Exact $T = 0$ Partition Functions for Potts Antiferromagnets on Sections of the Simple Cubic Lattice

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Abstract

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 $2 \times 4$ and boundary conditions (a) $(FBC_x, FBC_y, FBC_z)$ and (b) $(PBC_x, FBC_y, FBC_z)$, where $FBC$ ($PBC$) denote free (periodic) boundary conditions. In the limit of infinite-length, $L_z \rightarrow \infty$, 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 $L_z \rightarrow \infty$ 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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1 Introduction

The $q$-state Potts antiferromagnet (PAF) \[1, 2\] exhibits nonzero ground state entropy, $S_0 > 0$ (without frustration) for sufficiently large $q$ on a given lattice $\Lambda$ 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-mole), i.e., $S_0/R = 0.41 \pm 0.03$, where $R = N_{\text{Avog}} k_B$ \[5\]. 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

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

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

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

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 $q_s = 0, 1, .., \chi(G)$), one has the noncommutativity of limits \[\[11\]

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

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 \[\[1.3\], 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 $B$ intersects the (positive) real axis. For some families of graphs, $B$ 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, $B$ often includes complex-conjugate arcs with endpoints close to the positive real axis, and hence, in these cases, it can be useful to define a quantity $(q_c)_{\text{eff}}$ equal to the real part of the endpoints. 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 length $L_z$, for cross sections $L_x \times L_y = 3 \times 2$ and $4 \times 2$. These calculations are carried out for the cases (a) $(FBC_x, FBC_y, FBC_z)$ (rectangular solid) and (b) $(PBC_x, FBC_y, FBC_z)$ (homeomorphic to an annular cylindrical solid), where $FBC_i$ and $PBC_i$ denote free and periodic boundary conditions in the $i$'th direction, respectively. We shall use the notation $(L_i)_F$ and $(L_i)_P$ to denote free and periodic boundary conditions in the $i$'th 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 $3_F \times 2_F \times (L_z)_F$ and $3_P \times 2_F \times (L_z)_F$, respectively. For each family of graphs, taking the infinite-length limit $L_z \to \infty$, we calculate $W(\{G\}, q)$, $B$, 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 $q = 3$ [13]. 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 $(q_c)_{\text{eff}}$ 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 $q_c$ which 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, $\lim_{L_x,L_y \to \infty} q_c(s_c, (L_x)_{BCx} \times (L_y)_{BCy} \times F)$ is not equal to, but instead less than, the value $q_c(s_c)$ 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, $\lim_{L_y \to \infty} q_c((L_y)_P \times \infty_F) \approx 3.81967...$ 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 $\sim 3.82$. 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 2D lattice strips with free longitudinal boundary conditions (for both free and periodic transverse boundary conditions) [31, 43, 44, 47, 50]. Calculations for $L_P \times \infty_F$ (i.e. cylindrical) strips of the square lattice have been carried out in [31, 46, 47, 50] with widths $L$ extending.
up to 13 [51], with \( q_c(sq, 13\times\infty_F) \simeq 2.916 \). This value is within about 3\% of the value for the infinite square lattice, \( q_c(sq) = 3 \). As the width increases, the endpoints of the prongs do move in toward the real axis. These calculations for \( L_p \times \infty_F \) strips of the square lattice are consistent with either of the two possibilities, that \( \lim_{L \to \infty} q_c(sq, L_p \times \infty_F) \) is equal to, or slightly less than, \( q_c(sq) \).

It is interesting that the exact calculations of the singular loci \( B \) 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, 40, 49, 45]. For these families of strips it was found that \( B \) always crossed the positive real axis at \( q = 0 \) and at a maximal point, so \( q_c \) is always defined; furthermore, \( L_F \times \infty_P \), the value of \( q_c \) is a monotonically nondecreasing function of the width. For \( L_P \times \infty_P \) 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 \( \Delta \)-regular iff each of its vertices has the same degree, \( \Delta \). 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,

\[
\Delta_{\text{eff}} = \lim_{|V| \to \infty} \frac{2|E|}{|V|} .
\]

