

Ground-state entropy of Potts antiferromagnets: Bounds, series, and Monte Carlo measurements

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We report several results concerning $W(\Lambda, q) = \exp(S_0/k_B)$, the exponent of the ground-state entropy of the Potts antiferromagnet on a lattice Λ . First, we improve our previous rigorous lower bound on $W(\text{hc}, q)$ for the honeycomb (hc) lattice and find that it is extremely accurate; it agrees to the first 11 terms with the large- q series for $W(\text{hc}, q)$. Second, we investigate the heteropolygonal Archimedean $4 \cdot 8^2$ lattice, derive a rigorous lower bound, on $W(4 \cdot 8^2, q)$, and calculate the large- q series for this function to $O(y^{12})$ where $y = 1/(q-1)$. Remarkably, these agree exactly to all 13 terms calculated. We also report Monte Carlo measurements, and find that these are very close to our lower bound and series. Third, we study the effect of non-nearest-neighbor couplings, focusing on the square lattice with next-nearest-neighbor bonds. [S1063-651X(97)07509-0]

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I. INTRODUCTION

Nonzero ground-state disorder and associated entropy, $S_0 \neq 0$, is an important subject in statistical mechanics; a physical realization is provided by ice, for which $S_0 = 0.82 \pm 0.05$ cal/(K mol), i.e., $S_0/k_B = 0.41 \pm 0.03$ [1]. A particularly simple model exhibiting ground-state entropy without the complication of frustration is the q -state Potts antiferromagnet (AF) on a lattice Λ for sufficiently large q , [2,3]. This subject also has a deep connection with graph theory in mathematics [4–6] since the zero-temperature partition function of the q -state Potts AF on a lattice Λ satisfies $Z(\Lambda, q, T=0)_{\text{PAF}} = P(\Lambda, q)$ and hence $S_0/k_B = \ln W(\Lambda, q)$, where $P(G, q)$ is the chromatic polynomial, expressing the number of ways of coloring the vertices of a graph G with q colors such that no two adjacent vertices have the same color, and

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

where Λ_n denotes an n -vertex lattice of type Λ (with appropriate boundary conditions). Given the above connection, it is convenient to express our bounds on the ground-state entropy in terms of its exponent, $W(\Lambda, q)$. Recently, we studied the ground-state entropy in antiferromagnetic Potts models on various lattices, including both Monte Carlo measurements and rigorous upper and lower bounds, [7–10]. Here we continue this study. The reader is referred to Refs. [7–9] for further background and references.

II. IMPROVED LOWER BOUND ON $W(\text{hc}, q)$ FOR THE HONEYCOMB LATTICE

In Ref. [9], we derived lower and upper bounds on $W(\text{hc}, q)$ for the honeycomb (hc) lattice using a method applied by Biggs to obtain such bounds for the square lattice [11]. We showed that the upper and lower bounds rapidly

approached each other for large q and hence became very restrictive even for moderately large q . In particular, we obtained the lower bound, $W(\text{hc}, q) \geq W(\text{hc}, q)_{l'}$ for $q \geq 3$, where

