

High-Precision Entropy Values for Spanning Trees in Lattices

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Abstract. Shrock and Wu have given numerical values for the exponential growth rate of the number of spanning trees in Euclidean lattices. We give a new technique for numerical evaluation that gives much more precise values, together with rigorous bounds on the accuracy. In particular, the new values resolve one of their questions.

§1. Introduction.

Since the time of Kirchhoff (1847), physicists and mathematicians have been interested in enumerating spanning trees. One aspect of this endeavor has been to evaluate or to estimate asymptotics of the growth rate of the number of spanning trees in large graphs. Additional interest in the asymptotic growth rate arises in ergodic theory, since the exponential rate is also the entropy of a natural and important system, the so-called uniform spanning forest. See Pemantle (1991), Burton and Pemantle (1993), Benjamini, Lyons, Peres, and Schramm (2001), Lyons (1998), and Lyons (2003) for explanations and information about the uniform spanning forest. Some modern enumeration efforts include Burton and Pemantle (1993), Shrock and Wu (2000), Lyons (2003); see also the references therein. In many cases, one can express the main term of the asymptotics by an integral formula. For example, if $\tau(G)$ denotes the number of spanning trees of a graph G and if G_n are the graphs induced by cubes of side length n in the hypercubic lattice \mathbb{Z}^d , then it is well known (and rederived in both Burton and Pemantle (1993) and Shrock and Wu (2000)) that the thermodynamic limit

$$h_d := \lim_{n \rightarrow \infty} \frac{1}{n^d} \log \tau(G_n)$$

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can be expressed as

$$h_d = \int_{\mathbb{T}^d} \log \left(2d - 2 \sum_{i=1}^d \cos 2\pi x_i \right) dx = \log(2d) + \int_{\mathbb{T}^d} \log \left(1 - \frac{1}{d} \sum_{i=1}^d \cos 2\pi x_i \right) dx. \quad (1.1)$$

It is also well known (due to its connection with the dimer problem) that $h_2 = 4G/\pi$, where $G := \sum_{k=0}^{\infty} (-1)^k / (2k+1)^2$ is Catalan's constant (see, e.g., Kasteleyn (1961) or Montroll (1964)). No values of h_d for any $d \geq 3$ are known in simple terms of other known constants and functions. Shrock and Wu (2000) evaluated these integrals in higher dimensions by numerical methods and found one particularly intriguing value: $h_4 = 2.0000(5)$. They suggested that h_4 may be exactly 2, which would be quite surprising. Indeed, it would be extraordinary for a natural system without parameters to have a natural-log entropy that is a non-zero integer. This would have been the first such example to our knowledge. However, we shall see that h_4 is extraordinarily close to 2, but not, in fact, exactly 2. We shall also give more accurate values for other h_d with rigorous bounds on their accuracy.

The numerical evaluation of h_d is problematic if one wants to use the formula (1.1), due to the difficulty of accurate integration in higher dimensions. Therefore, Shrock and Wu (2000) gave an interesting large- d asymptotic expansion of h_d to order $1/d^6$; we have given more terms below, to show that not all coefficients are positive, as one might otherwise believe, and to illustrate that this is indeed only an asymptotic expansion, not a convergent series:

$$h_d = \log(2d) - \left[\frac{1}{4d} + \frac{3}{16d^2} + \frac{7}{32d^3} + \frac{45}{128d^4} + \frac{269}{384d^5} + \frac{805}{512d^6} + \frac{3615}{1024d^7} \right. \\ \left. + \frac{23205}{4096d^8} - \frac{144963}{10240d^9} - \frac{2187031}{8192d^{10}} - \frac{40225409}{16384d^{11}} - \frac{1277353077}{65536d^{12}} \right. \\ \left. - \frac{66817216455}{458752d^{13}} - \frac{271891453119}{262144d^{14}} + O\left(\frac{1}{d^{15}}\right) \right].$$

However, it is difficult to know how many terms of this expansion to use; Shrock and Wu (2000) used this series to report $h_5 = 2.243$ and $h_6 = 2.437$. For smaller d , Shrock and Wu (2000) used numerical integration to find that $h_3 = 1.6741481(1)$ and that $h_4 = 2.0000(5)$. However, the accuracy of h_3 is off by several orders of magnitude.

