Some Exact Results for Spanning Trees on Lattices

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Abstract.

For $n$-vertex, $d$-dimensional lattices $\Lambda$ with $d \geq 2$, the number of spanning trees $N_{ST}(\Lambda)$ grows asymptotically as $\exp(nz_{\Lambda})$ in the thermodynamic limit. We present an exact closed-form result for the asymptotic growth constant $z_{\text{bcc}(d)}$ for spanning trees on the $d$-dimensional body-centered cubic lattice. We also give an exact integral expression for $z_{\text{fcc}}$ on the face-centered cubic lattice and an exact closed-form expression for $z_{488}$ on the $4 \times 8 \times 8$ lattice.
1. Introduction

Let $G = (V, E)$ denote a connected graph (without loops) with vertex (site) and edge (bond) sets $V$ and $E$. Let $n = v(G) = |V|$ be the number of vertices and $e(G) = |E|$ the number of edges in $G$. A spanning subgraph $G'$ is a subgraph of $G$ with $v(G') = |V|$, and a tree is a connected subgraph with no circuits. A spanning tree is a spanning subgraph of $G$ that is a tree (and hence $e(G') = n - 1$). A problem of fundamental interest in mathematics and physics is the enumeration of the number of spanning trees on the graph $G$, $N_{ST}(G)$. This number can be calculated in several ways, including as a determinant of the Laplacian matrix of $G$ and as a special case of the Tutte polynomial of $G$ [1, 2]. In this paper we shall present an exact closed-form result for the asymptotic growth constant for spanning trees on the $d$-dimensional body-centered cubic lattice, denoted $bcc(d)$, with $bcc(3) \equiv bcc$. We shall also give an exact integral expression for the $z_{fcc}$ describing the face-centered cubic lattice and an exact closed-form expression $z_{88}$ for the $4 \cdot 8 \cdot 8$ lattice. A previous study on the enumeration of spanning trees and the calculation of their asymptotic growth constants was carried out in Ref. 3. In that work, closed-form integrals for these quantities were given, and from the integral for the $bcc(d)$ lattice, an infinite series representation was derived. Our present result for the $bcc(d)$ lattice is obtained by summing exactly this infinite series. Similarly, our present result for the $4 \cdot 8 \cdot 8$ lattice is obtained by an exact closed-form evaluation of the integral given for this lattice in Ref. 3.

2. Background and Method

We briefly recall some definitions and background on spanning trees and the calculational method that we use. For $G = G(V, E)$, the degree $k_i$ of a vertex $v_i \in V$ is the number of edges attached to it. A $k$-regular graph is a graph with the property that each of its vertices has the same degree $k$. Two vertices are adjacent if they are connected by an edge. The adjacency matrix $A(G)$ of $G$ is the $n \times n$ matrix with elements $A_{ij} = 1$ if $v_i$ and $v_j$ are adjacent and zero otherwise. The Laplacian matrix $Q = Q(G)$ is the $n \times n$ matrix $Q$ with $Q_{ij} = k_i \delta_{ij} - A_{ij}$. One of the eigenvalues of $Q(G)$ is always zero; let us denote the rest as $\lambda_i(G)$, $1 \leq i \leq n - 1$. A basic theorem is that $11 2$ $N_{ST}(G) = (1/n) \prod_{i=1}^{n-1} \lambda_i(G)$. Here we shall focus on $k$-regular $d$-dimensional lattices $\Lambda$. For these lattices, if $d \geq 2$, then in the thermodynamic limit, $N_{ST}$ grows exponentially with $n$ as $n \to \infty$; that is, there exists a constant $z_\Lambda$ such that $N_{ST}(\Lambda) \sim \exp(nz_\Lambda)$ as $n \to \infty$. The constant describing this exponential growth is thus given by

$$z_\Lambda = \lim_{n \to \infty} n^{-1} \ln N_{ST}(\Lambda).$$

(1)

