_{14} \\ T_{21} & T_{22} & T_{23} & T_{24} \\ 1 & 2(-3+q) & 12-6q+q^2 & -2(-4+q) \\ 0 & -2 & -4(-3+q) & 15-7q+q^2 \end{pmatrix}, \tag{3.1}$$

where

$$T_{11}=1089-1578q+1054q^2-417q^3+103q^4-15q^5+q^6, \tag{3.2}$$

$$T_{12}=6(-292+394q-231q^2+74q^3-13q^4+q^5), \tag{3.3}$$

$$T_{13}=6(110-117q+51q^2-11q^3+q^4), \tag{3.4}$$

$$T_{14}=3(154-149q+60q^2-12q^3+q^4), \tag{3.5}$$

$$T_{21}=-90+71q-20q^2+2q^3, \tag{3.6}$$

$$T_{22}=203-189q+71q^2-13q^3+q^4, \tag{3.7}$$

$$T_{23}=-109+80q-21q^2+2q^3, \tag{3.8}$$

$$T_{24}=-81+52q-12q^2+q^3. \tag{3.9}$$

The vectors $\mathbf{v}$ and $\mathbf{u}_{\rm id}$ are given by

$$\mathbf{v}=\begin{pmatrix} (-2+q)(-1+q)q(-13+14q-6q^2+q^3) \\ 6(-2+q)^3(-1+q)q \\ 6(-2+q)^2(-1+q)q \\ 3(-3+q)(-2+q)(-1+q)q \end{pmatrix}, \tag{3.10}$$

$$\mathbf{u}_{\rm id}=\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{3.11}$$

We remark that in this case the most general basis contains an additional partition: $\delta_{1,5}\delta_{2,6}\delta_{3,4}+\delta_{2,4}\delta_{3,5}\delta_{1,6}$. This one can be dropped, as it corresponds to a vanishing amplitude.

We have computed the chromatic zeros for $L_z=15$ and 30, i.e., $n=90$ and 180, respectively. These are shown in Fig. 3. The limiting curve $\mathcal{B}$ contains three pairs of self-conjugate arcs. Although the arcs do not cross the real axis, so that, strictly speaking, no q_c is defined, $(q_c)_{\rm eff} \simeq 3.33$, which is larger than the value $q_c=3$ for the square lattice-.The locus $\mathcal{B}$ has 12 endpoints: $q \simeq 0.5061 \pm 2.6413i$,

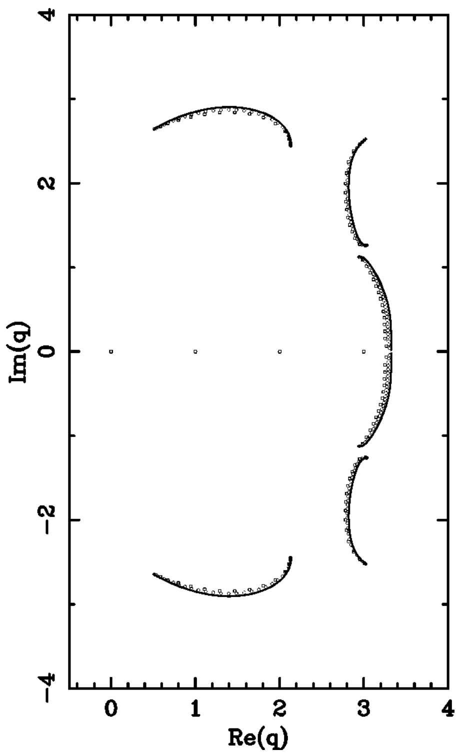

FIG. 3. Chromatic zeros for the $2_{\rm P}\times 3_{\rm P}\times (L_z)_{\rm F}$ section of the simple cubic lattice, for (a) $L_z=15$, i.e., $n=90$ (□), (b) $L_z=30$, i.e., $n=180$ (○).

