Knotting probabilities and pattern theorems for polygons in tubes

Nicholas Beaton

School of Mathematics and Statistics, University of Melbourne, Australia

Knots and Polymers
Ochanomizu University, Tokyo, Japan

August 9, 2017

THE UNIVERSITY OF MELBOURNE

Australian Government
Australian Research Council

Outline

Collaborators

Chris Soteros

Jeremy Eng

Koya Shimokawa

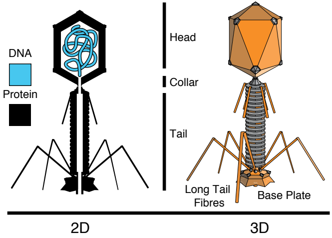
Kai Ishihara

Mahshid Atapour

Mariel Vazquez

Introduction I: Motivation

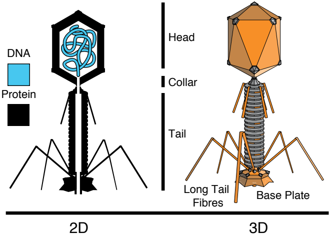
DNA molecules can be packed incredibly tightly in cell nuclei. For example, human DNA can be 2 m long but must fit inside a cell nucleus of diameter 10 μm. Similarly, bacteriophage DNA is packed into a hard capsid until it is injected into the host cell.



[1] Arsuaga et al, PNAS **99** (2002), 5373–5377.

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.

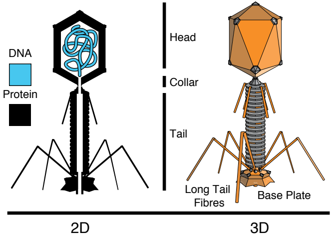


Some DNA molecules (like mitochondrial DNA) have a natural ring structure, while linear DNA can cyclise (the ends stick together) in the nucleus or after being released from confinement.

[1] Arsuaga et al, PNAS **99** (2002), 5373–5377.

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.



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.

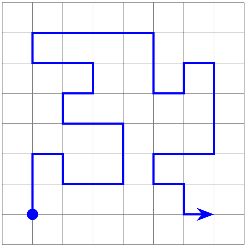
The tight packing within a cell or capsid may result in a high level of tangling, with lots of knots and/or links. Knotting rates of up to 95% have been observed for DNA released from certain bacteriophages.[1]

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

[1] Arsuaga et al, PNAS **99** (2002), 5373–5377.

Introduction II: Self-avoiding walks & polygons

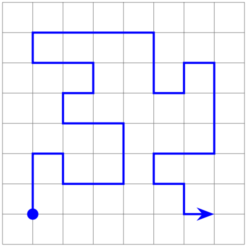
A self-avoiding walk (SAW) ω on a graph is a sequence $(\omega_0, \ldots, \omega_n)$ of distinct vertices with consecutive vertices adjacent on the graph.



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

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.



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

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

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

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

This can be used to show

Theorem (Hammersley 1957)

The limit

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

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

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

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

This can be used to show

Theorem (Hammersley 1957)

The limit

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

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

κ is known as the connective constant of the lattice.

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

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

This can be used to show

Theorem (Hammersley 1957)

The limit

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

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

κ is known as the connective constant of the lattice.

Corollary

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

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

$$\kappa_{\mathbb{Z}^2} \approx 0.970081147$$
$$\kappa_{\mathbb{Z}^3} \approx 1.54416097$$

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

$$\kappa_{\mathbb{Z}^2} \approx 0.970081147$$
$$\kappa_{\mathbb{Z}^3} \approx 1.54416097$$

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

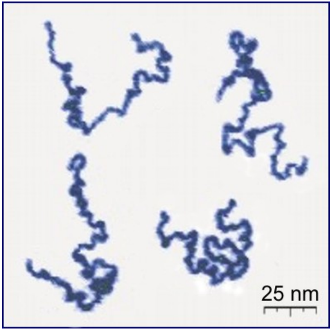
$$c_n \sim An^{\gamma-1}e^{\kappa n}$$

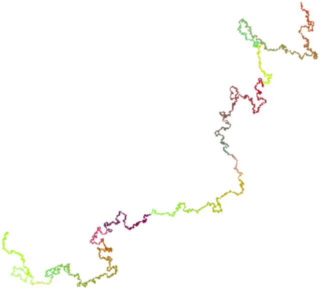
where A and κ depend on the lattice, γ depends only on the dimension. In 2D, expect that $\gamma = 43/32$, while in 3D $\gamma \approx 1.156957$.

Why use SAWs?

Why use SAWs?

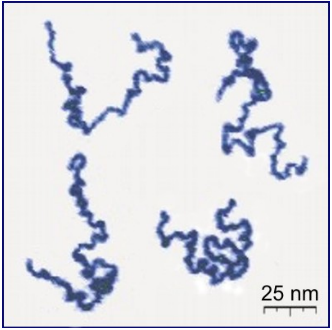
3D SAWs do a good job of modelling geometric properties of polymers in a good solvent (e.g. mean squared end-to-end distance)

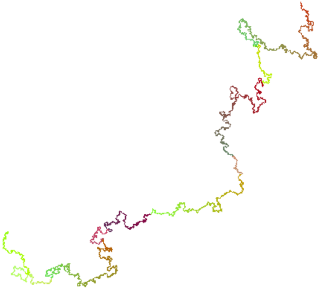




Why use SAWs?

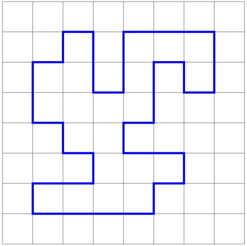
3D SAWs do a good job of modelling geometric properties of polymers in a good solvent (e.g. mean squared end-to-end distance)



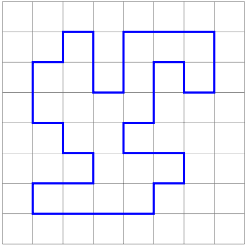


SAWs incorporate the excluded volume effect.

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

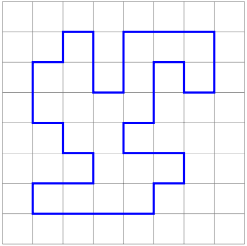


A self-avoiding polygon (SAP) is a simple closed loop on the edges of the lattice:



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.

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



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 (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 $\kappa = \sup_{n\geq 0} \frac{1}{n} \log\left(\frac{p_n}{d-1}\right)$.

In fact polygons have the same growth rate as walks:

Theorem (Hammersley 1961)

The limit

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

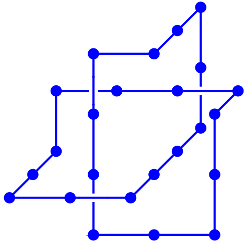
exists and is equal to κ, the connective constant of the lattice, where the limit is taken through even values of n. Moreover $\kappa = \sup_{n\geq 0} \frac{1}{n} \log \left(\frac{p_n}{d-1} \right)$.

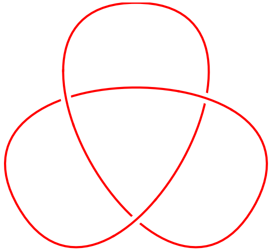
Expect similar power law subexponential terms:

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

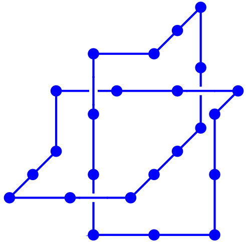
where B, κ depend on lattice and α depends on dimension. In 2D, expect $\alpha = 1/2$, while in 3D expect $\alpha \approx 0.23721$.

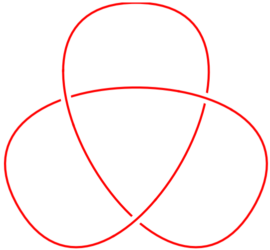
In 3D SAPs can be knotted:





In 3D SAPs can be knotted:



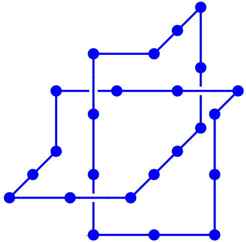


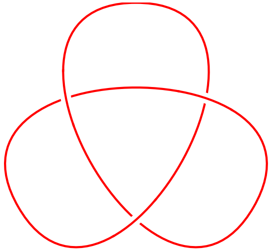
In fact, very long polygons are almost always knotted:

Theorem (Sumners & Whittington 1988)

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

In 3D SAPs can be knotted:





In fact, very long polygons are almost always knotted:

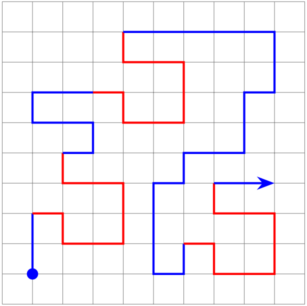
Theorem (Sumners & Whittington 1988)

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

This is proved using a pattern theorem.

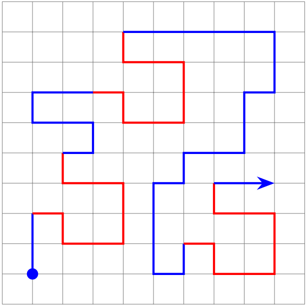
Introduction III: Pattern theorems

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.



Introduction III: Pattern theorems

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.



Theorem (Kesten 1963)

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

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

Sketch of (a) proof:

Sketch of (a) proof:

- Work on d-dimensional hypercubic lattice with coordinates $(x_1, \ldots, x_d)$.