$$W(\text{hc}, q)_{l'} = \frac{(q-1)^{3/2}}{q^{1/2}} \quad (2.1)$$

and found that this was very close to the actual value of $W(\text{hc}, q)$, as determined from Monte Carlo measurements [7–9,12]. (We also obtained similar bounds for the triangular lattice.) Accordingly, in this paper we shall focus on deriving rigorous lower bounds for several lattices Λ , which again turn out to be very accurate not just as bounds but as approximations for the $W(\Lambda, q)$ functions. In passing, we mention that, using the same methods as in Ref. [9], we could also derive rigorous upper bounds for additional lattices; however, we concentrate here on the lower bounds because of their very high accuracy as approximations for the $W(\Lambda, q)$ functions. We begin by sharpening our lower bound for the honeycomb lattice. We picture this lattice as a brick lattice with the long axis of the bricks horizontal, as in Fig. 1(a) of Ref. [9]. We consider a sequence of these lattices with m (n) sites in the horizontal (vertical) direction, denoted $(\text{hc})_{m \times n}$. In the thermodynamic limit the boundary conditions do not affect the bound, so for technical convenience, we take free (periodic) boundary conditions along the horizontal (vertical) directions. Further, to maintain the bipartite nature of the lattice and avoid frustration, we take n even. Our bounds in Ref. [9] were obtained by taking the vectors of color configurations to refer to the vertical lines; here we take them to refer to horizontal lines L . The number of allowed q colorings of this line of vertices is $\mathcal{N} = P(L_m, q) = q(q-1)^{m-1}$. One can then associate with two adjacent horizontal lines of sites L, L' , forming one layer of bricks, an $\mathcal{N} \times \mathcal{N}$ dimensional symmetric coloring matrix T with entries $T_{L, L'} = 1$ or 0 if the q colorings of these lines are or are not compatible. Here, by compatible q colorings we mean colorings that satisfy the constraint that no two adjacent vertices have the same color. Then (for fixed m, n) $P((\text{hc})_{m \times n}, q) = \text{Tr}(T^n)$. Since T is a nonnegative ma-

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trix, one can apply the Perron-Frobenius theorem [13] to conclude that T has a real positive maximal eigenvalue $\lambda_{\max,n}(q)$. Hence, for fixed m ,

$$\lim_{n \rightarrow \infty} \text{Tr}(T^n)^{1/(mn)} \rightarrow \lambda_{\max}^{1/m} \tag{2.2}$$

so that

$$W(\Lambda, q) = \lim_{m \rightarrow \infty} \lambda_{\max}^{1/m} \tag{2.3}$$

Denote the column sum $\kappa_j(T) = \sum_{i=1}^{\mathcal{N}} T_{ij}$ [equal to the row sum $\rho_j(T) = \sum_{i=1}^{\mathcal{N}} T_{ji}$ since $T^T = T$] and $S(T) = \sum_{i,j=1}^{\mathcal{N}} T_{ij}$; note that $S(T)/\mathcal{N}$ is the average row (column) sum. Combining the bounds for a general nonnegative $\mathcal{N} \times \mathcal{N}$ matrix A [13],

$$\min\{\gamma_j(A)\} \leq \lambda_{\max}(A) \leq \max\{\gamma_j(A)\} \quad \text{for } \gamma_j = \kappa_j \text{ or } \rho_j, \tag{2.4}$$

with the ($\nu=1$ case of the) more restrictive lower bound applicable to a symmetric nonnegative matrix [14],

$$\left[\frac{S(T^\nu)}{\mathcal{N}} \right]^{1/\nu} \leq \lambda_{\max} \quad \text{for } \nu = 1, 2, \dots, \tag{2.5}$$

we have

$$\frac{S(T)}{\mathcal{N}} \leq \lambda_{\max}(T) \leq \max\{\kappa_j(T)\}. \tag{2.6}$$

The sum $S(T)$ is given by the chromatic polynomial for the brick layer of length m , hence containing $2m$ vertices, which we calculate to be

$$P((\text{Ch})_{6,2m}, q) = q(q-1)D_6(q)^{(m-1)/2}, \tag{2.7}$$

where the notation [10] $(\text{Ch})_{k,2m}$ means a $2m$ -vertex chain of k -sided polygons, with each adjacent pair of k -gons intersecting along one common edge, and

$$D_k(q) = \sum_{s=0}^{k-2} (-1)^s \binom{k-1}{s} q^{k-2-s}. \tag{2.8}$$

Taking the $m \rightarrow \infty$ limit and applying the $\nu=1$ case of Eq. (2.5), we thus obtain the lower bound $W(\text{hc}, q) \geq W(\text{hc}, q)_l$ for $q \geq 3$ [12], where

$$W(\text{hc}, q)_l = \frac{D_6(q)^{1/2}}{q-1} = \frac{(q^4 - 5q^3 + 10q^2 - 10q + 5)^{1/2}}{q-1}. \tag{2.9}$$