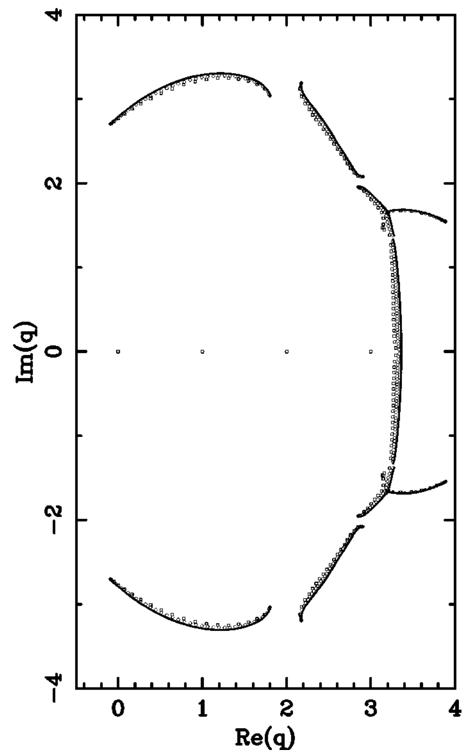

FIG. 4. Chromatic zeros for the $2_{\rm P}\times 4_{\rm P}\times (L_z)_{\rm F}$ section of the simple cubic lattice, for (a) $L_z=20$, i.e., $n=160$ (□), (b) $L_z=40$, i.e., $n=320$ (○).

$q\simeq 2.1301\pm 2.4407i$, $q\simeq 3.0251\pm 2.5249i$, $q\simeq 3.0412 \pm 1.2643i$, $q\simeq 2.9328\pm 1.1238i$, and $q\simeq 3.3255\pm 0.01839i$.

C. $4_P\times 2_P\times (L_z)_F$ section of simple cubic lattice

In this case we have 56 basis elements. However, there are 11 trivial basis element that lead to a vanishing amplitude. The transfer matrix and the vectors **v** and $\mathbf{u}_{\rm id}$ are listed in the MATHEMATICA file `transfer_sc.m`. Among the other 45 basis elements, we have numerical indications that there are 19 additional vanishing amplitudes.

The limiting curve $\mathcal{B}$ (see Fig. 4) contains eight self-conjugate arcs. As in the $4_{\rm P}\times 2_{\rm P}\times \infty_{\rm F}$ case, this locus does not actually cross the positive real q axis, but again has endpoints that lie very close to this axis, and we obtain $(q_c)_{\rm eff} \simeq 3.36$. As expected, this is larger than the value $(q_c)_{\rm eff} \simeq 3.33$ that we found for the tube $3_{\rm P}\times 2_{\rm P}\times \infty_{\rm F}$. There are nine pairs of complex-conjugate end points: $q\simeq -0.095 \pm 2.700i$, $q\simeq 1.803\pm 3.031i$, $q\simeq 2.176\pm 3.196i$, $q\simeq 2.841 \pm 1.954i$, $q\simeq 2.910\pm 2.080i$, $q\simeq 3.263\pm 1.333i$, $q\simeq 3.279 \pm 1.377i$, $q\simeq 3.362\pm 0.006i$, and $q\simeq 3.892\pm 1.542i$. Finally, there is one pair of complex-conjugate T points: $q\simeq 3.204 \pm 1.665i$.

Another property that was observed in our earlier calculations of chromatic polynomials for strips of 2D lattices is that, for a given type of transverse boundary conditions, for infinite-length strips with free longitudinal boundary conditions, as the width increases, the number of arcs on $\mathcal{B}$ increases and the end points of these arcs move in such a manner as to reduce the gaps between the arcs. Here we observe the same qualitative behavior as the area of the transverse cross section of the tube section increases. If this trend continues for progressively larger transverse widths or cross sectional areas, then the number of arcs could increase without bound as one approaches the respective infinite 2D or 3D lattices. Now in the two cases where the loci $\mathcal{B}$ have been calculated exactly for regular lattices, namely, the $d=1$ lattice (with periodic boundary conditions; for free boundary conditions, $\mathcal{B}=\emptyset$) and the triangular lattice (defined as the limit $L\to\infty$ of $L_{\rm P}\times\infty_F$ strips [23]), this locus has no prongs or endpoints. Thus, one could imagine that as the width or cross sectional area of the strips or tubes increases to infinity, the endpoints of arcs join so that the gaps between these arcs disappear, and prongs either have lengths that go to zero or have end points that join to form closed boundaries. We also observe that, for a given width or, for the present families of tube sections, for a given transverse cross sectional area, there tend to be fewer arcs when one uses periodic rather than free boundary conditions for the transverse direction(s). This is in accord with the fact that calculations for strips with periodic longitudinal boundary conditions [11,36,40,46,49,45] found no prongs (or line segments) on the respective loci $\mathcal{B}$, i.e., in all cases studied, these loci did not contain endpoints. Finally, our calculations are consistent with the expectation that as the area of the transverse cross section goes to infinity, the outer envelope of the locus $\mathcal{B}$ approaches a limit, which crosses the real axis at $q=0$, $q_c({\rm sc})$, and other point(s) between these two.

