ARTICLES

Ground-state degeneracy of Potts antiferromagnets on two-dimensional lattices: Approach using infinite cyclic strip graphs

Robert Shrock[1,*] and Shan-Ho Tsai[2,†]
[1]Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11794-3840
[2]Department of Physics and Astronomy, University of Georgia, Athens, Georgia 30602
(Received 25 February 1999)

The q-state Potts antiferromagnet on a lattice Λ 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 $W(\text{sq},q)$ 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 $W(\text{sq},q)$. Similar results are given for the kagomé lattice. [S1063-651X(99)01010-7]

PACS number(s): 05.50.+q, 05.20.−y, 64.60.Cn, 75.10.Hk

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) [2,3] exhibits nonzero ground-state entropy (without frustration) for sufficiently large q on a given lattice Λ, 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 $Z(G,q,T=0)_{PAF} = P(G,q)$, 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 [4,5]. Thus, $W(\{G\},q) = \lim_{n\to\infty} P(G,q)^{1/n}$, where $n = v(G)$ is the number of vertices of G [6,7] and $\{G\} = \lim_{n\to\infty} G$. $W(\{G\},q)$ has been calculated exactly for the triangular lattice [8] and various families of graphs [7,9–15]. The special values for the square (sq) and kagomé (kg) lattices $W(\text{sq},3)$ [16] and $W(\text{kg},3)$ (which can be extracted from [17,8]) are also known. However, aside from the triangular case, the exact calculation of $W(\Lambda,q)$ for general q on lattices Λ of dimensionality $d \geq 2$ remains an outstanding challenge. In this paper 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 two-dimensional (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, $q_c(\{G\})$ [7,18]. For a given $\{G\}$, we denote the continuous locus of nonanalyticities of W as $\mathcal{B}$. This locus $\mathcal{B}$ forms as the accumulation set of the zeros of $P(G,q)$ (chromatic zeros of G) as $n\to\infty$ [19–21,7] and satisfies $\mathcal{B}(q) = \mathcal{B}(q^*)$. In cases where $\mathcal{B}$ 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 $\mathcal{B}$ intersects the real axis, which can occur via $\mathcal{B}$ crossing this axis or via a line segment of $\mathcal{B}$ lying along the axis. The chromatic polynomial $P(G,q)$ has a general decomposition as $P(G,q) = c_0(q) + \Sigma_j c_j(q)(a_j(q))^{t_j n}$ 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" (ℓ) if it dominates the $n\to\infty$ limit of $P(G,q)$. The locus $\mathcal{B}$ occurs where there is an abrupt nonanalytic change in W as the leading terms a_ℓ changes; thus the locus $\mathcal{B}$ is the solution to the equation of degeneracy of magnitudes of leading terms. Hence, W is finite and continuous, although nonanalytic, across $\mathcal{B}$.

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 $n\to\infty$ [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 [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 [11,12,15]. For graphs that (a) contain global circuits, (b) cannot be written in the form $G = K_p + H$ [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

*Electronic address: robert.shrock@sunysb.edu
†Electronic address: tsai@hal.physast.uga.edu

free boundary conditions in the longitudinal direction (and free or periodic BC's in the transverse direction) [10,13], it is found that the resultant loci $\mathcal{B}$ consist of arcs (and possible real line segments) that, 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 properties (i)–(iv) hold for $W(\Lambda,q)$ and $\mathcal{B}$ on a lattice Λ (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 Λ 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_Λ. The generating function $\Gamma(G_\Lambda,q,x)$ yields the chromatic polynomials for finite-length strips of Λ as the coefficients in its Taylor-series expansion in the auxiliary variable x about $x=0$. Here, $\Gamma(G_\Lambda,q,x)=\mathcal{N}(G_\Lambda,q,x)/\mathcal{D}(G_\Lambda,q,x)$, where $\mathcal{N}$ and $\mathcal{D}$ are polynomials in x and q (with no common factors). The degrees of these, as polynomials in x, are denoted $j_{max}=\deg_x(\mathcal{N})$ and $k_{max}=\deg_x(\mathcal{D})$. The $\mathcal{N}$ are not needed here (they will be given elsewhere) since W and $\mathcal{B}$ are determined completely by $\mathcal{D}$, independent of $\mathcal{N}$ [10]. For a particular G_Λ, writing $\mathcal{D}=\prod_{j=1}^{j_{max}}(1-\lambda_j x)$, W is given in region R_1 and $|W|$ in other regions [24] by $W=(\lambda_{max})^t$ and $|W|=|\lambda_{max}|^t$, where λ_{max} denotes the λ 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 $L_y=1$, $\mathcal{B}$ 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 $\mathcal{B}$ separates the q plane into four regions, $q_c=2$, and $W=(q^2-3q+3)^{1/2}$ for $q\in R_1$ [7]. We have calculated the generating function for the $L_y=3$ case. This has $j_{max}=8$ and $k_{max}=10$ and is considerably more complicated than the $L_y=3$ open strip, where $j_{max}=1$ and $k_{max}=2$. For $\mathcal{D}$ we find