where $\Lambda$, when used as a subscript in this manner, implicitly refers to the thermodynamic limit of the lattice $\Lambda$. A regular $d$-dimensional lattice is comprised of repeated unit cells, each containing $\nu$ vertices. Define $a(\tilde{n}, \tilde{n}')$ as the $\nu \times \nu$ matrix describing the adjacency of the ($d$-dimensional) vertices of the unit cells $\tilde{n}$ and $\tilde{n}'$, the elements of which are given by $a(\tilde{n}, \tilde{n}')_{ij} = 1$ if $v_i \in \tilde{n}$ is adjacent to $v_j \in \tilde{n}'$ and 0 otherwise. Assuming that
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A given lattice has periodic boundary conditions, and using the resultant translational symmetry, we have \(a(\tilde{n}, \tilde{n}') = a(\tilde{n} - \tilde{n}')\), and we can therefore write \(a(\tilde{n}) = a(\tilde{n}_1, \cdots, \tilde{n}_d)\). In Ref. [3] a method was derived to calculate \(N_{ST}(\Lambda)\) and \(z_\Lambda\) in terms of a matrix \(M\) which is determined by these \(a(\tilde{n}, \tilde{n}')\). For a \(d\)-dimensional lattice, define

\[
M(\theta_1, \cdots, \theta_d) = k \cdot 1 - \sum_{\tilde{n}} a(\tilde{n})e^{i\tilde{n}\cdot\theta}
\]

where in this equation 1 is the unit matrix and \(\theta\) stands for the \(d\)-dimensional vector \((\theta_1, \cdots, \theta_d)\). Then [3]

\[
z_\Lambda = \frac{1}{\nu} \int_{-\pi}^{\pi} \left[ \prod_{j=1}^{d} \frac{d\theta_j}{2\pi} \right] \ln[\det(M(\theta_1, \cdots, \theta_d))] \tag{3}
\]

For a \(k\)-regular graph \(\Lambda\), a general upper bound is \(z_\Lambda \leq \ln k\). A stronger upper bound for a \(k\)-regular graph \(\Lambda\) with coordination number \(k \geq 3\) can be obtained from the bound [4, 5]

\[
N_{ST}(G) \leq \left(\frac{2\ln n}{nk\ln k}\right)(C_k)^n \tag{4}
\]

where

\[
C_k = \frac{(k - 1)^{k-1}}{[k(k - 2)]^{k-1}}. \tag{5}
\]

With eq. (1), this then yields [3]

\[
z_\Lambda \leq \ln(C_k). \tag{6}
\]

It is of interest to see how close the exact results are to these upper bounds. For this purpose, we define the ratio

\[
r_\Lambda = \frac{z_\Lambda}{\ln C_k} \tag{7}
\]

where \(k\) is the coordination number of \(\Lambda\).

3. bcc(\(d\)) Lattice

For the \(bcc(\(d\))\) lattice a unit cell contains \(\nu_{bcc(\(d\))} = 2\) vertices located at \(v_1 = (0, \cdots, 0)\) and \(v_2 = (\frac{1}{2}, \cdots, \frac{1}{2})\). This lattice has coordination number \(k_{bcc(\(d\))} = 2^d\). Using eq. (3), Ref. [3] obtained

\[
z_{bcc(\(d\))} = d \ln 2 + I_{bcc(\(d\))} \tag{8}
\]

where

\[
I_{bcc(\(d\))} = \frac{1}{2} \int_{-\pi}^{\pi} \left[ \prod_{j=1}^{d} \frac{d\theta_j}{2\pi} \right] \ln \left( 1 - \prod_{j=1}^{d} \cos^2(\theta_j/2) \right)
\]

\[
= \int_{-\pi}^{\pi} \left[ \prod_{j=1}^{d} \frac{d\theta_j}{2\pi} \right] \ln \left( 1 - \prod_{j=1}^{d} \cos \theta_j \right). \tag{9}
\]
Expanding the logarithm and carrying out the integration term by term yields the infinite series representation

$$I_{bcc}(d) = -\frac{1}{2} \sum_{\ell=1}^{\infty} \frac{1}{\ell} \left( \frac{(2\ell)!}{2^{2\ell} (\ell!)^2} \right)^d$$

(10)

We now sum this series exactly. First,

$$I_{bcc}(d) = -\frac{1}{2} \sum_{\ell=1}^{\infty} \frac{(\ell - 1)! \cdot [(2\ell)!]^d}{2^{2\ell d} (\ell!)^{2d+1}}$$

$$= -\frac{1}{2} \sum_{k=0}^{\infty} \frac{(k!)^2 \cdot [(2k + 2)!]^d}{2^{2k+1}(k+1)! \cdot [(k + 1)!]^{2d+1} k!}$$

$$= -\frac{1}{2^{d+1}} \sum_{k=0}^{\infty} \frac{\Gamma(k + 1)^2 \cdot \Gamma(2k + 3)}{\Gamma(k + 2)^{2d+1} k!}.$$  (11)