IV. FURTHER REMARKS ON THE STRUCTURE OF $\mathcal{B}$

In the introductory section, we discussed some differences in the locus $\mathcal{B}$ that depend on whether one uses periodic or free longitudinal boundary conditions. Here we include some further remarks relevant to our present results. It has been established that the structure of $\mathcal{B}$ inside its outer envelope and, in particular, the question of whether and where it crosses the positive real axis between $q=0$ and $q=q_c(\{G\})$ are dependent upon the boundary conditions used. For example, exact calculations for $L_{\rm F}\times\infty_{\rm P}$ and $L_{\rm P}\times\infty_{\rm P}$ strips of the triangular lattice show that the respective loci $\mathcal{B}$ cross the real axis at $q=2$ [36,45,49], corresponding to the fact that the Ising antiferromagnet has a (frustrated) $T=0$ critical point on these strips; however the loci $\mathcal{B}$ obtained in [23,31] for $L_{\rm P}\times\infty_{\rm F}$ strips or in [30] for $L_{\rm F}\times\infty_{\rm F}$ strips of the triangular lattice do not, in general, cross the real axis at $q=2$, nor is this crossing obtained for the infinite-width limit of the cylindrical strips calculated in [23]. Similarly, for $L_{\rm F}\times\infty_{\rm P}$ and $L_{\rm P}\times\infty_{\rm P}$ strips of the square lattice it was found that $\mathcal{B}$ passes through $q=0$, $q=2$, and a maximal value, $q=q_c(\{G\})$ [11,36,40,46]. In contrast, for the corresponding strips of the square lattice with free longitudinal boundary conditions, it has been found that $\mathcal{B}$ does not contain $q=0$ or, in general, $q=2$, and while the arc end points nearest to the origin move toward this point as the width increases (leading to the inference that for infinite width, $\mathcal{B}$ would pass through $q=0$), there is no analogous tendency of arcs on $\mathcal{B}$ to elongate toward $q=2$ [30,31,47,50]. There is also no tendency for the arcs on the loci $\mathcal{B}$ for our tube sections of the simple cubic lattice with free longitudinal boundary conditions to move toward $q=2$ as the cross sectional area increases.

A second point concerns the positions of the leftmost arcs. We find from the exact calculations reported here that for the infinite-length tube sections of the simple cubic lattice of the form $(L_x)_{\rm P}\times(L_y)_{\rm P}\times\infty_F$ with sufficiently large transverse cross section, namely $L_x=4$, $L_y=2$, $\mathcal{B}$ contains support in the $Re(q)<0$ half plane. This suggests that for this family of tube sections of the simple cubic lattice with periodic transverse boundary conditions, as the transverse area $L_xL_y\to\infty$, the complex-conjugate curves on $\mathcal{B}$ could approach the origin from the $Re(q)<0$ half plane, as happens for the limit $L\to\infty$ of $L_{\rm P}\times\infty_{\rm F}$ strips of the triangular lattice [23] and sufficiently wide strips of the square lattice of the form $L_{\rm F}\times\infty_{\rm F}$ [30,47], $L_{\rm P}\times\infty_{\rm F}$ [46,47,50], and $L_{\rm F}\times\infty_{\rm P}$ [36,38,46].

V. BEHAVIOR OF q_c FOR $\mathbb{E}^d$ WITH LARGE d

For the d-dimensional Cartesian lattice $\mathbb{E}^d$, Mattis suggested the ansatz [24]

$$W(\mathbb{E}^n,q)\simeq 1+\frac{(q-2)^d}{(q-1)^{d-1}}. \tag{5.1}$$

This agrees with the general results $W(\{C\},q)=q-1$ for $d=1$, and, for the square lattice $\mathbb{E}^2$ with $q=3$ yields the estimate $W(sq,q=3)=3/2$, which is within 4% of the known result $W(\mathbb{E}^2,q=3)=(4/3)^{3/2}=1.5396\ldots$ [16]. Mattis addressed the question of $d_c(q)$, i.e., the lower critical dimensionality of the q-state Potts antiferromagnet, below which it is disordered for $T\geq 0$. An equation yielding d_c as a function of q can also be solved to yield q_c as a function of d, so $d_c(q)$ and $q_c(d)$ constitute equivalent information about the system. Mattis argued that $d_c(q)$ could be estimated by noting that W is a measure of disorder, and if it is significantly greater than 1, then the system would be sufficiently disordered that one would not expect there to be a phase transition at $T\geq 0$. Taking the criterion that $W<2$ as the demarcation value for which a zero-temperature phase transition could occur, this yields the result