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

\[
\Delta_{\text{eff}}(sq, (L_x)_F \times (L_y)_F; L_x \to \infty) = 4 - \frac{2}{L_y} .
\]

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

\[
\Delta_{\text{eff}}(sq, (L_x)_F \times (L_y)_P; L_x \to \infty) = 4 .
\]

For the \((L_x)_F \times (L_y)_F \times (L_z)_F\) 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 \(2_F \times 2_F \times (L_z)_F\), there are no interior vertices in the 3D sense, so that

\[
\Delta_{\text{eff}}(sc, 2_F \times 2_F \times (L_z)_F; L_z \to \infty) = 4 .
\]
For the next case \((L_x)_F \times 2_F \times (L_z)_F\) with \(L_x \geq 3\) there are also no interior vertices in the 3D sense; in this case

\[
\Delta_{\text{eff}} (sc, (L_x)_F \times 2_F \times (L_z)_F; FBC_x, FBC_y, FBC_z; L_z \to \infty) = 5 - \frac{2}{L_x} .
\] (1.8)

For the \(L_z \to \infty\) limit of the \(L_x \times L_y \times L_z\) section with \(L_x \geq 3, L_y \geq 3\), we have

\[
\Delta_{\text{eff}} (sc, (L_x)_F \times (L_y)_F \times (L_z)_F; L_z \to \infty) = 6 - 2\frac{(L_x + L_y)}{L_x L_y} .
\] (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 \(E^d\), with \(L_i \to \infty, i = 1, ..., d\) and \(\lim_{L_i \to \infty} L_i / L_j\) equal to a finite nonzero constant, the effective degree is \(\Delta_{\text{eff}} (E^d) = 2d\) independent of boundary conditions.

In this case, although free boundary conditions in one or more directions entails 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

\[
\chi (sc, (L_x)_F \times (L_y)_F \times (L_z)_F) = 2
\] 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,

\[
\chi (sc, (L_x)_P \times (L_y)_F \times (L_z)_F) = \begin{cases} 
2 & \text{if } L_x \text{ is even} \\
3 & \text{if } L_x \text{ is odd} 
\end{cases}
\] (1.11)

For an infinite regular lattice having coordination number \(\Delta\), a rigorous upper bound on \(q_c\) was derived in \cite{13} using the Dobrushin theorem:

\[
q_c \leq 2\Delta .
\] (1.12)

Aside from the general property that, for cases where there is a \(q_c\), this point satisfies \(q_c \geq 2\), 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, \(B\) does not necessarily intersect or cross the real \(q\) axis, and for such a family, 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 \(B\) 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 \(n \to \infty\).
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 $\Delta_{eff}$. Thus, for the family of cyclic strips of the square lattice with free transverse boundary conditions, whose $1_F \times \infty_F$ case with $\Delta = 2$ and $q_c = 2$, one finds the following results: (i) $2_F \times \infty_F$ ($\Delta = 3$) yields $q_c = 2$ \[1\], (ii) $3_F \times \infty_F$ ($\Delta_{eff} = 10/3$) yields $q_c \approx 2.3365$ \[10\], (iii) $3_F \times \infty_F$ ($\Delta_{eff} = 7/2$) yields $q_c \approx 2.4928$ \[10\]. 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 $3_F \times \infty_P$ strip yields $q_c = 3$ \[10\] while the $4_F \times \infty_P$ strips yields the smaller value $q_c \approx 2.78$ \[49\].

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 $(q_c)_{eff}$, where the latter can be defined, is a monotonically increasing function of $L_y$, and since in these families of lattice strips, $\Delta_{eff}$ is a monotonically increasing function of $L_y$, this means that $(q_c)_{eff}$ is also a monotonically increasing function of $\Delta_{eff}$. Thus, for $1_F \times \infty_F$ with $\Delta_{eff} = 2$ and $2_F \times \infty_F$ with $\Delta_{eff} = 3$, $B = \emptyset$ and there is no $(q_c)_{eff}$, while $3_F \times \infty_F$ with $\Delta_{eff} = 10/3$ yields $q_c = 2$ \[30\], $4_F \times \infty_F$ with $\Delta_{eff} = 7/2$ yields $q_c \approx 2.3014$ \[30\], $5_F \times \infty_F$ with $\Delta_{eff} = 3.60$ yields $q_c \approx 2.428$ \[40, 47\], etc. up to $8_F \times \infty_F$ with $\Delta_{eff} = 3.75$, which yields arc endpoints at $q \approx 2.6603 \pm 0.0013i$ and hence $(q_c)_{eff} = 2.6603$ \[47\].