Sketch of (a) proof:

- Work on d-dimensional hypercubic lattice with coordinates $(x_1, \ldots, x_d)$.
- A SAW $\omega = (\omega_0, \ldots, \omega_n)$ is a bridge if $x_d(\omega_0) < x_d(\omega_i) \leq x_d(\omega_n)$ for all $i = 1, \ldots, n$. Let b_n be the number of bridges of length n.

Sketch of (a) proof:

- Work on d-dimensional hypercubic lattice with coordinates $(x_1, \ldots, x_d)$.
- A SAW $\omega = (\omega_0, \ldots, \omega_n)$ is a bridge if $x_d(\omega_0) < x_d(\omega_i) \leq x_d(\omega_n)$ for all $i = 1, \ldots, n$. Let b_n be the number of bridges of length n.
- Bridges can be freely concatenated without creating self-intersections. A bridge is irreducible if it cannot be written as the concatenation of two (non-empty) bridges. Let i_n be the number of irreducible bridges of length n.

Sketch of (a) proof:

- Work on d-dimensional hypercubic lattice with coordinates $(x_1, \ldots, x_d)$.
- A SAW $\omega = (\omega_0, \ldots, \omega_n)$ is a bridge if $x_d(\omega_0) < x_d(\omega_i) \leq x_d(\omega_n)$ for all $i = 1, \ldots, n$. Let b_n be the number of bridges of length n.
- Bridges can be freely concatenated without creating self-intersections. A bridge is irreducible if it cannot be written as the concatenation of two (non-empty) bridges. Let i_n be the number of irreducible bridges of length n.
- Define the generating functions $\mathcal{C}(z) = \sum_n c_n z^n$, and likewise $\mathcal{B}(z)$ and $\mathcal{I}(z)$. Then with inclusion and unfolding arguments it is straightforward to show

$$\mathcal{I}(z) \leq \mathcal{B}(z) \leq \mathcal{C}(z) \leq e^{2\mathcal{B}(z)} = e^{2\mathcal{I}(z)/(1-\mathcal{I}(z))}$$

Sketch of (a) proof:

- Work on d-dimensional hypercubic lattice with coordinates $(x_1, \ldots, x_d)$.
- A SAW $\omega = (\omega_0, \ldots, \omega_n)$ is a bridge if $x_d(\omega_0) < x_d(\omega_i) \leq x_d(\omega_n)$ for all $i = 1, \ldots, n$. Let b_n be the number of bridges of length n.
- Bridges can be freely concatenated without creating self-intersections. A bridge is irreducible if it cannot be written as the concatenation of two (non-empty) bridges. Let i_n be the number of irreducible bridges of length n.
- Define the generating functions $\mathcal{C}(z) = \sum_n c_n z^n$, and likewise $\mathcal{B}(z)$ and $\mathcal{I}(z)$. Then with inclusion and unfolding arguments it is straightforward to show

$$\mathcal{I}(z) \leq \mathcal{B}(z) \leq \mathcal{C}(z) \leq e^{2\mathcal{B}(z)} = e^{2\mathcal{I}(z)/(1-\mathcal{I}(z))}$$

- Likewise define $\mathcal{C}_{\bar{P}}(z), \mathcal{B}_{\bar{P}}(z)$ and $\mathcal{I}_{\bar{P}}(z)$. The same inequalities hold (unless P can be formed at the concatenation of two irreducible bridges... then more care must be taken)

Sketch of (a) proof (ct'd):

- $\mathcal{C}(z)$ has a dominant singularity at $z = z_c = e^{-\kappa}$, and $c_{m+n} \leq c_m c_n$ implies that $\mathcal{C}(z)$ diverges at least as strongly as a simple pole as $z \to z_c$. Hence $\mathcal{B}(z)$ also diverges as $z \to z_c$.

Sketch of (a) proof (ct'd):

- $\mathcal{C}(z)$ has a dominant singularity at $z = z_c = e^{-\kappa}$, and $c_{m+n} \leq c_m c_n$ implies that $\mathcal{C}(z)$ diverges at least as strongly as a simple pole as $z \to z_c$. Hence $\mathcal{B}(z)$ also diverges as $z \to z_c$.
- Since $\mathcal{B}(z) = \mathcal{I}(z)/(1 - \mathcal{I}(z))$, we have $\mathcal{I}(z_c) = 1$.

Sketch of (a) proof (ct'd):

- $\mathcal{C}(z)$ has a dominant singularity at $z = z_c = e^{-\kappa}$, and $c_{m+n} \leq c_m c_n$ implies that $\mathcal{C}(z)$ diverges at least as strongly as a simple pole as $z \to z_c$. Hence $\mathcal{B}(z)$ also diverges as $z \to z_c$.
- Since $\mathcal{B}(z) = \mathcal{I}(z)/(1 - \mathcal{I}(z))$, we have $\mathcal{I}(z_c) = 1$.
- But $\mathcal{I}_{\bar{P}}(z_c) < 1$, so the dominant singularity for $\mathcal{B}_{\bar{P}}(z)$ and $\mathcal{C}_{\bar{P}}(z)$ must be greater than z_c.

Sketch of (a) proof (ct'd):

- $\mathcal{C}(z)$ has a dominant singularity at $z = z_c = e^{-\kappa}$, and $c_{m+n} \leq c_m c_n$ implies that $\mathcal{C}(z)$ diverges at least as strongly as a simple pole as $z \to z_c$. Hence $\mathcal{B}(z)$ also diverges as $z \to z_c$.
- Since $\mathcal{B}(z) = \mathcal{I}(z)/(1 - \mathcal{I}(z))$, we have $\mathcal{I}(z_c) = 1$.
- But $\mathcal{I}_{\bar{P}}(z_c) < 1$, so the dominant singularity for $\mathcal{B}_{\bar{P}}(z)$ and $\mathcal{C}_{\bar{P}}(z)$ must be greater than z_c.
- So the growth rate for walks which do not contain P must be smaller than that of all walks!

Sketch of (a) proof (ct'd):

- $\mathcal{C}(z)$ has a dominant singularity at $z = z_c = e^{-\kappa}$, and $c_{m+n} \leq c_m c_n$ implies that $\mathcal{C}(z)$ diverges at least as strongly as a simple pole as $z \to z_c$. Hence $\mathcal{B}(z)$ also diverges as $z \to z_c$.
- Since $\mathcal{B}(z) = \mathcal{I}(z)/(1 - \mathcal{I}(z))$, we have $\mathcal{I}(z_c) = 1$.
- But $\mathcal{I}_{\bar{P}}(z_c) < 1$, so the dominant singularity for $\mathcal{B}_{\bar{P}}(z)$ and $\mathcal{C}_{\bar{P}}(z)$ must be greater than z_c.
- So the growth rate for walks which do not contain P must be smaller than that of all walks!

In fact a stronger result holds:

Theorem (Kesten 1963)

Let P be a Kesten pattern, and let $c_{n,\bar{P}}(\leq k)$ be the number of SAWs of length n which contain at most k occurrences of P. Then there exists an $\epsilon > 0$ such that

$$\limsup_{n\to\infty} \frac{1}{n} \log c_{n,\bar{P}}(\epsilon n) < \kappa.$$

Sketch of (a) proof (ct'd):

- $\mathcal{C}(z)$ has a dominant singularity at $z = z_c = e^{-\kappa}$, and $c_{m+n} \leq c_m c_n$ implies that $\mathcal{C}(z)$ diverges at least as strongly as a simple pole as $z \to z_c$. Hence $\mathcal{B}(z)$ also diverges as $z \to z_c$.
- Since $\mathcal{B}(z) = \mathcal{I}(z)/(1 - \mathcal{I}(z))$, we have $\mathcal{I}(z_c) = 1$.
- But $\mathcal{I}_{\bar{P}}(z_c) < 1$, so the dominant singularity for $\mathcal{B}_{\bar{P}}(z)$ and $\mathcal{C}_{\bar{P}}(z)$ must be greater than z_c.
- So the growth rate for walks which do not contain P must be smaller than that of all walks!

In fact a stronger result holds:

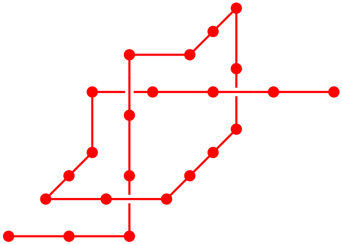
Theorem (Kesten 1963)

Let P be a Kesten pattern, and let $c_{n,\bar{P}}(\leq k)$ be the number of SAWs of length n which contain at most k occurrences of P. Then there exists an $\epsilon > 0$ such that

$$\limsup_{n \to \infty} \frac{1}{n} \log c_{n,\bar{P}}(\epsilon n) < \kappa.$$

Both results can easily be extended from SAWs to SAPs.

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



If this pattern occurs anywhere in a polygon, the polygon cannot be the unknot.

Conjectures

Let p_n^K be the number of SAPs in $\mathbb{Z}^3$ of length n and knot type K, and let $u_n = p_n^{0_1}$.

Conjectures

Let p_n^K be the number of SAPs in $\mathbb{Z}^3$ of length n and knot type K, and let $u_n = p_n^{0_1}$. Two unknots can be concatenated to give a bigger unknot, so

$$u_{m+n} \geq \frac{1}{2} u_m u_n.$$

(Not true for any other knot type!)

Conjectures

Let p_n^K be the number of SAPs in $\mathbb{Z}^3$ of length n and knot type K, and let $u_n = p_n^{0_1}$.
Two unknots can be concatenated to give a bigger unknot, so

$$u_{m+n} \geq \frac{1}{2} u_m u_n.$$

(Not true for any other knot type!)

