Entanglements in lattice polygons in tubes

Chris Soteros
University of Saskatchewan

I acknowledge that I live and work on Treaty 6 Territory and the Homeland of the Métis. I pay my respects to the First Nations and Métis ancestors of this place and reaffirm our relationship with one another.

A Tour of Combinatorics and Statistical Mechanics: In Memory of Richard Brak, February 7, 2022

Thanks to the organizers of the conference!

Nathan Clisby, Tim Garoni, Tony Guttmann, Aleks Owczarek

Collaborators: Nick Beaton (Melbourne); Jeremy Eng (SaskPoly) ; Kai Ishihara (Yamaguchi); Puttipong Pongtanapaisan (USask); Matthew Schmirler (USask); Koya Shimokawa (Saitama); Mariel Vazquez (Davis); Rob Scharein (Hypnagogic Software)

Student assistants: Jayda Jessee, Eithne Arsuaga-Vazquez, Mathew Zbitniff

Supporting Agencies: NSERC, PIMS, Compute Canada

Remembering Richard Brak …

- Met at conferences in North America early 90's via Stu Whittington – "Critical Phenomena in Polymer Physics" (Peterborough)
- Friendly Informal Workshop on Monte Carlo Simulation and Related Topics. June 20-24, 1994 Saskatoon
- Hosted me during first sabbatical 1995 Sept-Dec Melbourne

Inspired me to pursue "solvable" problems

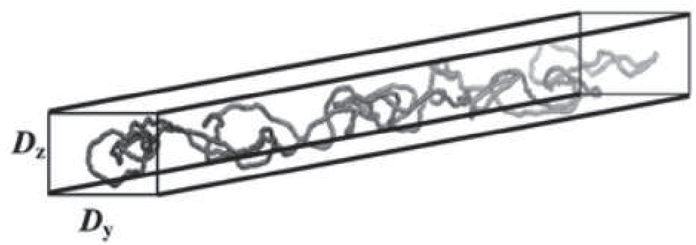
Learned about the beauty of Australia and saw koalas in the wild with Richard's family and Mireille

On anisotropic spiral self-avoiding walks, R Brak, A L Owczarek and C E Soteros 1998 J. Phys. A: Math. Gen. 31 4851

- During same sabbatical learned about Alm and Janson transfer-matrix results for SAWs in lattice tubes … led to my talk today

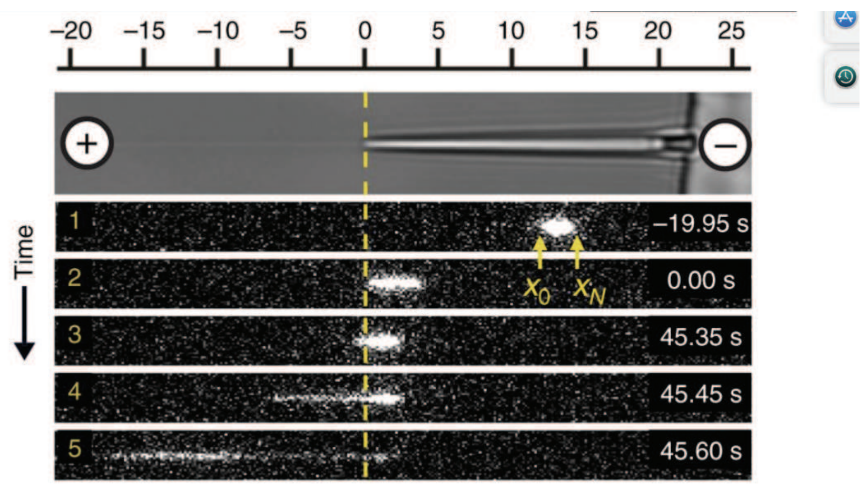
Richard provided great support to me and my career over the decades. From invitations to and discussions/talks at conferences as well as providing advice and listening to me gripe about academic politics.

DNA in Nano-channels and Nano-pores



Snapshot of a ring confined in a rectangular channel.

Z Benková, P Námera and P Cifraa (Soft Matter, 2016, 12, 8425), moleclular dynamics



J Zhou, et al (Nature Comm., 8, 807 (2017)), λ-phage DNA electrokinetically driven into nanochannel; fluorescence images of DNA stained with an intercalating dye.

The DNA (non-equilibrium) experiments point to Open Questions about the "characteristics" of knots and links at equilibrium in nanopore/nanochannel confinement:

- What is the typical "size" of the knotted/linked part relative to the length of the polymer?

  Leads to mathematical questions:

  How does one measure knot or link "size"?

  Are the knots/links "localized" and to what extent?

  For knot size m in a length n polymer, if $\frac{m}{n} \to 0$ as $n \to \infty$, knot is "localized".

  If as $n \to \infty$, $m \sim c$, "strongly localized", while if $m \sim cn^t$, $0 < t < 1$, knot is "weakly localized".

- Can one distinguish between different "modes" of knotting/linking and are some modes more probable than others?

  Leads to mathematical questions such as how to detect or define different geometrical configurations of knots/links.

We have been using lattice polygon models confined to tubular sublattices of the simple cubic lattice and transfer-matrix methods to address these questions both rigorously and via Monte Carlo simulations.

Simplest Case: Each SAP of size n (number of edges) is considered equally likely.

p_n - # of distinct (up to translation) n-edge SAPs in $\mathbb{Z}^3$

$p_n(\phi)$ - # of distinct (up to translation) n-edge UNKNOTTED SAPs in $\mathbb{Z}^3$ – $p_n(0_1)$

$p_n(K)$ - # of distinct (up to translation) n-edge knot type K SAPs in $\mathbb{Z}^3$

As $n \to \infty$ Sumners and Whittington (1988) (JPA **21**, 1689–94) $\Rightarrow$

$$Prob.\ of\ Knotting = 1 - \frac{p_n(\phi)}{p_n} = 1 - e^{-(\kappa - \kappa_o)n + o(n)}$$

Soteros, Sumners and Whittington (1992) (MathProcCambPhilSoc **111** 75) $\Rightarrow$

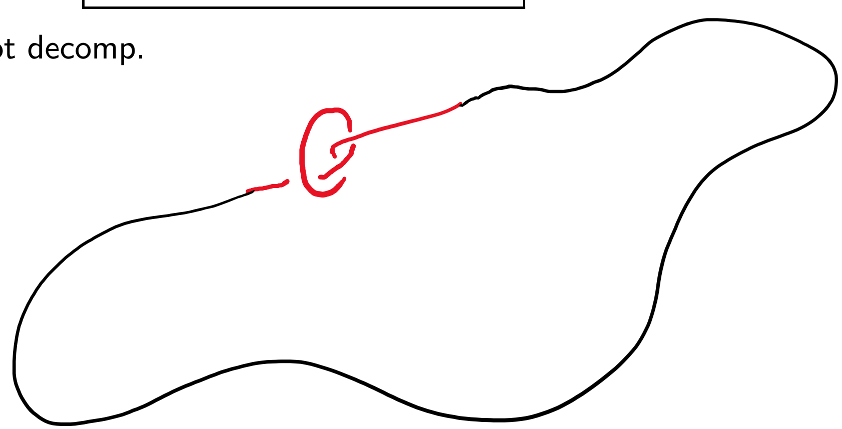
$$Prob.\ of\ Knot\text{-}type\ K = \frac{p_n(K)}{p_n} \to 0$$

Orlandini *et al* (1998) (IMA Vol.Math.Appl. **103** 9; JPA **31** 5953) Monte Carlo evidence consistent with

$$p_n(K) \sim A_K n^{\theta_o + f_K} e^{\kappa_o n}$$

f_K - # prime knots in K's knot decomp.

