Large-q series expansion for the ground-state degeneracy of the q-state Potts antiferromagnet on the $(3\cdot 12^2)$ lattice

Shan-Ho Tsai*

Institute for Theoretical Physics, State University of New York at Stony Brook, Stony Brook, New York 11794-3840

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We calculate the large-q series expansion for the ground-state degeneracy (= exponent of the ground-state entropy) per site of the q-state Potts antiferromagnet on the $(3\cdot 12^2)$ lattice, to order $O(y^{19})$, where $y=1/(q-1)$. We note a remarkable agreement, to $O(y^{18})$, between this series and a rigorous lower bound derived recently. [S1063-651X(98)09803-1]

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I. INTRODUCTION

Nonzero ground-state disorder and associated entropy, $S_0\neq 0$, is an important subject in statistical mechanics. 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 $R=N_{\rm Avog}k_B$ [1,2]. A particularly simple model exhibiting ground-state entropy without the complication of frustration is the q-state Potts antiferromagnet (AF) [3,4] on a lattice Λ, for $q\geqslant\chi(\Lambda)$, where $\chi(\Lambda)$ denotes the minimum number of colors necessary to color the vertices of the lattice such that no two adjacent vertices have the same color. This model has a deep connection with graph theory in mathematics, since the zero-temperature partition function of the above-mentioned q-state Potts antiferromagnet on a lattice Λ satisfies $Z(\Lambda,q,T=0)_{\rm PAF}=P(\Lambda,q)$, where $P(G,q)$ is the chromatic polynomial [5] expressing the number of ways of coloring the vertices of a graph G with q colors such that no two adjacent vertices (connected by a bond of the graph) have the same color. Hence, the ground-state entropy per site is given by $S_0/k_B=\ln W(\Lambda,q)$, where $W(\Lambda,q)$, the ground-state degeneracy per site, is

$$W(\Lambda,q)=\lim_{n\to\infty}P(\Lambda_n,q)^{1/n}. \tag{1.1}$$

Here, Λ_n denotes an n-vertex lattice of type Λ with appropriate (e.g., free) boundary conditions. Since nontrivial exact solutions for this function are known in only a very few cases (square lattice for $q=3$ [6], triangular lattice [7], and kagomé lattice for $q=3$ [8,4]), it is important to exploit and extend general approximate methods that can be applied to all cases. Such methods include rigorous upper and lower bounds, large-q series expansions, and Monte Carlo measurements. Recently, with R. Shrock, the present author studied the ground-state entropy in antiferromagnetic Potts models on various lattices and obtained further results with these three methods [9–11]. We derived a general lower bound on $W(\Lambda,q)$ [11] which applies to all Archimedean lattices and coincides to many orders with large-q series expansion of this function. Previous large-q series expansions include works by Baker [12], Nagle [13,14], Kim and Enting [15], Bakaev and co-workers [16], and work reported in [10,11]. Related work on series expansions for the ground-state degeneracy of ice was done by Nagle [17].

Large-q series expansions of the respective $W(\Lambda,q)$ functions on various Archimedean lattices were computed in Ref. [11]. In particular, $W(\Lambda,q)$ for $\Lambda=(3\cdot 12^2)$ was computed to $O(y^{13})$ [11]. In the present paper we extend this series to higher order, namely, to $O(y^{19})$. Our main motivation is to check the accuracy of the lower bound on $W((3\cdot 12^2),q)$ given in [11]. It is interesting that this lower bound coincides with the first 19 terms, i.e., to $O(y^{18})$, in the large-q series. We choose the lattice $\Lambda=(3\cdot 12^2)$ as an illustrative example of a heteropolygonal Archimedean lattice. The reader is referred to Refs. [9–11] for further background and references.

II. LARGE-q SERIES EXPANSION

Before proceeding, we recall that an Archimedean lattice is defined as a uniform tiling of the plane by regular polygons in which all vertices are equivalent [18]. Such a lattice is specified by the ordered sequence of polygons that one traverses in making a complete circuit around a vertex in a given (say counterclockwise) direction. This is incorporated in the mathematical notation for an Archimedean lattice Λ:

$$\Lambda=\left(\prod_i p_i^{a_i}\right), \tag{2.1}$$

where in the above circuit, the notation $p_i^{a_i}$ indicates that the regular polygon p_i occurs contiguously a_i times; it can also occur noncontiguously. We shall denote $a_{i,s}$ as the sum of the a_i's over all of the occurrences of the given p_i in the product. Because the starting point is irrelevant, the symbol is invariant under cyclic permutations. The number of polygons of type p_i per site is given by

$$\nu_{p_i}=\frac{a_{i,s}}{p_i}. \tag{2.2}$$

The coordination number for an Archimedean lattice is $\Delta=\Sigma_i a_{i,s}$. In particular, for the $(3\cdot 12^2)$ lattice considered in this paper, the number of triangles per site is $p_3=1/3$, the number of 12-gons per site is $p_{12}=1/6$, and the coordination number is $\Delta=3$. A section of this lattice is shown in Fig. 1.

