Entanglement statistics of polymers in a lattice tube and unknotting of 4-plats

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with

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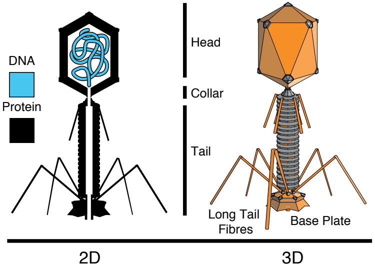
Monash Topology Seminar

Introduction I: Motivation

DNA molecules can be packed incredibly tightly in cell nuclei. For example, human DNA can be 2 m long but must fit inside a cell nucleus of diameter 10 μm. Similarly, bacteriophage DNA is packed into a hard capsid until it is injected into the host cell.



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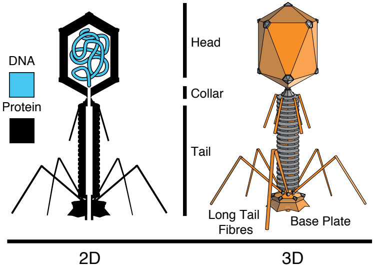

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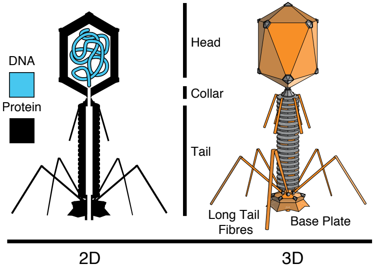

Some DNA molecules (like mitochondrial DNA) have a natural ring structure, while linear DNA can cyclise (the ends stick together) in the nucleus or after being released from confinement.

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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The topology of DNA is important because knots/links have been observed to impede biological processes like replication.

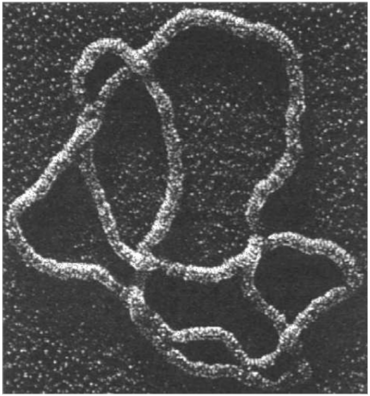

Figure: Knotted DNA (S.A. Wasserman et al, *Science* 1985)

Introduction I: More motivation

A major motivation for this work (and many others) is the following conjecture:

Conjecture 1 (Frisch & Wasserman (1961) and Delbrück (1962))

Almost all sufficiently long ring polymers in dilute solutions are knotted.

Or stated more explicitly:

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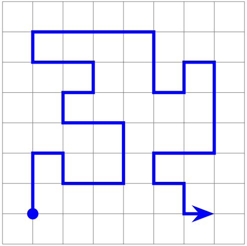
It has been proved in some settings – will return to this shortly.

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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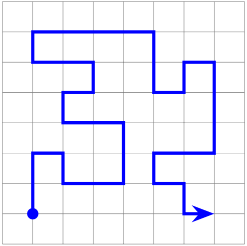

When the graph is infinite and has translational symmetry (i.e. a lattice), define SAWs up to translation.

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 $n = 79$.

Any SAW of length $m + n$ can be split into two smaller SAWs of lengths m and n. Thus the submultiplicative inequality

$$c_{m+n} \leq c_m c_n.$$

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This can be used to show

Theorem 1 (Hammersley 1957)

The limit

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

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Corollary 1

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

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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The subexponential factors are believed to have a power law form:

$$c_n \sim A n^{\gamma-1} \mu^n$$

where A and μ depend on the lattice, γ depends only on the dimension. (Extra logarithmic factor in dimension 4.) In 2D, expect that $\gamma = 43/32$, while in 3D $\gamma \approx 1.156957$.