$$d_c(q)=\frac{\ln(q-1)}{\ln\left(\frac{(q-1)}{(q-2)}\right)}. \tag{5.2}$$

As noted, this may equivalently be regarded as an equation for q_c as a function of d and for $d=3$, this ansatz gives

$$q_c(d=3)\simeq 4.15. \tag{5.3}$$

Our exact results W and q_c for tube sections of the simple cubic are consistent with this estimate from the ansatz (5.1).

It is also of interest to ask what the behavior of q_c is for large d on Cartesian lattices. The ansatz (5.1) yields the asymptotic behavior

$$q_c\sim\frac{d}{\ln d}\quad \text{for}\quad d\to\infty. \tag{5.4}$$

This is in agreement with the upper bound (1.12)

$$q_c\leq 4d \tag{5.5}$$

and evidently is a smaller and smaller fraction of this upper bound as d gets large, with

$$R_{q_c}\sim\frac{1}{4\ln d}\quad \text{for}\quad d\to\infty. \tag{5.6}$$

VI. FAMILY $(K_{m,m})^{L_z}$

It is also useful to calculate $\mathcal{B}$ and study the dependence of q_c on vertex degree for infinite-length limits of other families of tube graphs. We report calculations here for a family of tube graphs whose transverse cross section is the complete bipartite graph $K_{m,m}$. The graph $K_{m,m}$ is Δ-regular graph with $\Delta=m$. We construct our tubes with the $K_{m,m}$ transverse cross section connected lengthwise L_z times, so that each vertex of one $K_{m,m}$ subgraph is connected "vertically" to the corresponding vertex of the next $K_{m,m}$. This recursive family of graphs is denoted as $(K_{m,m})^{L_z}$. The value of $\Delta_{\rm eff}$ is for this family

$$\Delta_{\rm eff}((K_{m,m})^{L_z};{\rm FBC}_z;L_z\to\infty)=m+2. \tag{6.1}$$

The computational method is the same as in the simple cubic families: the transfer matrix and the partition function are computed using the same formulas (2.1)/(2.6). The only difference is the single-layer edge set E^0.

A. Family $(K_{2,2})^{L_z}$

The family $(K_{2,2})^{L_z}$ is trivially equivalent to the family sq$(4_{\rm P}\times L_{\rm F})$, so by Eq. (2.9) it is also equivalent to the family sc$(2_{\rm F}\times 2_{\rm F}\times (L_z)_{\rm F})$. The transfer matrix, written in the basis $\mathbf{P}=\{1,\delta_{1,2}+\delta_{3,4}\}$, takes the same form as Eq. (2.17); and the partition function is equivalent to Eq. (2.16).

B. Family $(K_{3,3})^{L_z}$

The transfer matrix for the family $(K_{3,3})^{L_z}$ has dimension 5. In the basis $\mathbf{P}=\{1,\delta_{1,2}+\delta_{1,3}+\delta_{2,3}+\delta_{4,5}+\delta_{4,6}+\delta_{5,6}, \delta_{1,2,3}+\delta_{4,5,6}, \delta_{1,2}\delta_{4,5}+\delta_{1,2}\delta_{4,6}+\delta_{1,2}\delta_{5,6}+\delta_{1,3}\delta_{4,5}+\delta_{1,3}\delta_{4,6}+\delta_{1,3}\delta_{5,6}+\delta_{2,3}\delta_{4,5}+\delta_{2,3}\delta_{4,6}+\delta_{2,3}\delta_{5,6}, \delta_{1,2,3}\delta_{4,5}+\delta_{1,2,3}\delta_{4,6}+\delta_{1,2,3}\delta_{5,6}+\delta_{4,5,6}\delta_{1,2}+\delta_{4,5,6}\delta_{1,3}+\delta_{4,5,6}\delta_{2,3}\}$, we can write the transfer matrix as