*Electronic address: tsai@insti.physics.sunysb.edu

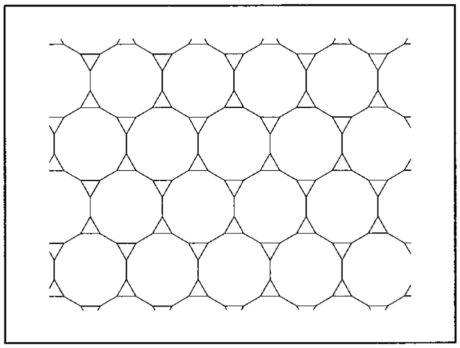

FIG. 1. Section of the $(3\cdot 12^2)$ Archimedean lattice.

A general upper bound on a chromatic polynomial for an n-vertex graph G is $P(G,q)\leqslant q^n$. This yields the corresponding upper bound $W(\{G\},q)<q$. Hence, as in our previous work [9–11], it is natural to define a reduced function that has a finite limit as $q\to\infty$,

$$W_r(\{G\},q)=q^{-1}W(\{G\},q). \tag{2.3}$$

When calculating large-q Taylor series expansions for W functions on regular lattices, it is most convenient to carry this out for the related function

$$\overline{W}(\Lambda,y)=\frac{W(\Lambda,q)}{q(1-q^{-1})^{\Delta/2}}, \tag{2.4}$$

for which the large-q series can be written in the form

$$\overline{W}(\Lambda,y)=1+\sum_{m=1}^{\infty} w_{\Lambda,m}y^m \tag{2.5}$$

with

$$y=\frac{1}{q-1}. \tag{2.6}$$

Our calculations of large-q series expansion use the method of Ref. [14]. The chromatic polynomial is written as the sum

$$P(G,q)=\frac{(q-1)^E}{q^{(E-n)}}\sum_{G_a\leqslant G}(-1)^e\frac{q^{(e-v)}}{(q-1)^e}m(G_a,q), \tag{2.7}$$

where E is the total number of edges of the n-vertex graph G, $m(G_a,q)$ are weights [19] of weak subgraphs G_a of G, and e and v are the numbers of edges and vertices, respectively, of G_a. The summation is over all weak subgraphs G_a. The weight function $m(G_a,q)$ vanishes if G_a has any vertices of degree one or if G_a has a bridge. Another property is that $m(G_a,q)$ does not change under the insertion or deletion of vertices of degree two in G_a. Thus in the summation of weak subgraphs, one effectively has to consider (connected and disconnected) subgraphs with no vertices of degree one and without bridges. One also has to consider graphs with articulation points. Weight functions $m(G_a,q)$ are independent of G and satisfy a simple recursion relation formula. Reference [14] gives the weights of all star graphs with cyclomatic number less or equal to four [20].

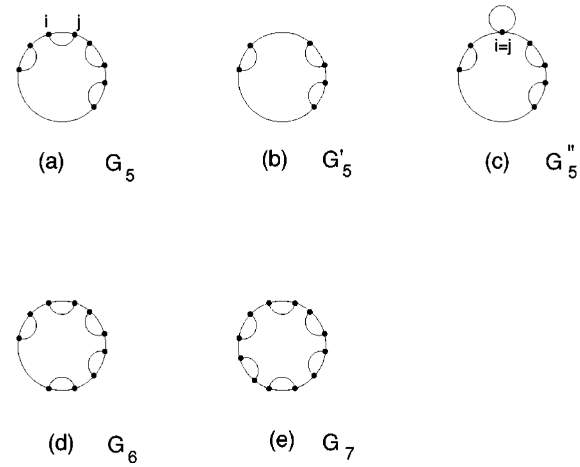

FIG. 2. Illustration of star graphs with cyclomatic number $c\leqslant 7$. (a) G_5 is a graph with $c=5$, (b) G_5' is derived from G_5 by omitting one edge between vertices i and j, and (c) G_5'' is the graph with vertices i and j identified. (d) G_6 is a graph with $c=6$ and (e) G_7 has $c=7$. Vertices of degree 2 are not shown.