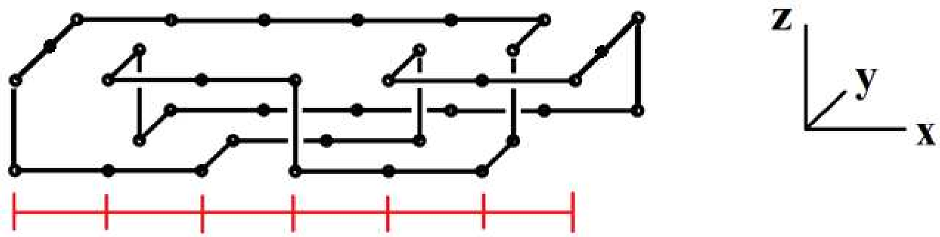
$\binom{n}{1} p_n(0_1)$



A Bonato, E Orlandini, SG Whittington, Asymptotics of multicomponent linked polygons. J. Phys. A: Math. Theor. 54, 235002 (2021).

Modelling Equilibrium Properties: Polygons in tubes and confined polymers

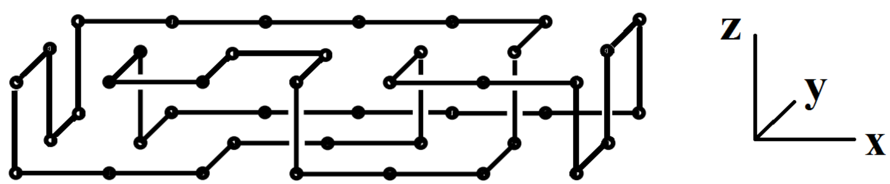
$\mathbb{T}_{L,M} \equiv \mathbb{T} = \{(x, y, z) : 0 \le y \le L, 0 \le z \le M\} = \mathbb{Z} \times \{0, ..., L\} \times \{0, ..., M\}$



A SAP with span $s = 6$

Polygons represent polymer configurations and in simplest model assume each polygon of the same "size" is equally likely.

For size=span, probability $= \dfrac{1}{p_{\mathbb{T}}(s)}$, $\boldsymbol{p}_{\mathbb{T}}(\boldsymbol{s})$: # of span $\boldsymbol{s}$ SAPs in $(\boldsymbol{L}, \boldsymbol{M})$-tube



Hamiltonian Polygons: densely packed proteins (Kloczkowski and Jernigan 1998 JCP 109 p5134;p5147)

August 24, 2020

Applying Transfer Matrices to SAPs in Tubes.

- The main tool used to study SAPs and 2SAPs was transfer matrices.
- SAPs and 2SAPs in an $L \times M$ tube can be viewed as a sequence of connected “1-patterns” that “grow” in the $+x$-direction.
- This allows for the use of *transfer matrices*.

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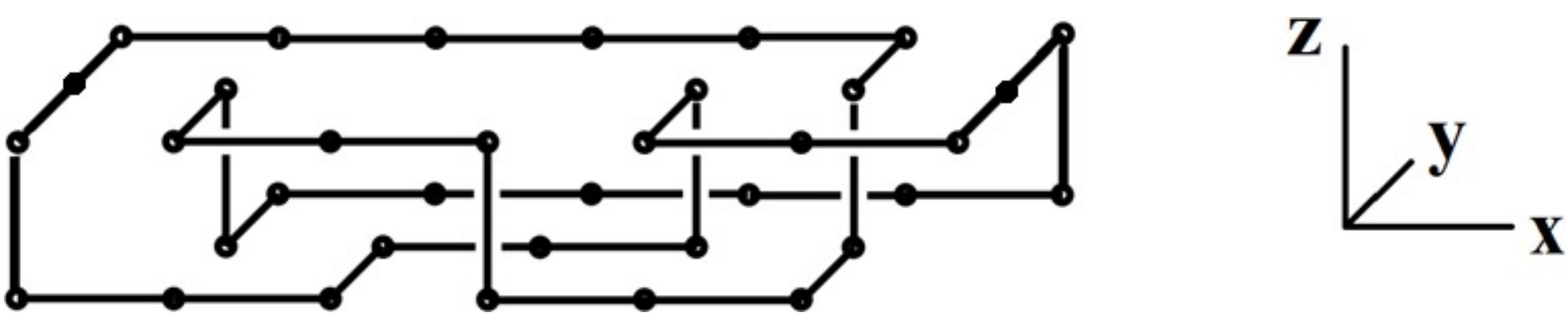

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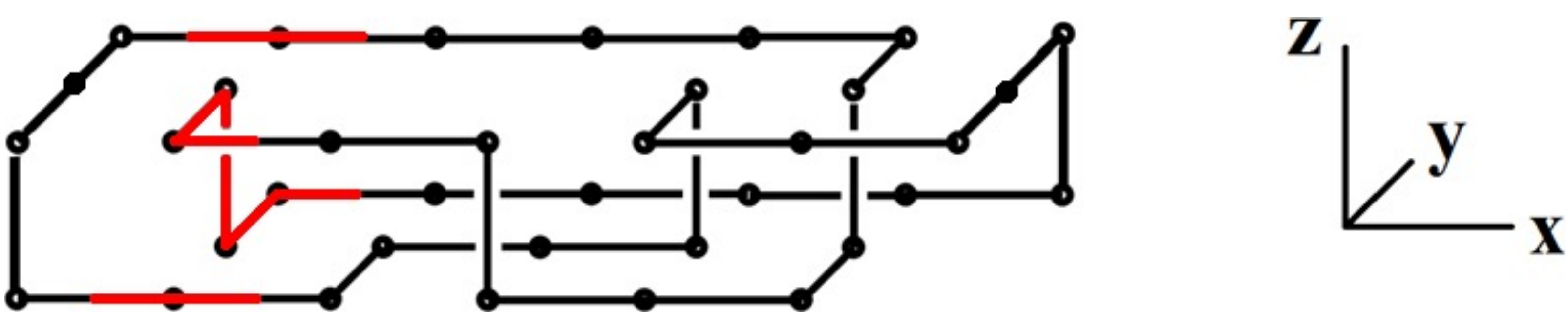

