Physical Knots

Nick Beaton

Highlights in Mathematical Physics Seminar

October 7, 2022

Combinatorial + Biological + Probabilistic + Computational Knots

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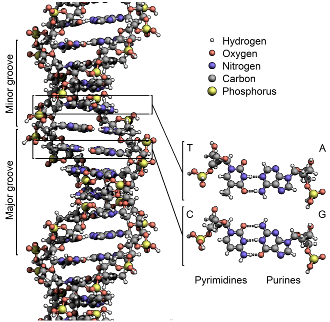
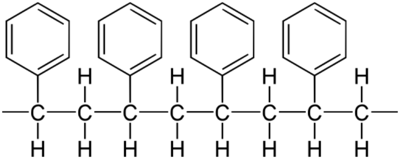
Motivation: Polymer knots

Polymers are large molecules made of many small repeating parts.

- Natural (e.g. DNA)
- Synthetic (e.g. polyethylene)

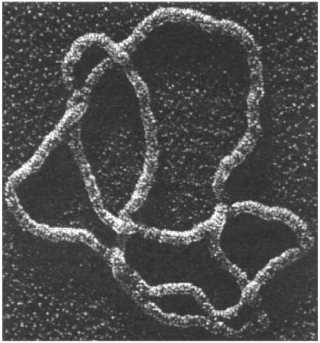




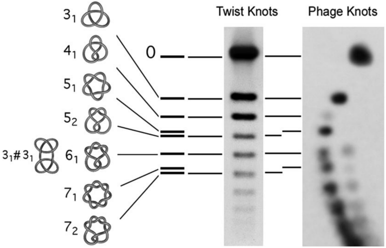
Motivation: Polymer knots

Polymers can have simple linear structure or more complicated, e.g. branching.

Can also form loops $\rightarrow$ knots and links.



Wasserman et al, *Science* 1985



Arsuaga et al, *PNAS* 2005

Motivation: Polymer knots

Knots and links in DNA can affect replication. Enzymes like topoisomerase can cut and join DNA to simplify topology, but how they work is poorly understood.

More generally the topology of polymer molecules affects their chemical and physical function.

"Physical" models of knots

Many different ways to build models of knots

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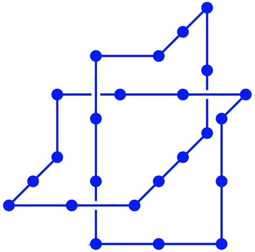
- Lattice models e.g. self-avoiding polygons etc.



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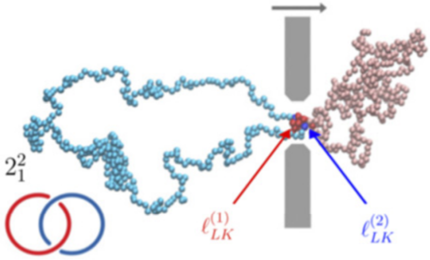
- Continuum models e.g. beads on a string



Orlandini & Micheletti, *J. Phys.: Condens. Matter* 2022

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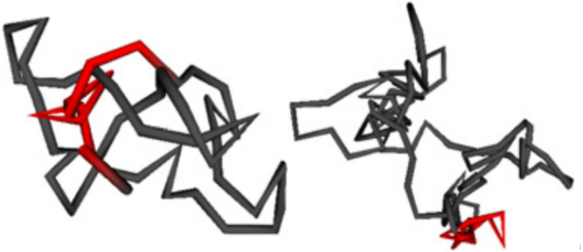
- Equilateral polygons in $\mathbb{R}^3$



Xiong et al, *J. Phys. A* 2021

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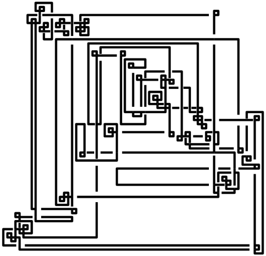

Chapman & Rechnitzer, *Experimental Math.* 2022

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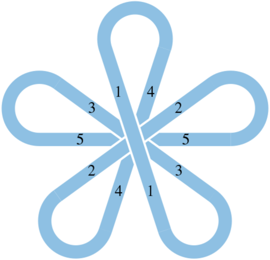

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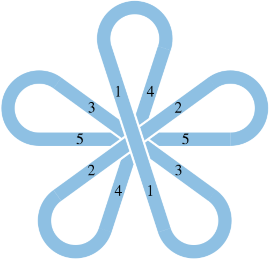

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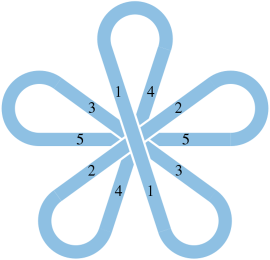


Reminder: Self-avoiding walks & polygons

A self-avoiding walk (SAW) in $\mathbb{Z}^d$ is a sequence of vertices

$$\omega = (\omega_0, \omega_1, \ldots, \omega_n)$$

such that $|\omega_{i+1} - \omega_i| = 1$ and $\omega_i \neq \omega_j$ for $i \neq j$.