$\Rightarrow$ Unknots have connective constant $\kappa_0 < \kappa$.

Conjectures

Let p_n^K be the number of SAPs in $\mathbb{Z}^3$ of length n and knot type K, and let $u_n = p_n^{0_1}$. Two unknots can be concatenated to give a bigger unknot, so

$$u_{m+n} \geq \frac{1}{2} u_m u_n.$$

(Not true for any other knot type!)

$\Rightarrow$ Unknots have connective constant $\kappa_0 < \kappa$.

Can concatenate unknot with knot type K to get bigger knot of type K, so

$$\liminf_{n\to\infty} \frac{1}{n} \log p_n^K \geq \kappa_0.$$

Conjectures

Let p_n^K be the number of SAPs in $\mathbb{Z}^3$ of length n and knot type K, and let $u_n = p_n^{0_1}$. Two unknots can be concatenated to give a bigger unknot, so

$$u_{m+n} \geq \frac{1}{2} u_m u_n.$$

(Not true for any other knot type!)

$\Rightarrow$ Unknots have connective constant $\kappa_0 < \kappa$.

Can concatenate unknot with knot type K to get bigger knot of type K, so

$$\liminf_{n\to\infty} \frac{1}{n} \log p_n^K \geq \kappa_0.$$

Generally believed that

Conjecture

$$\lim_{n\to\infty} \frac{1}{n} \log p_n^K = \kappa_0$$

for all K.

Conjectures

Let p_n^K be the number of SAPs in $\mathbb{Z}^3$ of length n and knot type K, and let $u_n = p_n^{0_1}$. Two unknots can be concatenated to give a bigger unknot, so

$$u_{m+n} \geq \frac{1}{2} u_m u_n.$$

(Not true for any other knot type!)

$\Rightarrow$ Unknots have connective constant $\kappa_0 < \kappa$.

Can concatenate unknot with knot type K to get bigger knot of type K, so

$$\liminf_{n\to\infty} \frac{1}{n} \log p_n^K \geq \kappa_0.$$

Generally believed that

Conjecture

$$\lim_{n\to\infty} \frac{1}{n} \log p_n^K = \kappa_0$$

for all K.

Idea: expect a very long knot of type K to "look" like an unknot except for a small K component somewhere.

Then expect

$$p_n^K \sim A_K n^{\gamma_K - 1} e^{\kappa_0 n}$$

for some constants A_K and γ_K.

Then expect

$$p_n^K \sim A_K n^{\gamma_K - 1} e^{\kappa_0 n}$$

for some constants A_K and γ_K.

Say K has $P(K)$ prime knot components. (With $P(0_1) = 0$.)

Then expect

$$p_n^K \sim A_K n^{\gamma_K - 1} e^{\kappa_0 n}$$

for some constants A_K and γ_K.

Say K has $P(K)$ prime knot components. (With $P(0_1) = 0$.) Generally believed that

Conjecture

$$\gamma_K = \gamma_{0_1} + P(K). \tag{1}$$

Then expect

$$p_n^K \sim A_K n^{\gamma_K - 1} e^{\kappa_0 n}$$

for some constants A_K and γ_K.

Say K has $P(K)$ prime knot components. (With $P(0_1) = 0$.) Generally believed that

Conjecture

$$\gamma_K = \gamma_{0_1} + P(K). \tag{1}$$

Idea: a long knot of type K should "look" like an unknot except for the $P(K)$ small prime components, and there are $\approx n^{P(K)}$ ways to "insert" them.

Then expect

$$p_n^K \sim A_K n^{\gamma_K - 1} e^{\kappa_0 n}$$

for some constants A_K and γ_K.

Say K has $P(K)$ prime knot components. (With $P(0_1) = 0$.) Generally believed that

Conjecture

$$\gamma_K = \gamma_{0_1} + P(K). \tag{1}$$

Idea: a long knot of type K should "look" like an unknot except for the $P(K)$ small prime components, and there are $\approx n^{P(K)}$ ways to "insert" them.

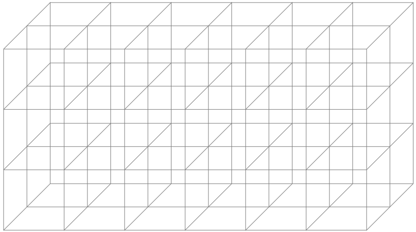
We will look at polygons in a subset of $\mathbb{Z}^3$ in order to (hopefully) prove results which are difficult on the whole lattice.

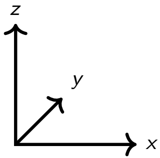
Polygons in lattice tubes

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 $L \geq M$.)





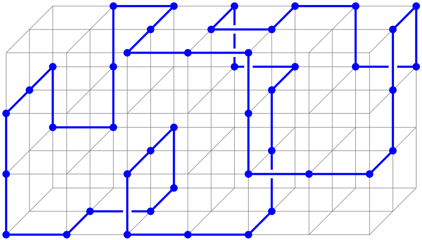
Polygons in lattice tubes

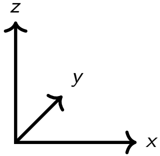
Let $\mathbb{T}_{L,M} \equiv \mathbb{T}$ be an $L \times M$ semi-infinite tube of $\mathbb{Z}^3$:

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

(Assume $L \geq M$.)

Let $\mathcal{P}_{\mathbb{T}}$ be the set of SAPs confined within $\mathbb{T}$, counted up to translation in the x direction.





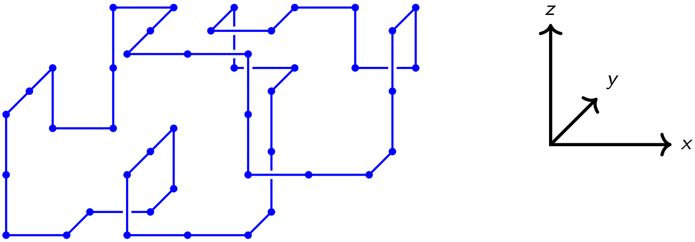
Polygons in lattice tubes

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

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

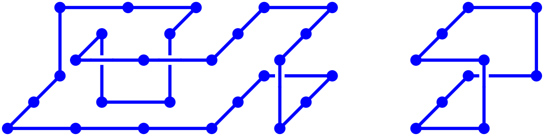
(Assume $L \geq M$.)

Let $\mathcal{P}_{\mathbb{T}}$ be the set of SAPs confined within $\mathbb{T}$, counted up to translation in the x direction.

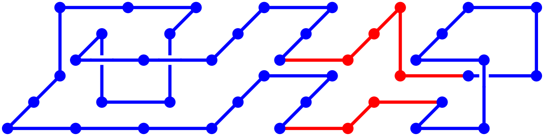


Let $p_{\mathbb{T},n}$ be the number of polygons in $\mathcal{P}_{\mathbb{T}}$ of length n.

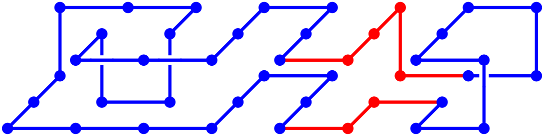
Then it's possible to concatenate two polygons in $\mathbb{T}$ of lengths m and n by adding a constant number of steps:



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



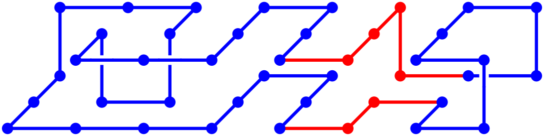
Then it's possible to concatenate two polygons in $\mathbb{T}$ of lengths m and n by adding a constant number of steps:



So

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

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



So

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

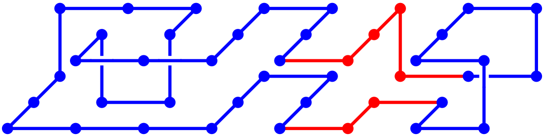
Theorem (Soteros & Whittington 1989)

The limit

$$\kappa_{\mathbb{T}} = \lim_{n\to\infty} \frac{1}{n} \log p_{\mathbb{T},n}$$

exists.

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



So

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

Theorem (Soteros & Whittington 1989)

The limit

$$\kappa_{\mathbb{T}} = \lim_{n\to\infty} \frac{1}{n} \log p_{\mathbb{T},n}$$

exists.

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

Transfer matrices

In fact we can do better:

Theorem (Soteros 1998)

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

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

Transfer matrices

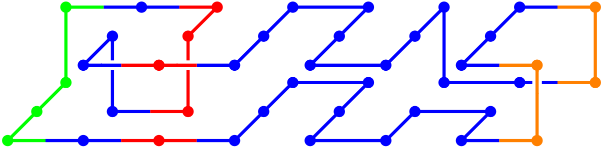
In fact we can do better:

Theorem (Soteros 1998)

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

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

This and other results are proved with transfer matrices:



A (1-)block is the portion of a polygon between $x = j$ and $x = j + 1$ for some $j \in \mathbb{Z} + 1/2$. A starting block is the first non-empty block, and a finishing block is the last non-empty block. Distinguish blocks not only by their edges and vertices, but also by how the incoming edges on the left are paired up.