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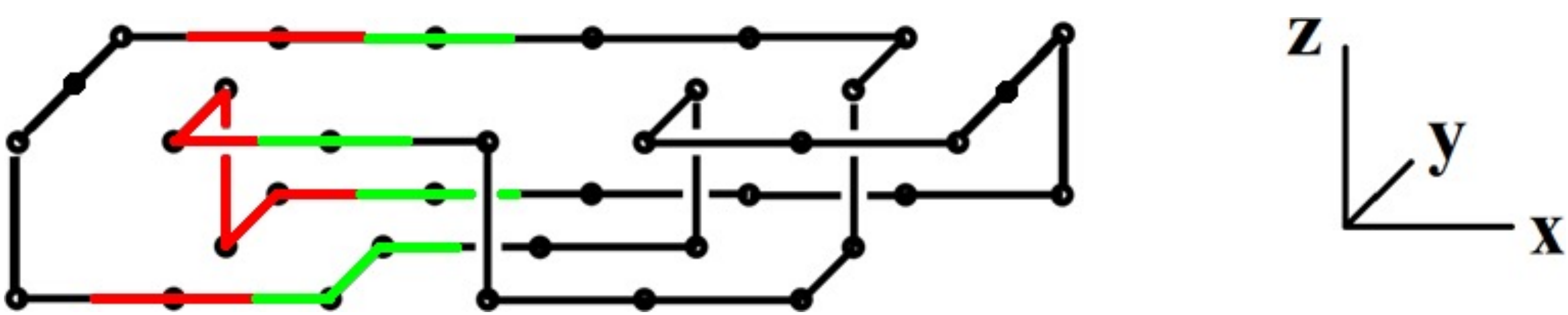

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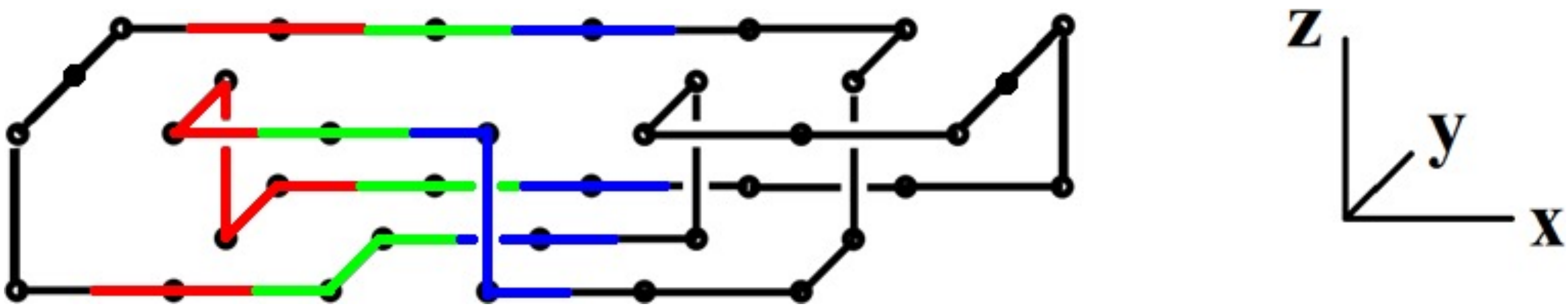

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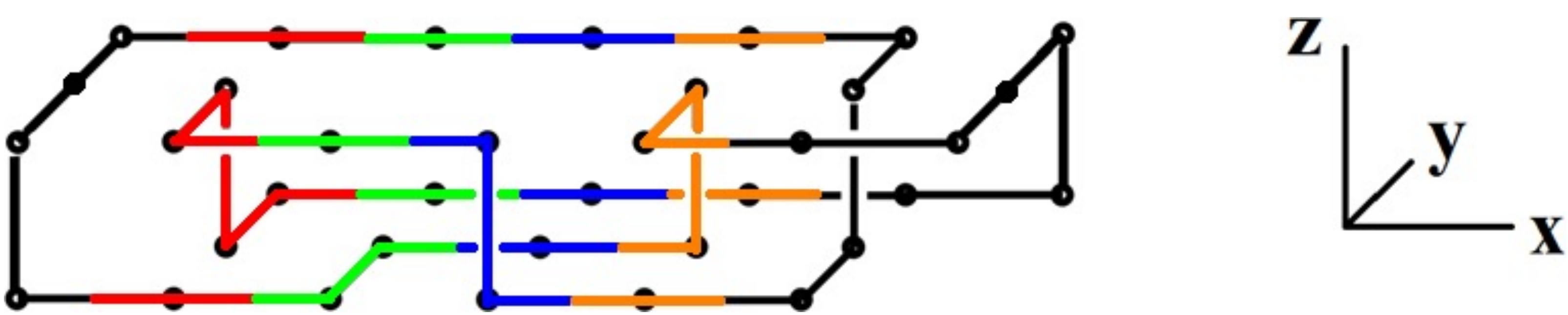

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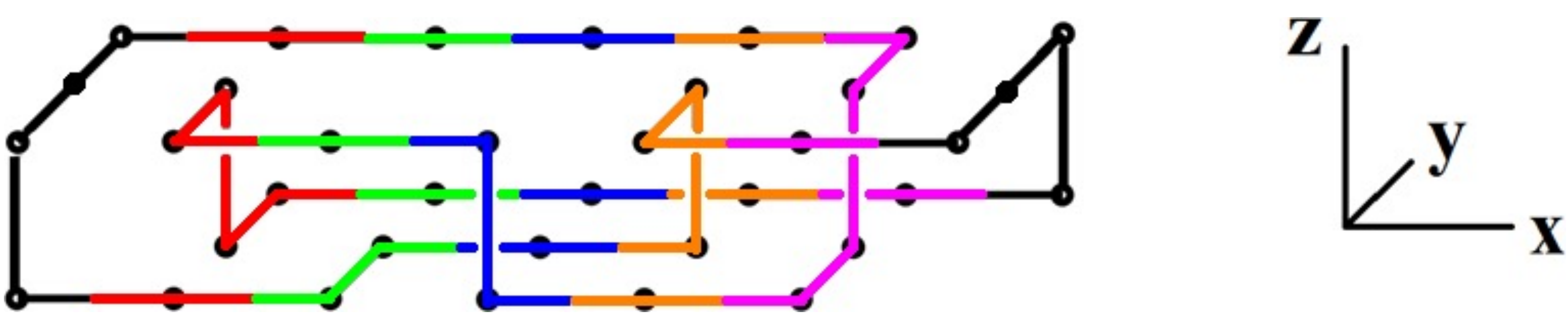

