On the universality of knot probability ratios

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Abstract. Let p_n denote the number of self-avoiding polygons of length n on a regular three-dimensional lattice, and let $p_n(K)$ be the number which have knot type K. The probability that a random polygon of length n has knot type K is $p_n(K)/p_n$ and is known to decay exponentially with length [1, 2]. Little is known rigorously about the asymptotics of $p_n(K)$, but there is substantial numerical evidence [3, 4, 5, 6] that $p_n(K)$ grows as

$$p_n(K) \simeq C_K \, \mu_\emptyset^n \, n^{\alpha-3+N_K}, \quad \text{as } n \to \infty,$$

where N_K is the number of prime components of the knot type K. It is believed that the entropic exponent, α, is universal, while the exponential growth rate, $\mu_\emptyset$, is independent of the knot type but varies with the lattice. The amplitude, C_K, depends on both the lattice and the knot type.

The above asymptotic form implies that the relative probability of a random polygon of length n having prime knot type K over prime knot type L is

$$\frac{p_n(K)/p_n}{p_n(L)/p_n} = \frac{p_n(K)}{p_n(L)} \simeq \left[\frac{C_K}{C_L}\right].$$

In the thermodynamic limit this probability ratio becomes an amplitude ratio; it should be universal and depend only on the knot types K and L. In this letter we examine the universality of these probability ratios for polygons in the simple cubic, face-centered cubic, and body-centered cubic lattices. Our results support the hypothesis that these are universal quantities. For example, we estimate that a long random polygon is approximately 28 times more likely to be a trefoil than be a figure-eight, independent of the underlying lattice, giving an estimate of the intrinsic entropy associated with knot types in closed curves.

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1. Introduction

A self-avoiding polygon (SAP) on a regular lattice $\mathbb{L}$ is the piecewise linear embedding of a simple closed curve as a sequence of distinct edges joining vertices in $\mathbb{L}$. The number of distinct unrooted polygons modulo translations is denoted p_n. It is known that $\lim_{n\to\infty} p_n^{1/n} = \mu$ exists, where μ is the self-avoiding walk growth constant [7, 8].

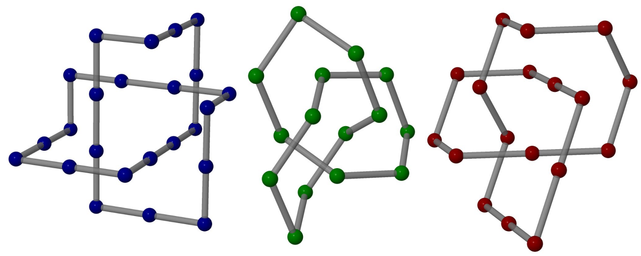

Figure 1. Minimal trefoils on the SC (left — 24 edges), FCC (middle — 15 edges) and BCC (right — 18 edges).

The knot type of polygons in three-dimensional lattices are well defined. Denote by $p_n(K)$ the number of unrooted polygons of length n and knot type K, modulo translations. Computing p_n or $p_n(K)$ is a very difficult combinatorial problem, though determining the minimal length n such that $p_n(K) > 0$ and the numbers of shortest embeddings is viable for knot types of low complexity. For example, there are 3 shortest unknots of length 4 in the simple cubic lattice (SC), 8 of length 3 in the face-centred cubic lattice (FCC), and 12 of length 4 in the body-centered cubic lattice (BCC). The simplest non-trivial knot type is the trefoil (denoted by 3_1, see Figure 1) and it is known that $p_n(3_1) = 0$ if $n < 24$ and $p_{24}(3_1) = 3328$ in the SC [9]. Data on polygons collected by the GAS algorithm [10] shows that $p_{15}(3_1) = 128$ in the FCC and $p_{18}(3_1) = 3168$ in the BCC (see Table 1); no shorter trefoils were observed.