In contrast, for strips with free longitudinal and periodic transverse boundary conditions, $\Delta_{eff}$ is fixed, e.g., equal to 4 for strips of the square lattice. Insofar as one expects $q_c$ or $(q_c)_{eff}$ to depend on $\Delta_{eff}$, it is not clear, a priori, how these quantities should behave as functions of $L_y$. Indeed, one finds that $q_c$ or $(q_c)_{eff}$ have no monotonic dependence on $L_y$. For example, for $3_F \times \infty_F$, $B = \emptyset$, 4$F \times \infty_F$ yields $q_c \approx 2.3517$ \[31\], 5$F \times \infty_F$ yields $q_c \approx 2.6917$ \[46, 17\], but 6$F \times \infty_F$ yields $q_c \approx 2.6132$ \[46, 17\]. For 7$F \times \infty_F$, $B$ has arc endpoints near the real axis at $q \approx 2.7515 \pm 0.0025i$, so $(q_c)_{eff} \approx 2.7515$ \[17\]. For the cases $(L_y)P \times \infty$ up to $L = 11$, it is found empirically that $q_c$ or $(q_c)_{eff}$ 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 $d \geq 2$ 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 \( \Delta_{\text{eff}} \) is. Therefore, as one increases \( \Delta_{\text{eff}} \) 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 \( d \geq 3 \).

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

\[
R_{q_c} = \frac{q_c}{2\Delta}.
\]

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, \( N_{\lambda} \leq \dim(T) \), where
dim(T) is the dimension of the transfer matrix in the Fortuin-Kasteleyn representation, and the difference, \( N_0 = \dim(T) - N_\lambda \), 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 \( q \)).

2 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 Section 3 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 \( v_P \) are indexed by partitions \( P \) of the single-layer vertex set \( V^0 \). We shall abbreviate delta functions \( \delta(\sigma_1, \sigma_3) \) as \( \delta_{1,3} \). Moreover, we shall also abbreviate partitions \( P \) by writing instead the corresponding product \( v_P \) of delta functions: e.g., in place of \( P = \{\{1, 3\}, \{2, 4\}, \{5\}\} \) we shall write simply \( P = \delta_{1,3}\delta_{2,4} \). The transfer matrix can be expressed as

\[
T = V H
\]  (2.1)

where the matrices \( H \) and \( V \) are defined as

\[
H = \prod_{<xx'> \in E^0} [I - J_{xx'}] \quad (2.2)
\]

\[
V = \prod_{x \in V^0} [-I + D_x] \quad (2.3)
\]

In these formulae \( E^0 \) 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 \( v_P \) is as follows

\[
J_{xx'} v_P = v_{P \bullet xx'} \quad (2.4)
\]

\[
D_x v_P = \begin{cases} v_{P \setminus x} & \text{if } \{x\} \notin P \\ q v_P & \text{if } \{x\} \in P \end{cases} \quad (2.5)
\]

where \( P \bullet xx' \) is the partition obtained from \( P \) by amalgamating the blocks containing \( x \) and \( x' \) (if they were not already in the same block); and \( P \setminus x \) is the partition obtained from \( P \) by detaching \( x \) from its block (and thus making it what we term a “singleton”). In eq. (2.5)
we have written the formulae 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

$$Z(L_x \times L_y \times L_z; q) = u^T \cdot H (VH)^{L_z-1} \cdot v_{id} \quad (2.6)$$

where “id” denotes the partition in which each site $x \in V^0$ is a singleton, and $u^T$ is defined by

$$u^T \cdot v_P = q^{|P|} \quad (2.7)$$

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 $T' = HVH$ in place of $T = VH$, and using the basis vectors

$$w_P = H v_P \quad (2.8)$$

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

The computation of the limiting curves $B$ was performed with either the resultant and 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].

