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2006 J. Phys. A: Math. Gen. 39 5653

(http://iopscience.iop.org/0305-4470/39/20/001)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 5653–5658 doi:10.1088/0305-4470/39/20/001

Some exact results for spanning trees on lattices

Shu-Chiuan Chang[1] **and Robert Shrock**[2]

[1] Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan
[2] C N Yang Institute for Theoretical Physics, State University of New York, Stony Brook, NY 11794, USA

Received 23 February 2006
Published 3 May 2006
Online at stacks.iop.org/JPhysA/39/5653

Abstract
For n-vertex, d-dimensional lattices Λ with $d \geqslant 2$, 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 $z_{bcc(d)}$ for spanning trees on the d-dimensional body-centred cubic lattice. We also give an exact integral expression for z_{fcc} on the face-centred cubic lattice and an exact closed-form expression for z_{488} on the 4 8 8 lattice.

PACS numbers: 02.10.Ox, 05.20.−y

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 which 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-centred 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-centred cubic lattice and an exact closed-form expression z_{488} for the 4 8 8 lattice. A previous study on the enumeration of spanning trees and the calculation of their asymptotic growth constants was carried out in [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 8 8 lattice is obtained by an exact closed-form evaluation of the integral given for this lattice in [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 $\lambda_i(G)$, $1 \leqslant i \leqslant n-1$. A basic theorem is that [1, 2] $N_{\mathrm{ST}}(G) = (1/n)\prod_{i=1}^{n-1}\lambda_i(G)$. Here we shall focus on k-regular d-dimensional lattices Λ. For these lattices, if $d \geqslant 2$, then in the thermodynamic limit, N_{ST} grows exponentially with n as $n \to \infty$; that is, there exists a constant z_Λ such that $N_{\mathrm{ST}}(\Lambda) \sim \exp(nz_\Lambda)$ as $n \to \infty$. The constant describing this exponential growth is thus given by

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

where Λ, when used as a subscript in this manner, implicitly refers to the thermodynamic limit of the lattice Λ. A regular d-dimensional lattice is comprised of repeated unit cells, each containing ν 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 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 $a(\tilde{n}) = a(\tilde{n}_1, \ldots, \tilde{n}_d)$. In [3] a method was derived to calculate $N_{\mathrm{ST}}(\Lambda)$ and z_Λ in terms of a matrix M which is determined by these $a(\tilde{n}, \tilde{n}')$. For a d-dimensional lattice, define

$$M(\theta_1, \ldots, \theta_d) = k \cdot 1 - \sum_{\tilde{n}} a(\tilde{n})\, \mathrm{e}^{\mathrm{i}\tilde{n}\cdot\theta} \tag{2}$$

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

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

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

$$N_{\mathrm{ST}}(G) \leqslant \left(\frac{2\ln n}{nk\ln k}\right)(C_k)^n, \tag{4}$$

where

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

With equation (1), this then yields [3]

$$z_\Lambda \leqslant \ln(C_k). \tag{6}$$

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 Λ.

3. bcc(d) lattice

For the bcc(d) lattice a unit cell contains $\nu_{\mathrm{bcc}(d)} = 2$ vertices located at $v_1 = (0, \ldots, 0)$ and $v_2 = \left(\frac{1}{2}, \ldots, \frac{1}{2}\right)$. This lattice has coordination number $k_{\mathrm{bcc}(d)} = 2^d$. Using equation (3), Shrock and Wu [3] obtained

$$z_{\mathrm{bcc}(d)} = d \ln 2 + I_{\mathrm{bcc}(d)} \tag{8}$$

where

$$\begin{aligned} I_{\mathrm{bcc}(d)} &= \frac{1}{2} \int_{-\pi}^{\pi} \left[\prod_{j=1}^{d} \frac{\mathrm{d}\theta_j}{2\pi} \right] \ln \left(1 - \prod_{j=1}^{d} \cos^2(\theta_j/2) \right) \\ &= \int_{-\pi}^{\pi} \left[\prod_{j=1}^{d} \frac{\mathrm{d}\theta_j}{2\pi} \right] \ln \left(1 - \prod_{j=1}^{d} \cos\theta_j \right). \end{aligned} \tag{9}$$