For $q \geq 4$, the difference between the lower bounds (2.1) and (2.9) decreases rapidly toward zero. The corresponding reduced W functions $W_r(\text{hc}, q) = q^{-1}W(\text{hc}, q)$ have large- q Taylor series which coincide up to order $O(q^{-4})$:

$$q^{-1}W(\text{hc}, q)_l = 1 - \frac{3}{2}q^{-1} + \frac{3}{8}q^{-2} + \frac{1}{16}q^{-3} + \frac{3}{128}q^{-4} + \frac{131}{256}q^{-5} + O(q^{-6}) \tag{2.10}$$

and

$$q^{-1}[W(\text{hc}, q)_l - W(\text{hc}, q)_r] = \frac{1}{2}q^{-5} + O(q^{-6}). \tag{2.11}$$

Since the quantity $y = 1/(q-1)$ is a natural variable for a large- q expansion, it is also useful to compare an expansion of our new lower bound with a small- y series. For a lattice Λ , this series has the form [15–17]

$$W(\Lambda, q) = q(1 - q^{-1})^{\zeta/2} \bar{W}(\Lambda, y), \tag{2.12}$$

where ζ is the lattice coordination number, and

$$\bar{W}(\Lambda, y) = 1 + \sum_{n=1}^{\infty} w_n y^n, \quad y = \frac{1}{q-1}. \tag{2.13}$$

Analogously, for the expansion of our lower bound, we define the reduced lower bound function $\bar{W}(\Lambda, y)_l$ via

$$W(\Lambda, q)_l = q(1 - q^{-1})^{\zeta/2} \bar{W}(\Lambda, y)_l. \tag{2.14}$$

From Eq. (2.9), we find the very simple result

$$\bar{W}(\text{hc}, y)_l = (1 + y^5)^{1/2}. \tag{2.15}$$

Expanding this in a Taylor series in y , we have

$$\bar{W}(\text{hc}, y)_l = 1 + \frac{1}{2}y^5 - \frac{1}{8}y^{10} + \frac{1}{16}y^{15} + O(y^{20}). \tag{2.16}$$

Although as a lower bound, this need not, *a priori*, agree with terms in the small- y Taylor series expansion of the actual function $\bar{W}(\text{hc}, y)$, we find that, remarkably, it does agree all the way up to $O(y^{10})$, i.e., for the first 11 terms. The small- y Taylor series expansion of $\bar{W}(\text{hc}, y)$, calculated to order $O(y^5)$ in Ref. [16] and to $O(y^{18})$ in Ref. [17], is

$$\bar{W}(\text{hc}, y)_l = 1 + \frac{1}{2}y^5 - \frac{1}{8}y^{10} + y^{11} + O(y^{12}). \tag{2.17}$$

To show how close our lower bound is to the actual function $W(\text{hc}, q)$, we give a comparison in Table I for $q=3$ through $q=10$. We determined the values of $W(\text{hc}, q)$ by Monte Carlo measurements, as discussed in detail in our previous work, Refs. [7, 8]. We also include a comparison with our slightly less stringent lower bound (2.1). Evidently, both lower bounds are quite close to the actual measurements, even for q as low as 3. In particular, the sharper lower bound (2.9) provides an extremely good approximation to the actual function $W(\text{hc}, q)$ for $q \geq 3$.