Next, we use the duplication formula for the Euler gamma function,

$$\Gamma(2z) = (2\pi)^{-1/2} \left( 2^{2z-1} \cdot \Gamma(z) \cdot \Gamma(z + \frac{1}{2}) \right)$$

(12)

with $z = k + \frac{3}{2}$, together with $\Gamma(1/2) = \sqrt{\pi}$, to express

$$\frac{\Gamma(2k + 3)}{2^{2k+1} \Gamma(k + 2)} = \frac{\Gamma(k + \frac{3}{2})}{\Gamma(\frac{3}{2})}.$$  (13)

Substituting this into eq. (11), we have

$$I_{bcc}(d) = -\frac{1}{2^{d+1}} \sum_{k=0}^{\infty} \frac{\Gamma(k + 1)^2 \cdot \Gamma(2k + 3)/\Gamma(\frac{3}{2})}{\Gamma(k + 2)^{2d+1} k!}$$

$$= -2^{-(d+1)} \cdot F_{d+1}(1, [1, 1, 3/2, \ldots, 3/2], [2, \ldots, 2], 1)$$

(14)

where there are $d + 2$ entries in first square bracket $[\cdots]$ and $d + 1$ entries in the second square bracket $[\cdots]$ in the argument, and $_pF_q$ is the generalized hypergeometric function,

$$_pF_q([a_1, \cdots, a_p], [b_1, \cdots, b_q], x) = \sum_{k=0}^{\infty} \left( \frac{\prod_{j=1}^{p} (a_j)_k}{\prod_{r=1}^{q} (b_r)_k} \right) \frac{x^k}{k!}$$

(15)

where $c_n = \Gamma(c + n)/\Gamma(c)$. Hence,

$$z_{bcc(d)} = d \ln 2 - 2^{-(d+1)} \cdot F_{d+1}(1, [1, 1, 3/2, \cdots, 3/2], [2, \cdots, 2], 1) .$$  (16)

We comment on some special cases. For $d = 1$, the $bcc(1)$ lattice with free (periodic) boundary conditions degenerates effectively to a line (circuit) graph, for which, respectively, $N_{ST} = 1$ and $N_{ST} = n$; in both cases, it follows that $z_{bcc(1)} = 0$. Using the value $3F_2([1, 1, 3/2], [2, 2], 1) = 4 \ln 2$, we recover this elementary result. For $d = 2$, the $bcc(2)$ lattice is equivalent to the square lattice, for which $z_{sq} = (4/\pi)\beta(2) = 1.1662436$. [6, 7], where $\beta(s) = \sum_{n=0}^{\infty} (-1)^n (2n+1)^{-s}$ and $\beta(2) = C = 0.915965594177..$ is the Catalan constant. The general result [8] with [14] evaluated for $d = 2$ agrees with this, since $4F_2([1, 1, 3/2, 3/2], [2, 2, 2], 1) = 16(\ln 2 - (2C/\pi))$. Our general exact result for $z_{bcc(d)}$ provides quite accurate values for higher values of $d$, which we list in Table II together with the corresponding ratios [7] which give a comparison with the upper bound (6). Evidently, the exact values are very close to this upper bound and move closer as $d$ increases.
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Table 1. Values of $z_{\text{bcc}}(d)$ and $r_{\text{bcc}}(d)$.

| $d$ | $z_{\text{bcc}}(d)$                  | $r_{\text{bcc}}(d)$                  |
|-----|-------------------------------------|-------------------------------------|
| 1   | 0                                   | -                                   |
| 2   | 1.166243616123275                   | 0.9587702228064145                 |
| 3   | 1.9901911418271941                  | 0.9912457055306051                 |
| 4   | 2.732957535477362                   | 0.9977089878275579                 |
| 5   | 3.447331914522398                   | 0.9993413280070963                 |
| 6   | 4.150116933352462                   | 0.9998002121159708                 |
| 7   | 4.847789269805724                   | 0.9999373061649456                 |
| 8   | 5.543104959793989                   | 0.9999798500846987                 |
| 9   | 6.237305017795394                   | 0.9999934053622532                 |
| 10  | 6.930967870288660                   | 0.9999978103135475                 |