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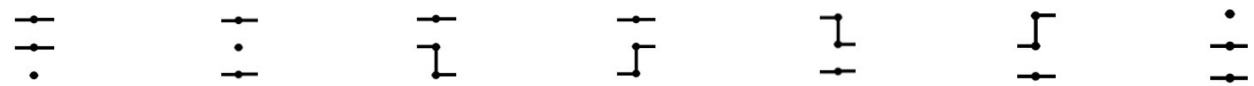
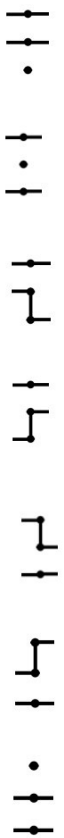
Transfer Matrix Example



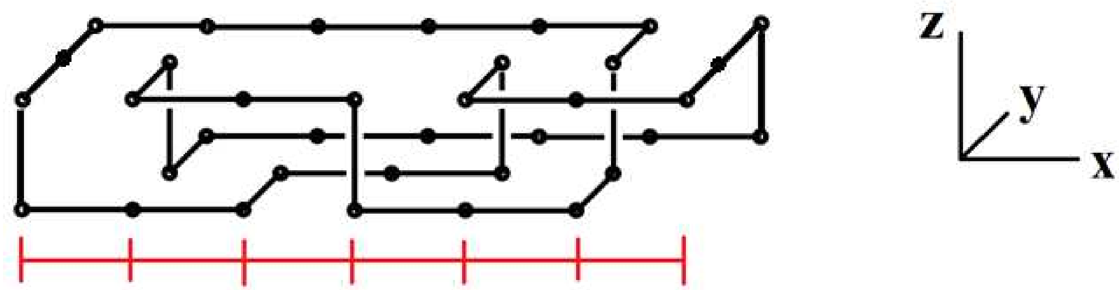


$$
\begin{bmatrix}
x^2 & 0 & x^2 & 0 & 0 & 0 & 0 \\
0 & x^2 & 0 & x^2 & x^2 & 0 & 0 \\
0 & x^3 & 0 & x^3 & x^3 & 0 & 0 \\
x^3 & 0 & x^3 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & x^3 & x^3 \\
0 & x^3 & 0 & x^3 & x^3 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & x^2 & x^2
\end{bmatrix}
$$

Figure: The 2×0 tube transfer matrix

Modelling Equilibrium Properties: Polygons in tubes and confined polymers

$$\mathbb{T}_{L,M} \equiv \mathbb{T} = \{(x,y,z) : 0 \le y \le L, 0 \le z \le M\} = \mathbb{Z} \times \{0,\ldots,L\} \times \{0,\ldots,M\}$$



A SAP with span $s = 6$

Grand Canonical Partition Function for polygons in (L, M)-Tube

$$H(x,y) = \sum_n \sum_s p_{\mathbb{T},n}(s) x^n y^s = \sum_n \sum_s p_{\mathbb{T},n}(s) e^{gn} e^{fs} =$$

$$\boxed{\sum_i \sum_j \left[B(x)\left(I + yG(x) + y^2G^2(x) + y^3G^3(x) + \ldots\right) C(x)\right]_{i,j} \propto \frac{1}{\det(I - yG(x))}}$$

$\boldsymbol{p_{\mathbb{T},n}(s)}$: # of n-edge, span s polygons in (L, M)-tube

$\boldsymbol{G(x)}$: Transfer-Matrix

Two possible models depending on what is used for polygon "size" - edges n or span s

Table A.1 The approximate amount of resources required to create the transfer matrices for SAPs in each of the above cases. Cases larger than the 2×2 tube were run on Compute Canada's Graham and Cedar clusters. The amount of time required for generating each set of sampled SAPs at different spans is also available upon request.

Type	Tube	CPU Time (dd:hh:mm)	RAM
SAP	2x1	00:00:02	<1 GB
SAP	3x1	00:00:11	<1 GB
SAP	2x2	00:00:24	<1 GB
SAP	4x1	00:04:00	5 GB
SAP	5x1	05:22:52	350 GB
SAP	3x2	06:21:35	400 GB
Ham. SAP	2x1	00:00:02	<1 GB
Ham. SAP	3x1	00:00:05	<1 GB
Ham. SAP	2x2	00:00:07	<1 GB
Ham. SAP	4x1	00:01:00	2 GB
Ham. SAP	5x1	02:01:13	110 GB
Ham. SAP	3x2	02:06:30	150 GB

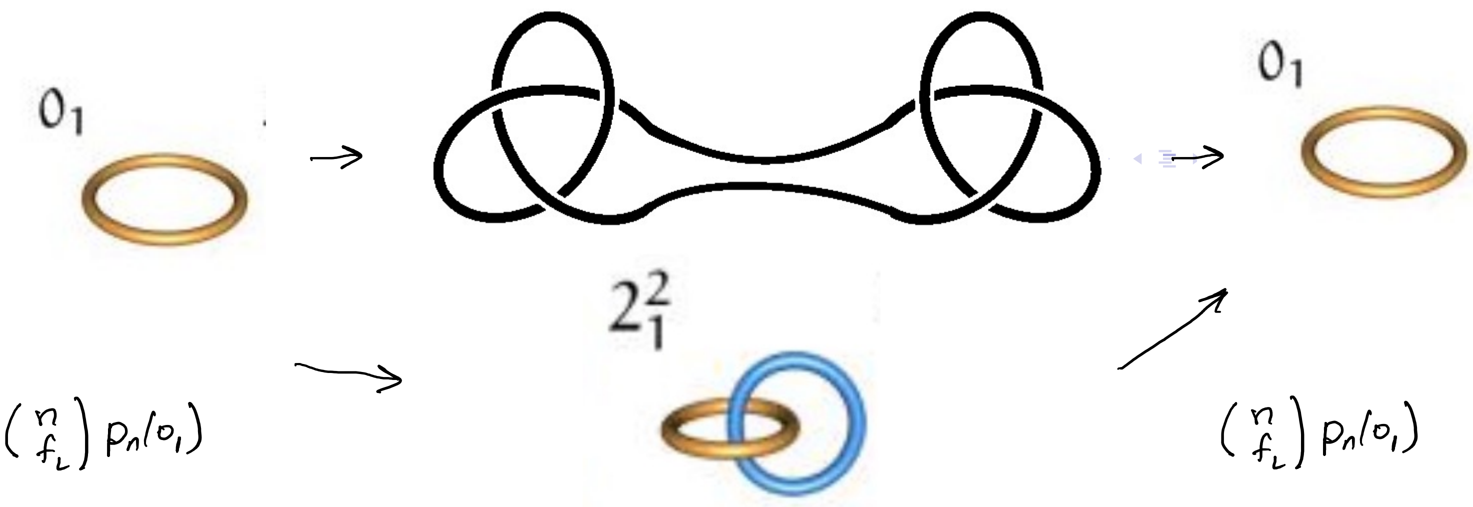
Jeremy Eng PhD Thesis 2020 https://harvest.usask.ca/handle/10388/13022