Let $\mathbf{G}_{\mathbb{T}}(z)$ be the matrix with terms

$$g_{ij} = \begin{cases} z^{\#\text{edges in } j} & \text{if block } j \text{ can follow block } i \\ 0 & \text{otherwise.} \end{cases}$$

Let $\mathbf{G}_{\mathbb{T}}(z)$ be the matrix with terms

$$g_{ij} = \begin{cases} z^{\#\text{edges in } j} & \text{if block } j \text{ can follow block } i \\ 0 & \text{otherwise.} \end{cases}$$

Let $\mathbf{A}_{\mathbb{T}}(z)$ be the vector with

$$a_j = \sum_{\substack{\text{starting block } i \\ \text{can precede block } j}} z^{\#\text{edges in } i}$$

Let $\mathbf{G}_{\mathbb{T}}(z)$ be the matrix with terms

$$g_{ij} = \begin{cases} z^{\#\text{edges in } j} & \text{if block } j \text{ can follow block } i \\ 0 & \text{otherwise.} \end{cases}$$

Let $\mathbf{A}_{\mathbb{T}}(z)$ be the vector with

$$a_j = \sum_{\substack{\text{starting block } i \\ \text{can precede block } j}} z^{\#\text{edges in } i}$$

Let $\mathbf{B}_{\mathbb{T}}(z)$ be the vector with

$$b_i = \sum_{\substack{\text{finishing block } j \\ \text{can follow block } i}} z^{\#\text{edges in } j}$$

Let $\mathbf{G}_{\mathbb{T}}(z)$ be the matrix with terms

$$g_{ij} = \begin{cases} z^{\#\text{edges in } j} & \text{if block } j \text{ can follow block } i \\ 0 & \text{otherwise.} \end{cases}$$

Let $\mathbf{A}_{\mathbb{T}}(z)$ be the vector with

$$a_j = \sum_{\substack{\text{starting block } i \\ \text{can precede block } j}} z^{\#\text{edges in } i}$$

Let $\mathbf{B}_{\mathbb{T}}(z)$ be the vector with

$$b_i = \sum_{\substack{\text{finishing block } j \\ \text{can follow block } i}} z^{\#\text{edges in } j}$$

Then the generating function $F_{\mathbb{T}}(z)$ for polygons in $\mathbb{T}$ with z conjugate to length is (for polygons of span ≥ 2)

$$F_{\mathbb{T}}(z) = \mathbf{A}_{\mathbb{T}}(z).(\mathbf{I} - \mathbf{G}_{\mathbb{T}}(z))^{-1}.\mathbf{B}_{\mathbb{T}}(z)$$

Let $\mathbf{G}_{\mathbb{T}}(z)$ be the matrix with terms

$$g_{ij} = \begin{cases} z^{\#\text{edges in } j} & \text{if block } j \text{ can follow block } i \\ 0 & \text{otherwise.} \end{cases}$$

Let $\mathbf{A}_{\mathbb{T}}(z)$ be the vector with

$$a_j = \sum_{\substack{\text{starting block } i \\ \text{can precede block } j}} z^{\#\text{edges in } i}$$

Let $\mathbf{B}_{\mathbb{T}}(z)$ be the vector with

$$b_i = \sum_{\substack{\text{finishing block } j \\ \text{can follow block } i}} z^{\#\text{edges in } j}$$

Then the generating function $F_{\mathbb{T}}(z)$ for polygons in $\mathbb{T}$ with z conjugate to length is (for polygons of span ≥ 2)

$$F_{\mathbb{T}}(z) = \mathbf{A}_{\mathbb{T}}(z).(\mathbf{I} - \mathbf{G}_{\mathbb{T}}(z))^{-1}.\mathbf{B}_{\mathbb{T}}(z)$$

Since polygons can be concatenated, $\mathbf{G}_{\mathbb{T}}$ is irreducible, and since there are blocks which can follow themselves, $\mathbf{G}_{\mathbb{T}}$ is primitive (aperiodic). The dominant singularity of $F_{\mathbb{T}}(z)$ is $z_{\mathbb{T}} = e^{-\kappa_{\mathbb{T}}}$ = the value of z which makes the dominant eigenvalue of $\mathbf{G}_{\mathbb{T}}(z)$ equal to 1.

Knots in tubes

Theorem (Soteros 1998)

For any $L \times M$ tube $\mathbb{T}$ with $L \geq 2$, $M \geq 1$ the probability of a random n-step polygon in $\mathbb{T}$ being knotted approaches 1 as $n \to \infty$.

(Knots cannot occur in the 1×1 tube.)

Knots in tubes

Theorem (Soteros 1998)

For any $L \times M$ tube $\mathbb{T}$ with $L \geq 2$, $M \geq 1$ the probability of a random n-step polygon in $\mathbb{T}$ being knotted approaches 1 as $n \to \infty$.

(Knots cannot occur in the 1×1 tube.)

This also follows from a pattern theorem.

Knots in tubes

Theorem (Soteros 1998)

For any $L \times M$ tube $\mathbb{T}$ with $L \geq 2$, $M \geq 1$ the probability of a random n-step polygon in $\mathbb{T}$ being knotted approaches 1 as $n \to \infty$.

(Knots cannot occur in the 1×1 tube.)

This also follows from a pattern theorem. Generalise $\mathbf{G}, \mathbf{A}$ and $\mathbf{B}$ so that their entries correspond to k-blocks: segments of a polygon between $x = j$ and $x = j + k$ for some $j \in \mathbb{Z} + 1/2$.

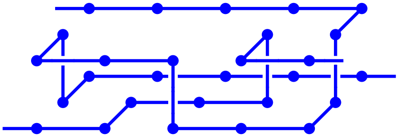
Knots in tubes

Theorem (Soteros 1998)

For any $L \times M$ tube $\mathbb{T}$ with $L \geq 2$, $M \geq 1$ the probability of a random n-step polygon in $\mathbb{T}$ being knotted approaches 1 as $n \to \infty$.

(Knots cannot occur in the 1×1 tube.)

This also follows from a pattern theorem. Generalise $\mathbf{G}, \mathbf{A}$ and $\mathbf{B}$ so that their entries correspond to k-blocks: segments of a polygon between $x = j$ and $x = j + k$ for some $j \in \mathbb{Z} + 1/2$. Then (if k is large enough) some k-patterns guarantee knotting:



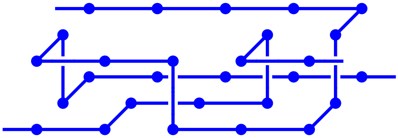
Knots in tubes

Theorem (Soteros 1998)

For any $L \times M$ tube $\mathbb{T}$ with $L \geq 2$, $M \geq 1$ the probability of a random n-step polygon in $\mathbb{T}$ being knotted approaches 1 as $n \to \infty$.

(Knots cannot occur in the 1×1 tube.)

This also follows from a pattern theorem. Generalise $\mathbf{G}, \mathbf{A}$ and $\mathbf{B}$ so that their entries correspond to k-blocks: segments of a polygon between $x = j$ and $x = j + k$ for some $j \in \mathbb{Z} + 1/2$. Then (if k is large enough) some k-patterns guarantee knotting:



Theorem (Schaefer 1974)

The dominant eigenvalue of a non-negative irreducible matrix $\mathbf{M}$ *is a strictly increasing function of all of* $\mathbf{M}$*'s elements.*

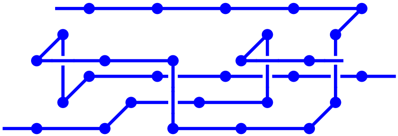
Knots in tubes

Theorem (Soteros 1998)

For any $L \times M$ tube $\mathbb{T}$ with $L \geq 2$, $M \geq 1$ the probability of a random n-step polygon in $\mathbb{T}$ being knotted approaches 1 as $n \to \infty$.

(Knots cannot occur in the 1×1 tube.)

This also follows from a pattern theorem. Generalise $\mathbf{G}, \mathbf{A}$ and $\mathbf{B}$ so that their entries correspond to k-blocks: segments of a polygon between $x = j$ and $x = j + k$ for some $j \in \mathbb{Z} + 1/2$. Then (if k is large enough) some k-patterns guarantee knotting:



Theorem (Schaefer 1974)

The dominant eigenvalue of a non-negative irreducible matrix $\mathbf{M}$ *is a strictly increasing function of all of* $\mathbf{M}$*'s elements.*

So removing any knotted k-pattern results in a smaller growth rate!

What can we say about the growth of polygons with a fixed knot type?

What can we say about the growth of polygons with a fixed knot type?

Theorem (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

If K is a knot type that can occur in the 2×1 tube $\mathbb{T}$ (a 2-bridge knot), then

$$\lim_{n\to\infty} \frac{1}{n} \log p^K_{\mathbb{T},n} = \kappa_{\mathbb{T},0}.$$

What can we say about the growth of polygons with a fixed knot type?

Theorem (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

If K is a knot type that can occur in the 2×1 tube $\mathbb{T}$ (a 2-bridge knot), then

$$\lim_{n\to\infty} \frac{1}{n} \log p^K_{\mathbb{T},n} = \kappa_{\mathbb{T},0}.$$

Lower bound already established.

What can we say about the growth of polygons with a fixed knot type?

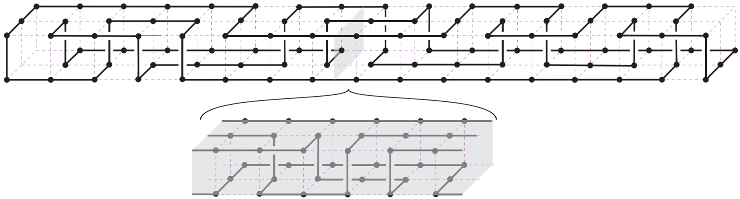
Theorem (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

If K is a knot type that can occur in the 2×1 tube $\mathbb{T}$ (a 2-bridge knot), then

$$\lim_{n \to \infty} \frac{1}{n} \log p_{\mathbb{T},n}^{K} = \kappa_{\mathbb{T},0}.$$

Lower bound already established.