Numerical studies [3, 4, 6, 5, 10] have shown that $p_n(K)$ behaves as

$$p_n(K) \simeq C_K\, \mu_\emptyset^n\, n^{\alpha-3+N_K}, \quad \text{as } n \to \infty, \tag{1}$$

where N_K is the number of prime components of the knot type K. The exponent is thought to be universal, while the growth rate, $\mu_\emptyset$, depends on the lattice but not the knot type. The amplitude, C_K, depends on both the lattice and the knot type. Unfortunately very little of this form can be proven rigorously — the exponential growth rate is only known to exist when K is the unknot. A pattern-theorem [1, 2] shows that the growth rate of unknots, $\mu_\emptyset$, is strictly smaller than μ. The same argument also shows that the probability that a polygon of length n has knot type K, given by $p_n(K)/p_n$, decays exponentially with length.

In this paper we consider the asymptotic behaviour of ratios of knotting probabilities. In particular, for two prime knot types K and L one has $N_K = N_L = 1$ and the ratio of probabilities is given by

$$\frac{p_n(K)/p_n}{p_n(L)/p_n} = \frac{p_n(K)}{p_n(L)} \simeq \left[\frac{C_K}{C_L}\right], \quad \text{as } n \to \infty. \tag{2}$$

Hence, the limiting ratio of probabilities approaches a constant. Since this limit is an *amplitude ratio* we expect it to be universal — depending only on the knot types and the universality class of the underlying model.

Such ratios were studied previously on the SC [10] (by the methods used in this paper) and in [11] (by very different methods). Here, we use the GAS algorithm to estimate $p_n(K)$ for various prime knots on the SC, FCC and BCC lattices. Our results indicate that the above ratio is dependent on the knot types, but independent of the underlying lattices, and so, universal.

2. Atmospheric moves on cubic lattices

The GAS algorithm [12] samples along sequences of conformations that evolve through local elementary transitions called atmospheric moves (see eg. [13]). The algorithm is a generalisation of the Rosenbluth algorithm [14, 15], and is an approximate enumeration algorithm.

The GAS algorithm was used to estimate the number of knotted polygons on the SC [10] using BFACF moves [16, 17, 18] as atmospheric moves. This implementation relies on a result in [19] that the irreducibility classes of the BFACF elementary moves applied to SC polygons are the classes of polygons of fixed knot types [19].

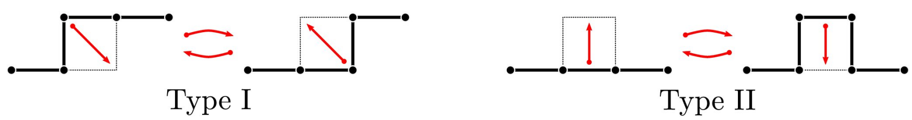

Figure 2. Elementary moves of the BFACF algorithm on the SC lattice.

BFACF elementary moves (see Figure 2) are either neutral (or Type I) operating on two adjacent orthogonal edges of a SC polygon, or the are of Type 2 which are positive or negative length changing moves. A neutral moves exchanges two adjacent edges over a unit lattice square which defines a *neutral atmospheric plaquette*. A *negative move* replaces three edges in a $\sqcap$ conformation by a single edge and so defines a *negative atmospheric plaquette*. Similarly a *positive move* replaces a single edge of the polygon by three edges in a $\sqcap$ arrangement; these edges define a *positive atmospheric plaquette*. Let $a_+(\varphi), a_0(\varphi), a_-(\varphi)$ be the total numbers positive, neutral and negative atmospheric moves of a SC lattice polygon φ.

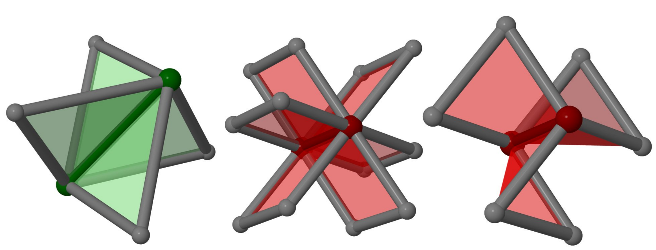

Figure 3. (Left) There are 4 elementary triangular plaquettes incident to each edge in the FCC lattice. (Middle and right) Each edge in the BCC lattice is incident to 12 plaquettes; 6 planar and 6 non-planar (the remaining 3 are reflections of the 3 displayed).