<u>New Result for 2 x 1 Tube:</u> (M Atapour (CapilanoU), NR Beaton (UMelbourne), JW Eng (USaskatchewan), K Ishihara (YamaguchiU), K Shimokawa (SaitamaU), CE Soteros (USaskatchewan), M Vazquez (UCDavis)) Let L be any non-split link embeddable in $\mathbb{T}^*$ and let $p_{\mathbb{T}^*,m}(L)$ be the number of m-edge embeddings in $\mathbb{T}^*$ with link type L. Then, for non-trivial L there exist positive constants $\epsilon \in (0,1)$, $b_L \in \mathbb{R}$, $d_L \in \mathbb{Z}$, $e_L \in \mathbb{Z}$ (independent of n) and an integer $N_{L,\epsilon} > 0$ such that for any $n \geq N_{L,\epsilon}$, we have lower and upper bounds on the number of n-edge embeddings of L in $\mathbb{T}^*$ as follows:

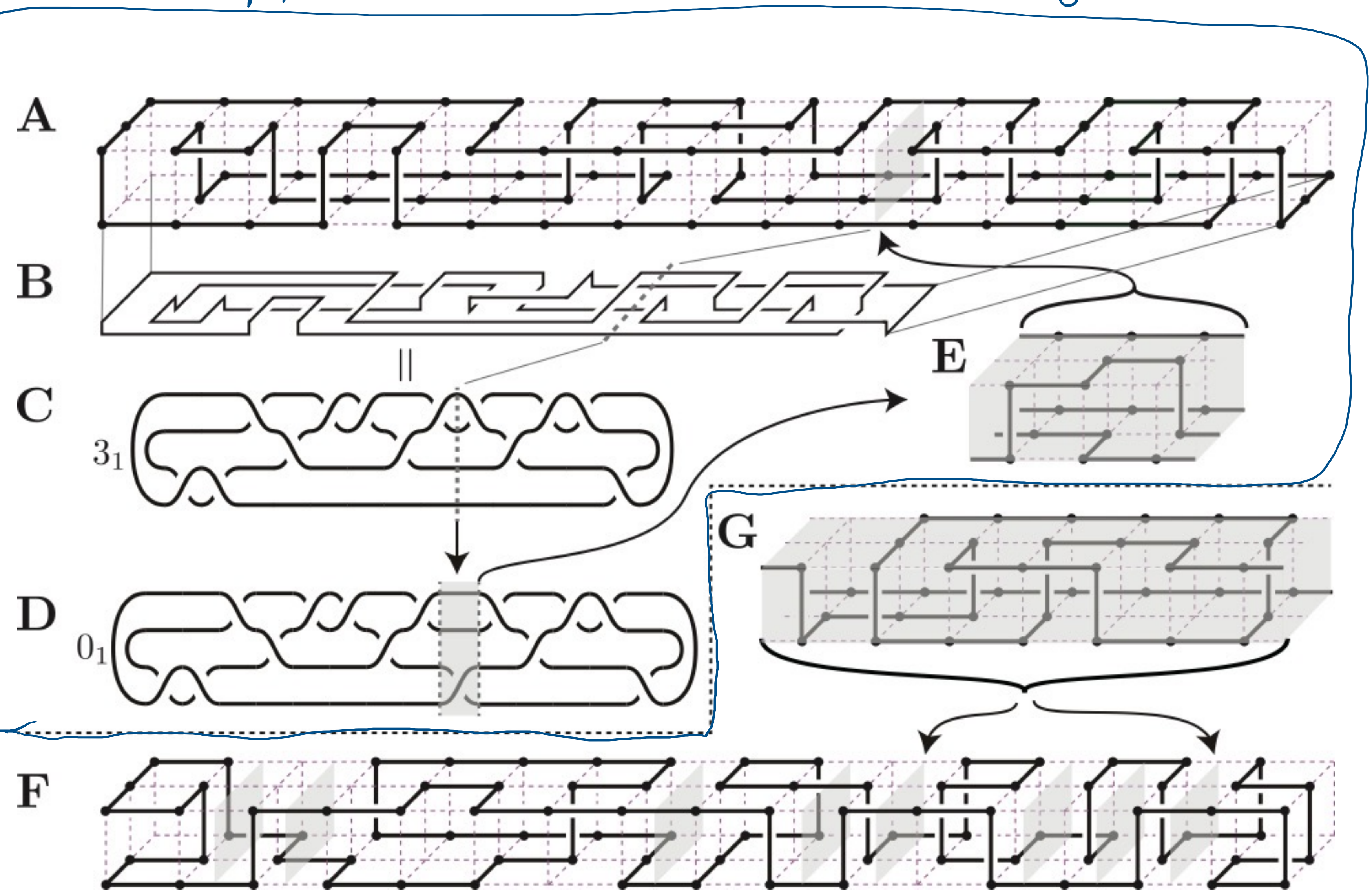
$$\begin{aligned} \frac{1}{2}\binom{\lfloor \epsilon(n-e_L)\rfloor}{f_L} p_{\mathbb{T}^*,n-e_L}(0_1) &\leq p_{\mathbb{T}^*,n}(L) \\ &\leq b_L \binom{n}{f_L} p_{\mathbb{T}^*,n+d_L}(0_1). \end{aligned} \tag{1}$$

