Ground State Degeneracy of Potts Antiferromagnets on 2D Lattices: Approach Using Infinite Cyclic Strip Graphs

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The \(q\)-state Potts antiferromagnet on a lattice \(\Lambda\) exhibits nonzero ground state entropy \(S_0 = k_B \ln W\) for sufficiently large \(q\) and hence is an exception to the third law of thermodynamics. An outstanding challenge has been the calculation of \(W(sq, q)\) on the square (sq) lattice. We present here an exact calculation of \(W\) on an infinite-length cyclic strip of the square lattice which embodies the expected analytic properties of \(W(sq, q)\). Similar results are given for the kagomé lattice.

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Nonzero ground state entropy, $S_0 \neq 0$, is an important subject in statistical mechanics as an exception to the third law of thermodynamics (e.g., [1]). This is equivalent to a ground state degeneracy per site $W > 1$, since $S_0 = k_B \ln W$. The $q$-state Potts antiferromagnet (AF) exhibits nonzero ground state entropy (without frustration) for sufficiently large $q$ on a given lattice $\Lambda$, or more generally, a given graph $G$, and serves as a valuable model for the study of this phenomenon. The zero-temperature partition function of the above-mentioned $q$-state Potts AF on $G$ satisfies $Z(G, q, T = 0)_{P_{AF}} = P(G, q)$, where $P(G, q)$ is the chromatic polynomial (in $q$) expressing the number of ways of coloring the vertices of the graph $G$ with $q$ colors such that no two adjacent vertices have the same color [2,3]. Thus, $W(G, q) = \lim_{n \to \infty} P(G, q)^{1/n}$, where $n = v(G)$ is the number of vertices of $G$ and $\{G\} = \lim_{n \to \infty} G$. $W(G, q)$ has been calculated exactly for the triangular lattice [4] and various families of graphs [5, 6, 7]. The special values for the square (sq) and kagomé (kg) lattices $W(sq, 3)$ [8] and $W(kg, 3)$ (which can be extracted from [17,8]) are also known. However, aside from the triangular case, the exact calculation of $W(A, q)$ for general $q$ on lattices $A$ of dimensionality $d \geq 2$ remains an outstanding challenge. In this work we report exact calculations of $W$ on infinite-length, finite-width strips of the square and kagomé lattices that exhibit the analytic properties expected for the $W$ functions on the respective full 2D lattices and, in this sense, constitute the closest exact results that one has to these $W$ functions.

Let us describe these analytic properties. Denote $\lim_{n \to \infty} G = \{G\}$. Since $P(G, q)$ is a polynomial, one can generalize $q$ from $\mathbb{Z}_+ \to \mathbb{R}$ and indeed $\mathbb{C}$. $W(G, q)$ is a real analytic function for real $q$ down to a minimum value, $q_c(\{G\})$ [4,5]. For a given $\{G\}$, we denote the continuous locus of non-analyticities of $W$ as $B$. This locus $B$ forms as the accumulation set of the zeros of $P(G, q)$ (chromatic zeros of $G$) as $n \to \infty$ [19, 21, 22] and satisfies $B(q) = B(q^*)$. In cases where $B$ serves as a natural boundary, dividing the $q$ plane into different regions, $W$ has different analytic forms in these different regions. The point $q_c$ is the maximal point where $B$ intersects the real axis, which can occur via $B$ crossing this axis or via a line segment of $B$ lying along the axis. The chromatic polynomial $P(G, q)$ has a general decomposition as $P(G, q) = c_0(q) + \sum_j c_j(q)(a_j(q))^{t_j^q}$ where the $a_j(q)$ and $c_j \neq 0(q)$ are independent of $n$, while $c_0(q)$ may contain $n$-dependent terms, such as $(-1)^n$, but does not grow with $n$ like $(\text{const.})^n$ with $|\text{const.}| > 1$, and $t_j$ is a $G$-dependent constant. A term $a_\ell(q)$ is “leading”($\ell$) if it dominates the $n \to \infty$ limit of $P(G, q)$. The locus $B$ occurs where there is an abrupt nonanalytic change in $W$ as the leading terms $a_\ell$ changes; thus the locus $B$ is the solution to the equation of degeneracy of magnitudes of leading terms. Hence, $W$ is finite and continuous, although nonanalytic, across $B$.