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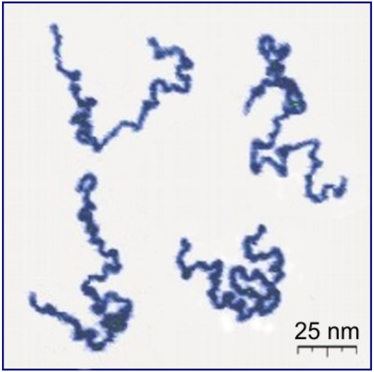

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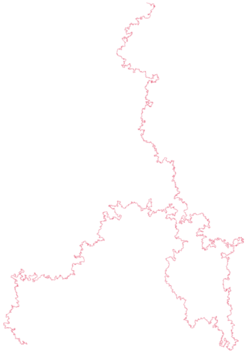

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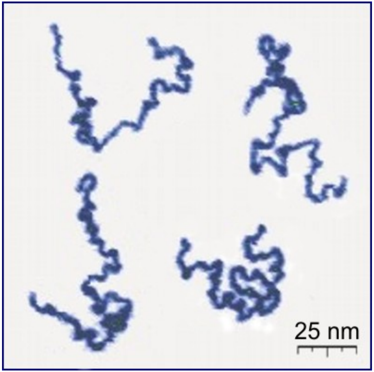

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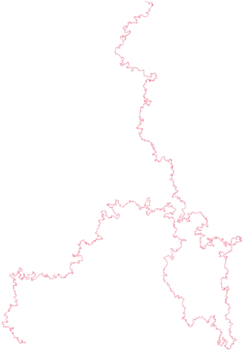

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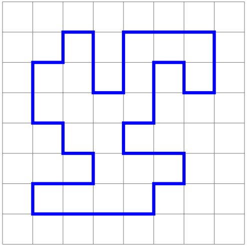
SAWs incorporate the excluded volume effect.

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



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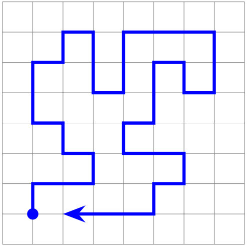

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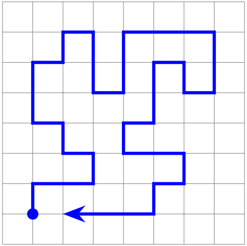

A SAP of n edges can be associated with a SAW of $n-1$ edges by selecting a vertex and a direction. There are $2n$ ways to do this.

Let p_n be the number of SAPs of length n. (Note that on any bipartite lattice like $\mathbb{Z}^2$ or $\mathbb{Z}^3$, $p_n = 0$ if n is odd, so henceforth always assume n is even.) Then two polygons of length m and n can be concatenated to give a polygon of length $m+n$ (may have to rotate the second one), so we have the supermultiplicative inequality

$$p_{m+n} \geq \frac{1}{d-1} p_m p_n.$$

So polygons also have an exponential growth rate.

In fact polygons have the same growth rate as walks:

Theorem 2 (Hammersley 1961)

The limit

$$\lim_{n\to\infty} \frac{1}{n} \log\left(\frac{p_n}{d-1}\right) = \lim_{n\to\infty} \frac{1}{n} \log p_n$$

exists and is equal to κ, the connective constant of the lattice, where the limit is taken through even values of n. Moreover $\kappa = \sup_{n\geq 0} \frac{1}{n} \log\left(\frac{p_n}{d-1}\right)$.

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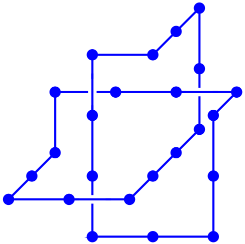
Expect similar power law subexponential terms:

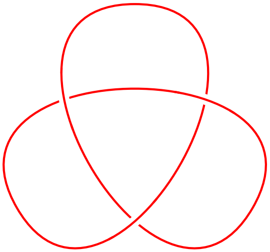
$$p_n \sim B n^{\alpha-3} \mu^n$$

where B, μ depend on lattice and α depends on dimension. In 2D, expect $\alpha = 1/2$, while in 3D expect $\alpha \approx 0.23721$.