The series expansion for $W((3\cdot 12^2),q)$ to $O(y^{19})$ involves star graphs with cyclomatic number up to 7. The graphs with cyclomatic number equal to 5, 6, and 7, which enter in the series expansion to this order are shown in Figs. 2(a), 2(d), and 2(e), respectively. To derive the weights of these graphs, we use theorems III and VII of Ref. [14]. Theorem III states that if a graph G consists of two pieces G_1 and G_2 that have just one vertex in common, its weight is given by

$$m(G,q)=\frac{1}{q}m(G_1,q)m(G_2,q). \tag{2.8}$$

Theorem VII states that

$$m(G,q)=-\frac{1}{q}m(G',q)+m(G'',q), \tag{2.9}$$

where G' is derived from G by omitting the edge between two vertices, say i and j, and G'' is the graph with vertices i and j identified. As an example, consider the graphs G_5, G_5' and G_5'' depicted in Figs. 2(a), 2(b), and 2(c). G_5'' has an articulation point and, using Eq. (2.8), we can write its weight as $m(G_5'',q)=q^{-1}m(P,q)m(G_5',q)$, where P here stands for polygon. The weights for P and G_5' are $m(P,q)=(q-1)$ and $m(G_5',q)=(q-1)(q-2)^3/q^3$ [14]. Hence, Eq. (2.9) yields

$$m(G_5,q)=-\frac{1}{q}m(G_5',q)+m(G_5'',q)=\frac{1}{q^4}(q-1)(q-2)^4. \tag{2.10}$$

Note that vertices of degree two have been omitted in Fig. 2.

The weights of the graphs with higher cyclomatic numbers, shown in Figs. 2(d) and 2(e), can be similarly determined to be

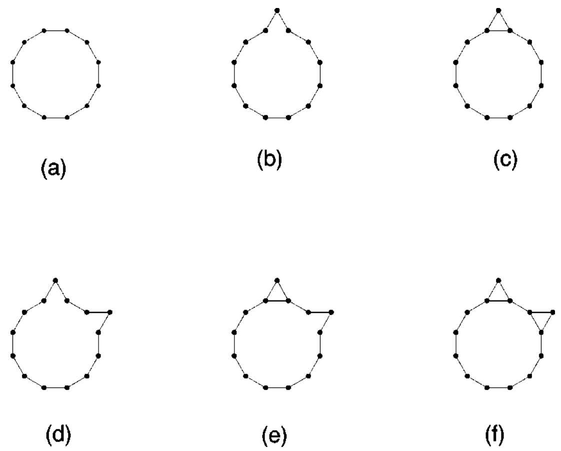

FIG. 3. Illustration of some graphs that enter in the large-q series for $W((3\cdot 12^2),q)$. Graphs (a), (b), and (c) enter in series to $O(y^{12})$, while graphs (d), (e), and (f) contribute to $O(y^{13})$ and higher.

$$m(G_6,q)=\frac{1}{q^5}(q-1)(q-2)^5 \tag{2.11}$$

and

$$m(G_7,q)=\frac{1}{q^6}(q-1)(q-2)^6, \tag{2.12}$$

respectively.

The subgraphs which contribute to the series to $O(y^{12})$ are (i) graphs formed by t disconnected triangles, where $t=1,2,\ldots,6$, (ii) polygons with 12 vertices (12-gons), as shown in Fig. 3(a), (iii) graphs formed by a triangle connected to a 12-gon, as shown in Figs. 3(b) and 3(c). Let us refer to the edge in the overlap between a triangle and a 12-gon as an internal edge. Internal edges can be part of the subgraph [as in Fig. 3(c)] or not [as in Fig. 3(b)].

Further subgraphs which contribute to $O(y^{13})$ are (i) graphs formed by one 12-gon and one disconnected triangle and (ii) graphs formed by two triangles connected to a 12-gon. In the latter case, one has to consider graphs with no internal edges [as in Fig. 3(d)], one internal edge [as in Fig. 3(e)], and two internal edges [as in Fig. 3(f)]. Moreover, one has to consider all the distinguishable permutations in the positions of the two triangles. In the remaining of this paper, when we refer to t triangles connected to 12-gons, we are including all possible distinguishable permutations of the triangles and all cases where i internal edges belong to the subgraph, with $i=0,1,\ldots,t$.

To $O(y^{14})$ other subgraphs that enter in the series are (i) graphs formed by seven disconnected triangles, (ii) graphs formed by three triangles connected to a 12-gon, and (iii) graphs formed by one triangle connected to a 12-gon and one disconnected triangle.

