Lower Bounds on the Ground State Entropy of the Potts Antiferromagnet on Slabs of the Simple Cubic Lattice

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We calculate rigorous lower bounds for the ground state degeneracy per site, W, of the q-state Potts antiferromagnet on slabs of the simple cubic lattice that are infinite in two directions and finite in the third and that thus interpolate between the square (sq) and simple cubic (sc) lattices. We give a comparison with large-q series expansions for the sq and sc lattices and also present numerical comparisons.

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I. INTRODUCTION

Nonzero ground state entropy (per lattice site), $S_0 \neq 0$, is an important subject in statistical mechanics, as an exception to the third law of thermodynamics and a phenomenon involving large disorder even at zero temperature. Since $S_0 = k_B \ln W$, where $W = \lim_{n\to\infty} W_{tot.}^{1/n}$ and n denotes the number of lattice sites, $S_0 \neq 0$ is equivalent to $W > 1$, i.e., a total ground state degeneracy $W_{tot.}$ that grows exponentially rapidly as a function of n. One physical example is provided by H_2O ice, for which the residual entropy per site (at 1 atm. pressure) is measured to be $S_0 = (0.41 \pm 0.03)k_B$, or equivalently, $W = 1.51 \pm 0.05$ [1]-[3]. A salient property of ice is that the ground state entropy occurs without frustration; i.e., each of the ground state configurations of the hydrogen atoms on the bonds between oxygen atoms minimizes the internal energy of the crystal [4].

A model that also exhibits ground state entropy without frustration and hence provides a useful framework in which to study the properties of this phenomenon is the q-state Potts antiferromagnet [5]-[7] on a given lattice Λ or, more generally, a graph G, for sufficiently large q. Consider a graph $G = (V, E)$, defined by its vertex (site) and edge (bond) sets V and E. Denote the cardinalities of these sets as $n(G) = |V| \equiv n$ and $e(G) = |E|$, and let $\{G\} \equiv \lim_{n(G)\to\infty} G$. An important connection with graph theory is the fact that the zero-temperature partition function of the q-state Potts antiferromagnet on the graph G satisfies $Z(G, q, T = 0) = P(G, q)$, 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 (called a proper q-coloring of G) [8, 9]. Thus,

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

In general, for certain special values of q, denoted q_s, one has the following noncommutativity of limits [10]

$$\lim_{n\to\infty} \lim_{q\to q_s} P(G, q)^{1/n} \neq \lim_{q\to q_s} \lim_{n\to\infty} P(G, q)^{1/n} \ , \qquad (1.2)$$

and hence it is necessary to specify which order of limits that one takes in defining $W(\{G\}, q)$. Here by $W(\{G\}, q)$ we mean the function obtained by setting q to the given value first and then taking $n \to \infty$. For the $n \to \infty$ limit of a bipartite graph $G_{bip.}$, an elementary lower bound is $W(\{G_{bip.}\}, q) \geq \sqrt{q-1}$, so that for $q > 2$, the Potts antiferromagnet has a nonzero ground state entropy on such a lattice. A better lower bound for the square lattice is $W(sq, q) \geq (q^2-3q+3)/(q-1)$ [11]. In previous work [12]-[15] one of us and Tsai derived lower and upper bounds on W for a variety of different two-dimensional lattices. It was found that these lower bounds are quite close to the actual values as determined with reasonably good accuracy from large-q series expansions and/or Monte Carlo measurements.

In the present paper we generalize these lower bounds on two-dimensional lattice graphs by deriving lower bounds on $W(\{G\}, q)$ for sections of a three-dimensional lattice, namely the simple cubic lattice, which are of infinite extent in two directions (taken to lie along the x and y axes) and finite in the third direction, z. By comparison with large-q expansions and numerical evaluations, we show how the lower bounds for the W functions for these slabs interpolate between the values for the (respective thermodynamic limits of the) square and simple cubic lattices. These bounds are of interest partly because one does not know the exact functions $W(sq, q)$ or $W(sc, q)$ for general q.

II. CALCULATIONAL METHOD

Let us consider a section (slab) of the simple cubic lattice of dimensions $L_x \times L_y \times L_z$ vertices, which we denote $sc[(L_x)_{BCx} \times (L_y)_{BCy} \times (L_z)_{BCz}]$, where the boundary conditions (BC) in each direction are indicated by the subscripts. The chromatic polynomial of this lattice will be denoted $P(sc[(L_x)_{BCx} \times (L_y)_{BCy} \times (L_z)_{BCy}], q)$. We will calculate lower bounds for $W(sc[(L_x)_{BCx} \times (L_y)_{BCy} \times (L_z)_{BCz}], q)$ in the limit $L_x \to \infty$ and $L_y \to \infty$ with L_z fixed. These are independent of the boundary conditions imposed in the directions in which the slab is of infinite extent, and hence, for brevity of nota-