From exact calculations of $W$ on a number of families of graphs we have inferred several
general results on $\mathcal{B}$: (i) for a graph $G$ with well-defined lattice structure, a sufficient condition for $\mathcal{B}$ to separate the $q$ plane into different regions is that $G$ contains at least one global circuit, defined as a route following a lattice direction which has the topology of the circle $S^1$ and a length $\ell_{g.c.}$ that goes to infinity as $n \to \infty$ \cite{10,22}. For a $d$-dimensional lattice graph, the existence of global circuits is equivalent to having periodic boundary conditions (BC’s) in at least one direction. Further, (ii) the general condition for a family $\{G\}$ to have a locus $\mathcal{B}$ that is noncompact (unbounded) in the $q$ plane \cite{11} shows that a sufficient (not necessary) condition for $\{G\}$ to have a compact, bounded locus $\mathcal{B}$ is that it is a regular lattice \cite{11,12,15}. The third and fourth general features are that for graphs that (a) contain global circuits, (b) cannot be written in the form $G = K_p + H$ \cite{9,23}, and (c) have compact $\mathcal{B}$, we have observed that $\mathcal{B}$ (iii) passes through $q = 0$ and (iv) crosses the positive real axis, thereby always defining a $q_c$.

From exact calculations of $W$ for a number of infinite-length, finite-width (homogeneous) strips of 2D lattices with free boundary conditions in the longitudinal direction (and free or periodic BC’s in the transverse direction) \cite{10,13}, it is found that the resultant loci $\mathcal{B}$ consist of arcs (and possible real line segments) which, although compact, do not separate the $q$ plane into different regions, do not pass through $q = 0$ and, for the arcs, do not necessarily intersect the real $q$ axis. These calculations showed that as the strip width $L_y$ increases, the complex-conjugate (c.c.) arcs comprising $\mathcal{B}$ tend to elongate so that the gaps between them decrease, and the left endpoints of the c.c. arcs nearest to $q = 0$ move toward this point, thereby leading to the inference that in the limit $L_y \to \infty$, these arcs will close to form one or more regions, and $\mathcal{B}$ will pass through $q = 0$ and will cross the positive real axis at one or more points, thereby defining a $q_c$. In turn, this motivates the conclusion that the properties (i)-(iv) hold for $W(\Lambda, q)$ and $\mathcal{B}$ on a lattice $\Lambda$ (in the thermodynamic limit, independent of the boundary conditions used). The advantage of cyclic strip graphs is that these properties are present for each finite $L_y$ rather than only being approached in the limit $L_y \to \infty$ as for open strips.

Our method for obtaining exact $W$ functions that exhibit the analytic properties expected for $W$ on a 2D lattice is as follows. We calculate $P(G_\Lambda, q)$ on $L_x \times L_y$ strips of the lattice $\Lambda$ with periodic (i.e., cyclic) BC’s in the longitudinal ($L_x$) direction, then take $L_x \to \infty$ and calculate $W$ and the resultant $\mathcal{B}$. By construction, these $W$ functions and the associated loci $\mathcal{B}$ embody the four general properties given above. For each strip, the exterior of $\mathcal{B}$ in the $q$ plane, denoted as the region $R_1$, is the maximal region into which one can analytically continue $W$ from the real interval $q > q_c$. The calculation of $W$ for a cyclic strip of a given width is considerably more difficult and the result more complicated than that for the open strip (free $L_x$ BC) of the same width; the value of the cyclic strips is that the resultant $W$
exhibits the analytic features of the full 2D $W$ function. The boundary condition in the transverse direction is not important for these results since the width is finite; for simplicity we use free transverse BC’s.

We use an extension of the generating function method of Ref. [10] from open to cyclic strip graphs $G_{\Lambda}$. The generating function $\Gamma(G_{\Lambda}, q, x)$ yields the chromatic polynomials for finite-length strips of $\Lambda$ as the coefficients in its Taylor series expansion in the auxiliary variable $x$ about $x = 0$. Here, $\Gamma(G_{\Lambda}, q, x) = N(G_{\Lambda}, q, x)/D(G_{\Lambda}, q, x)$, where $N$ and $D$ are polynomials in $x$ and $q$ (with no common factors). The degrees of these, as polynomials in $x$, are denoted $j_{\text{max}} = \deg x(N)$ and $k_{\text{max}} = \deg x(D)$. The $N$ are not needed here (they will be given elsewhere) since $W$ and $B$ are determined completely by $D$, independent of $N$ [10].