Upper bound is proved by showing that a knot of type K can be unknotted by inserting "untwisting" blocks:



The number of insertions is bounded above by the crossing number $c(K)$, giving

$$p_{\mathbb{T},n}^{K} \leq a_K \binom{n}{c(K)} p_{\mathbb{T},n+b_K}^{0_1}$$

for some numbers a_K and b_K.

The number of insertions is bounded above by the crossing number $c(K)$, giving

$$p^K_{\mathbb{T},n} \leq a_K \binom{n}{c(K)} p^{0_1}_{\mathbb{T},n+b_K}$$

for some numbers a_K and b_K.

Moreover, if $K = K_1 \# K_2 \# \ldots \# K_p$, with each of the K_i having unknotting number 1, then the number of insertions required is only p. In this case,

$$p^K_{\mathbb{T},n} \leq a_K n^p u_{\mathbb{T},n+b(K)}.$$

The number of insertions is bounded above by the crossing number $c(K)$, giving

$$p^K_{\mathbb{T},n} \leq a_K \binom{n}{c(K)} p^{0_1}_{\mathbb{T},n+b_K}$$

for some numbers a_K and b_K.

Moreover, if $K = K_1 \# K_2 \# \ldots \# K_p$, with each of the K_i having unknotting number 1, then the number of insertions required is only p. In this case,

$$p^K_{\mathbb{T},n} \leq a_K n^p u_{\mathbb{T},n+b(K)}.$$

This establishes the upper bound for (1) – can we get a lower bound?

The number of insertions is bounded above by the crossing number $c(K)$, giving

$$p^K_{\mathbb{T},n} \leq a_K \binom{n}{c(K)} p^{0_1}_{\mathbb{T},n+b_K}$$

for some numbers a_K and b_K.

Moreover, if $K = K_1 \# K_2 \# \ldots \# K_p$, with each of the K_i having unknotting number 1, then the number of insertions required is only p. In this case,

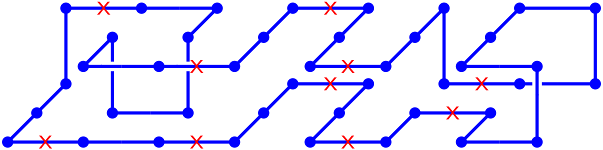
$$p^K_{\mathbb{T},n} \leq a_K n^p u_{\mathbb{T},n+b(K)}.$$

This establishes the upper bound for (1) – can we get a lower bound?

This would require showing that there are (on average) at least const.$\times n^p$ ways to convert an unknot to a knot of type K.

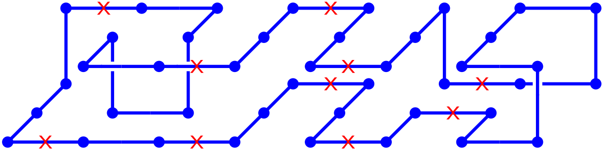
A "pattern theorem" for unknots in $\mathbb{T}$

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:



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

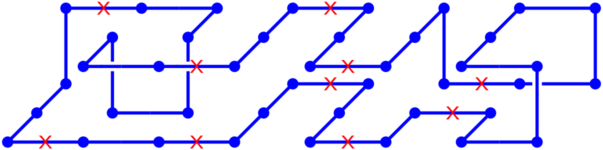
A 2-string in a polygon π occurs at position $x^* \in \mathbb{Z} + 1/2$ if π intersects the plane $x = x^*$ in only 2 places:



If π has a 2-string at $x = x^*$, then we can break it at that point, close up the two halves to get π_1 and π_2, and know that the knot type $K(\pi)$ is $K(\pi_1)\#K(\pi_2)$.

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:

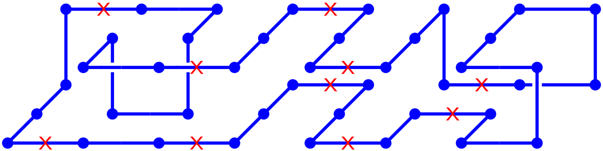


If π has a 2-string at $x = x^*$, then we can break it at that point, close up the two halves to get π_1 and π_2, and know that the knot type $K(\pi)$ is $K(\pi_1)\#K(\pi_2)$.

We can also insert a polygon π^* in the middle, concatenate π_1, π^*, π_2, and get something of knot type $K(\pi_1)\#K(\pi^*)\#K(\pi_2)$.

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:



If π has a 2-string at $x = x^*$, then we can break it at that point, close up the two halves to get π_1 and π_2, and know that the knot type $K(\pi)$ is $K(\pi_1)\#K(\pi_2)$.

We can also insert a polygon π^* in the middle, concatenate π_1, π^*, π_2, and get something of knot type $K(\pi_1)\#K(\pi^*)\#K(\pi_2)$.

So if unknots have a lot (ie. $O(n)$) of 2-strings, there should be a lot (ie. $O(n^p)$) of ways to insert the p knot components into an unknot to get a knot of type $K = K_1\# \dots \#K_p$.

Lemma (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

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

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

Lemma (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

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

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

The proof that almost all long polygons in $\mathbb{T}$ are knotted [Soteros 1998] followed easily from the transfer matrix.

Lemma (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

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

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

The proof that almost all long polygons in $\mathbb{T}$ are knotted [Soteros 1998] followed easily from the transfer matrix. But there is no finite transfer matrix for unknots. So we need another way.

Lemma (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

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

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

The proof that almost all long polygons in $\mathbb{T}$ are knotted [Soteros 1998] followed easily from the transfer matrix. But there is no finite transfer matrix for unknots. So we need another way.

Can prove it numerically!

Lemma (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

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

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

The proof that almost all long polygons in $\mathbb{T}$ are knotted [Soteros 1998] followed easily from the transfer matrix. But there is no finite transfer matrix for unknots. So we need another way.

Can prove it numerically! Unknots in the 2×1 tube can be concatenated with the addition of 6 edges. So

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

and hence

$$\kappa_{\mathbb{T},0} = \lim_{n\to\infty} \frac{1}{n} \log u_{\mathbb{T},n} = \sup_{n} \frac{1}{n} \log u_{\mathbb{T},n-6}.$$

Lemma (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

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

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

The proof that almost all long polygons in $\mathbb{T}$ are knotted [Soteros 1998] followed easily from the transfer matrix. But there is no finite transfer matrix for unknots. So we need another way.

Can prove it numerically! Unknots in the 2×1 tube can be concatenated with the addition of 6 edges. So

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

and hence

$$\kappa_{\mathbb{T},0} = \lim_{n\to\infty} \frac{1}{n} \log u_{\mathbb{T},n} = \sup_{n} \frac{1}{n} \log u_{\mathbb{T},n-6}.$$

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

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

On the other hand, we can construct a transfer matrix for all polygons (not just unknots) which excludes 2-strings.

On the other hand, we can construct a transfer matrix for all polygons (not just unknots) which excludes 2-strings. Bounds on the dominant eigenvalue can be calculated, which show that the growth rate for polygons with no 2-strings is at most 0.446287.

On the other hand, we can construct a transfer matrix for all polygons (not just unknots) which excludes 2-strings. Bounds on the dominant eigenvalue can be calculated, which show that the growth rate for polygons with no 2-strings is at most 0.446287. So

$$\limsup_{n\to\infty} \frac{1}{n} \log u_{\mathbb{T},n}(0) \leq 0.446287 < \kappa_{\mathbb{T},0}.$$

On the other hand, we can construct a transfer matrix for all polygons (not just unknots) which excludes 2-strings. Bounds on the dominant eigenvalue can be calculated, which show that the growth rate for polygons with no 2-strings is at most 0.446287. So

$$\limsup_{n\to\infty} \frac{1}{n} \log u_{\mathbb{T},n}(0) \leq 0.446287 < \kappa_{\mathbb{T},0}.$$

But we need something stronger:

Theorem (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

There exists $\epsilon^* > 0$ such that

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

On the other hand, we can construct a transfer matrix for all polygons (not just unknots) which excludes 2-strings. Bounds on the dominant eigenvalue can be calculated, which show that the growth rate for polygons with no 2-strings is at most 0.446287. So

$$\limsup_{n\to\infty} \frac{1}{n} \log u_{\mathbb{T},n}(0) \leq 0.446287 < \kappa_{\mathbb{T},0}.$$

But we need something stronger:

Theorem (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

There exists $\epsilon^* > 0$ such that

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

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.

If $\epsilon < 1/4$ then

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

If $\epsilon < 1/4$ then

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

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

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

which is less than $\kappa_{\mathbb{T},0}$ for sufficiently small ϵ, and hence ϵ^* exists.

If $\epsilon < 1/4$ then

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

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

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

which is less than $\kappa_{\mathbb{T},0}$ for sufficiently small ϵ, and hence ϵ^* exists.

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 $K = K_1\#\ldots\#K_p$ in at least $\binom{\epsilon^* n}{p} = O(n^p)$ ways.

If $\epsilon < 1/4$ then

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

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

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

which is less than $\kappa_{\mathbb{T},0}$ for sufficiently small ϵ, and hence ϵ^* exists.

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 $K = K_1\#\ldots\#K_p$ in at least $\binom{\epsilon^* n}{p} = O(n^p)$ ways. So for sufficiently large n there exist numbers $a(K), b(K), c(K), d(K)$ such that

$$c(K)n^p u_{\mathbb{T},n-d(K)} \leq p_{\mathbb{T},n}(K) \leq a(K)n^p u_{\mathbb{T},n+b(K)}$$

and (1) follows.