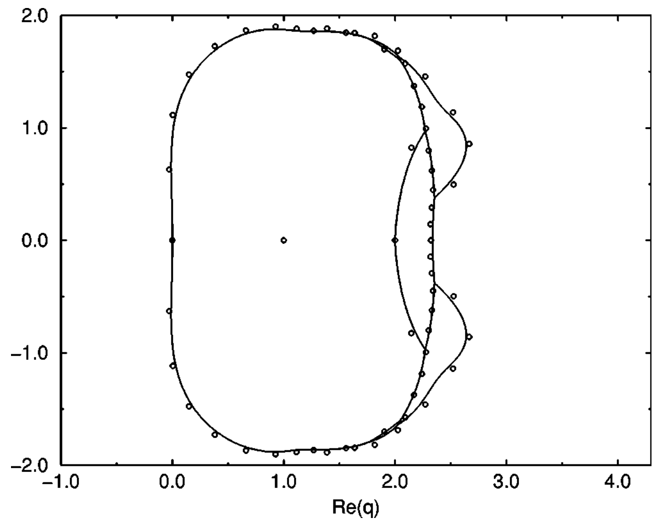

FIG. 1. Locus $\mathcal{B}$ for W for the $\infty\times3$ cyclic strip of square lattice. Chromatic zeros for $L_x=20$ (i.e., $n=60$) are also shown.

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

where

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

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

$$b_{\mathrm{sq},21}=2q^2-9q+12, \qquad (4)$$

$$b_{\mathrm{sq},22}=q^4-10q^3+36q^2-56q+31, \qquad (5)$$

$$b_{\mathrm{sq},23}=-(q-1)(q^4-9q^3+29q^2-40q+22). \qquad (6)$$

The boundary $\mathcal{B}$ is shown in Fig. 1. It divides the q plane into several regions and crosses the positive real axis at $q_c=2.336\,54$ 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., $q_c=3$ [7]. In region R_1 including the real interval $q>q_c$,

$$\begin{aligned}W(\{G_{\mathrm{sq}(L_y=3)}\},q\in R_1)&\\ =2^{-1/3}\{(q-2)(q^2-3q+5)+[(q^2-5q+7)&\\ \times(q^4-5q^3+11q^2-12q+8)]^{1/2}\}^{1/3}.& \qquad (7)\end{aligned}$$

At q_c, $W=1.184\,87$. 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 $q=2.4\pm0.9i$, $|W|$ is given by the respective maximal cube roots of the equation $\xi^3+b_{\mathrm{sq},21}\xi^2+b_{\mathrm{sq},22}\xi+b_{\mathrm{sq},23}$

$=0$. As an algebraic curve, $\mathcal{B}$ 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 [10] for the open strip). Γ has $j_{max}=8$ and $k_{max}=9$ as compared with $j_{max}=1$, $k_{max}=2$ for the open strip of the same width [10]. We calculate

$$\mathcal{D}(\text{kg}(L_y=2),q,x) = (1+b_{\text{kg},11}x+b_{\text{kg},12}x^2)(1+b_{\text{kg},21}x+b_{\text{kg},22}x^2) \times(1+b_{\text{kg},31}x+b_{\text{kg},32}x^2)[1-(q-2)x] \times[1-(q-4)x][1-(q-1)(q-2)^2x], \tag{8}$$

where

$$b_{\text{kg},11}=-(q-2)(q^4-6q^3+14q^2-16q+10), \tag{9}$$

$$b_{\text{kg},12}=(q-1)^3(q-2)^3, \tag{10}$$

$$b_{\text{kg},21}=-q^3+7q^2-19q+20, \tag{11}$$

$$b_{\text{kg},22}=(q-1)(q-2)^3, \tag{12}$$

$$b_{\text{kg},31}=11-9q+2q^2, \tag{13}$$

$$b_{\text{kg},32}=-(q-1)(q-2)^2. \tag{14}$$

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

$$W(\{G_{\text{kg}(L_y=2)}\},q)=2^{-1/5}(q-2)^{1/5}\{q^4-6q^3+14q^2 -16q+10+[q^8-12q^7+64q^6 -200q^5+404q^4-548q^3+500q^2 -292q+92]^{1/2}\}^{1/5}. \tag{15}$$

