Self-avoiding polygons in confined geometries

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Outline

Introduction I: Motivation

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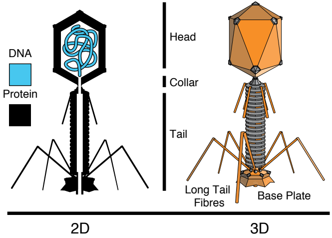

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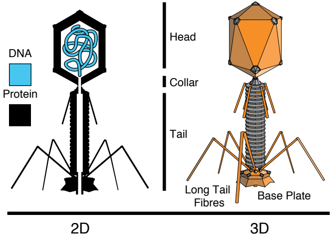

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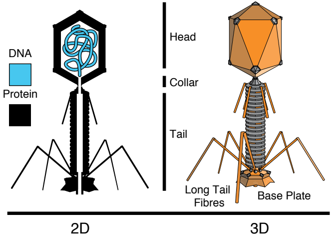

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The tight packing within a cell or capsid may result in a high level of tangling, with lots of knots and/or links. Knotting rates of up to 95% have been observed for DNA released from certain bacteriophages.[1]

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Moreover, it has also been observed that the knot types of randomly cyclised DNA from bacteriophages do not appear to be completely randomly distributed.[2] In particular, chiral knots appear more frequently than in random equilateral polygons.

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Goal: Investigate the thermodynamic and topological properties of a model of tightly packed polymers which incorporates the excluded volume effect.

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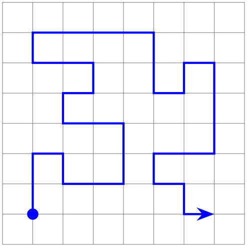
Introduction II: Self-avoiding walks & polygons

A self-avoiding walk (SAW) ω on a graph is a sequence $(\omega_0, \ldots, \omega_n)$ of distinct vertices with consecutive vertices adjacent on the graph.



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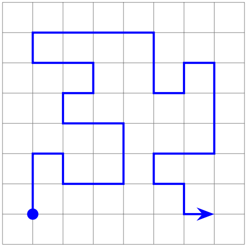

When the graph is infinite and has translational symmetry (i.e. a lattice), define SAWs up to translation.

For a given lattice, c_n is the number of SAWs of length n (n edges $\iff$ $n+1$ vertices).

On $\mathbb{Z}^2$, $\{c_n\}_{n\geq 0} = 1, 4, 12, 36, 100, 284, \ldots$ Known up to $n = 79$.

Theorem (Hammersley 1957)

The limit

$$\lim_{n\to\infty} \frac{1}{n} \log c_n = \kappa$$

exists and is equal to $\inf_{n\geq 0} \frac{1}{n} \log c_n$.

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Corollary

$$c_n = e^{o(n)} \mu^n.$$

μ is known exactly only for 2-dimensional honeycomb lattice. For the square $\mathbb{Z}^2$ and cubic $\mathbb{Z}^3$ lattices,

$$\mu_{\mathbb{Z}^2} \approx 2.63815853031$$
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Also interested in the geometric properties of SAWs. Various measures of size, e.g. mean squared end-to-end distance, radius of gyration, etc. are believed to obey a power law:

$$\langle d^2_{\text{end-end}} \rangle_n \sim \text{const.} \times n^{2\nu}$$

where ν depends only on dimension. In 2D, expect $\nu = 3/4$, while in 3D $\nu \approx 0.587597$.