4. fcc Lattice

The face-centered cubic (fcc) lattice has coordination number $k_{\text{fcc}} = 12$ and a unit cell consisting of the $v_{\text{fcc}} = 4$ vertices $(0,0,0)$, $(0,\frac{1}{2},\frac{1}{2})$, $(\frac{1}{2},0,\frac{1}{2})$, and $(\frac{1}{2},\frac{1}{2},0)$. For this lattice, $M(\theta_1, \theta_2, \theta_3)$ is

$$M(\theta_1, \theta_2, \theta_3) = \begin{pmatrix} 12 & -(v_2 v_3)^* & -(v_1 v_3)^* & -(v_1 v_2)^* \\ -v_2 v_3 & 12 & -v_1^* v_2 & -v_1^* v_3 \\ -v_1 v_3 & -v_1 v_2^* & 12 & -v_2^* v_3 \\ -v_1 v_2 & -v_1 v_3^* & -v_2 v_3^* & 12 \end{pmatrix}$$

(17)

where $v_j = 1 + e^{i \theta_j}$, $j = 1, 2, 3$. The evaluation of the determinant yields

$$z_{\text{fcc}} = \ln(12) + \frac{1}{4} \int_{-\pi}^{\pi} \frac{d\theta_1}{2\pi} \int_{-\pi}^{\pi} \frac{d\theta_2}{2\pi} \int_{-\pi}^{\pi} \frac{d\theta_3}{2\pi} \ln F(\theta_1, \theta_2, \theta_3)$$

(18)

where, with the abbreviation $c_j \equiv \cos(\theta_j/2)$,

$$F(\theta_1, \theta_2, \theta_3) = \left[ 1 + \frac{1}{3}(-c_2 c_3 + c_3 c_1 + c_1 c_2) \right] \left[ 1 + \frac{1}{3}(c_2 c_3 - c_3 c_1 + c_1 c_2) \right]$$

$$\times \left[ 1 + \frac{1}{3}(c_2 c_3 + c_3 c_1 - c_1 c_2) \right] \left[ 1 - \frac{1}{3}(c_2 c_3 + c_3 c_1 + c_1 c_2) \right]$$

$$= 1 - \frac{2}{9}(c_1 c_2)^2 + (c_2 c_3)^2 + (c_3 c_1)^2 - \frac{8}{27}(c_1 c_2 c_3)^2$$

$$- \frac{2}{81}(c_1 c_2 c_3)^2(c_1^2 + c_2^2 + c_3^2) + \frac{1}{81}[(c_1 c_2)^4 + (c_2 c_3)^4 + (c_3 c_1)^4].$$

(19)

(This corrects an algebraic error in eq. (5.3.3) of Ref. [3]). Evaluating this numerically, we find that $z_{\text{fcc}} \simeq 2.41292$. Substituting $z_{\text{fcc}}$ into eq. (17), we get $r_{\text{fcc}} \simeq 0.98915$, so that the upper bound (17) is very close to the actual value of the growth constant.
5. 4·8·8 Lattice

An Archimedean lattice is a uniform tiling of the plane by regular polygons in which all vertices are equivalent. Such a lattice can be defined by the ordered sequence of polygons that one traverses in making a complete circuit around the local neighborhood of any vertex. This is indicated by the notation $\Lambda = (\prod_i p_i^{a_i})$, meaning that in this circuit, a regular $p_i$-sided polygon occurs contiguously $a_i$ times. We consider here the 4·8·8 lattice involving the tiling of the plane by squares and octagons. In eq. (4.11) of Ref. [3], the asymptotic growth constant for this lattice was calculated to be

$$z_{488} = \frac{1}{4} \ln 2 + \frac{1}{4} \int_{-\pi}^{\pi} \frac{d\theta_1}{2\pi} \int_{-\pi}^{\pi} \frac{d\theta_2}{2\pi} \ln \left[ 7 - 3(\cos \theta_1 + \cos \theta_2) - \cos \theta_1 \cos \theta_2 \right]$$

$$= \frac{1}{4} \ln 2 + \frac{1}{4\pi} \int_{0}^{\pi} d\theta \ln \left[ 7 - 3 \cos \theta + 4 \sin(\theta/2)\sqrt{5 - \cos \theta} \right]$$

where the integral on the second line of eq. (20) is obtained by doing one of the two integrations in the expression on the first line. These integrals were evaluated numerically to obtain the result $z_{488} = 0.786684(1)$, where the number in parentheses indicates the estimated error in the last digit.