Introduction III: Knotted polygons & pattern theorems

In 3D SAPs can be knotted:





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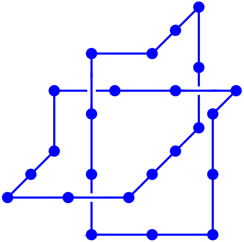

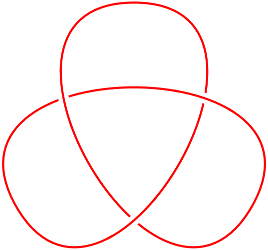

In fact, very long polygons are almost always knotted:

Theorem 3 (Sumners & Whittington 1988)

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

That is, the Frisch-Wasserman-Delbrück (FWD) conjecture is true for SAPs on the cubic lattice. (Also proved for other 3D lattices.)

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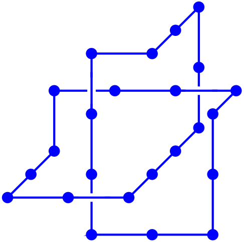

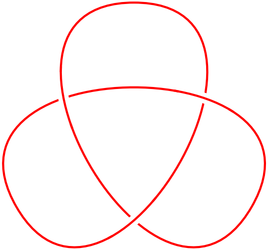

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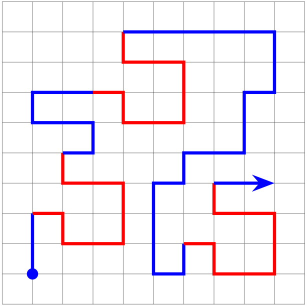
The Sumners-Whittington proof uses a pattern theorem.

A pattern is a (sub)walk which can occur as part of a larger SAW. A Kesten pattern is one which can occur in (at least) three (possibly overlapping) places in a SAW.



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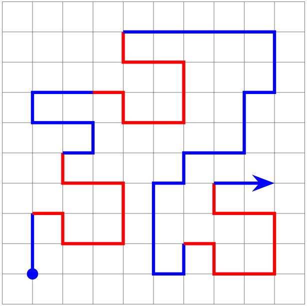
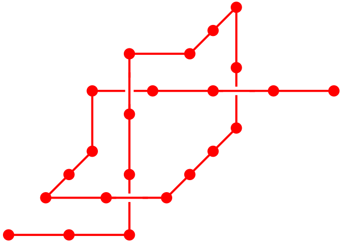


Theorem 4 (Kesten 1963)

Let P be a Kesten pattern, and let $c_{n,\overline{P}}$ be the number of SAWs of length n which do not contain any occurrences of P. Then

$$\limsup_{n\to\infty} \frac{1}{n} \log c_{n,\overline{P}} < \kappa.$$

Whittington and Sumners show that unknots are exponentially rare by letting P be a tight trefoil pattern:



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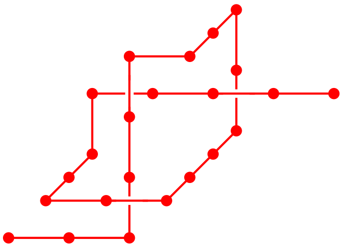

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Let u_n be the number of unknot polygons with n edges. Since unknots can be concatenated to create bigger unknots, we have

Lemma 1

The limit

$$\lim_{n\to\infty} \frac{1}{n} \log u_n = \kappa_0$$

exists, and (by Sumners and Whittington) $\kappa_0 < \kappa$.

Fixed knot type

However, any other fixed knot type is not preserved under concatenation. So what can we say about other knot types?