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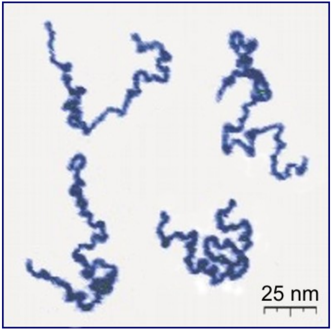

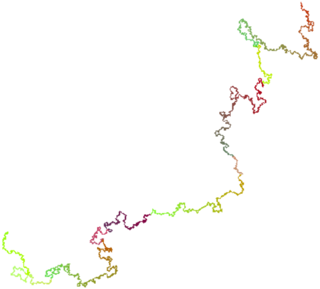

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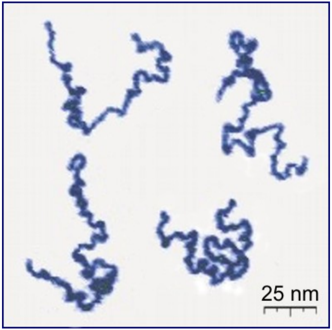
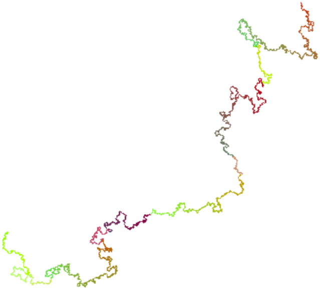
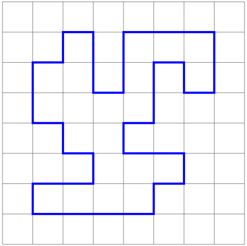




SAWs incorporate the excluded volume effect.

A self-avoiding polygon (SAP) is a simple closed loop on the edges of the lattice:



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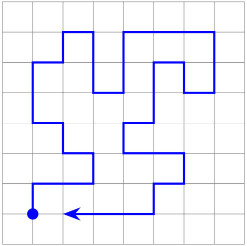

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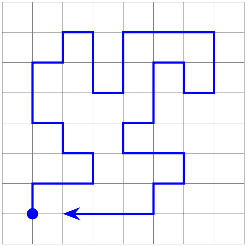

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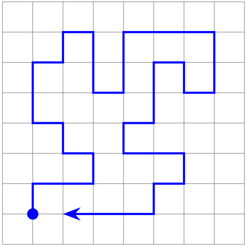

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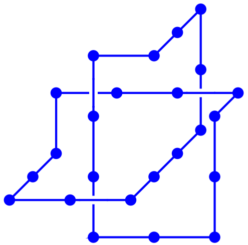
Theorem (Hammersley 1961)

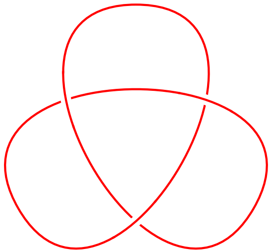
The limit

$$\lim_{n\to\infty} \frac{1}{n} \log p_n$$

exists and is equal to κ, the connective constant of the lattice, where the limit is taken through even values of n.

In 3D SAPs can be knotted:





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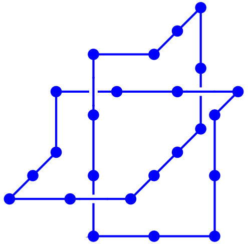
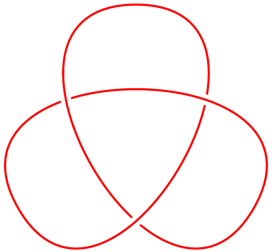




In fact, very long polygons are almost always knotted:

Theorem (Sumners & Whittington 1988)

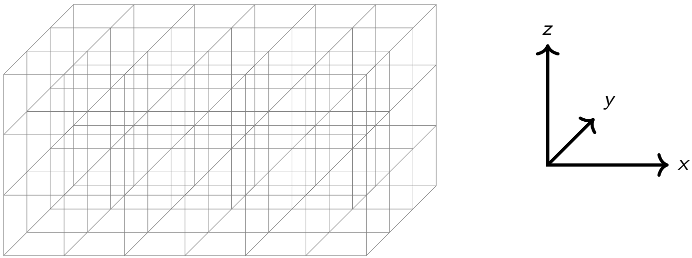
All except exponentially few sufficiently long SAPs on the cubic lattice are knotted.