If $\epsilon < 1/4$ then

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

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

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

which is less than $\kappa_{\mathbb{T},0}$ for sufficiently small ϵ, and hence ϵ^* exists.

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 $K = K_1\#\ldots\#K_p$ in at least $\binom{\epsilon^* n}{p} = O(n^p)$ ways. So for sufficiently large n there exist numbers $a(K), b(K), c(K), d(K)$ such that

$$c(K)n^p u_{\mathbb{T},n-d(K)} \leq p_{\mathbb{T},n}(K) \leq a(K)n^p u_{\mathbb{T},n+b(K)}$$

and (1) follows.

Theorem (Atapour, NRB, Eng, Ishihara, Shimokawa, Soteros & Vazquez 2017)

If $K = K_1\#\ldots\#K_p$ with all K_p being 2-bridge knots with unknotting number 1, then in the 2×1 tube $\mathbb{T}$,

$$\frac{p_{\mathbb{T},n}(K)}{u_{\mathbb{T},n}} \sim \mathit{const.} \times n^p.$$

Beyond the 2×1 tube?

The enumeration argument used to show the density of 2-strings works the 3×1 tube too, but have to enumerate unknots to length 28. For larger tubes, would have to go further $\Rightarrow$ infeasible at present.

The "untwisting" algorithm has not been developed beyond the 2×1 tube, but it may work in some cases.

Random sampling

Transfer matrices cannot be used to estimate $\kappa_{\mathbb{T},0}$ directly, and counting polygons of a given knot type quickly becomes infeasible.

Random sampling

Transfer matrices cannot be used to estimate $\kappa_{\mathbb{T},0}$ directly, and counting polygons of a given knot type quickly becomes infeasible.

So instead we will try to use Monte Carlo methods.

Random sampling

Transfer matrices cannot be used to estimate $\kappa_{\mathbb{T},0}$ directly, and counting polygons of a given knot type quickly becomes infeasible.

So instead we will try to use Monte Carlo methods. The transfer matrices can be used to generate uniformly random polygons of a given span or length, built up one 1-block at a time.

Roughly, the idea (adapted from [Alm & Janson 1990]) is that the correct transition probability from 1-block i to 1-block j is

$$e^f z_c^{|j|} \frac{\xi_j(z_c)}{\xi_i(z_c)},$$

where $|j|$ is the number of edges in j, $z_c = e^{-\kappa_{\mathbb{T}}}$, and $\xi(z_c)$ is the corresponding right eigenvector.

(Some other stuff has to happen at the leftmost and rightmost blocks.)

Some results

Knots turn out to be exceedingly rare in the 2×1 tube $\Rightarrow$ focus on the 3×1 tube.

Some results

Knots turn out to be exceedingly rare in the 2×1 tube $\Rightarrow$ focus on the 3×1 tube.

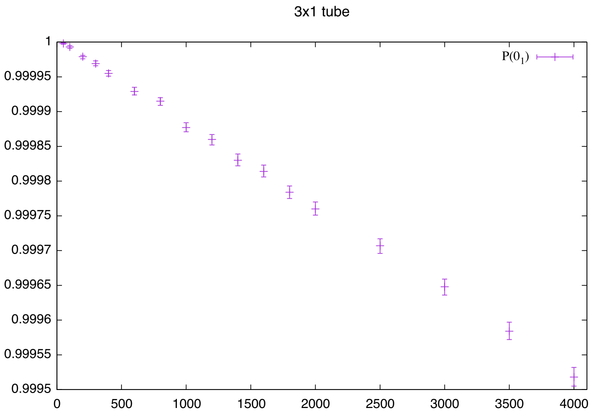


Figure: Probably of unknot in the 3×1 tube.

Some results

Knots turn out to be exceedingly rare in the 2×1 tube $\Rightarrow$ focus on the 3×1 tube.

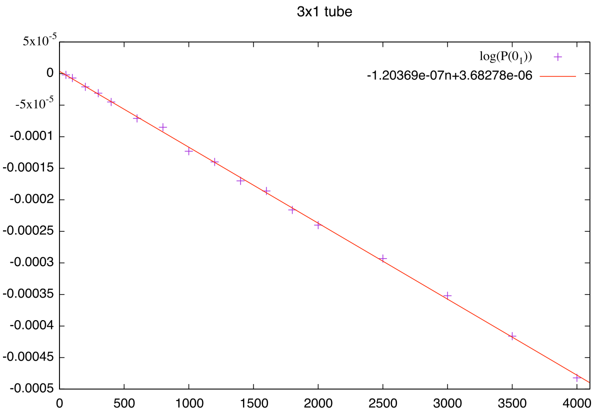


Figure: Straight line fit to $\log(\cdot)$.

Some results

Knots turn out to be exceedingly rare in the 2×1 tube $\Rightarrow$ focus on the 3×1 tube.

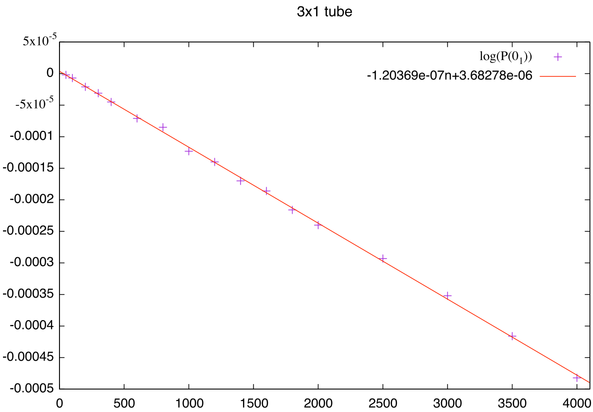


Figure: Straight line fit to $\log(\cdot)$.

So $\kappa_{\mathbb{T},0} \approx \kappa_{\mathbb{T}} - 1.204 \times 10^{-7}$. In $\mathbb{Z}^3$ the difference has been estimated to be $\approx 4.15 \times 10^{-6}$ [Whittington & Janse van Rensburg 1992].

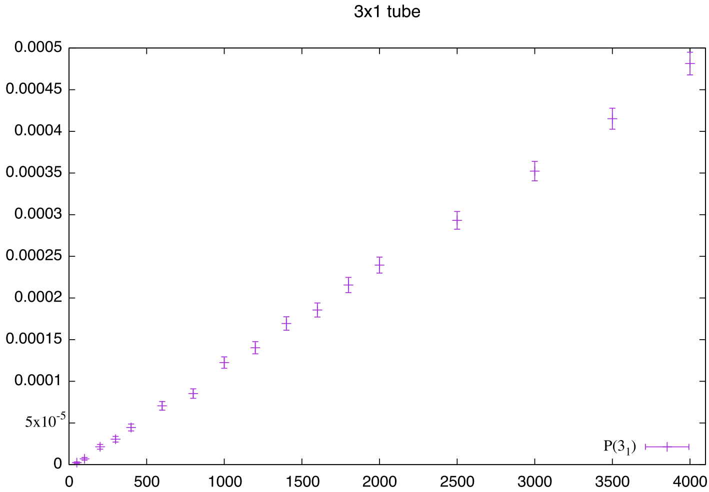


Figure: Probably of trefoil in the 3×1 tube.

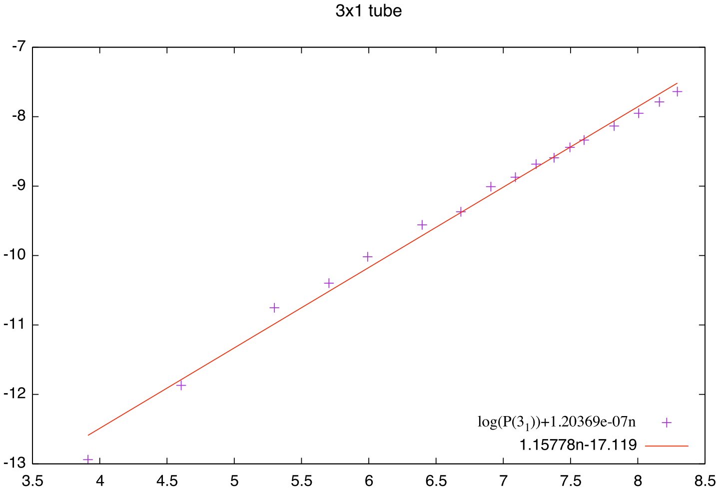


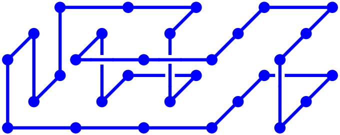
Figure: Straight line fit to log-log plot $+1.204 \times 10^{-7} n$.

Hamiltonian polygons

Knots in 3×1 are still very very rare!

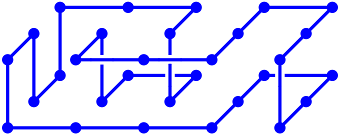
Hamiltonian polygons

Knots in 3×1 are still very very rare! We see a lot more knots if we instead only focus on Hamiltonian polygons: polygons which visit every box in an $L \times M \times S$ box.



Hamiltonian polygons

Knots in 3×1 are still very very rare! We see a lot more knots if we instead only focus on Hamiltonian polygons: polygons which visit every box in an $L \times M \times S$ box.



All of the theorems proved so far work for these too (in fact some are easier).