III. 4 · 8² LATTICE

Another interesting question in statistical mechanics and graph theory is the Potts AF ground-state entropy and the related asymptotic behavior of the chromatic polynomial on heteropolygonal lattices, i.e., Archimedean lattices [18] involving tiling of the plane by more than one regular polygon such that all vertices are equivalent. In standard mathematical notation [18,19], an Archimedean lattice is defined by the set $p_1 \cdot p_2 \cdots p_n$ of polygons that one traverses in a circuit

TABLE I. Comparison of lower bounds for $W(\text{hc}, q)$ and ratios of bounds to Monte Carlo measurements for $3 \leq q \leq 10$. The estimated uncertainty from the MC measurements for the entries in the $W(\text{hc}, q)_l / W(\text{hc}, q)_{\text{MC}}$ and $W(\text{hc}, q)_{l'} / W(\text{hc}, q)_{\text{MC}}$ entries is 3×10^{-4} .

q	$W(\text{hc}, q)_{\text{MC}}$	$W(\text{hc}, q)_l$	$W(\text{hc}, q)_l / W(\text{hc}, q)_{\text{MC}}$	$W(\text{hc}, q)_{l'}$	$W(\text{hc}, q)_{l'} / W(\text{hc}, q)_{\text{MC}}$
3	1.6600(5)	1.6583124	0.99898	1.6329932	0.98373
4	2.6038(7)	2.6034166	0.99985	2.5980762	0.99780
5	3.5796(10)	3.5794553	0.99996	3.5777088	0.99947
6	4.5654(15)	4.5650849	0.99993	4.56435465	0.99977
7	5.5556(17)	5.5552778	0.99994	5.5549206	0.99988
8	6.5479(20)	6.5480952	1.00003	6.5479004	1.00000
9	7.5424(22)	7.5425874	1.00002	7.5424723	1.00001
10	8.5386(25)	8.5382220	0.99996	8.5381497	0.99995

around a vertex (site) of the lattice. For a homopolygonal lattice, these are all the same (e.g., in this notation, the square, honeycomb, and triangular lattices are 4^4 , 6^3 , and 3^6). We consider here the $4 \cdot 8^2$ lattice.

A. Lower bound on $W(4 \cdot 8^2, q)$

It is convenient to represent the $4 \cdot 8^2$ lattice as a generalized brick lattice, containing two types of bricks at each hori-

zontal level: square bricks and rectangular ones with (length,height)=(3,1). In the next layer up, a square brick is located in the center above a (3,1) brick, and a (3,1) brick is located with its center above a square brick, and so forth for successive levels. Using the same general method as before, we construct a coloring matrix defined between adjacent horizontal rows of bricks and obtain the lower bound $W(4 \cdot 8^2, q) \geq W(4 \cdot 8^2, q)_l$ for $q \geq 3$ [12], where

$$W(4 \cdot 8^2, q)_l = \frac{[D_4(q)D_8(q)]^{1/4}}{q-1} = \frac{[(q^2-3q+3)(q^6-7q^5+21q^4-35q^3+35q^2-21q+7)]^{1/4}}{q-1}. \quad (3.1)$$

Dividing by the asymptotic behavior as before [9], this has the large- q expansion

$$q^{-1}W(4 \cdot 8^2, q)_l = 1 - \frac{3}{2}q^{-1} + \frac{3}{8}q^{-2} + \frac{5}{16}q^{-3} + \frac{51}{128}q^{-4} + O(q^{-5}). \quad (3.2)$$

The corresponding reduced function $\bar{W}(4 \cdot 8^2, y)_l$ is

$$\begin{aligned} \bar{W}(4 \cdot 8^2, y)_l &= (1+y^3+y^7+y^{10})^{1/4} = [(1+y^3)(1+y^7)]^{1/4} \\ &= (1+y)^{1/2} [(1-y+y^2) \\ &\quad \times (1-y+y^2-y^3+y^4-y^5+y^6)]^{1/4}. \end{aligned} \quad (3.3)$$

B. Large- q series expansion

Using standard methods [15], we have calculated the large- q expansion, i.e., the small- y expansion, of the reduced function $\bar{W}(4 \cdot 8^2, y)$. We find

$$\begin{aligned} \bar{W}(4 \cdot 8^2, y) &= 1 + \frac{1}{4}y^3 - \frac{3}{2^5}y^6 + \frac{1}{4}y^7 + \frac{7}{2^7}y^9 + \frac{1}{2^4}y^{10} \\ &\quad - \frac{77}{2^{11}}y^{12} + O(y^{13}). \end{aligned} \quad (3.4)$$