Expanding the logarithm and carrying out the integration term by term yields the infinite series representation [3]

$$I_{\mathrm{bcc}(d)} = -\frac{1}{2} \sum_{\ell=1}^{\infty} \frac{1}{\ell} \left(\frac{(2\ell)!}{2^{2\ell}(\ell!)^2} \right)^d. \tag{10}$$

We now sum this series exactly. First,

$$\begin{aligned} I_{\mathrm{bcc}(d)} &= -\frac{1}{2} \sum_{\ell=1}^{\infty} \frac{(\ell-1)![(2\ell)!]^d}{2^{2\ell d}(\ell!)^{2d+1}} \\ &= -\frac{1}{2} \sum_{k=0}^{\infty} \frac{(k!)^2[(2k+2)!]^d}{2^{2(k+1)d}[(k+1)!]^{2d+1}k!} \\ &= -\frac{1}{2^{d+1}} \sum_{k=0}^{\infty} \frac{[\Gamma(k+1)]^2[\Gamma(2k+3)]^d}{2^{(2k+1)d}[\Gamma(k+2)]^{2d+1}k!}. \end{aligned} \tag{11}$$

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

$$\Gamma(2z) = (2\pi)^{-1/2}\, 2^{2z-\frac{1}{2}} \Gamma(z) \Gamma\left(z + \tfrac{1}{2}\right) \tag{12}$$

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

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

Substituting this into equation (11), we have

$$\begin{aligned} I_{\mathrm{bcc}(d)} &= -\frac{1}{2^{d+1}} \sum_{k=0}^{\infty} \frac{[\Gamma(k+1)]^2[\Gamma\left(k+\frac{3}{2}\right)/\Gamma\left(\frac{3}{2}\right)]^d}{[\Gamma(k+2)]^{d+1}k!} \\ &= -2^{-(d+1)}\, {}_{d+2}F_{d+1}([1, 1, 3/2, \ldots, 3/2], [2, \ldots, 2], 1) \end{aligned} \tag{14}$$

where there are $d+2$ entries in the 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

$${}_pF_q([a_1, \ldots, a_p], [b_1, \ldots, b_q], x) = \sum_{k=0}^{\infty} \left(\frac{\prod_{j=1}^{p}(a_j)_k}{\prod_{r=1}^{q}(b_r)_k} \right) \frac{x^k}{k!} \tag{15}$$

Table 1. Values of $z_{\mathrm{bcc}(d)}$ and $r_{\mathrm{bcc}(d)}$.

d	$z_{\mathrm{bcc}(d)}$	$r_{\mathrm{bcc}(d)}$
1	0	–
2	1.166 243 616 123 275	0.958 770 222 806 4145
3	1.990 191 418 271 941	0.991 245 705 530 6051
4	2.732 957 535 477 362	0.997 709 897 827 5579
5	3.447 331 914 522 398	0.999 341 328 007 0963
6	4.150 116 933 352 462	0.999 800 212 115 9708
7	4.847 789 269 805 724	0.999 937 306 164 9456
8	5.543 104 959 793 989	0.999 979 850 084 6987
9	6.237 305 017 795 394	0.999 993 405 362 2532
10	6.930 967 870 288 660	0.999 997 810 313 5475

where $c_k = \Gamma(c+k)/\Gamma(c)$. Hence,

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

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, $N_{\mathrm{ST}} = 1$ and $N_{\mathrm{ST}} = n$; in both cases, it follows that $z_{\mathrm{bcc}(1)} = 0$. 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 $z_{\mathrm{sq}} = (4/\pi)\beta(2) = 1.1662436..$ [6, 7], where $\beta(s) = \sum_{n=0}^{\infty}(-1)^n(2n+1)^{-s}$ and $\beta(2) = C = 0.915\,965\,594\,177..$ is the Catalan constant. The general result (8) with (14) evaluated for $d = 2$ agrees with this, since ${}_4F_3([1, 1, 3/2, 3/2], [2, 2, 2], 1) = 16(\ln 2 - (2C/\pi))$. Our general exact result for $z_{\mathrm{bcc}(d)}$ provides quite accurate values for higher values of d, which we list in table 1, 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.