The model: Polygons in lattice tubes

Let $\mathbb{T}_{L,M} \equiv \mathbb{T}$ be an $L \times M$ semi-infinite tube of $\mathbb{Z}^3$:

$$\mathbb{T} = \{(x, y, z) : x \geq 0, 0 \leq y \leq L, 0 \leq z \leq M\}.$$

(Assume $L \geq M$.)



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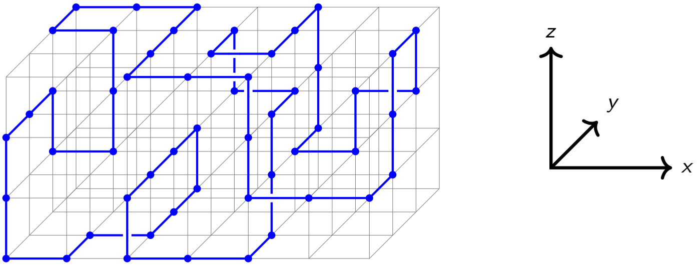

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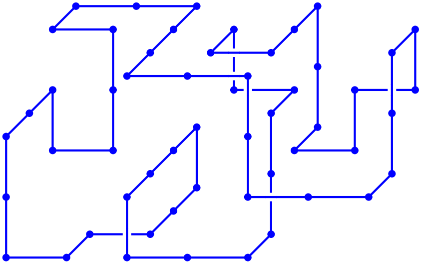

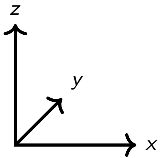

Let $p_{\mathbb{T},n}$ be the number of polygons in $\mathcal{P}_{\mathbb{T}}$ of length n.

Theorem (Soteros & Whittington 1989)

The limit

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Note: Unlike in $\mathbb{Z}^2$ or $\mathbb{Z}^3$, in general SAWs and SAPs in the tube have different growth rates. We will not consider SAWs in $\mathbb{T}$.

Compressing/pulling force

To examine polygons which are tightly packed in a small space, we introduce a force. If π is a polygon in $\mathbb{Z}^3$ or $\mathbb{T}$, let $s(\pi)$ be its span in the x-direction.

To model a force f acting on polygons, we associate a weight of $e^{fs(\pi)}$ with each polygon. The partition function of polygons of length n in $\mathbb{T}$ is then

$$Z_{\mathbb{T},n}(f) = \sum_{\substack{\pi \in \mathbb{T} \\ |\pi| = n}} e^{fs(\pi)} = \sum_s p_{\mathbb{T},n}(s) e^{fs}$$

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Theorem (Atapour, Soteros & Whittington 2009)

The free energy

$$\mathcal{F}_{\mathbb{T}}(f) = \lim_{n\to\infty} \frac{1}{n} \log Z_{\mathbb{T},n}(f)$$

exists for all f. It is a continuous, convex function of f, and is almost-everywhere differentiable.

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The expected span of a polygon of length n at a given f (under the Boltzmann distribution) is

$$\frac{d}{df} \log Z_{\mathbb{T},n}(f)$$

so that the expected "span density" (span per unit length) in the limit of long polygons is

$$\frac{d}{df} \mathcal{F}_{\mathbb{T}}(f).$$

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Theorem (NRB, Eng & Soteros 2016)

As $f \to \infty$, the free energy $\mathcal{F}_{\mathbb{T}}(f)$ is asymptotic to $f/2$. That is,

$$\lim_{f \to \infty} (\mathcal{F}_{\mathbb{T}}(f) - f/2) = 0.$$

Note: This result also holds if polygons in $\mathbb{T}$ are replaced by all polygons in $\mathbb{Z}^d$.

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Note: This result also holds if polygons in $\mathbb{T}$ are replaced by all polygons in $\mathbb{Z}^d$.