To obtain greater accuracy and enable us to prove that $h_4 \neq 2$, we shall use a new formula, namely,

$$h_d = \log(2d) - \sum_{k=1}^{\infty} p_d(k)/k, \quad (1.2)$$

where $p_d(k)$ is the probability that simple nearest-neighbor random walk on the hypercubic lattice \mathbb{Z}^d returns to its starting point after k steps. (A generalization of this formula is due to Lyons (2003).) Even this formula is slightly problematic to use, since $p_d(k)$ is the sum of a large number of binomial coefficients for large k . Because of the large number of small terms, it is important to calculate the sum as an exact rational before converting to a real approximation. Fortunately, there is a simple recursion formula that enables quicker computation. In addition, we explain how to estimate the tail of the series in (1.2).

In the remainder of this note, we first state our numerical results and then derive the simple but crucial (1.2). Next, we explain how to compute $p_d(k)$ quickly and how to approximate the error, and finally prove rigorous bounds. We shall also briefly discuss body-centered cubic lattices. We end by discussing an alternative approach that was brought to our attention after a first version of this article was submitted.

§2. Results.

The numerical results are, to an accuracy we believe includes all reported digits, in the following table:

d	h_d	d	h_d
3	1.67338930297	12	3.1557714292824
4	1.999707644517	13	3.2376421551842
5	2.2424880598113	14	3.31330031802725
6	2.43662696200071	15	3.383624540390254
7	2.5986763042	16	3.449318935201
8	2.73786766385	17	3.510956551787645
9	2.859910142340	18	3.56901006528479
10	2.968594484443	19	3.62387396384455
11	3.066571824248	20	3.67588091671257

These arise as follows. To prove (1.2), use the Maclaurin series for $\log(1 - z)$ to find

$$\begin{aligned}
 \int_{\mathbb{T}^d} \log \left(1 - \frac{1}{d} \sum_{i=1}^d \cos 2\pi x_j \right) dx &= - \sum_{k=1}^{\infty} \frac{1}{k} \int_{\mathbb{T}^d} \left[\frac{1}{d} \sum_{i=1}^d \cos 2\pi x_j \right]^k dx. \\
 &= - \sum_{k=1}^{\infty} \frac{1}{k} \int_{\mathbb{T}^d} \left[\frac{1}{2d} \sum_{i=1}^d \left(e^{2\pi i x_j} + e^{-2\pi i x_j} \right) \right]^k dx \\
 &= - \sum_{k=1}^{\infty} \frac{1}{k} p_d(k).
 \end{aligned}$$

Clearly, we have $p_d(k) = 0$ for k odd and $p_1(2k) = \binom{2k}{k}/2^{2k}$. It is well known that $p_2(2k) = p_1(2k)^2$ (e.g., one step of a random walk in \mathbb{Z}^2 can be made by taking one step in each of the directions $\pm(1/\sqrt{2}, 1/\sqrt{2})$ and $\pm(1/\sqrt{2}, -1/\sqrt{2})$, independently). For fast computation of other return probabilities, write $f(d, k) := (2d)^{2k} p_d(2k)$ for the number of nearest-neighbor walks of length $2k$ in \mathbb{Z}^d that start and end at the origin. Such a walk has the property that its projection to the first d_1 coordinates also starts and ends at the origin, while the number of steps in the first d_1 directions may be any even number between 0 and $2k$. Similar reasoning shows that

$$f(d_1 + d_2, k) = \sum_{r=0}^k \binom{2k}{2r} f(d_1, r) f(d_2, k - r).$$

This allows one to reduce the computation of $p_d(\bullet)$ to the values of $p_{\lfloor d/2 \rfloor}(\bullet)$ and $p_{\lceil d/2 \rceil}(\bullet)$.