The series to $O(y^{15})$ includes (i) graphs formed by four triangles connected to a 12-gon, (ii) graphs formed by two triangles connected to a 12-gon and one disconnected triangle, and (iii) two disconnected triangles and one 12-gon.

To $O(y^{16})$, extra subgraphs are (i) graphs comprised of eight disconnected triangles, (ii) graphs formed by five triangles connected to a 12-gon, (iii) graphs composed of a triangle connected to a 12-gon and two disconnected triangles, and (iv) graphs formed by three triangles connected to a 12-gon and one disconnected triangle.

To $O(y^{17})$, other subgraphs are (i) graphs formed by six triangles connected to a 12-gon, (ii) three disconnected triangles and one 12-gon, (iii) two triangles connected to a 12-gon and two disconnected triangles, and (iv) four triangles connected to a 12-gon and one disconnected triangle.

To $O(y^{18})$, further subgraphs are (i) graphs formed by nine disconnected triangles, (ii) graphs formed by one triangle connected to a 12-gon and three disconnected triangles, (iii) graphs comprised of three triangles connected to a 12-gon and two disconnected triangles, and (iv) graphs formed by five triangles connected to a 12-gon and one disconnected triangle.

To $O(y^{19})$, new subgraphs are (i) graphs formed by four disconnected triangles and one 12-gon, (ii) graphs formed by two triangles connected to a 12-gon and three disconnected triangles, (iii) graphs formed by four triangles connected to a 12-gon and two disconnected triangles, (iv) graphs formed by six triangles connected to a 12-gon and one disconnected triangle, and (v) 20-gons.

To this order, we obtain

$$\begin{aligned}\overline{W}((3\cdot 12^2),y)=1&-\frac{1}{3}y^2-\frac{1}{9}y^4-\frac{5}{3^4}y^6-\frac{10}{3^5}y^8-\frac{22}{3^6}y^{10}\\&+\frac{1}{6}y^{11}-\frac{154}{3^8}y^{12}-\frac{1}{18}y^{13}-\frac{374}{3^9}y^{14}\\&-\frac{1}{54}y^{15}-\frac{935}{3^{10}}y^{16}-\frac{5}{486}y^{17}-\frac{21505}{3^{13}}y^{18}\\&+\frac{719}{1458}y^{19}+O(y^{20}).\end{aligned} \tag{2.13}$$

The lower bound of Ref. [11], namely,

$$\overline{W}((3\cdot 12^2),y)_l=(1-y^2)^{1/3}(1+y^{11})^{1/6}, \tag{2.14}$$

coincides with the first 19 terms of the series given in Eq. (2.13), i.e., to $O(y^{18})$. This is remarkable and shows that this lower bound is indeed a very accurate approximation to the exact solution for the $\overline{W}$ function. The lower bound first differs from the large-q expansion for the exact $\overline{W}$ function at order y^{19}: the Taylor series expansion of this lower bound gives $-(5/729)y^{19}$ whereas the large-q series expansion of $\overline{W}$ yields $(719/1458)y^{19}$.

It is interesting to note that the lowest order in y in which the bound (2.14) differs from the series is an order in which subgraphs involving two adjacent 12-gons, i.e., 20-gons, first contribute in the series expansion. If one were to calculate the series expansion without considering the contribution of 20-gons to $O(y^{19})$, one would get a result that coincides with the coefficient of the $O(y^{19})$ term in the Taylor series of the bound (2.14).

III. CONCLUSIONS

We report on large-q series expansion for the ground-state degeneracy of the Potts antiferromagnet on the $(3\cdot 12^2)$ lattice, to $O(y^{19})$. It is remarkable that the lower bound derived previously coincides with the first 19 terms of the series, i.e., to $O(y^{18})$. It is worthwhile to perform similar series expansions to high orders for other types of lattices.

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[19] In Ref. [14] the weights $m(G_a,q)$ are called reduced weights and denoted by $w(G_a,q)$. A total weight is also defined therein. However, in the present paper we shall not refer to the total weight.
[20] The expansion of the chromatic polynomial $P(G,q)$ in terms of subgraphs in Eq. (2.7) can be regarded as a special case of the low-temperature series expansion of the partition function of the Potts model on the dual graph $\mathcal{D}(G)$ [4]. In this formulation, for planar subgraphs G_a, the weights $m(G_a,q)$ in Eq. (2.7) are simply given by $m(G_a,q)=P(\mathcal{D}(G_a),q)/q^{e-v+1}$, where $P(\mathcal{D}(G_a),q)$ is the chromatic polynomial on the graph dual to G_a; and e and v are the number of edges and vertices, respectively, of G_a [4]. We thank Professor F. Y. Wu for this comment.