Lower bound is straightforward: the maximum span for a polygon of length n is $(n-2)/2$, and there is always at least one with this span, so

$$Z_{\mathbb{T},n}(f) \geq e^{f(n-2)/2} \qquad \Rightarrow \qquad F_{\mathbb{T}}(f) \geq f/2.$$

Upper bound (sketch): divide polygons of length n into m pieces of size $r = \lfloor n/m \rfloor$ (maybe with leftover piece of length $q < r$).

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Let $t = \alpha n$. The $f \to \infty$ limit of the free energy is connected (in a non-trivial way) with the limits $n \to \infty$, $\alpha \to 1/2$. As $\alpha \to 1/2$, the "other" pieces become negligible, and the only contribution to the upper bound is by polygons with (almost) all x-steps, whose free energy $\to f/2$.

Large forces: $f \to -\infty$

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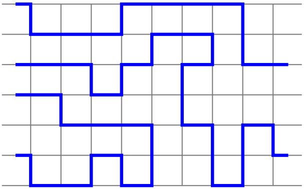
An *s*-block of $\mathbb{T}$ is the section of any polygon between planes $x = k + 1/2$ and $x = k + s + 1/2$ for some k (with at least one vertex in each plane $x = k+1, k+2, \ldots, k+s$). The length is the total number of occupied vertices.



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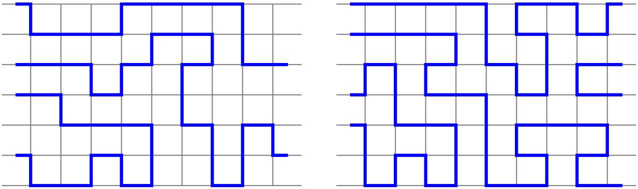

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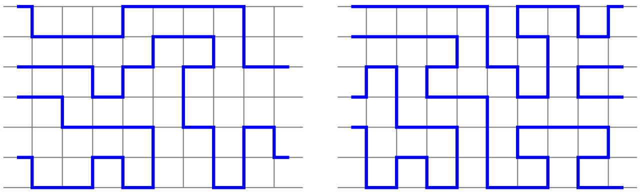

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Let $b_{\mathbb{T},s}$ be the number of s-blocks in $\mathbb{T}$, and $b^{\mathrm{F}}_{\mathbb{T},s}$ the number of full s-blocks.

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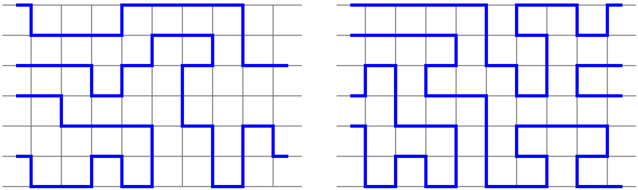

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Lemma

The following limits exist and are finite:

$$\beta_{\mathbb{T}} = \lim_{s\to\infty} \frac{1}{s} \log b_{\mathbb{T},s} \qquad \textit{and} \qquad \beta^{\mathsf{F}}_{\mathbb{T}} = \lim_{s\to\infty} \frac{1}{s} \log b^{\mathsf{F}}_{\mathbb{T},s}.$$

Theorem (NRB, Eng & Soteros 2016)

The free energy $\mathcal{F}_{\mathbb{T}}(f)$ is asymptotic to $(f + \beta_{\mathbb{T}}^{\mathsf{F}})/W$ as $f \to -\infty$, ie.

$$\lim_{f \to -\infty} (\mathcal{F}_{\mathbb{T}}(f) - f/W) = \beta_{\mathbb{T}}^{\mathsf{F}}/W.$$

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The upper bound is similar to the $f \to \infty$ case, except instead of dividing the polygons up into disjoint subwalks, we divide them into disjoint blocks. As $f \to -\infty$, the PHP implies that most must be full.

Why blocks and not polygons?

The $f \to -\infty$ asymptote is written in terms of $\beta_{\mathbb{T}}^{\mathsf{F}}$, the growth rate for full s-blocks. Why not a growth rate of "full" polygons?

