Ground State Entropy in Potts Antiferromagnets and Chromatic Polynomials

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We discuss recent results on ground state entropy in Potts antiferromagnets and connections with chromatic polynomials. These include rigorous lower and upper bounds, Monte Carlo measurements, large-\(q\) series, exact solutions, and studies of analytic properties. Some related results on Fisher zeros of Potts models are also mentioned.

1. Introduction

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. \cite{1}). A physical example is ice. A simple model exhibiting ground state entropy is the \(q\)-state Potts antiferromagnet (PAF) on a lattice, or more generally a graph \(G\), for sufficiently large \(q\). The zero-temperature partition function satisfies

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

where \(P(G, q)\) 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. Let \(\{G\} = \lim_{n \to \infty} G\). The ground state degeneracy per site \(W\), given by

\[
S_0 = k_B \ln W,
\]

is

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

There are very few nontrivial exact solutions for \(W\). We have obtained a number of new results on \(W\), including rigorous bounds, large-\(q\) series expansions, Monte Carlo measurements, exact solutions, and studies of analytic properties \cite{2-10}. Besides physical (positive integral) \(q\), it is of interest to consider \(W\) as a function of complex \(q\;

\[
W\text{ is an analytic function of } q \text{ except on a continuous locus } B \text{ (} B \text{ may be null, and there may also be isolated singularities of } W\). As } n \to \infty, \text{ the locus } B \text{ forms via coalescence of a subset of zeros of } P(G, q). W \text{ is determined via } (2) \text{ in the region } R_1 \text{ reached by analytic continuation from the real } q \text{ axis for } q > \chi(G), \text{ where } \chi(G) \text{ is the chromatic number of } G, \text{ i.e., the minimum number of colors needed to color } G \text{ with the above constraint. In other regions separated from } R_1 \text{ by nonanalytic boundaries comprising } B, \text{ only } |W| \text{ can be determined. There is a subtlety in the definition of } W, \text{ since at certain special points one encounters the noncommutativity of limits } \]

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

At such points, we use the second order of limits to define \(W\). Physically, one finds \(W > 1\), i.e., \(S_0 > 0\) for \(q > \chi(G)\).

2. Bounds, Series, and Monte Carlo Measurements

We have proved rigorous lower and upper bounds on \(W\) for a number of lattices \(\Lambda\). As an example, for the honeycomb \((hc)\) lattice, we get

\[
W(hc, q)_{\ell} \leq W(hc, q) \leq W(hc, q)_{u}
\]

where

\[
W(hc, q)_{\ell} = \frac{(q^4 - 5q^3 + 10q^2 - 10q + 5)^{1/2}}{q - 1}
\]

\[
W(hc, q)_{u}
\]
and
\[ W(hc, q) = (q^2 - 3q + 3)^{1/2} \] (6)

These bounds are very restrictive even for moderate \( q \), as is clear from the fact that the first three terms in a large-\( q \) expansion coincide. Although a bound on a given function need not, \textit{a priori}, coincide with a series expansion of that function, we find that the lower bound (3) coincides with the first eleven terms of the large-\( q \) expansion for \( W(hc, q) \).

Accordingly, we have extended our study of the lower bound and have discovered and proved a generalization applicable to the full set of Archimedean lattices \( \mathcal{A} \). An Archimedean lattice is a uniform tiling of the plane with one or more regular polygons such that all vertices are equivalent to each other. It can be specified by the ordered sequence of polygons \( p_i \) traversed by a circuit around any vertex: \( \Lambda = \prod_i p_i^a_i \). Let \( \sum a_i = a_{is} \) and \( \nu_i = a_{is}/p_i \). Then our general lower bound is
\[ W\left(\prod_i p_i^{a_i}, q\right) \geq \frac{1}{q-1} \prod_i D_{p_i}(q)^{\nu_{p_i}} \] (7)

with
\[ D_k(q) = \sum_{s=0}^{k-2} (-1)^s \binom{k-1}{s} q^{k-2-s} \] (8)

We have calculated large-\( q \) series expansions for a number of Archimedean lattices and have compared the lower bounds with these series \( \mathcal{F} \). For the square, triangular, and honeycomb lattices we have carried out Monte Carlo measurements of \( W(\Lambda, q) \) for \( q \) values up to 10 and have found that even for moderate values of \( q \), the upper and lower bounds bracket the measured values quite closely \( \mathcal{F} \).