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Lemma 2

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Generally believed (but unproven) that

Conjecture 2

$$u_n \sim \textit{const.} \times n^{\gamma_0} e^{\kappa_0 n}$$

for some $\gamma_0 \in \mathbb{R}$ and

$$\frac{p_n(K)}{u_n} \sim \textit{const.} \times n^{f_K} \qquad (*)$$

where f_K is the number of (non-trivial) prime knots in the decomposition of K.

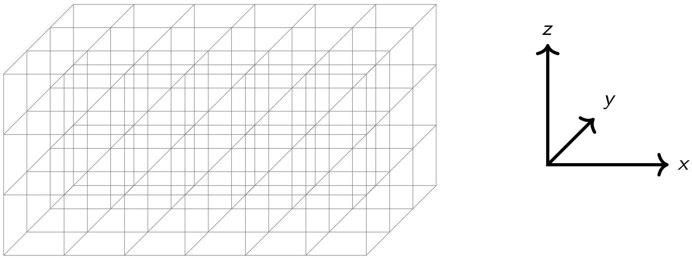
Polygons in lattice tubes

In order to say more, we now restrict to 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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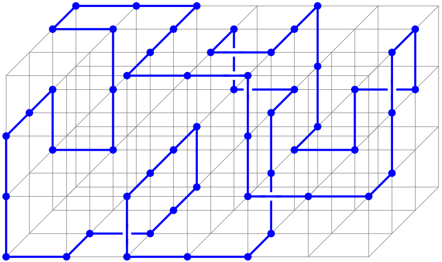

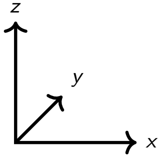

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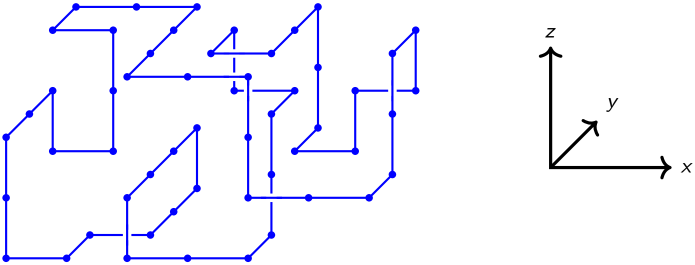
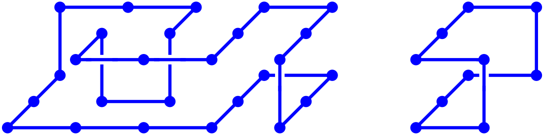


Let $p_{\mathbb{T},n}$ be the number of polygons in $\mathcal{P}_{\mathbb{T}}$ of length n.

Then it's possible to concatenate two polygons in $\mathbb{T}$ of lengths m and n by adding a constant number of steps:



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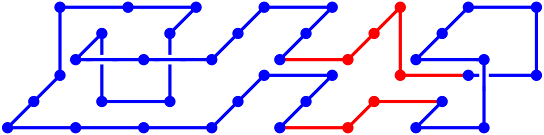

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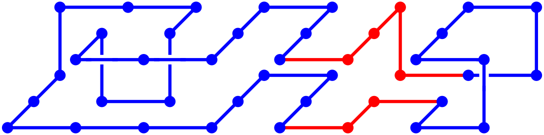

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$$p_{\mathbb{T},m+n+c} \geq p_{\mathbb{T},m} p_{\mathbb{T},n} \qquad \Rightarrow \qquad p_{\mathbb{T},m+n-c} \geq p_{\mathbb{T},m-c} p_{\mathbb{T},n-c}.$$

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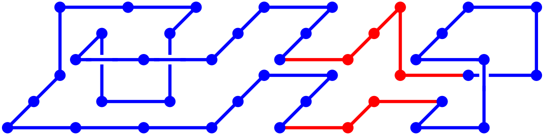

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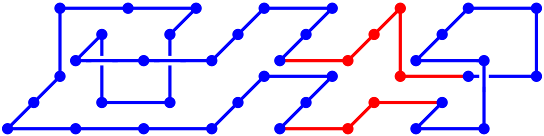

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exists.