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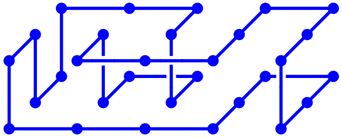
A polygon in $\mathbb{T}$ is Hamiltonian if it has span s and length $n = W(s+1)$. Equivalently, it occupies every vertex in a $L \times M \times s$ box of $\mathbb{Z}^3$.



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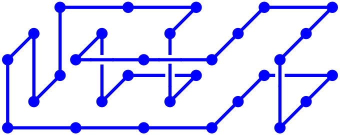

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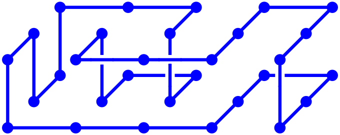

Let $p^{\mathrm{H}}_{\mathbb{T},n}$ be the number of Hamiltonian polygons in $\mathbb{T}$ of length n. Note that $p^{\mathrm{H}}_{\mathbb{T},n} = 0$ if n is not a multiple of W.

Theorem (Eng 2014)

The limit

$$\kappa^{\mathrm{H}}_{\mathbb{T}} = \lim_{n\to\infty} \frac{1}{n} \log p^{\mathrm{H}}_{\mathbb{T},n}$$

(taken through values of n which are multiples of W) exists and is finite.

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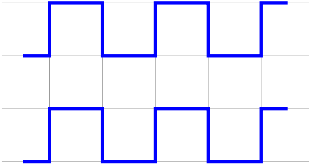

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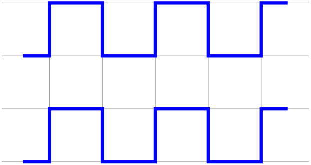

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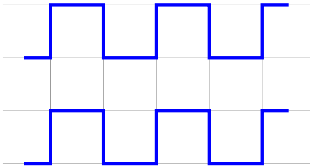

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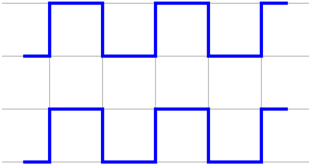

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Conjecture

The growth rates of Hamiltonian polygons and full s-blocks (counted by length instead of span) are the same, ie.

$$\kappa_{\mathbb{T}}^{\mathsf{H}} = \frac{\beta_{\mathbb{T}}^{\mathsf{F}}}{W}.$$

Knots

Theorem (Soteros 1998; Atapour, Soteros & Whittington 2009)

For any $L \times M$ tube $\mathbb{T}$ with $L \geq 2$, $M \geq 1$, and for any finite f, the probability of a random n-step polygon in $\mathbb{T}$ (sampled from the Boltzmann distribution) being knotted approaches 1 as $n \to \infty$.

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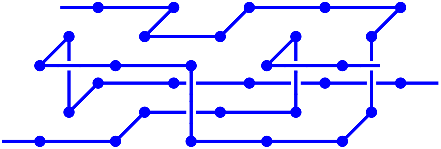
Like the result in $\mathbb{Z}^3$, both proofs use a pattern theorem: there are patterns which guarantee knotting, and which are found in all but exponentially few long polygons.



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But the transfer matrices cannot be used to characterise all knotted or unknotted polygons.

Random sampling via the transfer matrix

The transfer matrices can be used to generate random polygons of a given span, built up one 1-block at a time. Idea (adapted from [Alm & Janson 1990]):