For a particular $G_{\Lambda}$, writing $D = \prod_{j=1}^{j_{\text{max}}}(1 - \lambda_j x)$, $W$ is given in region $R_1$ and $|W|$ in other regions [24] by $W = (\lambda_{\text{max}}')^t$ and $|W| = |\lambda_{\text{max}}'|^t$, where $\lambda_{\text{max}}$ denotes the $\lambda$ in $P$ with maximal magnitude in the respective region and $t = L_x/n = 1/L_y$ for the square strip and 1/5 for the kagomé strip considered here.

We first consider cyclic strips of the square lattice. For $L_y = 1$, $B$ consists of the unit circle $|q - 1| = 1$ so that $q_c = 2$, and $W = q - 1$ for $q \in R_1$. For $L_y = 2$, from the known $P$ [19], we found that $B$ separates the $q$ plane into four regions, $q_c = 2$, and $W = (q^2 - 3q + 3)^{1/2}$ for $q \in R_1$ [3]. We have calculated the generating function for the $L_y = 3$ case. This has $j_{\text{max}} = 8$ and $k_{\text{max}} = 10$ and is considerably more complicated than the $L_y = 3$ open strip, where $j_{\text{max}} = 1$ and $k_{\text{max}} = 2$. For $D$ we find

$$D(sq(L_y = 3), q, x) = (1 + b_{sq,11}x + b_{sq,12}x^2)(1 + b_{sq,21}x + b_{sq,22}x^2 + b_{sq,23}x^3) \times (1 + x)[1 + (q - 2)^2x][1 - (q - 2)x][1 - (q - 4)x][1 - (q - 1)x]$$

where

$$b_{sq,11} = - (q - 2)(q^2 - 3q + 5)$$

$$b_{sq,12} = (q - 1)(q^3 - 6q^2 + 13q - 11)$$

$$b_{sq,21} = 2q^2 - 9q + 12$$

$$b_{sq,22} = q^4 - 10q^3 + 36q^2 - 56q + 31$$

$$b_{sq,23} = - (q - 1)(q^4 - 9q^3 + 29q^2 - 40q + 22)$$
FIG. 1. Locus $B$ for $W$ for the $\infty \times 3$ cyclic strip of square lattice. Chromatic zeros for $L_x = 20$ (i.e., $n = 60$) are also shown.

The boundary $B$ is shown in Fig. 1. It divides the $q$ plane into several regions and crosses the positive real axis at $q_c = 2.33654$ and $q = 2$. Thus, this $L_y = 3$ cyclic strip is the first one sufficiently wide as to yield a value of $q_c$ above $q = 2$; indeed, the value of $q_c$ for this strip is only about 20% below the value for the full 2D lattice, viz., $q_c = 3$ \cite{7}. In region $R_1$ including the real interval $q > q_c$,

$$W(\{G_{sq(L_y=3)}, q \in R_1\}) = 2^{-1/3}\left[(q - 2)(q^2 - 3q + 5) + \left[(q^2 - 5q + 7)(q^4 - 5q^3 + 11q^2 - 12q + 8)\right]^{1/2}\right]^{1/3} \tag{7}$$

At $q_c$, $W = 1.18487$. In the region that includes the real interval $2 < q < q_c$, $|W| = |q - 4|^{1/3}$. In the region that includes the real interval $0 < q < 2$ and in the regions centered at roughly $q = 2.4 \pm 0.9i$, $|W|$ is given by the respective maximal cube roots of the equation $\xi^3 + b_{sq,21}\xi^2 + b_{sq,22}\xi + b_{sq,23} = 0$. As an algebraic curve, $B$ has several multiple points (defined as points where several branches of this curve cross intersect).