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

In fact we can do better:

Theorem 6 (Soteros 1998)

There exists a constant $\alpha_{\mathbb{T}}$ *such that*

$$p_{\mathbb{T},n} = \alpha_{\mathbb{T}} e^{\kappa_{\mathbb{T}} n} \left(1 + O(1/n)\right).$$

In fact we can do better:

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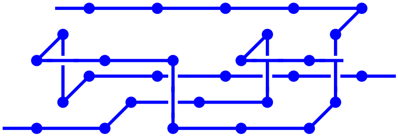

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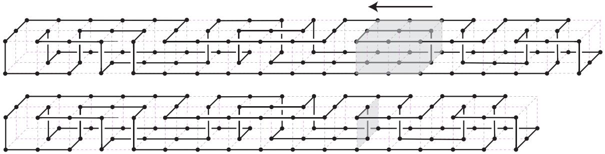
Upper bound is trickier: need to be able to get from any knot type K (which fits in 2×1 tube) to the unknot without adding too many edges.

Tube polygons and 4-plats

Polygons in a 2×1 tube can have 6 'strands' in the x direction, but those occurrences can be 'squashed'.



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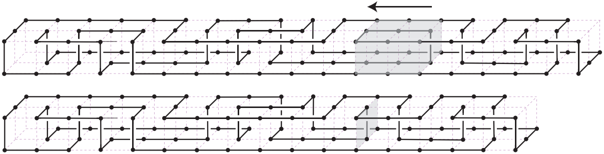

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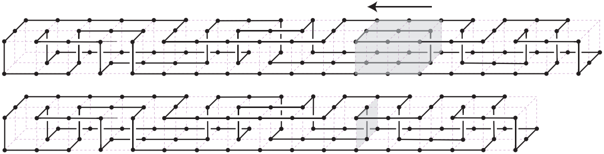

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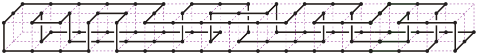

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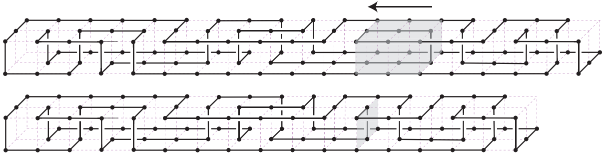

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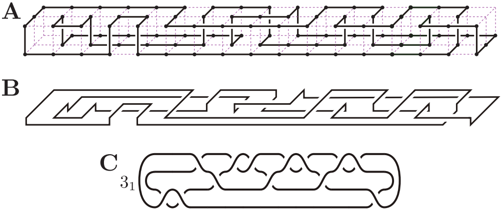

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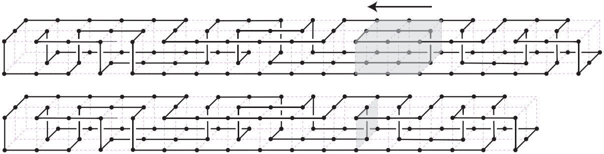

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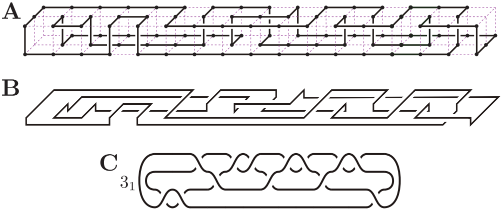

Conversely, any 4-plat can be embedded in the 2×1 tube, and the span in the x direction is at most $3 \times$ (number of crossings). (Actually could be a link – will talk about this later!)