$$T(K_{33})=\begin{pmatrix} T_{11} & T_{12} & T_{13} & T_{14} & T_{15} \\ T_{21} & T_{22} & T_{23} & T_{24} & T_{25} \\ T_{31} & T_{32} & T_{33} & T_{34} & T_{35} \\ 1 & 2(-3+q) & 0 & T_{44} & 2(-2+q) \\ 0 & 1 & 0 & -3 & 2-q \end{pmatrix}, \tag{6.2}$$

where

$$T_{11}=1234-1747q+1137q^2-437q^3+105q^4-15q^5+q^6, \tag{6.3}$$

$$T_{12}=6(-252+337q-198q^2+65q^3-12q^4+q^5), \tag{6.4}$$

$$T_{13}=2(36-56q+33q^2-9q^3+q^4), \tag{6.5}$$

$$T_{14}=9(89-94q+43q^2-10q^3+q^4), \tag{6.6}$$

$$T_{15}=6(-25+24q-8q^2+q^3), \tag{6.7}$$

$$T_{21}=-113+91q-27q^2+3q^3, \tag{6.8}$$

$$T_{22}=174-153q+54q^2-10q^3+q^4, \tag{6.9}$$

$$T_{23}=-10+13q-6q^2+q^3, \tag{6.10}$$

$$T_{24}=3(-40+28q-8q^2+q^3), \tag{6.11}$$

$$T_{25}=29-21q+4q^2, \tag{6.12}$$

$$T_{31}=55-27q+3q^2, \tag{6.13}$$

$$T_{32}=-3(29-17q+3q^2), \tag{6.14}$$

$$T_{33}=9-12q+6q^2-q^3, \tag{6.15}$$

$$T_{34}=-18(-3+q), \tag{6.16}$$

$$T_{35}=-3(7-5q+q^2), \tag{6.17}$$

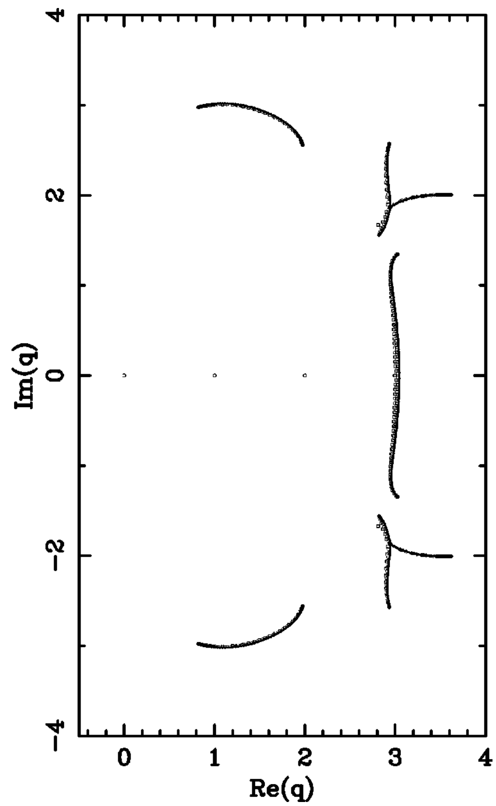

FIG. 5. Chromatic zeros for the $(K_{3,3})^m$ graph for (a) $m=L_z=15$, i.e., $n=90$ (□), (b) $m=L_z=30$, i.e. $n=180$ (○).

$$T_{44}=12-5q+q^2, \tag{6.18}$$

Finally,

$$\mathbf{v}=\begin{pmatrix} (-1+q)q(31-47q+28q^2-8q^3+q^4) \\ 6(-1+q)q(-7+10q-5q^2+q^3) \\ 2(-1+q)^3 q \\ 9(-1+q)q(3-3q+q^2) \\ 6(-1+q)^2 q \end{pmatrix}, \tag{6.19}$$

$$\mathbf{u}_{\rm id}=\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{6.20}$$

We remark that in this case there is an additional element of the basis $\delta_{1,2,3}\delta_{4,5,6}$ that should be taken into account in general. However, it corresponds to a vanishing amplitude.

Chromatic zeros for $(K_{3,3})^{L_z}$ with $L_z=15$ and $L_z=30$ are shown in Fig. 5, as well as the limiting curve $\mathcal{B}$. The limiting curve $\mathcal{B}$ contains six connected pieces. None of them crosses the real axis. Thus, strictly speaking, there is no q_c defined. However, by extrapolating the closest points to the real axis we get $q_c \simeq 3.045$, which is slightly greater than the value for the square lattice $q_c=3$.