A (undirected, unrooted) self-avoiding polygon (SAP) in $\mathbb{Z}^d$ is a simple closed loop on the edges of $\mathbb{Z}^d$.

Let c_n be the number of n-step SAWs and p_n be the number of n-edge SAPs (both counted up to translation).

Reminder: Self-avoiding walks & polygons

Theorem (Hammersley & Morton 1954, Hammersley 1961)

For a given dimension d the limits

$$\log \mu = \lim_{n \to \infty} \frac{1}{n} \log c_n = \lim_{n \to \infty} \frac{1}{2n} \log p_{2n}$$

exist and are equal to $\inf_n \frac{1}{n} \log c_n$.

Proof.

Any SAW of length $m+n$ can be split into two SAWs of lengths m, n, but concatenating any two of lengths m, n may not give a SAW.

$$c_{m+n} \leq c_m c_n \qquad \Rightarrow \qquad \log c_{m+n} \leq \log c_m + \log c_n$$

So $\{\log c_n\}$ is a subadditive sequence.

Then we need a result about subadditive sequences... $\square$

Reminder: Self-avoiding walks & polygons

Conjecture

In 2D and 3D,

$$c_n = An^{\gamma-1}\mu^n(1+o(1)) \qquad \text{and} \qquad p_{2n} = Bn^{\alpha-3}\mu^{2n}(1+o(1))$$

Conjectures/estimates:

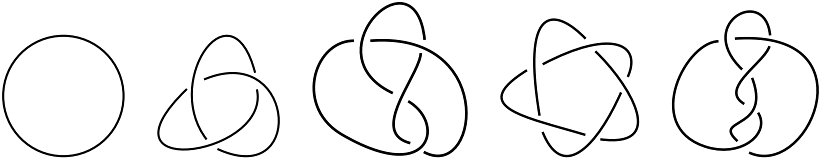
$$\mu = \begin{cases} 2.63815853032790(3) & d=2 \\ 4.684039931(27) & d=3 \end{cases}$$

$$\gamma = \begin{cases} \frac{43}{32} & d=2 \\ 1.15695300(95) & d=3 \end{cases}$$

$$\alpha = \begin{cases} \frac{1}{2} & d=2 \\ 0.23721 & d=3 \end{cases}$$

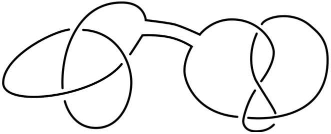
Knotted SAPs

Simplest prime knot types:



unknot (0_1) trefoil (3_1) figure-eight (4_1) cinquefoil (5_1) three-twist (5_2)

Can also have composite knots:



For a given knot type K define $p_{2n}(K)$ as the number of $2n$-edge polygons of knot type K.

The number of unknotted SAPs

Since two unknots can be concatenated to give another unknot, the limit

$$\log \mu_0 = \lim_{n\to\infty} \frac{1}{2n} \log p_{2n}(0_1)$$

exists.

Theorem (Sumners & Whittington 1988)

$$\mu_0 < \mu.$$

That is, unknots are exponentially rare among all SAPs.

Proof.

A pattern theorem... $\square$

The Frisch-Wasserman-Delbrück conjecture

Confirms the (SAP version of) a conjecture by Frisch and Wasserman (1962) and Delbrück (1962).

Later proved (Diao et al 1995) for random equilateral polygons in $\mathbb{R}^3$.

More precisely it is believed that

$$p_{2n}(0_1) = B_0 n^{\alpha-3} \mu_0^{2n}(1 + o(1))$$

where α is the same exponent as for all SAPs in 3D. (Supported by numerical evidence.)