Once we have these values, it is simple to compute partial sums for (1.2). Since all terms of the series are positive, each such partial sum gives a rigorous upper bound for the true value of h_d . Merely summing the first 13 terms of the series in (1.2) for $d = 4$ gives a rigorous proof that $h_4 < 2$. To get an lower bound for h_d , it suffices to bound above the remainder. It is well known (see, e.g., Spitzer (1976), Section 7) that

$$p_d(2k) \sim 2 \left(\frac{d}{4\pi k} \right)^{d/2}. \quad (2.1)$$

A more accurate approximation is

$$p_d(2k) \approx 2 \left(\frac{d}{4\pi k} \right)^{d/2} \left(1 - \frac{d}{8k} \right), \quad (2.2)$$

as shown by Ball and Sterbenz (2003). As this suggests, we believe that the right-hand side of (2.1) is actually larger than the left-hand side; indeed, this appears to be true for all d and k , not merely for large k , though it has been proved only for large k and small d . That is, we have

$$p_d(2k) \leq 2 \left(\frac{d}{4\pi k} \right)^{d/2} \quad (2.3)$$

for all k when $1 \leq d \leq 6$ and for all large k (if not all k) when $d \geq 7$; see Ball and Sterbenz (2003). Since the sum over $k \geq r$, any $r > 0$, of the right-hand sides of either (2.1) or (2.2) can be expressed via the Hurwitz zeta function, for which Euler-Maclaurin summation approximations are readily available, we obtain the very accurate values reported in the tables above by summing relatively few terms. Excellent accuracy is already available after just 10 terms, but we have used 1000 terms for $3 \leq d \leq 6$, 100 terms for $7 \leq d \leq 10$, and

80 terms for $11 \leq d \leq 20$. In addition, by using (2.3) and partial sums of 1000 terms, we get the rigorous bounds

$$\begin{aligned} 1.6733893024176978 &\leq h_3 \leq 1.6733917596720884 \\ 1.9997076445004571 &\leq h_4 \leq 1.9997076951104138 \\ 2.242488059810819 &\leq h_5 \leq 2.2424880610724065 \\ 2.436626962000695 &\leq h_6 \leq 2.4366269620369234. \end{aligned}$$

One can use similar estimates to improve the accuracy of the asymptotics for body-centered hypercubic lattices. As shown by Shrock and Wu (2000), the exponential growth rate of the number of spanning trees in d dimensions is

$$h_d^{\text{bcc}} = d \log 2 - \frac{1}{2} \sum_{k=1}^{\infty} \frac{1}{k} p_1(k)^d. \quad (2.4)$$

It is straightforward to show that

$$p_1(2k) \geq 2 \left(\frac{1}{4\pi k} \right)^{1/2} \left(1 - \frac{1}{8k} \right) \quad (2.5)$$

by use of Stirling's approximation. We sum 1000 terms of (2.4) and bound the remainder. Using (2.3) for a lower bound and (2.5) for an upper bound, we find

$$\begin{aligned} 1.9901914178466 &\leq h_3^{\text{bcc}} \leq 1.9901914178472 \\ 2.732957535468933 &\leq h_4^{\text{bcc}} \leq 2.7329575354689455. \end{aligned}$$

These agree with the estimates of Shrock and Wu (2000), but give about 3 times as many digits.

After a first version of this article was submitted for publication, Alan Sokal kindly brought to our attention some related calculations by Sokal and Starinets (2001). Up to a constant, the entropy h_d studied here is equal to the free energy $g_d(1/d)$ studied there (see equation (A.2) of their paper). Their formula (A.6) shows, then, that

$$h_d = \log(2d) + \int_0^{\infty} \frac{e^{-t}}{t} [1 - I_0(t/d)^d] dt, \quad (2.6)$$

where I_0 is the modified Bessel function. In this way, h_d can be estimated by numerical integration in only one dimension, which can be accomplished very quickly. The disadvantage, however, is that the integrand decays rather slowly. As noted in Appendix A.2

of Sokal and Starinets (2001), one can improve the precision dramatically by numerical integration up to some cut-off, then symbolic integration of the tail with an asymptotic formula replacing I_0 . Even so, not all the numerical values reported in Sokal and Starinets (2001) are correct in all their digits, as can be seen by comparison with our tables and our rigorous bounds. The second disadvantage of (2.6) is that it is less straightforward to provide rigorous bounds. For this purpose, one has to treat carefully the technique of numerical integration, as well as evaluation and bounding of I_0 . Some of this is discussed in Appendix B of Hara and Slade (1992). By comparison, our technique requires only the calculation of rational numbers, as well as one simple logarithm calculation.

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