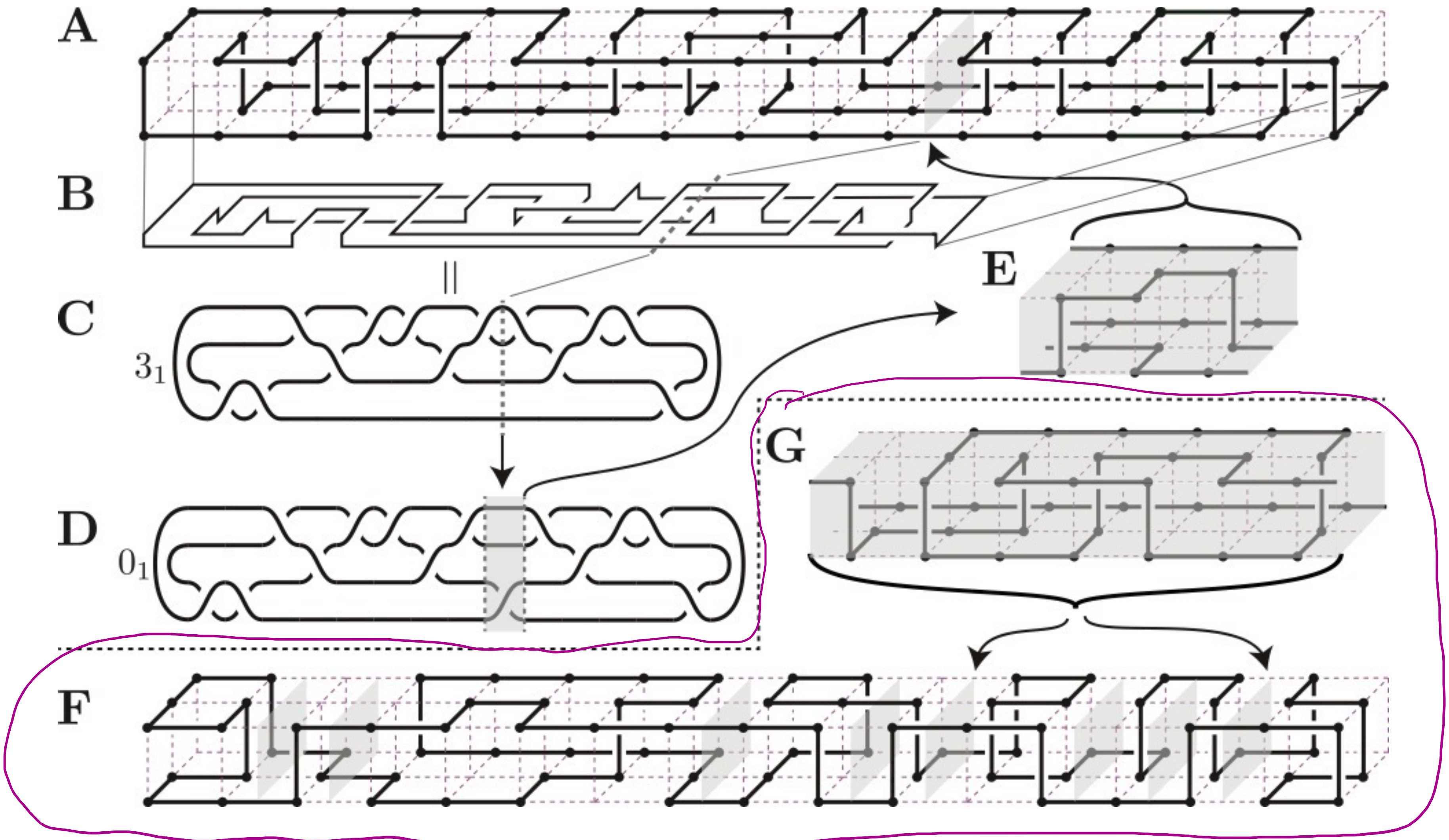
Furthermore, there exist constants C_1 and C_2 such that for all sufficiently large n

$$C_1 n^{f_L} p_{\mathbb{T}^*,n}(0_1) \leq p_{\mathbb{T}^*,n}(L) \leq C_2 n^{f_L} p_{\mathbb{T}^*,n}(0_1). \tag{2}$$



Upper Bound – New Knot Theory





LOWER BOUND - NEW PATTERN THEOREM

- New Knot Theory – a 4-braid word can be determined from a minimal diagram of the link that can be used to unknot any diagram of the link upon insertion of the word – a type of unknotting operation
- New Pattern Theorem for Unknots – use exact counts of unknot polygons and calculated bounds from the transfer matrix to proved that all but exponentially few sufficiently long unknot polygons contain a positive density of “2-sections” – from this can prove a general pattern theorem for unknot polygons

Pattern Theorems for unknots and fixed link-type 2×1 Tube:

Let $p_{\mathbb{T}^*,n}(0_1, \leq k)$ be the number of unknots of length n in $\mathbb{T}^*$ which contain at most k 2-sections. Then there exists an $\epsilon > 0$ such that

$$\limsup_{n\to\infty} \frac{1}{n} \log p_{\mathbb{T}^*,n}(0_1, \leq \epsilon n) < \lim_{n\to\infty} \frac{1}{n} \log p_{\mathbb{T}^*,n}(0_1) \equiv \kappa_{\mathbb{T}^*,0_1}.$$

Proof:

Delete all patterns corresponding to 2-sections from transfer matrix, standard upper bound for the spectral radius of a matrix, $\tau_M \leq \|M^k\|^{1/k}$ for any $k \geq 1$, where $\|\cdot\|$ is the maximum absolute row sum $\implies$

$$\limsup_{n\to\infty} \frac{1}{n} \log p_{\mathbb{T}^*,n}(0_1, 0) = \hat{\kappa}_{\mathbb{T}^*}(0_1) \leq \lim_{n\to\infty} \frac{1}{n} \log p_{\mathbb{T}^*,n}(0) = \hat{\kappa}_{\mathbb{T}^*} < 0.446287.$$

Concatenation $\implies$ $\log p_{\mathbb{T}^*,n-6}(0_1)$ *superadditive* $\implies$

$$\kappa_{\mathbb{T}^*}(0_1) = \lim_{n\to\infty} \frac{1}{n} \log p_{\mathbb{T}^*,n-6}(0_1) = \sup_{n\geq 0} \frac{1}{n} \log p_{\mathbb{T}^*,n-6}(0_1).$$

Exact enumeration $p_{\mathbb{T}^*,24}(0_1) = 119,796,593$

$$\hat{\kappa}_{\mathbb{T}^*}(0_1) \leq \hat{\kappa}_{\mathbb{T}^*} < 0.446287 < 0.620044 \leq \kappa_{\mathbb{T}^*}(0_1) \tag{3}$$

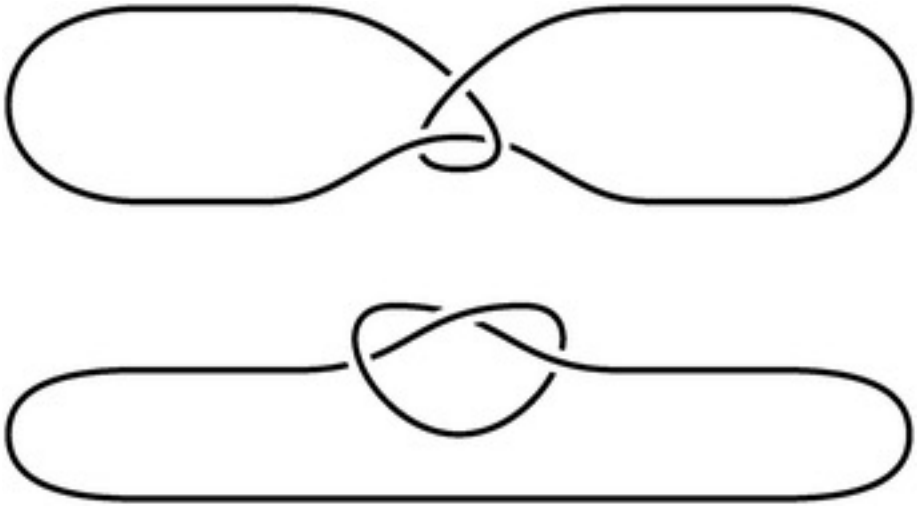
$\implies$ Unknots without 2-sections are exponentially rare amongst unknot polygons.