We have derived an exact closed form expression for this integral. We begin by recasting the integral in the equivalent form.

$$z_{488} = \frac{1}{4} \ln 2 + \frac{1}{2\pi} \int_{0}^{\pi} d\theta \ln \left( 2 \sin(\theta/2) + \sqrt{4 + 2\sin^2(\theta/2)} \right)$$

$$= \frac{3}{4} \ln 2 + \frac{1}{\pi} \int_{0}^{\pi/2} d\phi \ln \left( \sin(\phi) + \sqrt{1 + (1/2)\sin^2(\phi)} \right).$$

That is,

$$z_{488} = \frac{3}{4} \ln 2 + I(1/\sqrt{2})$$

where

$$I(a) = \frac{1}{\pi} \int_{0}^{\pi/2} d\phi \ln \left( \sin \phi + \sqrt{1 + a^2 \sin^2 \phi} \right).$$

In eq. (23), with no loss of generality, we take $a$ to be nonnegative. We will give a general result for $I(a)$ and then specialize to our case $a = 1/\sqrt{2}$. First, we note that $I(1) = C/\pi$, where $C$ is the Catalan constant. Next, assume $0 \leq a < 1$. Taking the derivative with respect to $a$ and doing the integral over $\phi$ in eq. (23), we get

$$I'(a) = \frac{-a/2 + (2/\pi) \tan^{-1} a}{1 - a^2}.$$  

To calculate $I(a)$, we then use $I(a) - I(0) = \int_{0}^{a} I'(x) dx$ and observe that

$$I(0) = \frac{1}{\pi} \int_{0}^{\pi/2} d\phi \ln(\sin(\phi) + 1) = -\frac{\ln 2}{2} + \frac{2C}{\pi}$$

We also make use of the integrals

$$\int_{0}^{a} \frac{x}{(1 - x^2)} dx = -\frac{1}{2} \ln(1 - a^2)$$
and
\[ \int_{0}^{a} \frac{\tan^{-1} x}{1-x^2} \, dx = -\frac{C}{2} - \frac{\pi}{8} \ln \left( \frac{1+a}{1-a} \right) + \frac{1}{2} \text{Ti}_2 \left( \frac{1+a}{1-a} \right) \] (27)
to obtain
\[ I(a) = \frac{C}{\pi} + \frac{1}{2} \ln \left( \frac{1-a}{2} \right) + \frac{1}{\pi} \text{Ti}_2 \left( \frac{1+a}{1-a} \right) \quad \text{if} \quad 0 \leq a < 1, \] (28)
where \( \text{Ti}_2(x) \) is the inverse tangent integral \[^8\],
\[ \text{Ti}_2(x) = \int_{0}^{x} \frac{\tan^{-1} y}{y} \, dy \]
\[ = x \left[ \text{ _3F_2}[1, 1/2, 1/2; 3/2, 3/2; -x^2] \right]. \] (29)
(Here the arctangent is taken to lie in the range \(-\pi/2 < \tan^{-1} y < \pi/2\).) Evaluating our result (28) for \( I(a) \) at \( a = 1/\sqrt{2} \) and substituting into eq. (22), we obtain the exact, closed-form expression
\[ z_{488} = \frac{C}{\pi} + \frac{1}{2} \ln(\sqrt{2} - 1) + \frac{1}{\pi} \text{Ti}_2(3 + 2\sqrt{2}). \] (30)
The numerical evaluation of eq. (30) agrees with the evaluation given in Ref. \[3\] to the accuracy quoted there and allows one to obtain higher accuracy; for example, to 15 significant figures, \( z_{488} = 0.786684275378832 \). We note that the \( \text{Ti}_2 \) function also appears at intermediate stages in the derivation of \( z_{\text{tri}} \) for the triangular lattice \[^9\]. For completeness, we have also calculated \( I(a) \) for \( a > 1 \) with the result
\[ I(a) = \frac{C}{\pi} + \frac{1}{2} \ln \left[ \frac{(a+1)^2}{2(a-1)} \right] + \frac{1}{\pi} \text{Ti}_2 \left( \frac{1+a}{1-a} \right) \quad \text{if} \quad a > 1. \] (31)

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