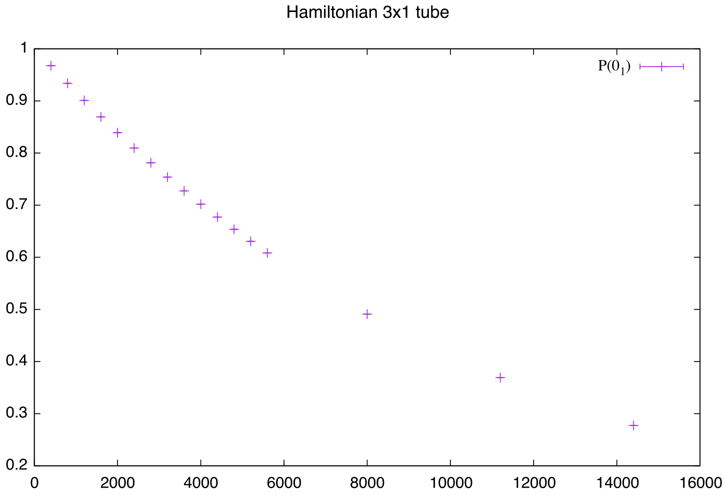


Figure: Probably of Hamiltonian unknot in the 3×1 tube.

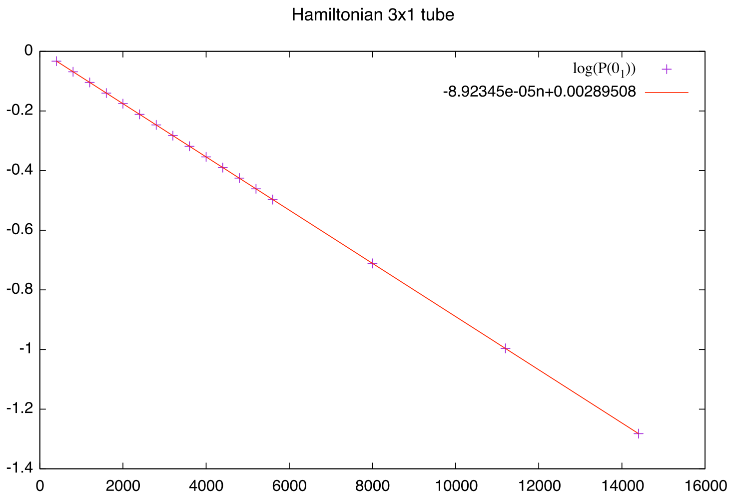


Figure: Straight line fit to $\log(\cdot)$.

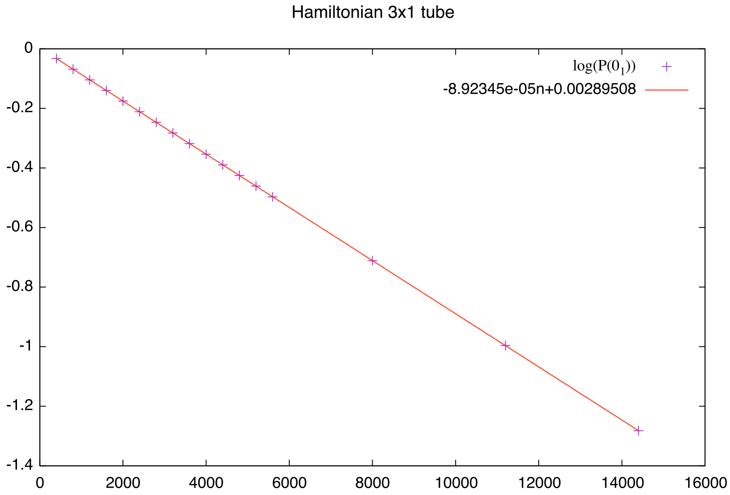


Figure: Straight line fit to $\log(\cdot)$.

So here $\kappa^{\mathsf{H}}_{\mathbb{T},0} \approx \kappa^{\mathsf{H}}_{\mathbb{T}} - 8.923 \times 10^{-5}$.

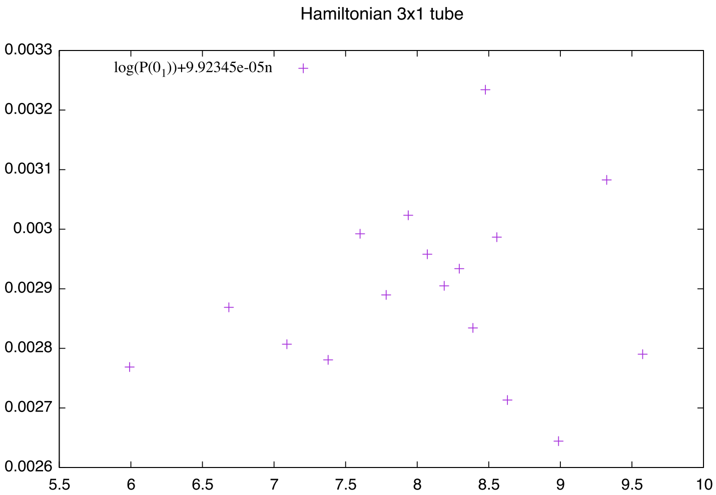


Figure: log-log plot $+8.923 \times 10^{-5} n$.

So here $\kappa^{\mathrm{H}}_{\mathbb{T},0} \approx \kappa^{\mathrm{H}}_{\mathbb{T}} - 8.923 \times 10^{-5}$. Taking a log-log plot and subtracting the exponential term just gives noise, suggesting that $\gamma_0 = 0$ in $\mathbb{T}$.

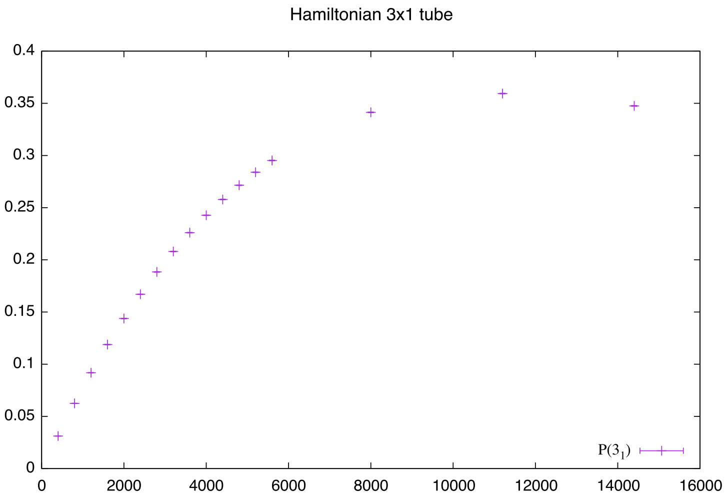


Figure: Probably of trefoil in the 3×1 tube.

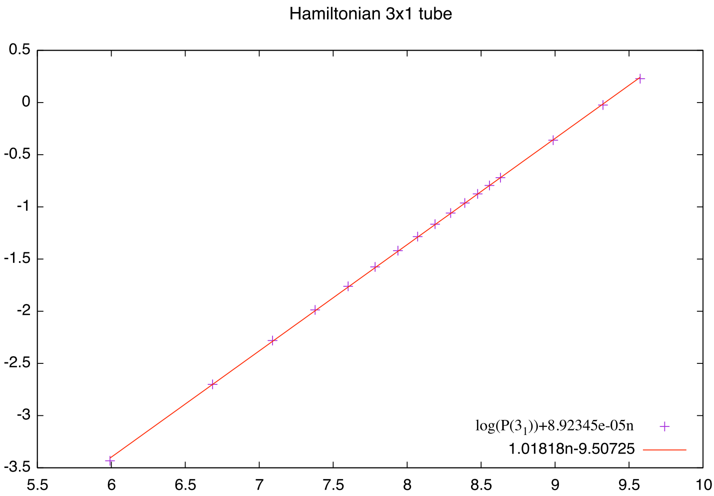


Figure: Straight line fit to log-log plot $+8.923 \times 10^{-5} n$.

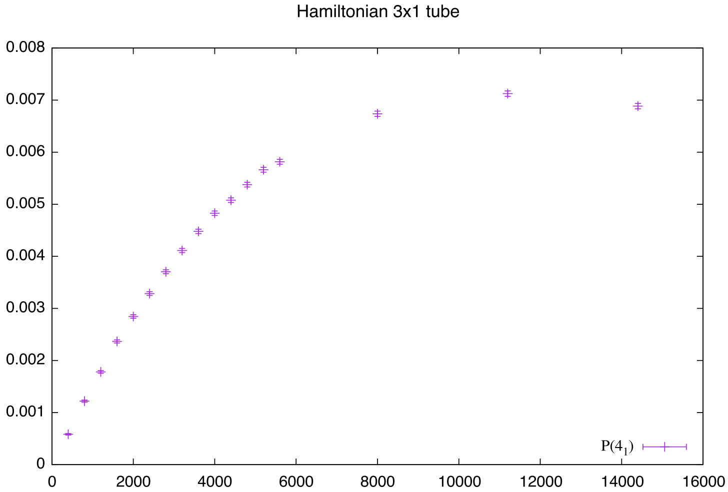


Figure: Probably of figure-eight in the 3×1 tube.