2.1 $2_F \times 2_F \times (L_z)_F$ Section of the Simple Cubic Lattice

Before proceeding to our new results, we note the identity

$$sc(2_F \times 2_F \times (L_z)_F) = sq(4_F \times (L_z)_F) \quad (2.1.1)$$

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 section 7 of [31] and, in the infinite-length limit, $W$ and $B$ 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 [31]-[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:

$$\Gamma(G_s, q, z) = \sum_{m=0}^{\infty} P((G_s)_m, q) z^m, \quad (2.1.2)$$
This generating function is a rational function of $q$ and $z$. For the strip considered here, of length $L_z = m$ edges,

$$\Gamma(G_s, q, z) = \frac{a_0 + a_1 z}{1 + b_1 z + b_2 z^2}$$

where

$$a_0 = q(q - 1)(q^2 - 3q + 3)$$

$$a_1 = -q(q - 1)(q^4 - 7q^3 + 16q^2 - 13q + 5)$$

$$b_1 = -q^4 + 8q^3 - 29q^2 + 55q - 46$$

$$b_2 = q^6 - 12q^5 + 61q^4 - 169q^3 + 269q^2 - 231q + 85$$

(Here we have converted the numerator coefficients from [31] to be in accord with the labelling convention of eq. (2.1.2); in the labelling convention of [31], the strip with length $m + 1$ edges.) The chromatic polynomial can equivalently be written as in 2.6: in the basis $P = \{1, \delta_1, 4 + \delta_2, 3\}$ it is given by

$$Z(2F \times 2F \times (L_z)_F; q) = \left( \begin{array}{c} q(q - 1)(q^2 - 3q + 3) \\ 2q(q - 1)^2 \end{array} \right)^T \cdot T(2F \times 2F)^{L_z - 1} \cdot \left( \begin{array}{c} 1 \\ 0 \end{array} \right)$$

The transfer matrix $T(2F \times 2F)$ is equal to

$$T(2F \times 2F) = \left( \begin{array}{cc} 41 - 51q + 28q^2 - 8q^3 + q^4 & 2(-12 + 14q - 6q^2 + q^3) \\ -5 + 2q & 5 - 4q + q^2 \end{array} \right)$$

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 (2.1.1) is planar and $\delta_{1,4}\delta_{3,2}$ is a crossing partition.

For this family, $B$ consists of two complex-conjugate arcs, a self-conjugate arc that crosses the real axis at $q \approx 2.3026$, and a line segment on this axis extending from $q \approx 2.2534$ to $q \approx 2.3517$, which latter point is thus $q_c$. It should be noted also that although this graph is included here as the minimal-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 $B$; two of them are given by the real values $q \approx 2.3026$ and $q \approx 2.3517$; the other six endpoints are the complex-conjugate pairs $q \approx 0.7098 \pm 2.0427 i$, $q \approx 1.9923 \pm 1.5942 i$, and $q \approx 2.9953 \pm 1.4266 i$.

## 2.2 3F × 2F × (Lz)F Section of Simple Cubic Lattice

The section of the simple cubic lattice with the next larger transverse cross section is the $3F \times 2F \times (L_z)_F$, or equivalently, $2F \times 3F \times (L_z)_F$, 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 \( B \). As is generally true, for the larger value of \( L_z \), and hence \( n \), the chromatic zeros move slightly outward, approaching the limiting curve \( B \) from smaller values of \(|q|\).

![Zeros sc lattice](image)

Figure 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., \( n = 180 \) (○).