The plaquettes in the FCC and BCC lattice (see Figure 3) define elementary moves in the FCC and BCC analogous to the BFACF moves. Since the FCC plaquettes are triangles they define positive and negative moves, while the BCC plaquettes are quadrilaterals and so also give neutral moves. These generalisations are discussed at length in [20] and it is shown that on each lattice the irreducibility classes of the moves coincide with classes of polygons of fixed knot types.

3. GAS sampling of knotted polygons

We have implemented the GAS algorithm using the atmospheric moves described above. Let φ_0 be a lattice polygon, then the GAS algorithm samples along a sequence of polygons $(\varphi_0, \varphi_1, \ldots)$, where φ_{j+1} is obtained from φ_j by an atmospheric move.

Each atmospheric move is chosen uniformly from the possible moves, so that if φ_j has length ℓ_j then

$$\Pr(+) \propto \beta_{\ell_j} a_+(\varphi_j), \quad \Pr(0) \propto a_0(\varphi_j), \quad \Pr(-) \propto a_-(\varphi_j). \tag{3}$$

where β_ℓ is a parameter that is chosen to be approximately $\frac{\langle a_+ \rangle_\ell}{\langle a_- \rangle_\ell}$. This parameter can be chosen so that on average the probability of making a positive move is roughly the same as that of making a negative move. This produces a sequence $\langle \varphi_j \rangle$ of states and we assign a weight to each state:

$$W(\varphi_n) = \frac{a_-(\varphi_0) + a_0(\varphi_0) + \beta_{\ell_0} a_+(\varphi_0)}{a_-(\varphi_n) + a_0(\varphi_n) + \beta_{\ell_n} a_+(\varphi_n)} \times \prod_{j=0}^{n} \beta_{\ell_j}^{(\ell_j - \ell_{j+1})}. \tag{4}$$

The probabilities and weights are functions of the number of possible atmospheric moves and so the algorithm must recalculate these efficiently. Since the elementary moves only involve local changes, executing a move and updating the polygon takes $O(1)$ time.

The resulting data were analysed by computing the mean weight $\langle W \rangle_n$ of polygon of length n edges and then using the result (from [12])

$$\frac{\langle W \rangle_n}{\langle W \rangle_m} = \frac{p_n(K)}{p_m(K)}. \tag{5}$$

This gives approximations to the number of polygons of any given length n, provided the number of polygons is known exactly at another length m.

4. Results

We collected data on the prime knots $3_1, 4_1, 5_1$ and 5_2 on the three lattices. In order to use equation (5) we computed the total number minimal length polygons of fixed given knot type — see Table 1. We did this by collecting them while performing the simulation (or in independent runs); this idea was used in [9] and [10] and our SC results agree. Typically, the algorithm quickly found all realisations of minimal knots (within hours) and then failed to find new conformations after another few days of CPU time. We note that the result for trefoils in the SC has been proved [21, 9].

Using the data in Table 1 and equation (5) we were able to estimate $p_n(K)$ for each knot type in each of the three lattices. Each simulation ran for 1 week on a single node of WestGrid's Glacier cluster‡. The implementation was particularly simple and efficient in the FCC lattice and the SC simulations were faster than the BCC lattice simulations. Each simulation was composed of approximately 400 chains of length 2^{27} polygons on the FCC lattice, 1400 chains of 2^{23} polygons on the simple cubic lattice

‡ See `http://www.westgrid.ca`

Knot	SC		FCC		BCC	
	length	number	length	number	length	number
0_1	4	3	3	8	4	12
3_1	24	3328	15	64	18	1584
4_1	30	3648	20	2796	20	12
5_1	34	6672	22	96	26	14832
5_2	36	114912	23	768	26	4872

Table 1. The number of minimal length polygons of fixed knot types in the SC, FCC and BCC lattices.

and 500 chains of 2^{23} polygons on the BCC lattice. In each simulation we limited the maximum length of the polygons to 512 edges.