Unknotting 4-plats

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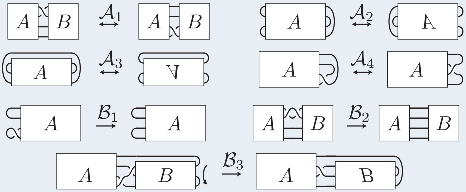
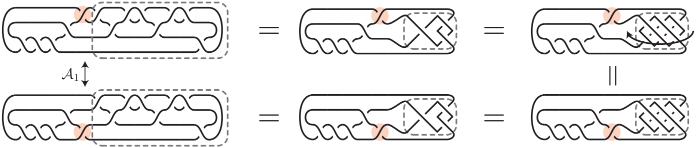
The goal now is to convert any 4-plat into the unknot by inserting something small(ish). First, a lemma:

Lemma 3

Suppose that two 4-plat diagrams D_1 and D_2 are related by one of the moves $\mathcal{A}_1$, $\mathcal{A}_2$, $\mathcal{A}_3$, $\mathcal{A}_4$, $\mathcal{B}_1$, $\mathcal{B}_2$ and $\mathcal{B}_3$. Then D_1 and D_2 represent the same knot type.





In particular $\mathcal{A}_1$ means a 4-plat can be written as a 3-braid, and $\mathcal{B}_1$–$\mathcal{B}_3$ reduce the number of crossings.

If w is a 3-braid word (on the alphabet $\sigma_1, \sigma_1^{-1}, \sigma_2, \sigma_2^{-1}$) then let $\overline{w}$ be the reverse word and $\widehat{w}$ be the flipped word (switch 1's and 2's).

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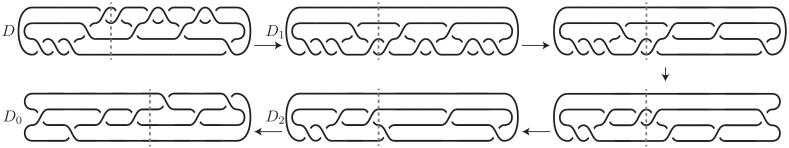

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Now back to the lattice. Each prime component can be unknotted by inserting something, so we get

Theorem 10

Any lattice embedding of a knot K in $\mathbb{T}^*$ can be converted to a lattice polygon of the unknot in $\mathbb{T}^*$ by f_K insertions of braid s-blocks. The span (s) is bounded above by $3c + 8$, where c is the maximum crossing number of the prime factors of K.

The upper bound

The number of insertions is bounded above by f_K, giving

$$p_{\mathbb{T},n}(K) \leq a_K \binom{n}{f_K} u_{\mathbb{T},n+b_K}$$

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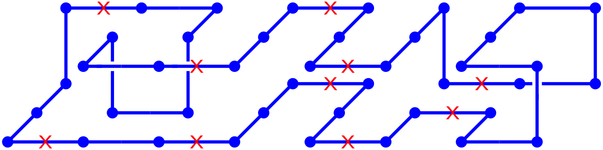
A corresponding lower bound requires something stronger than the previous argument. It requires showing that there are (on average) at least const.$\times n^{f_K}$ ways to convert an unknot to a knot of type K.

A “pattern theorem” for unknots in $\mathbb{T}$

A 2-string in a polygon π occurs at position $x^* \in \mathbb{Z} + 1/2$ if π intersects the plane $x = x^*$ in only 2 places:



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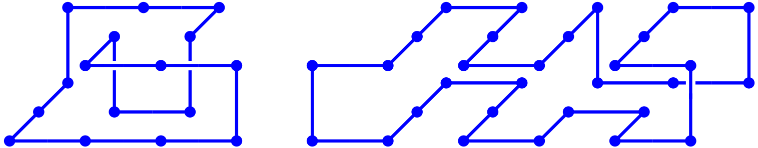

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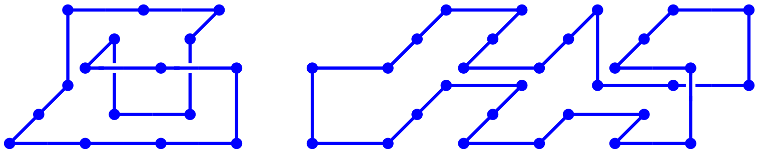