Next, in order to assess the accuracy for large q of our lower bound, we have expanded the corresponding reduced lower bound function $\bar{W}(4 \cdot 8^2, y)_l$, Eq. (3.3), in a series in y . Remarkably, the small- y series expansion of our lower bound agrees to $O(y^{12})$, i.e., to all 13 terms that we have calculated, with the small- y expansion of the true $\bar{W}(4 \cdot 8^2, y)$ function in Eq. (3.4). This shows that for even moderately large q , our lower bound $W(4 \cdot 8^2, q)_l$ actually provides an extremely accurate approximation to the true function $W(4 \cdot 8^2, q)$. Of course, it is straightforward to calculate the series (3.4) to higher order in y , and at $O(y^{13})$ or above the series for $\bar{W}(4 \cdot 8^2, y)$ and $\bar{W}(4 \cdot 8^2, y)_l$ could differ; nevertheless, the agreement to $O(y^{12})$ is already quite striking.

C. Monte Carlo measurements

To get further information on $W(4 \cdot 8^2, q)$, we have carried out Monte Carlo (MC) measurements of the Potts AF ground-state entropy S_0 and hence obtained $W = \exp(S_0/k_B)$, for $3 \leq q \leq 10$. Our methods are similar to those used in our previous works [7,8]. We present our results in Table II, including comparisons with our rigorous lower bound and our series calculation to $O(y^{12})$ (to which order they coincide). Evidently, the agreement is extremely good, even for q as low as 3.

TABLE II. Exponential of ground-state entropy, from Monte Carlo measurements, and comparison with lower bound, for the Potts antiferromagnet with $3 \leq q \leq 10$ on the $4 \cdot 8^2$ lattice. The estimated uncertainty from the MC measurements for the entries in the $W(4 \cdot 8^2, q)_l / W(4 \cdot 8^2, q)_{MC}$ column is 3×10^{-4} .

q	$W(4 \cdot 8^2, q)_{MC}$	$W(4 \cdot 8^2, q)_l / W(4 \cdot 8^2, q)_{MC}$
3	1.68575(60)	0.99959
4	2.62226(75)	0.99994
5	3.5918(10)	0.99995
6	4.5737(14)	0.99996
7	5.5618(16)	0.99992
8	6.5530(20)	0.99995
9	7.5466(23)	0.99995
10	8.5413(26)	0.99998

IV. SQUARE LATTICE WITH DIAGONAL NEXT-NEAREST-NEIGHBOR COUPLINGS

An interesting question concerns the effect of non-nearest-neighbor interactions on the ground-state entropy of the Potts antiferromagnet and the corresponding $W(\Lambda, q)$ function. We explore this question here by considering the Potts AF on a square lattice with next-nearest-neighbor couplings along both diagonals, defined by the Hamiltonian

$$\mathcal{H} = - \sum_{n, n'} J_{nn'} \delta_{\sigma_n, \sigma_{n'}}, \quad (4.1)$$

where $J_{n, n'} = J < 0$ if the sites n and n' are nearest neighbors along a row or column, and $J_{n, n'} = J_d < 0$ if n and n' are diagonally opposite sites on a given square of the lattice [with each such pair counted only once in the sum (4.1)]. We further define $K = \beta J$ and $K_d = \beta J_d$ and consider the $T \rightarrow 0$ limit, so that the color on each site n is required to be different from the colors of each of its nearest neighbors on the rows and columns of the lattice, and also each of its next-nearest neighbors along the diagonals of the lattice. Then $Z((sq)_d, q, T=0)_{PAF} = P((sq)_d, q)$, where $(sq)_d$ denotes the nonplanar graph formed from a square lattice by adjoining bonds connecting diagonally opposite sites on each square [20]. Note that the $(sq)_d$ lattice has coordination number $\zeta = 8$ and girth $\gamma = 3$, where ‘‘girth’’ γ of a graph G denotes the length of the shortest circuit on G . We find that the chromatic number of this lattice (for free boundary conditions or periodic boundary conditions that preserve the bipartite structure of the underlying square lattice before inclusion of diagonal bonds) is