Other knots

For other knot types even the existence of a growth rate has not been proved. However concatenating an unknot does not change knot type, so it follows that

$$\liminf_{n\to\infty} \frac{1}{2n} \log p_{2n}(K) \geq \log \mu_0.$$

Generally believed that

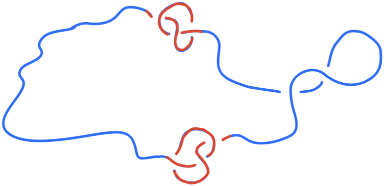
$$p_{2n}(K) \sim B'_K n^{f_K} p_{2n}(0_1)(1 + o(1)) = B_K n^{\alpha - 3 + f_K} \mu_0^{2n}(1 + o(1))$$

where f_K is the number of prime components in the knot decomposition of K.

This has been proved (NRB, Ishihara, Atapour, Eng, Shimokawa, Soteros & Vazquez 2022) for knotted SAPs in the 2×1 tube (narrowest tube that admits knots).

The shape of knots

The fact that the entropic exponent increases by 1 for each prime component corresponds to the idea that the “knotted parts” of a large knot are relatively small:



Numerical evidence (Marcone et al 2005) suggests that the length of the knotted part scales as n^t where $t \approx 0.75$, independent of knot type.

Other lattices & universality

Many other 3D lattices, e.g. face-centred cubic (FCC) and body-centred cubic (BCC).

Growth rates μ, μ_0 and amplitudes B, B_K expected to be different but exponent α should be universal.

Moreover for two prime knot types K, L, the ratio

$$\frac{p_{2n}(K)}{p_{2n}(L)} \sim \frac{B_K}{B_L}$$

is also expected to be universal. For example numerical evidence (Rechnitzer & Janse van Rensburg 2011)

$$\frac{B_{3_1}}{B_{4_1}} \approx 28 \qquad \frac{B_{3_1}}{B_{5_1}} \approx 400 \qquad \frac{B_{3_1}}{B_{5_2}} \approx 280$$

$$\frac{B_{4_1}}{B_{5_1}} \approx 15 \qquad \frac{B_{4_1}}{B_{5_2}} \approx 9$$

$$\frac{B_{5_1}}{B_{5_2}} \approx 0.67$$

Numerical methods

Computing and analysing series for c_n and p_{2n} is one of the most powerful methods in 2D, but not very effective in 3D.

In narrow tubes of $\mathbb{Z}^3$ we have finite transfer matrices $\rightarrow$ longer series, some proofs.

But in the bulk the best methods use Monte Carlo random sampling.

Monte Carlo methods

The state of the art for sampling long SAWs and SAPs is the pivot algorithm:

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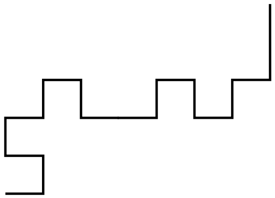

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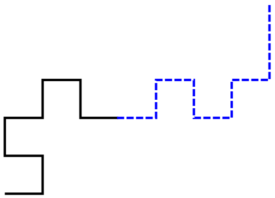

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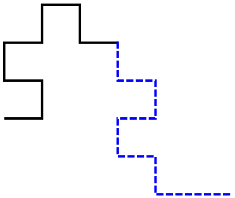

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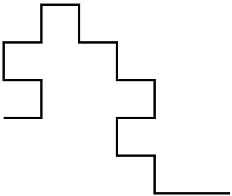

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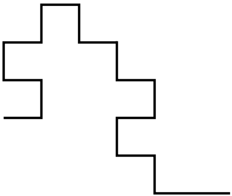


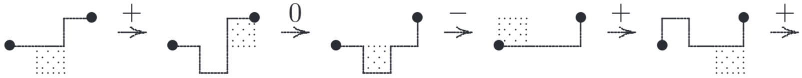
Proposed moves are rarely successful, but when they do succeed they make big changes. Clisby's algorithm (2010+) requires only $O(\log n)$ time per attempted move $\rightarrow$ can sample SAWs with billions of steps.

Works for SAPs too. However it is very difficult to control topology $\rightarrow$ need to check all possible crossings during the pivot.

Monte Carlo methods

Can instead use "local" moves which only change a small section at once $\rightarrow$ easier to control topology.

Canonical method is BFACF:



Then the ergodicity classes are the knot types.

With BFACF the size fluctuates $\rightarrow$ must be combined with an algorithm for flat-histogram sampling, e.g.

- multiple Markov chain (MMC)
- pruned/enriched Rosenbluth method (PERM)
- generalised atmospheric Rosenbluth method (GARM)
- generalised atmospheric sampling (GAS)
- Wang-Landau method
- etc.

Monte Carlo methods

Some current work (NRB, Clisby, Rechnitzer) looking at adapting the pivot algorithm to equilateral polygons in $\mathbb{R}^3$ while controlling topology. (Actually easier than SAWs.)

Thank you!