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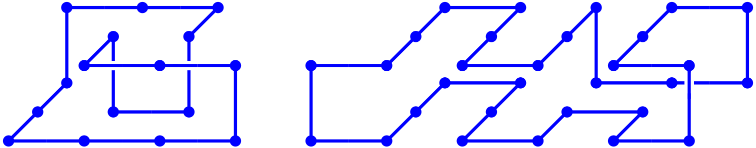

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So if unknots have a lot (ie. $O(n)$) of 2-strings, there should be a lot (ie. $O(n^{f_K})$) of ways to insert the f_K knot components into an unknot to get a knot of type K.

Lemma 4

Let $u_{\mathbb{T},n}(j)$ be the number of unknots in $\mathbb{T}$ of length n with j 2-strings. Then

$$\limsup_{n\to\infty} \frac{1}{n} \log u_{\mathbb{T},n}(0) < \kappa_{\mathbb{T},0}.$$

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$$u_{\mathbb{T},m} u_{\mathbb{T},n} \leq u_{\mathbb{T},m+n+6}$$

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There are 119,796,593 unknots of length 24 in $\mathbb{T}$, so we know

$$\kappa_{\mathbb{T},0} \geq 0.620044.$$

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$$\limsup_{n\to\infty} \frac{1}{n} \log u_{\mathbb{T},n}(\leq \epsilon^* n) < \kappa_{\mathbb{T},0}.$$

To prove this, we show that an unknot with $\leq j$ 2-strings can be converted into one with no 2-strings with the addition of a bounded number of edges. There are at most $n/2$ 2-strings in a polygon, so

$$u_{\mathbb{T},n}(\leq \epsilon n) \leq \sum_{j=0}^{\epsilon n} \binom{n/2}{j} u_{\mathbb{T},n+cj}(0)$$

for a constant c.

The main theorem

If $\epsilon < 1/4$ then

$$u_{\mathbb{T},n}(\leq \epsilon n) \leq (1+\epsilon n)\binom{n/2}{\epsilon n} u_{\mathbb{T},(1+c\epsilon)n}(0).$$

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Take logs, divide by n, apply Stirling's approximation, then

$$\limsup_{n\to\infty} u_{\mathbb{T},n}(\leq \epsilon n) \leq -\frac{1}{2}\log 2 - \left(\frac{1}{2}-\epsilon\right)\log\left(\frac{1}{2}-\epsilon\right) - \epsilon\log\epsilon + (1+c\epsilon)\times 0.446287$$

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Since unknots with fewer than $\epsilon^* n$ 2-strings are exponentially rare, we can take (almost) any unknot of length n and turn it into a knot of type K in at least $\binom{\epsilon^* n}{f_K} = O(n^{f_K})$ ways.

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Theorem 12

If K fits in the 2×1 tube $\mathbb{T}$ (i.e. it is 2-bridge) and has f_K prime components, then there exist constants C_1, C_2 such that for sufficiently large n,

$$C_1 n^{f_K} u_{\mathbb{T},n} \leq p_{\mathbb{T},n}(K) \leq C_2 n^{f_K} u_{\mathbb{T},n}.$$

Further results

The result is actually more general – it holds for non-split links which fit in $\mathbb{T}$.

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Parts of this can be extended to larger tubes, but there are problems with both lower and upper bounds:

- Upper bound: something can be said about which knots fit in larger tubes, but characterising the unknotting insertions for 6-plats, etc. is much more complicated
- Lower bound: computing transfer matrices, eigenvalues, etc. quickly becomes untenable (probably possible for a few larger tubes)

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In other works we have done numerical work on distributions of knot types, etc. in larger tubes.

Thank you for listening!

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