The limiting curve \( B \) 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
Table 1: Results for tube graphs of the simple cubic lattice. The table shows the relation between the degree (coordination number) \( \Delta \) of a \( \Delta \)-regular family or the effective degree \( \Delta_{\text{eff}} \), 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 \( B \) does not actually cross the real axis, so that, strictly speaking, no \( q_c \) is defined, but arcs on \( B \) end very close to the real axis, at the positions given. Similar results are listed for the tubes with \( K_{m,m} \) cross sections.

| \( G_s \) | \( \Delta \) | \( \Delta_{\text{eff}} \) | \( q_c \) | 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 ± 0.0184i* | here |
| sc, \( 4_P \times 2_P \times \infty_F \) | – | 5 | 3.3623 ± 0.0061i* | here |
| \( K_{2,2} \times \infty_F \) | – | 4 | 2.3517 | [31] |
| \( K_{3,3} \times \infty_F \) | – | 5 | 3.0452 ± 0.0082i* | here |
| \( K_{4,4} \times \infty_F \) | – | 6 | 3.6743 ± 0.0085i* | here |

is listed, together with that from other lattices, in Table [1]. 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: \( q \simeq 0.2943 ± 1.9150i \), \( q \simeq 1.9371 ± 2.4040i \), \( q \simeq 2.6374 ± 1.0937i \), \( q \simeq 2.8250 ± 1.4087i \), \( q \simeq 2.6255 ± 1.4647i \), \( q \simeq 3.2410 ± 1.2920i \), and \( q \simeq 2.2645 ± 2.4605i \). Finally, there are four T points at \( q \simeq 2.670 ± 1.117i \) and \( q \simeq 2.689 ± 1.500i \).

### 2.3 \( 4_F \times 2_F \times (L_z)_F \) 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 \( \mathbf{u}_{ld} \) can be found in the MATHEMATICA file \texttt{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. [4].

The limiting curve \( B \) 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 \( (q_c)_{\text{eff}} \approx 3.1498 \). 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 endpoints: \( q \simeq 0.073 ± 1.747i \), \( q \simeq 1.582 ± 2.845i \), \( q \simeq 1.684 ± 2.871i \), \( q \simeq
Figure 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., $n = 320$ (○).
2.379 ± 2.503i, q ≃ 2.513 ± 1.569i, q ≃ 2.661 ± 1.816i, q ≃ 2.697 ± 1.889i, q ≃ 3.034 ± 1.367i, q ≃ 3.035 ± 1.385i, q ≃ 3.150 ± 0.002i, and q ≃ 3.383 ± 1.157i. Finally, there are three pairs of complex-conjugate T points: q ≃ 2.381 ± 2.404i, q ≃ 2.695 ± 1.793i, and q ≃ 2.972 ± 1.578i.

3 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 Section 2. The only difference is that we enlarge the single-layer edge set $E^0$.

3.1 $2p \times 2p \times (L_z)_F$ Section of Simple Cubic Lattice

This family has (trivially) the same chromatic polynomials as the family $sc(2p \times 2p \times (L_z)_F$. (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 (2.1) and (2.6).

3.2 $3p \times 2p \times (L_z)_F$ 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 $B$ 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 $P = \{1, \delta_{2,4} + \delta_{2,6} + \delta_{1,5} + \delta_{3,5} + \delta_{1,6} + \delta_{3,4}, \delta_{1,5} \delta_{2,6} + \delta_{2,4} \delta_{3,5} + \delta_{3,4} \delta_{1,5} + \delta_{3,4} \delta_{2,6} + \delta_{1,6} \delta_{3,5} + \delta_{1,6} \delta_{2,4}, \delta_{1,6} \delta_{3,4} + \delta_{1,5} \delta_{2,4} + \delta_{2,6} \delta_{3,5}\}$, the transfer matrix can be written as

$$T(3p \times 2p) = \begin{pmatrix} T_{11} & T_{12} & T_{13} & T_{14} \\ T_{21} & T_{22} & T_{23} & T_{24} \\ 1 & 2(-3 + q) & 12 - 6q + q^2 & -2(-4 + q) \\ 0 & -2 & -4(-3 + q) & 15 - 7q + q^2 \end{pmatrix} \quad \text{(3.2.1)}$$

where

$$T_{11} = 1089 - 1578q + 1054q^2 - 417q^3 + 103q^4 - 15q^5 + q^6 \quad \text{(3.2.2)}$$