4. fcc lattice

The face-centred cubic (fcc) lattice has coordination number $k_{\mathrm{fcc}} = 12$ and a unit cell consisting of the $\nu_{\mathrm{fcc}} = 4$ vertices $(0, 0, 0)$, $\left(0, \frac{1}{2}, \frac{1}{2}\right)$, $\left(\frac{1}{2}, 0, \frac{1}{2}\right)$ and $\left(\frac{1}{2}, \frac{1}{2}, 0\right)$. For this lattice, $M(\theta_1, \theta_2, \theta_3)$ is [3]

$$M(\theta_1, \theta_2, \theta_3) = \begin{pmatrix} 12 & -(v_2v_3)^* & -(v_1v_3)^* & -(v_1v_2)^* \\ -v_2v_3 & 12 & -v_1^*v_2 & -v_1^*v_3 \\ -v_1v_3 & -v_1v_2^* & 12 & -v_2^*v_3 \\ -v_1v_2 & -v_1v_3^* & -v_2v_3^* & 12 \end{pmatrix} \tag{17}$$

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

$$z_{\mathrm{fcc}} = \ln(12) + \frac{1}{4}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta_1}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta_2}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta_3}{2\pi}\ln F(\theta_1, \theta_2, \theta_3) \tag{18}$$

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

$$F(\theta_1, \theta_2, \theta_3) = \left[1 + \tfrac{1}{3}(-c_2c_3 + c_3c_1 + c_1c_2)\right]\left[1 + \tfrac{1}{3}(c_2c_3 - c_3c_1 + c_1c_2)\right]$$
$$\times \left[1 + \tfrac{1}{3}(c_2c_3 + c_3c_1 - c_1c_2)\right]\left[1 - \tfrac{1}{3}(c_2c_3 + c_3c_1 + c_1c_2)\right]$$
$$= 1 - \tfrac{2}{9}[(c_1c_2)^2 + (c_2c_3)^2 + (c_3c_1)^2] - \tfrac{8}{27}(c_1c_2c_3)^2$$
$$- \tfrac{2}{81}(c_1c_2c_3)^2\left(c_1^2 + c_2^2 + c_3^2\right) + \tfrac{1}{81}[(c_1c_2)^4 + (c_2c_3)^4 + (c_3c_1)^4]. \tag{19}$$

(This corrects an algebraic error in equation (5.3.3) of [3].) Evaluating this numerically, we find that $z_{\rm fcc} \simeq 2.412\,92$. Substituting $z_{\rm fcc}$ into equation (7), we get $r_{\rm fcc} \simeq 0.989\,15$, so that the upper bound (7) 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 neighbourhood of any vertex. This is indicated by the notation $\Lambda = \left(\prod_i p_i^{a_i}\right)$, 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 equation (4.11) of [3], the asymptotic growth constant for this lattice was calculated to be

$$z_{488} = \frac{1}{2}\ln 2 + \frac{1}{4}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta_1}{2\pi}\int_{-\pi}^{\pi}\frac{\mathrm{d}\theta_2}{2\pi}\ln[7 - 3(\cos\theta_1 + \cos\theta_2) - \cos\theta_1\cos\theta_2]$$
$$= \frac{1}{4}\ln 2 + \frac{1}{4\pi}\int_0^{\pi}\mathrm{d}\theta\,\ln[7 - 3\cos\theta + 4\sin(\theta/2)\sqrt{5 - \cos\theta}], \tag{20}$$

where the integral on the second line of equation (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 $z_{488} = 0.786\,684(1)$, 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.