$$p_{\mathbb{T}^*,n}(0_1, \leq k) = \sum_{t=0}^{k} p_{\mathbb{T}^*,n}(0_1, t) \leq \sum_{t=0}^{k} 2^t \binom{\frac{n}{2}}{t} p_{\mathbb{T}^*,n+Et}(0_1, 0) \tag{4}$$

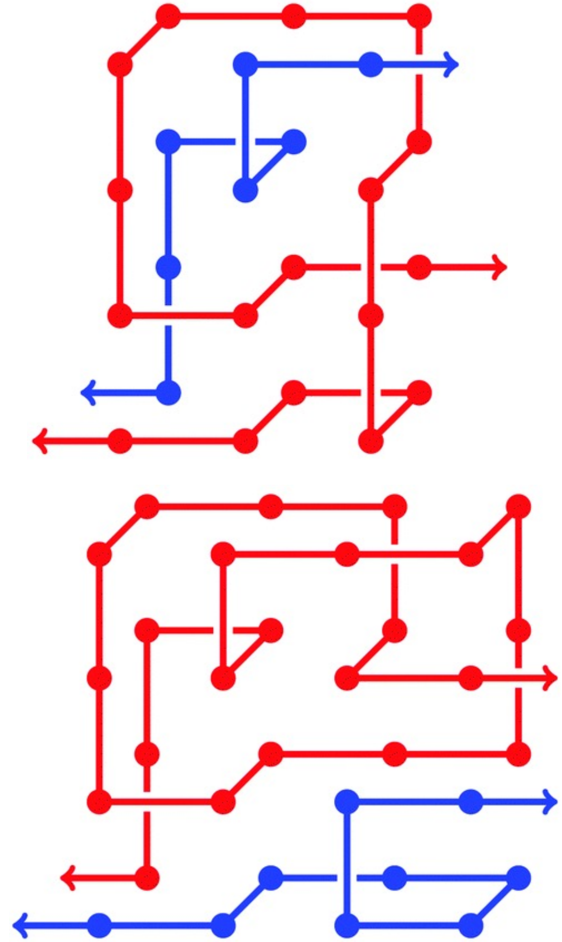
for a constant E $\implies$ a density of 2-sections in unknot polygons.

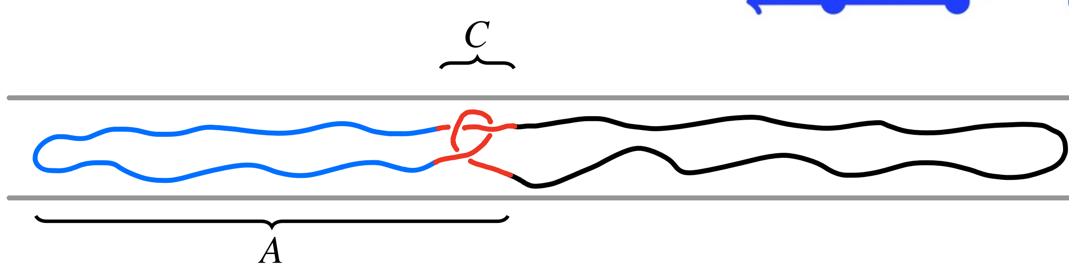
Equilibrium lattice model predicts two “modes” of knots