$$T_{12} = 6(-292 + 394q - 231q^2 + 74q^3 - 13q^4 + q^5) \quad \text{(3.2.3)}$$

$$T_{13} = 6(110 - 117q + 51q^2 - 11q^3 + q^4) \quad \text{(3.2.4)}$$

$$T_{14} = 3(154 - 149q + 60q^2 - 12q^3 + q^4) \quad \text{(3.2.5)}$$
\[ T_{21} = -90 + 71q - 20q^2 + 2q^3 \] (3.2.6)  
\[ T_{22} = 203 - 189q + 71q^2 - 13q^3 + q^4 \] (3.2.7)  
\[ T_{23} = -109 + 80q - 21q^2 + 2q^3 \] (3.2.8)  
\[ T_{24} = -81 + 52q - 12q^2 + q^3 \] (3.2.9)

The vectors \( \mathbf{v} \) and \( \mathbf{u}_{id} \) are given by

\[
\mathbf{v} = \begin{pmatrix} \frac{(-2 + q)(-1 + q)(-13 + 14q - 6q^2 + q^3)}{6(-2 + q)^3(-1 + q)q} \\
\frac{6(-2 + q)^3(-1 + q)q}{6(-2 + q)^2(-1 + q)q} \\
\frac{3(-3 + q)(-2 + q)(-1 + q)q}{1} \\
0 \\
0 \\
0 \end{pmatrix}
\] (3.2.10)

\[
\mathbf{u}_{id} = \begin{pmatrix} 1 \\
0 \\
0 \end{pmatrix}
\] (3.2.11)

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 \( B \) contains three pairs of self-conjugated arcs. Although the arcs do not cross the real axis, so that, strictly speaking, no \( q_c \) is defined, \((q_c)_{eff} \approx 3.33\), which is larger than the value \( q_c = 3 \) for the square lattice. The locus \( B \) has 12 endpoints: \( q \approx 0.5061 \pm 2.6413i \), \( q \approx 2.1301 \pm 2.4407i \), \( q \approx 3.0251 \pm 2.5249i \), \( q \approx 3.0412 \pm 1.2643i \), \( q \approx 2.9328 \pm 1.1238i \), and \( q \approx 3.3255 \pm 0.01839i \).

### 3.3 4p \( \times \) 2p \( \times \) (\( L_z \))\( F \) 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 \( \mathbf{v} \) and \( \mathbf{u}_{id} \) 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 \( B \) (see Fig. 4) contains eight self-conjugate arcs. As in the 4p \( \times \) 2p \( \times \) \( \infty_F \) 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 \((q_c)_{eff} \approx 3.36\). As expected, this is larger than the value \((q_c)_{eff} \approx 3.33\) that we found for the tube 3p \( \times \) 2p \( \times \) \( \infty_F \). There are nine pairs of complex-conjugate endpoints: \( q \approx -0.095 \pm 2.700i \), \( q \approx 1.803 \pm 3.031i \), \( q \approx 2.176 \pm 3.196i \), \( q \approx 2.841 \pm 1.954i \), \( q \approx 2.910 \pm 2.080i \), \( q \approx 3.263 \pm 1.333i \), \( q \approx 3.279 \pm 1.377i \), \( q \approx 3.362 \pm 0.006i \), and \( q \approx 3.892 \pm 1.542i \). Finally, there is one pair of complex-conjugate T points: \( q \approx 3.204 \pm 1.665i \).
Figure 3: Chromatic zeros for the $2_p \times 3_p \times (L_z)_P$ section of the simple cubic lattice, for (a) $L_z = 15$, i.e., $n = 90$ (□), (b) $L_z = 30$, i.e., $n = 180$ (○).
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 endpoints 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 $L_P \times \infty_F$ 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 endpoints 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, 45, 49, 47] 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 $q = 0$, $q_c(sc)$, and other point(s) between these two.