3. Analytic Structure of \( W(\{G\}, q) \)

We have calculated exact solutions for \( W(\{G\}, q) \) for a number of families of graphs and have studied their analytic structure. A general form for \( P(G, q) \) is
\[ P(G, q) = c_0(q) + \sum_{j=1}^{N_k} c_j(q)(a_j(q))^{k/n} \] (9)

where \( c_j(q) \) and \( a_j(q) \) are certain functions of \( q \). Here the \( a_j(q) \) and \( c_j \) 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 \(|\text{const.}| > 1\). A term \( a_\ell(q) \) is leading if it dominates the \( n \rightarrow \infty \) limit of \( P(G, q) \); in particular, if \( N_k \geq 2 \), then it satisfies \( |a_\ell(q)| \geq 1 \) and
\[ |a_\ell(q)| > \min_{j \neq \ell} |a_j(q)| \] for \( j \neq \ell \), so that
\[ |W| = |a_\ell|^5. \] The locus \( \mathcal{B} \) occurs where there is a nonanalytic change in \( W \) as the leading terms \( a_\ell \) in eq. (3) changes. For a given \( \{G\} \) one can ask various questions about \( \mathcal{B} \): (i) does it separate the \( q \) plane into separate regions? (ii) is it compact or noncompact? (iii) how many disjoint components does it contain? (iv) does it have multiple points where several branches cross? (v) does it cross the positive real axis or contain a segment lying along this axis, and if so, what is the maximal real value, \( q_0 \), in \( \mathcal{B} \)? We have answered these questions for various families \( \mathcal{F} \).

For example, such families as circuit and ladder graphs yield \( \mathcal{B} \) that do separate the \( q \) plane into various regions. With M. Röck, we have used a generating functional method to obtain exact solutions for \( W \) on infinitely long, finite-width homogeneous strip graphs \( \mathcal{F} \). For these we find that the loci \( \mathcal{B} \) consist of arcs that do not separate regions.

In general, the zeros of \( P(G, q) \) only merge to form \( \mathcal{B} \) in the \( n \rightarrow \infty \) limit, but for an interesting set of families, they actually lie exactly on \( \mathcal{B} \) even for finite \( n \). We have constructed an infinite set of these families, called \( p \)-wheels, \( (Wh)_{n}^{(p)} = K_{p} + C_{n-p} \), where \( K_{r} \) is the “complete” graph (each of whose vertices is connected to all others), \( C_{r} \) is the circuit graph, and \( G + H \) connotes joining of vertices of \( G \) to those of \( H \).

We proved that the zeros of \( P((Wh)_{n}^{(p)}, q) \) lie precisely on \( \mathcal{B} \), which is the circle \(|q - (p + 1)| = 1 \) \( \mathcal{F} \). This is reminiscent of the Yang-Lee circle theorem \( \mathcal{F} \) although different in certain respects.

For \( \{G\} \) with noncompact \( \mathcal{B} \) passing through \( z = 1/q = 0 \), no large-\( q \) series expansions exist. Since these series are very useful for regular lattices, it is important to understand the properties of a family \( \{G\} \) that yield a noncompact \( \mathcal{B} \). We have given a general condition for \( \mathcal{B} \) to be non-
compact and have constructed a number of these families \[G = (K_p)_b + H\]; one simple infinite set of families is \(G = (K_p)_b + H\), where \(b\) signifies the removal of \(b\) bonds from a vertex of \(K_p\). For example, for \(1 \leq b \leq p - 1\) and \(H = T_r\) (the tree graph on \(r\) vertices), in the limit \(r \to \infty\), \(B\) is the vertical line with \(Re(q) = p + \frac{1}{2}\), or equivalently, in the \(z = 1/q\) plane, the circle \(|z - z_c| = z_c\) with \(z_c = 2/(2p + 1)\). Additional families can be generated by various types of homeomorphic expansions of the basic \(G = (K_p)_b + H\) (homeomorphic expansion = insertion of degree-2 vertex on a bond).

4. Approach to 2D thermodynamic limit

Using exact solutions of \(W\) for infinitely long strip graphs of finite width \(L_y\), we have explored the approach of \(W\) to its 2D thermodynamic limit \[1\]. We showed that the approach of \(W\) to its 2D thermodynamic limit as \(L_y\) increases is quite rapid; for moderate values of \(q\) and \(L_y \simeq 4\), \(W(\Lambda, (L_x = \infty) \times L_y, q)\) is within about \(O(10^{-3})\) of the 2D value \(W(\Lambda, (L_x = \infty) \times (L_y = \infty), q)\) for periodic transverse boundary conditions (b.c.). The approach of \(W\) to the 2D thermodynamic limit was proved to be monotonic (non-monotonic) for free (periodic) transverse b.c. An application to compute central charges for cases with critical ground states was noted.

5. Complex-temperature properties

We have calculated Fisher zeros of the partition function for the Potts model on the square lattice for several \(q\) values and related the inferred CT phase boundaries to locations of singularities in the thermodynamic functions obtained from analyses of low-temperature series expansions \[12\]. These studies have been extended to honeycomb, triangular, kagomé, and diced lattices \[13\]. Although in general CT singularities have rather different properties than physical critical singularities in spin models, such as violation of universality \[13\], we have found an exact mapping that relates the free energy of the \(q\)-state Potts antiferromagnet on a lattice \(\Lambda\) for the full temperature interval \(0 \leq T \leq \infty\) and the free energy of the \(q\)-state Potts model on the dual lattice for a semi-infinite CT interval, \(-\infty \leq a_d \leq -(q - 1)\), where \(a_d = (a + q - 1)/(a - 1)\) and \(a = e^K\). Hence, for this interval, CT singularities of the free energy are equivalent to physical critical singularities. Effects of next-nearest-neighbor couplings were studied in Ref. \[10\].

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