$$z_{488} = \frac{1}{4}\ln 2 + \frac{1}{2\pi}\int_0^{\pi}\mathrm{d}\theta\,\ln(2\sin(\theta/2) + \sqrt{4 + 2\sin^2(\theta/2)})$$
$$= \frac{3}{4}\ln 2 + \frac{1}{\pi}\int_0^{\pi/2}\mathrm{d}\phi\,\ln(\sin(\phi) + \sqrt{1 + (1/2)\sin^2(\phi)}). \tag{21}$$

That is,

$$z_{488} = \tfrac{3}{4}\ln 2 + I(1/\sqrt{2}) \tag{22}$$

where

$$I(a) = \frac{1}{\pi}\int_0^{\pi/2}\mathrm{d}\phi\,\ln(\sin\phi + \sqrt{1 + a^2\sin^2\phi}). \tag{23}$$

In equation (23), with no loss of generality, we take a to be non-negative. 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 $0 \leqslant a < 1$. Taking the derivative with respect to a and doing the integral over ϕ in equation (23), we get

$$I'(a) = \frac{-a/2 + (2/\pi)\tan^{-1}a}{(1 - a^2)}. \tag{24}$$

To calculate $I(a)$, we then use $I(a) - I(0) = \int_0^a I'(x)\mathrm{d}x$ and observe that

$$I(0) = \frac{1}{\pi}\int_0^{\pi/2} \mathrm{d}\phi \ln(\sin(\phi) + 1) = -\frac{\ln 2}{2} + \frac{2C}{\pi}. \tag{25}$$

We also make use of the integrals

$$\int_0^a \frac{x}{(1-x^2)}\,\mathrm{d}x = -\frac{1}{2}\ln(1-a^2) \tag{26}$$

and

$$\int_0^a \frac{\tan^{-1}x}{(1-x^2)}\,\mathrm{d}x = -\frac{C}{2} - \frac{\pi}{8}\ln\left(\frac{1+a}{1-a}\right) + \frac{1}{2}\mathrm{Ti}_2\left(\frac{1+a}{1-a}\right) \tag{27}$$

to obtain

$$I(a) = \frac{C}{\pi} + \frac{1}{2}\ln\left(\frac{1-a}{2}\right) + \frac{1}{\pi}\mathrm{Ti}_2\left(\frac{1+a}{1-a}\right) \qquad \text{if} \quad 0 \leqslant a < 1, \tag{28}$$

where $\mathrm{Ti}_2(x)$ is the inverse tangent integral [8]

$$\mathrm{Ti}_2(x) = \int_0^x \frac{\tan^{-1}y}{y}\,\mathrm{d}y = x[{}_3F_2([1, 1/2, 1/2], [3/2, 3/2], -x^2)]. \tag{29}$$

(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 equation (22), we obtain the exact, closed-form expression

$$z_{488} = \frac{C}{\pi} + \frac{1}{2}\ln(\sqrt{2} - 1) + \frac{1}{\pi}\mathrm{Ti}_2(3 + 2\sqrt{2}). \tag{30}$$

The numerical evaluation of equation (30) agrees with the evaluation given in [3] to the accuracy quoted there and allows one to obtain higher accuracy; for example, to 15 significant figures, $z_{488} = 0.786\,684\,275\,378\,832$. We note that the Ti_2 function also appears at intermediate stages in the derivation of z_{tri} for the triangular lattice [9]. For completeness, we have also calculated $I(a)$ for $a > 1$ with the result

$$I(a) = \frac{C}{\pi} + \frac{1}{2}\ln\left[\frac{(a+1)^2}{2(a-1)}\right] + \frac{1}{\pi}\mathrm{Ti}_2\left(\frac{1+a}{1-a}\right) \qquad \text{if} \quad a > 1. \tag{31}$$

Acknowledgments

SCC thanks C-H Chen for use of computer facilities and software. R S thanks Professor F Y Wu for the collaboration on [3]. This research was partially supported by the Taiwan NSC grant NSC-94-2112-M-006-013 (SCC) and the US NSF grant PHY-00-98527 (RS).

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