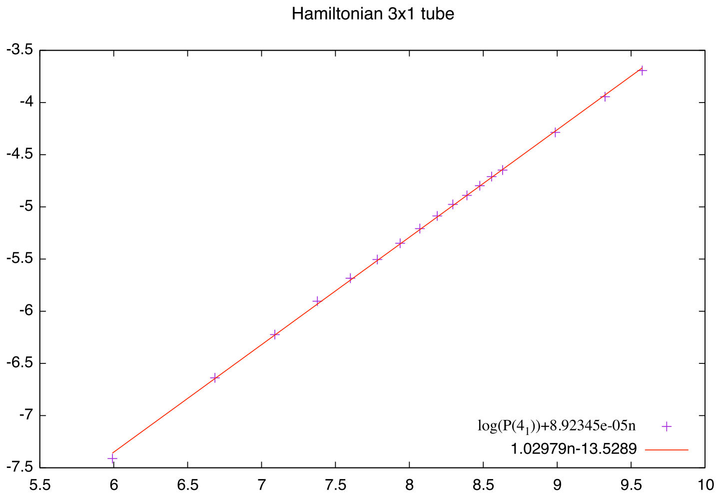


Figure: Straight line fit to log-log plot $+8.923 \times 10^{-5} n$.

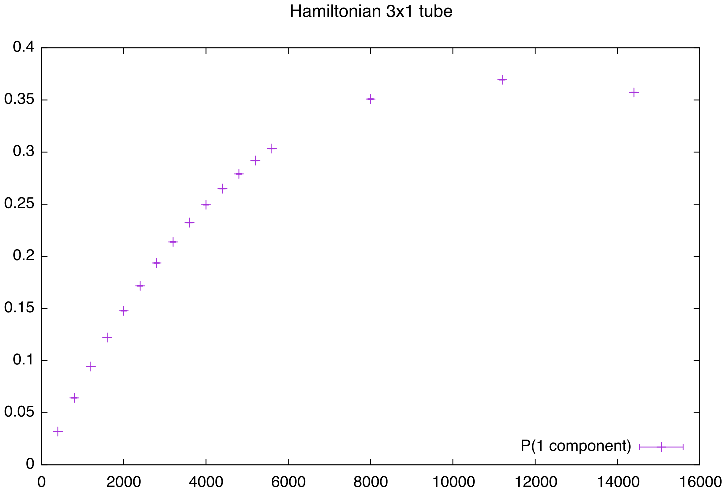


Figure: Probably of single-component knot in the 3×1 tube.

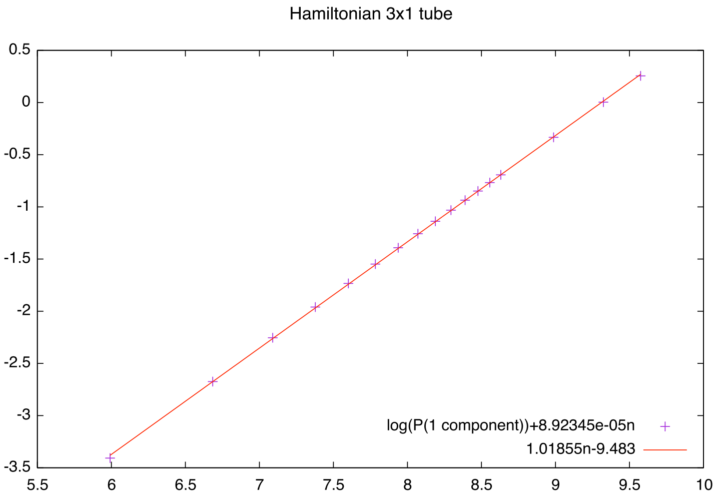


Figure: Straight line fit to log-log plot $+8.923 \times 10^{-5} n$.

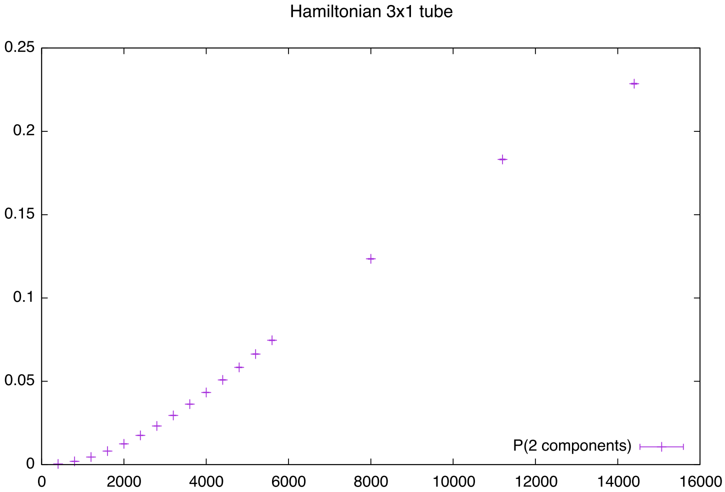


Figure: Probably of two-component knot in the 3×1 tube.

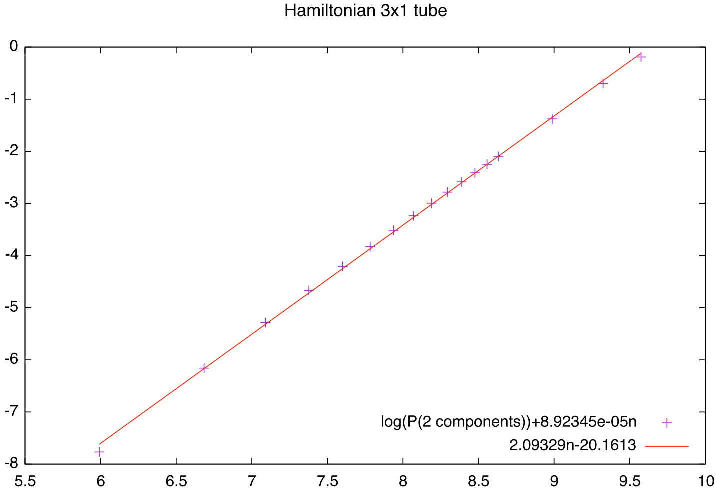


Figure: Straight line fit to log-log plot $+8.923 \times 10^{-5} n$.

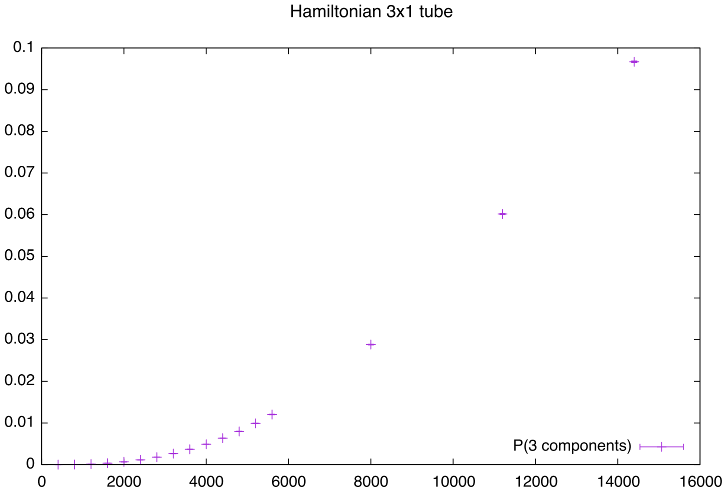


Figure: Probably of three-component knot in the 3×1 tube.

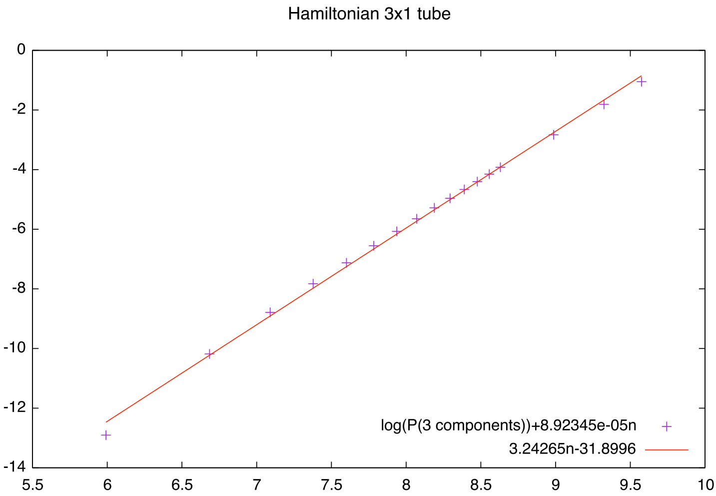


Figure: Straight line fit to log-log plot $+8.923 \times 10^{-5} n$.

Ongoing & future work

Investigate:

- how knotting probability behaves for larger tube sizes
- how large knot components tend to be
- whether knot components are "local" (occupy a small part along the chain) or "global"
- incorporate stretching & compressing forces; nearest-neighbour interactions; writhe
- In cases where the transfer matrix is too big to be used, develop new method (Markov chain?) for sampling Hamiltonian polygons

NRB, J. Eng & C. Soteros, Polygons in restricted geometries subjected to infinite forces. *Journal of Physics A* **49** (2016), 424002.

NRB, J. Eng & C. Soteros, Characterizing knotting properties of polymers in nanochannels, in preparation.

M. Atapour, NRB, J. Eng, K. Ishihara, K. Shimokawa, C. Soteros & M. Vazquez, Unknotting operations on 4-plat diagrams and the entanglement statistics of polygons in a lattice tube, in preparation.

NRB, J. Eng & C. Soteros, Polygons in restricted geometries subjected to infinite forces. *Journal of Physics A* **49** (2016), 424002.

NRB, J. Eng & C. Soteros, Characterizing knotting properties of polymers in nanochannels, in preparation.

M. Atapour, NRB, J. Eng, K. Ishihara, K. Shimokawa, C. Soteros & M. Vazquez, Unknotting operations on 4-plat diagrams and the entanglement statistics of polygons in a lattice tube, in preparation.

Thank you!