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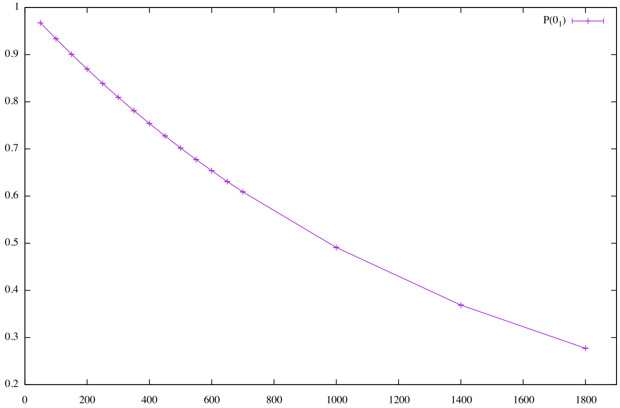
To accommodate this, we re-weight each sample by a factor of

$$\frac{N(b_0)\xi^{\mathrm{F}}_{\mathbb{T}}(b_1) N_{\text{end}}(b_{s-1})}{\xi^{\mathrm{F}}_{\mathbb{T}}(b_{s-1})}.$$

(Some) results

Probability of unknot (0_1) for Hamiltonian polygons in 3×1 tube (horizontal axis is span):



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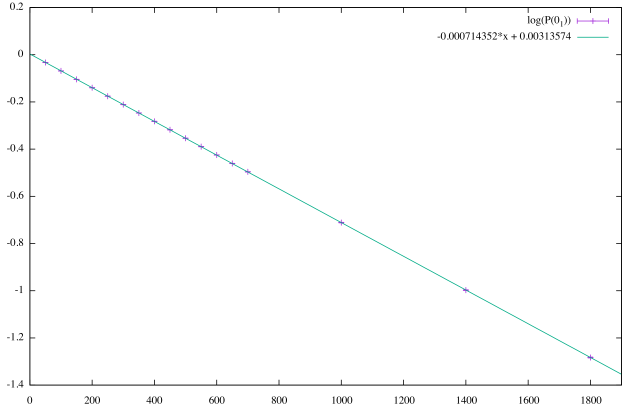

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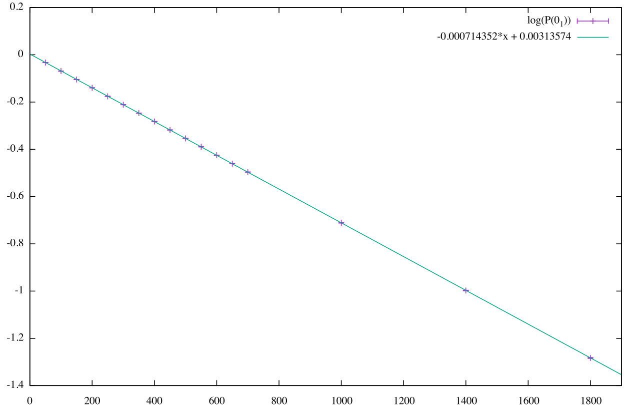

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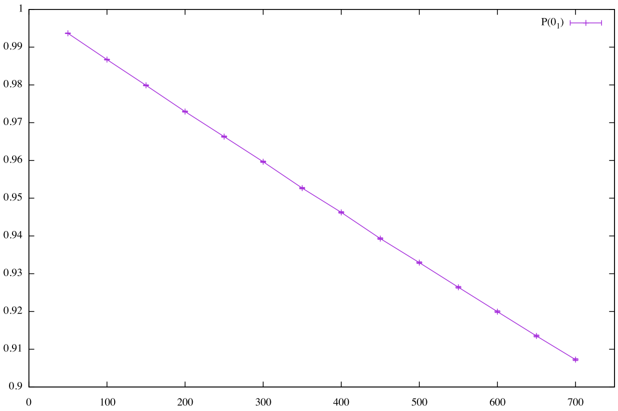
In $\mathbb{Z}^3$, it has been estimated $P(0_1) \sim \exp(-4.15 \times 10^{-6} n)$.