4 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 of 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 $L_F \times \infty_P$ and $L_P \times \infty_P$ 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 $L_P \times \infty_F$ strips or in [31] for $L_F \times \infty_F$ strips of the triangular lattice do not, in general, cross the real axis at $q = 2$, nor is
Figure 4: Chromatic zeros for the $2_p \times 4_p \times (L_z)_F$ section of the simple cubic lattice, for (a) $L_z = 20$, i.e., $n = 160$ (□), (b) $L_z = 40$, i.e., $n = 320$ (○).
this crossing obtained for the infinite-width limit of the cylindrical strips calculated in [23]. Similarly, for $L_F \times \infty_P$ and $L_P \times \infty_P$ 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 endpoints 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 $(L_x)_P \times (L_y)_P \times \infty_F$ with sufficiently large transverse cross section, namely $L_x = 4$, $L_y = 2$, $\mathcal{B}$ contains support in the $\text{Re}(q) < 0$ 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 $L_x L_y \to \infty$, the complex-conjugate curves on $\mathcal{B}$ could approach the origin from the $\text{Re}(q) < 0$ half-plane, as happens for the limit $L \to \infty$ of $L_P \times \infty_F$ strips of the triangular lattice [23] and sufficiently wide strips of the square lattice of the form $L_F \times \infty_F$ [30, 17], $L_P \times \infty_F$ [46, 17, 50], and $L_F \times \infty_P$ [36, 38, 16].

5 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]

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

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 $W(\mathbb{E}^2, q = 3) = (4/3)^{3/2} = 1.5396..$ [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
\[ d_c(q) = \frac{\ln(q - 1)}{\ln\left(\frac{(q-1)}{(q-2)}\right)}. \] (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
\[ q_c(d = 3) \approx 4.15 \] (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
\[ q_c \sim \frac{d}{\ln d} \quad \text{for} \quad d \to \infty. \] (5.4)

This is in agreement with the upper bound (1.12)
\[ q_c \leq 4d \] (5.5)

and evidently is a smaller and smaller fraction of this upper bound as \( d \) gets large, with
\[ R_{q_c} \sim \frac{1}{4\ln d} \quad \text{for} \quad d \to \infty. \] (5.6)

6 Family \( (K_{m,m})^{L_z} \)

It is also useful to calculate \( B \) 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 \( \Delta \)-regular graphs 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 \( \Delta_{\text{eff}} \) is for this family
\[ \Delta_{\text{eff}} \left( (K_{m,m})^{L_z}; FBC_z; L_z \to \infty \right) = m + 2. \] (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 formulae (2.1)/(2.7). The only difference is the single-layer edge set \( E^0 \).
6.1 Family \((K_{2,2})^{L_z}\)

The family \((K_{2,2})^{L_z}\) is trivially equivalent to the family \(sq(4_P \times L_F)\), so by (2.1.1) it is also equivalent to the family \(sc(2_F \times 2_F \times (L_2)_F)\) The transfer matrix, written in the basis \(P = \{1, \delta_{1,2} + \delta_{3,4}\}\), takes the same form as (2.1.9); and the partition function is equivalent to (2.1.8).

6.2 Family \((K_{3,3})^{L_z}\)

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

\[
T(K_{33}) = \begin{pmatrix}
T_{11} & T_{12} & T_{13} & T_{14} & T_{15} \\
T_{21} & T_{22} & T_{23} & T_{24} & T_{25} \\
T_{31} & T_{32} & T_{33} & T_{34} & T_{35} \\
1 & 2(-3 + q) & 0 & T_{44} & 2(-2 + q) \\
0 & 1 & 0 & -3 & 2 - q
\end{pmatrix} \quad (6.2.1)
\]