The estimates of $p_n(K)$ in each lattice were used to extrapolate the ratios $p_n(K)/p_n(L)$ for fixed prime knots K, L. In earlier work on SC polygons [10] we observed that the logarithm of these ratios were approximately linear in n^{-1}. In Figures 4, 5 and 6 we plot the logarithm of the ratio against n^{-1} for various pairs of prime knots.

In Figure 4 we show that there is strong agreement between the FCC and BCC data. In addition, the three extrapolated curves appear to have approximately the same limit. This is strong numerical support for the hypothesis that the limiting ratio is universal.

Linear fits of the data gives y-intercepts of 3.34(3), 3.35(3), 3.29(3) for the SC, the FCC and the BCC lattices (respectively). These results includes each other within 95% confidence intervals. Exponentiating these results estimates the limiting amplitude ratio to be 27 ± 2. If we exclude the BCC data, since it is not as well converged at large n, we obtain a limiting ratio of 28 ± 1.

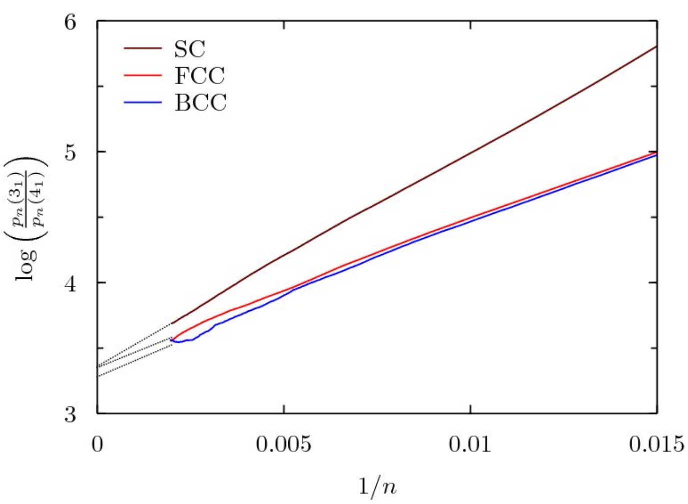

Figure 4. Plots of the logarithm of the ratio of the number of 3_1 to 4_1 knots. The dotted lines indicate the extrapolations. Note that the FCC and BCC data are nearly the same. The intercept indicates that the limiting ratio is approximately $e^{3.32} \approx 28$.

Turning to the ratio of 4_1 to 5_2 plotted in Figure 5 we find similar results, though the data are not as well converged and our estimates are not as good. Linear fits lead to an estimate of 9 ± 1 for the limiting ratio. The estimates on all three lattices agree, supporting the hypothesis of universality. In the final plot we show the ratio of 5_1 to 5_2 knots. Again we find similar results and estimate the limiting ratio to be 0.67(3).

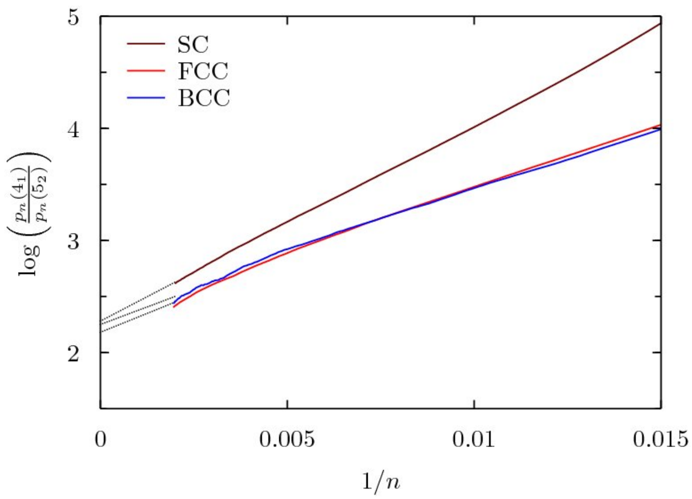

Figure 5. Plots of the logarithm of the ratio of the number of 4_1 to 5_2 knots. The linear extrapolations are indicated by dotted lines. The intercept indicates that the limiting ratio is approximately $e^{2.2} \approx 9$.