We next consider a cyclic strip of the kagomé lattice comprised of $m$ hexagons with each pair sharing two triangles as adjacent polygons (as in Fig. 1 in \cite{10} for the open strip). $\Gamma$
has $j_{\text{max}} = 8$ and $k_{\text{max}} = 9$ as compared with $j_{\text{max}} = 1$, $k_{\text{max}} = 2$ for the open strip of the same width [10]. We calculate

$$D(kg(L_y = 2), q, x) = (1 + b_{kg,11}x + b_{kg,12}x^2)(1 + b_{kg,21}x + b_{kg,22}x^2)(1 + b_{kg,31}x + b_{kg,32}x^2) \times
\left[1 - (q - 2)x\right]\left[1 - (q - 4)x\right]\left[1 - (q - 1)(q - 2)^2x\right]$$

(8)

where

$$b_{kg,11} = -(q - 2)(q^4 - 6q^3 + 14q^2 - 16q + 10)$$

(9)

$$b_{kg,12} = (q - 1)^3(q - 2)^3$$

(10)

$$b_{kg,21} = -q^3 + 7q^2 - 19q + 20$$

(11)

$$b_{kg,22} = (q - 1)(q - 2)^3$$

(12)

$$b_{kg,31} = 11 - 9q + 2q^2$$

(13)

$$b_{kg,32} = -(q - 1)(q - 2)^2$$

(14)

Define $\lambda_{kg,j,\pm} = (1/2)[-b_{kg,j1} \pm (b_{kg,j1}^2 - 4b_{kg,j2})^{1/2}]$. Again, $B$ divides the $q$ plane into several regions (Fig. 2). In region $R_1$, $W$ is determined by $\lambda_{kg,1,\pm}$:

$$W(G_{kg(L_y=2)}, q) = 2^{-1/5}(q - 2)^{1/5}\left[q^4 - 6q^3 + 14q^2 - 16q + 10 + \left[q^8 - 12q^7 + 64q^6 - 200q^5 + 404q^4 - 548q^3 + 500q^2 - 292q + 92\right]^{1/2}\right]^{1/5}$$

(15)

As is evident from Fig. 2, the value of $q_c$ is within about 10% of the inferred exact value $q_c = 3$ for the 2D kagomé lattice [14]. It is impressive that an infinite strip of width $L_y = 2$ yields a $q_c$ this close to the value for the full 2D lattice.
Another interesting feature of these results is the fact that the chromatic zeros and their accumulation set $\mathcal{B}$ contain support for $\Re(q) < 0$. This is in contrast with the situation for strips with free longitudinal BC’s \cite{12} and provides further support for our earlier conjecture that a necessary condition for this $\Re(q) < 0$ feature is that the graph family have global circuits.

We have also computed $W$ and $\mathcal{B}$ for the cyclic strip of the triangular strip with $L_y = 2$. We find $\mathcal{D} = (1 - x)[1 - (q - 2)x][1 + (2q - 5)x + (q - 2)^2x^2]$. $\mathcal{B}$ separates the $q$ plane into three regions and crosses the positive real axis at $q_c = 3$ and at $q = 2$. The $q_c$ value for this strip is one unit less than the value $q_c = 4$ for the full 2D lattice.

Similar calculations can be carried out for infinite-length cyclic strips $G_\Lambda$ of greater widths. Our method can also be applied to lattices with $d \geq 3$. To do this, one would use the generating function method to calculate $P$ for tubes with longitudinal PBC’s and successively larger $(d - 1)$-dimensional cross sections. We believe that this application, as well as that to other 2D lattices, is promising.

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[5] The minimum number of colors needed for this coloring of $G$ is called its chromatic number, $\chi(G)$.

[6] At certain special points $q_s$ (typically $q_s = 0, 1, \ldots, \chi(G)$), one has the noncommutativity of limits $\lim_{q \to q_s} \lim_{n \to \infty} P(G, q)^{1/n} \neq \lim_{n \to \infty} \lim_{q \to q_s} P(G, q)^{1/n}$, and hence it is necessary to specify the order of the limits in the definition of $W(\{G\}, q_s)$ \[7\]. As in Ref. \[7\], we shall use the first order of limits here; this has the advantage of removing certain isolated discontinuities in $W$.

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[22] Some families of graphs that do not have regular lattice directions have noncompact loci $B$ that separate the $q$ plane into different regions [11,12,15].

[23] The complete graph on $p$ vertices, denoted $K_p$, is the graph in which every vertex is adjacent to every other vertex. The “join” of graphs $G_1$ and $G_2$, denoted $G_1 + G_2$, is defined by adding bonds linking each vertex of $G_1$ to each vertex in $G_2$. Graph families with $B$ not including $q = 0$ are given in [11,12,15].

[24] For real $q < q_c(G)$, as well as other regions of the $q$ plane that cannot be reached by analytic continuation from the real interval $q > q_c(G)$, one can only determine the magnitude $|W(G, q)|$ unambiguously [7].