Probability of unknot (0_1) for all polygons in 3×1 tube:



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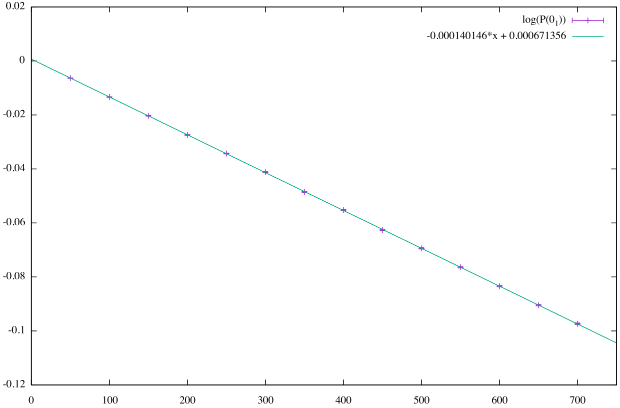
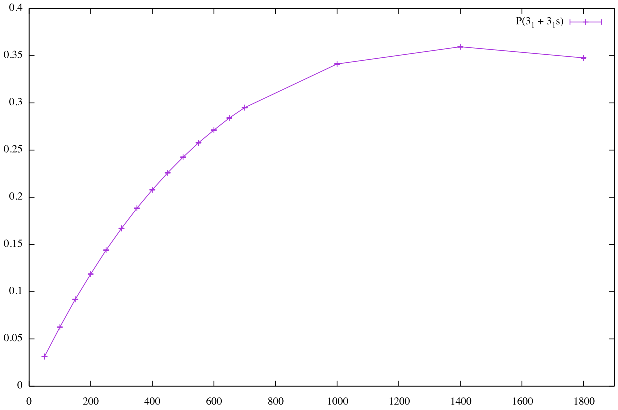


By taking the log, we see that

$$P(0_1) \sim \exp(-1.40 \times 10^{-4} s)$$

Probability of trefoil ($3_1^{\pm}$) for Hamiltonian polygons in 3×1 tube:



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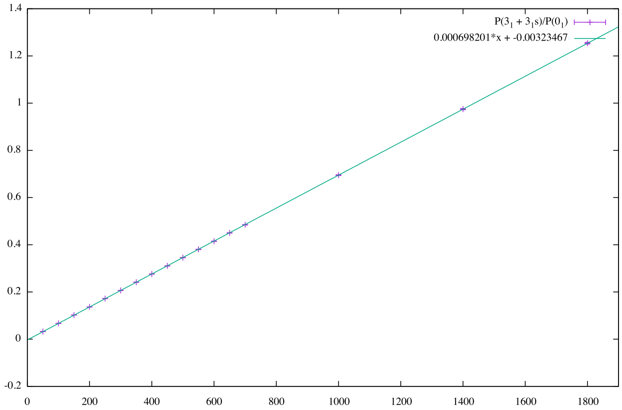

By taking $P(3_1^{\pm})/P(0_1)$, we see that

$$P(3_1^{\pm}) \sim 6.98 \times 10^{-4} s P(0_1) \sim 8.73 \times 10^{-5} n \exp(-4.15 \times 10^{-6} n).$$

This relationship seems to hold for any prime knot type (with different constants).

Further analysis (in progress) appears to confirm the expectation that if knot type K is the connected sum of k prime knots, then

$$P(K) \sim const. \times n^k P(0_1).$$

Similar results also hold for non-Hamiltonian polygons in $\mathbb{T}$. However, the transfer matrix is much bigger, so it is harder to get good estimates from the data.

Ongoing work

- Determine how knotting probability behaves for larger tube sizes
- The "knotted part" of a polygon in $\mathbb{T}$ tends to be very small – look at the distribution of its location/size
- Include the force f in the simulations, and examine how knotting probability etc. changes with force
- Examine writhe, twisting, etc. and how they affect knotting
- In cases where the transfer matrix is too big to be used, develop new method (Markov chain?) for sampling Hamiltonian polygons

arXiv:1604.07465 – NRB, Jeremy Eng and Chris Soteros, Polygons in restricted geometries subjected to infinite forces. To appear in *Journal of Physics A: Mathematical and Theoretical.*

More work in preparation.

Thank you!