where

\[
T_{11} = 1234 - 1747q + 1137q^2 - 437q^3 + 105q^4 - 15q^5 + q^6 \quad (6.2.2)
\]
\[
T_{12} = 6(-252 + 337q - 198q^2 + 65q^3 - 12q^4 + q^5) \quad (6.2.3)
\]
\[
T_{13} = 2(36 - 56q + 33q^2 - 9q^3 + q^4) \quad (6.2.4)
\]
\[
T_{14} = 9(89 - 94q + 43q^2 - 10q^3 + q^4) \quad (6.2.5)
\]
\[
T_{15} = 6(-25 + 24q - 8q^2 + q^3) \quad (6.2.6)
\]
\[
T_{21} = -113 + 91q - 27q^2 + 3q^3 \quad (6.2.7)
\]
\[
T_{22} = 174 - 153q + 54q^2 - 10q^3 + q^4 \quad (6.2.8)
\]
\[
T_{23} = -10 + 13q - 6q^2 + q^3 \quad (6.2.9)
\]
\[
T_{24} = 3(-40 + 28q - 8q^2 + q^3) \quad (6.2.10)
\]
\[
T_{25} = 29 - 21q + 4q^2 \quad (6.2.11)
\]
\[
T_{31} = 55 - 27q + 3q^2 \quad (6.2.12)
\]
\[
T_{32} = -3(29 - 17q + 3q^2) \quad (6.2.13)
\]
\[
T_{33} = 9 - 12q + 6q^2 - q^3 \quad (6.2.14)
\]
\[
T_{34} = -18(-3 + q) \quad (6.2.15)
\]
\[
T_{35} = -3(7 - 5q + q^2) \quad (6.2.16)
\]
\[ T_{44} = 12 - 5q + q^2 \]  \hspace{1cm} (6.2.17)

Finally,

\[
\mathbf{v} = \begin{pmatrix}
(-1 + q)(31 - 47q + 28q^2 - 8q^3 + q^4) \\
6(-1 + q)(-7 + 10q - 5q^2 + q^3)
\end{pmatrix}
\]

\[
\mathbf{u}_{id} = \begin{pmatrix}
1 \\
0 \\
0 \\
0
\end{pmatrix}
\]  \hspace{1cm} (6.2.18)

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. 3, as well as the limiting curve \(B\). The limiting curve \(B\) 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 \(q_c \approx 3.045\), which is slightly greater than the value for the square lattice \(q_c = 3\).

There are 14 endpoints: \(q \approx 0.8197 \pm 2.9764i\), \(q \approx 1.9761 \pm 2.5559i\), \(q \approx 2.8190 \pm 1.5587i\), \(q \approx 2.9364 \pm 2.5742i\), \(q \approx 3.6220 \pm 2.0051i\), \(q \approx 3.0283 \pm 1.3476i\), and \(q \approx 3.0452 \pm 0.008246i\).

There are two complex-conjugated T points at \(q \approx 2.949 \pm 1.870i\).

### 6.3 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 \textsc{Mathematica} file \texttt{transfer.Knn_tube.m} that is available with this paper in the LASL cond-mat archive.

There are eight connected pieces (See Figure 3), 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 \(q \approx 3.567 \pm 3.158i\).
Figure 5: Chromatic zeros for the \((K_{3,3})^m\) graph for (a) \(m = L_z = 15\), i.e., \(n = 90\), \(\bullet\), (b) \(m = L_z = 30\), i.e. \(n = 180\), \(\circ\).
Figure 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. \(n = 640\) (○).
7 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 \( B \) which is the continuous accumulation set of the chromatic zeros. In particular, we have calculated the value of \( q_c \) or \( (q_c)_{\text{eff}} \) 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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[12] We comment here on cases where \(q_c(\{G\})\) is non-integral. The Potts antiferromagnet can formally be defined for positive real, as well as integral, \(q\), via the formula

\[
Z(G, q, v) = \sum_{G' \subseteq G} q^{k(G')} v^{e(G')},
\]

where \(G'\) is a spanning subgraph of \(G\) (i.e. a subgraph containing all of the vertices and a subset of the edges of \(G\)), and \(k(G')\) and \(e(G')\) denote the number of connected components and edges in \(G'\). However, since \(-1 \leq v \leq 0\) for the Potts antiferromagnet, this model does not, in general, have a Gibbs measure for non-integral \(q\), and this can lead to unphysical behavior \([13, 14]\) such as negative specific heat and non-existence of a thermodynamic limit independent of boundary conditions.

In contrast, for positive integral \(q\), one can always define the partition function for the Potts antiferromagnet as

\[
Z(G, q, v) = \sum_{\sigma} \exp(-\beta H)\]

where \(\beta = (k_B T)^{-1}\) and

\[
H = -J \sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j}
\]

with \(J < 0\), which obviously has a Gibbs measure.

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