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

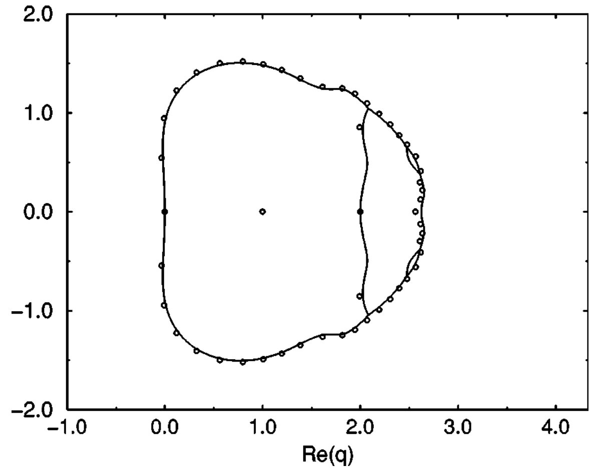

FIG. 2. Locus $\mathcal{B}$ for W for $\infty\times 2$ cyclic strip of the Kagomé lattice. Chromatic zeros for $m=10$ ($n=50$) are also shown.

$L_y=2$ 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 $\text{Re}(q)<0$. This is in contrast with the situation for strips with free longitudinal BC's [10] and provides further support for our earlier conjecture that a necessary condition for this $\text{Re}(q)<0$ 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 $\mathcal{D}=(1-x)[1-(q-2)^2x][1+(2q-5)x+(q-2)^2x^2]$. $\mathcal{B}$ 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_Λ of greater widths. Our method can also be applied to lattices with $d\geqslant 3$. To do this, one would use the generating function method to calculate P for tubes with longitudinal periodic BC's and successively larger $(d-1)$-dimensional cross sections. We believe that this application, as well as that to other 2D lattices, is promising.

This research was supported in part by the NSF Grant No. PHY-97-22101.

[1] M. Aizenman and E. H. Lieb, J. Stat. Phys. **24**, 279 (1981); Y. Chow and F. Y. Wu, Phys. Rev. B **36**, 285 (1987).

[2] R. B. Potts, Proc. Cambridge Philos. Soc. **48**, 106 (1952).

[3] F. Y. Wu, Rev. Mod. Phys. **54**, 235 (1982); **55**, 315(E) (1983).

[4] R. C. Read, J. Comb. Theory, Ser. A **4**, 52 (1968); R. C. Read and W. T. Tutte, in *Selected Topics in Graph Theory, 3*, edited by L. W. Beineke and R. J. Wilson (Academic Press, New York, 1988).

[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.

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

[8] R. J. Baxter, J. Phys. A **20**, 5241 (1987).

[9] R. Shrock and S.-H. Tsai, Phys. Rev. E **56**, 1342 (1997).

[10] M. Roček, R. Shrock, and S.-H. Tsai, Physica A **252**, 505 (1998); **259**, 367 (1998).

[11] R. Shrock and S.-H. Tsai, Phys. Rev. E **56**, 3935 (1997); **56**, 4111 (1997).

[12] R. Shrock and S.-H. Tsai, J. Phys. A **31**, 9641 (1998).
[13] R. Shrock and S.-H. Tsai, Physica A **259**, 315 (1998).
[14] R. Shrock and S.-H. Tsai, Phys. Rev. E **58**, 4332 (1998); e-print cond-mat/9808057. In the absence of exact solutions, these values of $W(\Lambda,q)$ are determined by Monte Carlo measurements and large-q series.
[15] R. Shrock and S.-H. Tsai, Physica A **265**, 186 (1999); J. Phys. A **32**, L195 (1999).
[16] E. H. Lieb, Phys. Rev. **162**, 162 (1967).
[17] R. J. Baxter, J. Math. Phys. **11**, 784 (1970).
[18] R. Shrock and S.-H. Tsai, J. Phys. A **30**, 495 (1997).
[19] N. L. Biggs, R. M. Damerell, and D. A. Sands, J. Comb. Theory, Ser. B **12**, 123 (1972); N. L. Biggs and G. H. Meredith, *ibid.* **20**, 5 (1976).
[20] S. Beraha, J. Kahane, and N. Weiss, J. Comb. Theory, Ser. B **28**, 52 (1980).
[21] R. C. Read and G. F. Royle, in *Graph Theory, Combinatorics, and Applications* (Wiley, New York, 1991), Vol. 2, p. 1009.
[22] Some families of graphs that do not have regular lattice directions have noncompact loci $\mathcal{B}$ 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 $\mathcal{B}$ not including $q=0$ are given in [9,11,12,15].
[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].