$$\chi((sq)_d) = 4 \quad (4.2)$$

[$\chi(G)$ is defined in Ref. [12].] These are to be compared with $\zeta = \gamma = 4$ and $\chi(sq) = 2$ for the square lattice. From our earlier discussion, one thus has $W((sq)_d, q) \leq W(sq, q)$. Indeed, we find that there is an especially strong difference with respect to the square lattice for the case $q = \chi((sq)_d) = 4$. Here, we calculate that for a $(sq)_d$ lattice $\Lambda_{L_1 \times L_2}$ of length L_1 in the x direction and L_2 in the y direction,

TABLE III. Exponential of ground-state entropy, from Monte Carlo measurements, and comparison with lower bound, for the Potts antiferromagnet with $5 \leq q \leq 10$ on the square lattice with diagonal next-nearest-neighbor couplings. The estimated uncertainty from the MC measurements in the entries for $W(sq_d, q)_l / W(sq_d, q)_{MC}$ is 1×10^{-3} .

q	$W(sq_d, q)_{MC}$	$W(sq_d, q)_l / W(sq_d, q)_{MC}$	$W(sq, q)_{MC}$
5	1.5781(16)	0.95051	3.2510(10)
6	2.4460(24)	0.98119	4.2003(12)
7	3.3660(33)	0.99029	5.1669(15)
8	4.3093(43)	0.99453	6.1431(20)
9	5.2680(53)	0.99658	7.1254(22)
10	6.2363(62)	0.99774	8.1122(25)

$$P(\Lambda_{L_1 \times L_2}, 4) \sim 2^{L_1 + L_2} \quad (4.3)$$

in the thermodynamic limit. Although this diverges, it does not diverge rapidly enough to yield a finite entropy. With the ordering of limits

$$W(\Lambda, q_s) \equiv \lim_{n \rightarrow \infty} \lim_{q \rightarrow q_s} P(G, q)^{1/n} \quad (4.4)$$

as discussed in Ref. [8], we thus obtain the exact result

$$W((sq)_d, q=4) = 1, \quad \text{i.e.,} \quad S_0((sq)_d, q=4) = 0. \quad (4.5)$$

This may be compared with the value for the usual square lattice, for which $W(sq, 4) = 2.3370(7)$ [8], corresponding to the nonzero ground-state entropy $S_0(sq, 4) = 0.8489(3)$. [Indeed, even without any detailed calculation, one knows that $S_0(sq, 4)$ is nonzero from the elementary rigorous lower bound on a bipartite lattice, $S_0(\Lambda_{\text{bip}}, q) > (1/2) \ln(q-1)$.]

Using the same type of coloring matrix method as above, we obtain the rigorous lower bound $W((sq)_d, q) \geq W((sq)_d, q)_l$, where

$$W((sq)_d, q)_l = \frac{(q-2)(q-3)}{q-1} \quad \text{for } q \geq 4. \quad (4.6)$$

For large q , we have the Taylor series expansion

$$q^{-1} W((sq)_d, q)_l = 1 - 4q^{-1} + 2[q^{-2} + q^{-3} + q^{-4} + O(q^{-5})]. \quad (4.7)$$

From Eq. (2.14) we have

$$\bar{W}(sq_d, y)_l = (1-y)(1-2y)(1+y)^3. \quad (4.8)$$

The MC measurements are given in Table III. For comparison, we include also our MC measurements of $W(sq, q)$ [8]. The lower bound (4.6) steadily approaches the measured values $W((sq)_d, q)$ as q increases and is quite close to them for q greater than about 6. The inequality $W((sq)_d, q) \leq W(sq, q)$ is also evident.

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