There are 14 end points: $q \simeq 0.8197 \pm 2.9764i$, $q \simeq 1.9761 \pm 2.5559i$, $q \simeq 2.8190 \pm 1.5587i$, $q \simeq 2.9364 \pm 2.5742i$, $q \simeq 3.6220 \pm 2.0051i$, $q \simeq 3.0283 \pm 1.3476i$, and $q \simeq 3.0452 \pm 0.008246i$. There are two complex-conjugate T points at $q \simeq 2.949 \pm 1.870i$.

C. Family $(K_{4,4})^{L_z}$

In this case the transfer matrix has 15 elements. However, three of them correspond to null amplitudes, so we have an effective 12-dimensional transfer matrix. This matrix is listed in the MATHEMATICA file `transfer_Knn_tube.m` that is available with this paper in the LASL cond-mat archive.

There are eight connected pieces (see Fig. 6), and none of them crosses the real axis. The closest points to that axis are the complex-conjugated pair $q \approx 3.6743 \pm 0.0085i$. There are ten endpoints (that were computed using the resultant method): $q \approx 1.0084 \pm 3.7740i$, $q \approx 1.9104 \pm 3.4341i$, $q \approx 2.9457 \pm 3.2436i$, $q \approx 3.0385 \pm 2.8658i$, $q \approx 3.5456 \pm 1.3512i$, $q \approx 3.6006 \pm 3.2332i$, $q \approx 3.6260 \pm 1.4516i$, $q \approx 3.6743 \pm 0.0085i$, $q \approx 3.7857 \pm 2.3839i$, and $q \approx 3.8460 \pm 2.7980i$. There are four T points at $q \approx 3.070 \pm 2.904i$, and $q \approx 3.567 \pm 3.158i$.

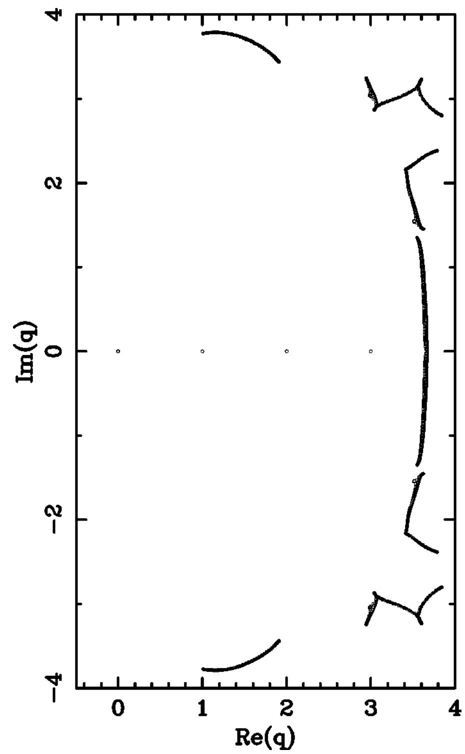

FIG. 6. Chromatic zeros for the $(K_{4,4})^m$ graph for (a) $m = L_z = 40$, i.e., $n = 320$ (□), (b) $m = L_z = 80$, i.e. $n = 640$ (○).

VII. CONCLUSIONS

In this paper we have reported exact solutions for the zero-temperature partition function of the q-state Potts antiferromagnet on tubes of the simple cubic lattice with various transverse cross sections and boundary conditions and with arbitrarily great length. We have used these to calculate, in the infinite-length limit, the resultant ground-state degeneracy per site W and the singular locus $\mathcal{B}$ which is the continuous accumulation set of the chromatic zeros. In particular, we have calculated the value of q_c or $(q_c)_{\rm eff}$ for these infinite-length tubes. Our results show quantitatively how this quantity increases as the effective coordination number for a given family of graphs increases and are a step toward determining q_c is for the infinite simple cubic lattice. We have also presented similar calculations for another interesting family of tube graphs whose transverse cross section is formed from the complete bipartite graph $K_{m,m}$.

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can always define the partition function for the Potts antiferromagnet as $Z(G,q,v)=\Sigma_{\sigma_i}\exp(-\beta\mathcal{H})$ where $\beta=(k_BT)^{-1}$ and $\mathcal{H}=-J\Sigma_{\langle ij\rangle}\delta_{\sigma_i,\sigma_j}$ with $J<0$, which obviously has a Gibbs measure.
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