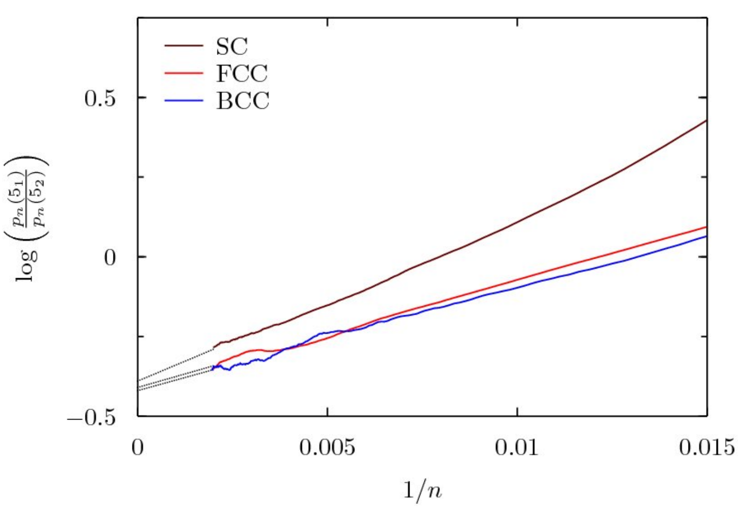

Figure 6. Plots of the logarithm of the ratio of the number of 5_1 to 5_2 knots. The linear extrapolations are indicated by dotted lines. The intercept indicates that the limiting ratio is approximately $e^{-0.4} \approx 0.67$.

We have also studied the other ratios and find similar support for their universality. In summary:

$$\begin{aligned} {}^{C_{3_1}}\!/_{C_{4_1}} &= 28(1) & {}^{C_{3_1}}\!/_{C_{5_1}} &= 400(20) & {}^{C_{3_1}}\!/_{C_{5_2}} &= 280(20) \\ & & {}^{C_{4_1}}\!/_{C_{5_1}} &= 15(1) & {}^{C_{4_1}}\!/_{C_{5_2}} &= 9(1) \\ & & & & {}^{C_{5_1}}\!/_{C_{5_2}} &= 0.67(3). \end{aligned} \tag{6}$$

These numbers are self-consistent within the stated error bars. Curiously, in each case we found that the curves for the FCC and BCC lie close together while that of the SC stands apart; we would like to understand this better, but have no explanation at this time.

Some caution is needed when comparing these results to previous studies of knot probability amplitudes such as [22, 23, 11]. Any estimate of the amplitude will have sensitive dependence on the estimate of the exponent. Indeed, unless the estimated exponents are equal, the ratio of the estimated probabilities will tend to zero or infinity.

Mindful of this, we may compare the ratio of estimated amplitudes for SC polygons from [11] we find $C_{3_1}/C_{4_1} \approx 22$ which is close to our estimate, but not within mutual error bars. The ratio of estimated amplitudes for off-lattice polygons from [22] and [23] give quite different results. However, it is not clear that our models are in the same universality class as these off-lattice models. In addition, the comparison may also be affected by differences in estimated entropic exponents in these studies.

5. Conclusions

We have studied the ratio of probabilities of different knot types. The scaling assumption in equation (1) indicates that the limit of this ratio should be an amplitude ratio and thus universal. Using the GAS algorithm we have formed direct estimates of the number of polygons of various prime knot types on three different lattices. Extrapolating from these estimates provides numerical evidence that the probability ratios are universal — depending only on the knot types and the universality class of the underlying model. In particular we find that a long polygon is about 28 times more likely to be a trefoil than a figure-eight.

There are a number of extensions of this work that we would like to pursue — extending these results to composite knots and links, and also to perform similar analyses of data from off-lattice models.

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