Non-local



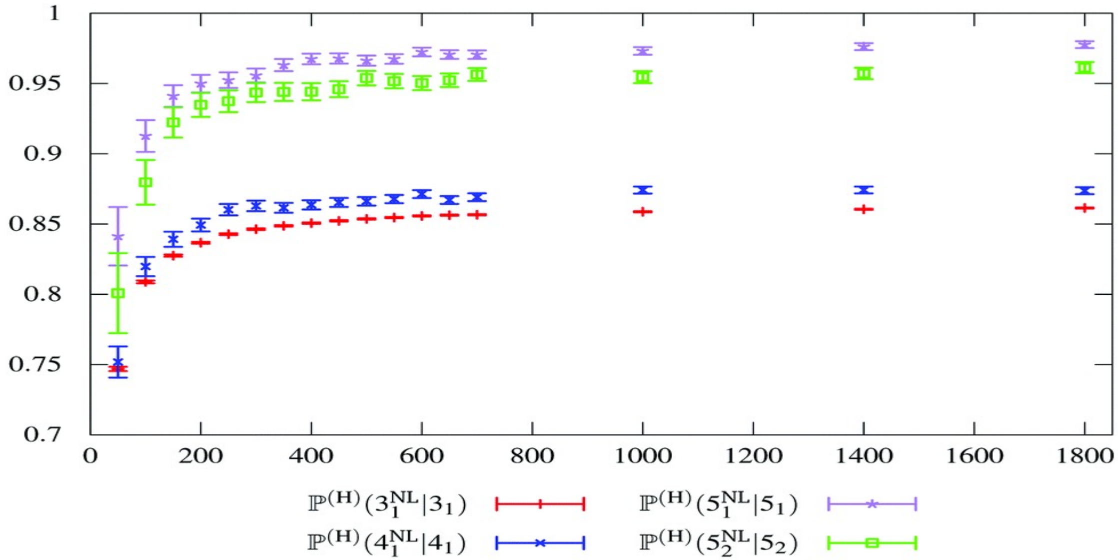
Local

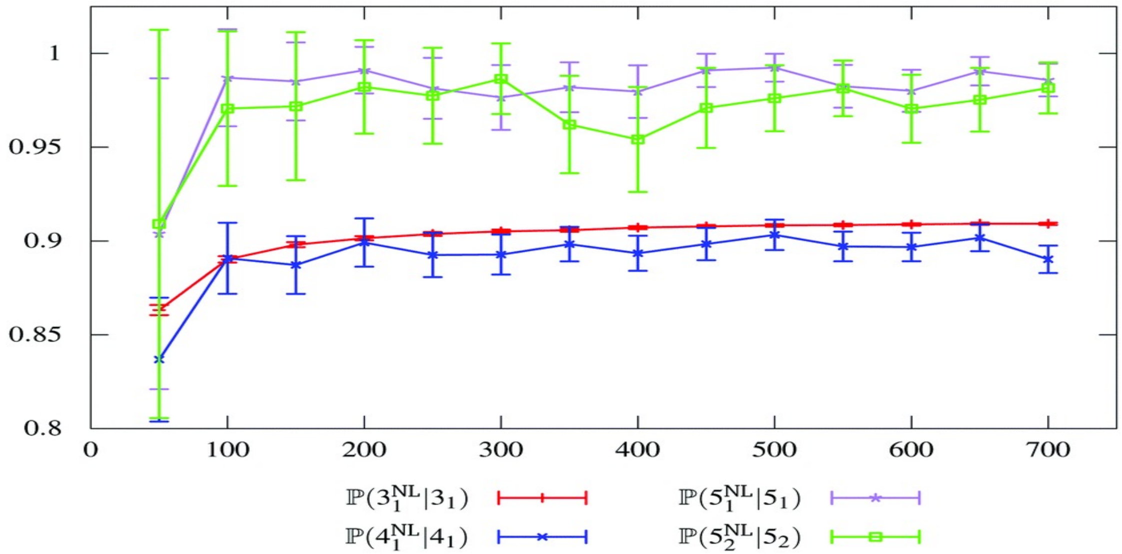


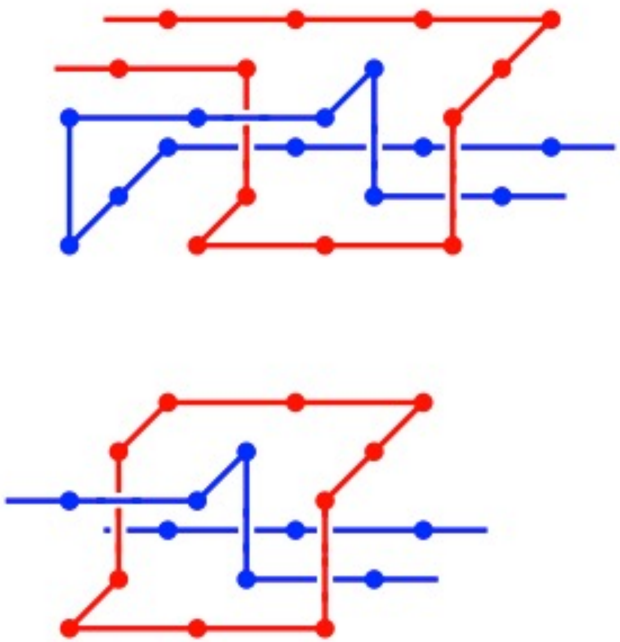


Lattice Model Results

Equilibrium small tube sizes: Beaton et al ***Soft Matter***, 2018,**14**, 5775





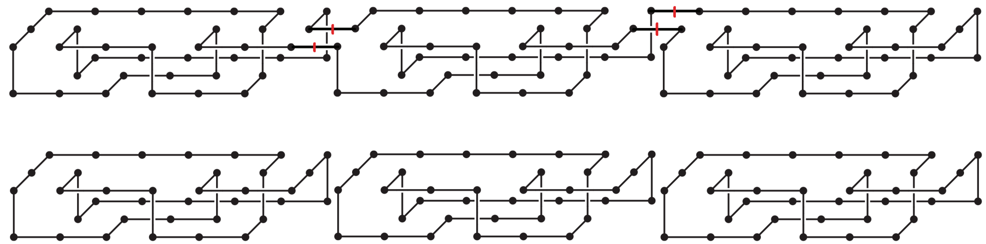


Two modes of the Hopf link: the two polygon mode (top) appears to require more edges than the one polygon mode (bottom).

Summary of Results for SAPs in Tubes:

1. *FWD Holds:* All but exponentially few large SAPs are knotted (CS 1998).
2. *Knot Identification Simplified in Tubes:*

Breaking at 2-sections gives connect summands. Useful for knot id/ knot pattern def^n.

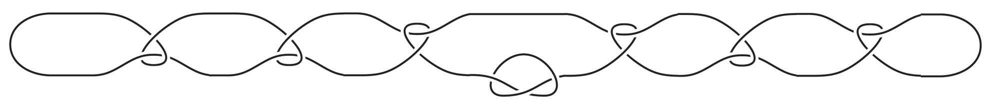


3. *Knot Localization and Knot Statistics of Polygons in $\mathbb{T}_{L,M}$:*

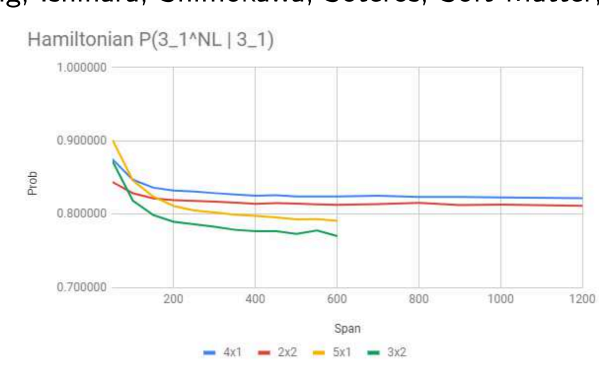
$$p_{\mathbb{T},n}(K) \sim p_{\mathbb{T},n}(0_1)\binom{n}{f_K} \sim p_{\mathbb{T},n}(0_1)n^{f_K} \sim \mu_{0_1}^n n^{f_K}$$

Monte Carlo Evidence: Beaton N, Eng J, Soteros C, (2019) JPhysA, 52(14): 144003.

Proof in 1×2 tube: Atapour, Beaton, Eng, Ishihara, Shimokawa, Soteros, Vazquez *in prep*)

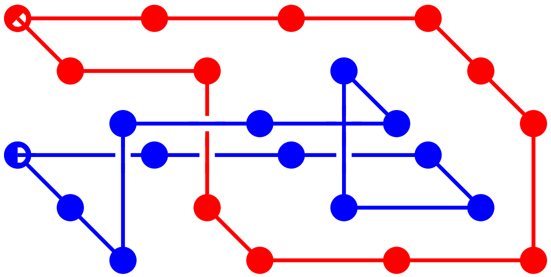


Two Modes Identified: Beaton, Eng, Ishihara, Shimokawa, Soteros, Soft Matter, 2018, 14, 5775

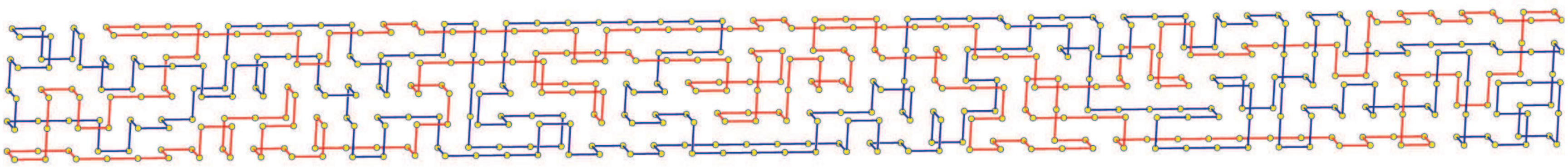


2SAPs: Pairs of SAPs which "Span" $\mathbb{T}$

$q_{\mathbb{T},s}$ - the number of pairs of mutually avoiding SAPs in $\mathbb{T}$ which have the same left-most and right-most planes and span s.



Linked 2SAP in (2,1)-tube with span 3



A 2SAP in (1,4)-tube with span 50