Knotting statistics for polygons in lattice tubes

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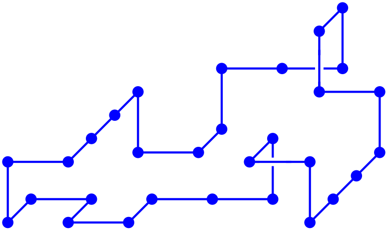
SAPs in $\mathbb{Z}^3$

A self-avoiding polygon (SAP) is a simple closed walk on the edges of $\mathbb{Z}^3$:



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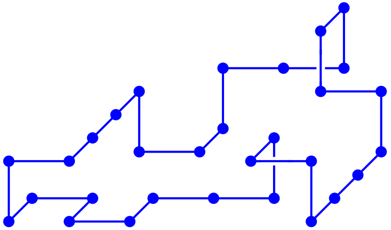

Let p_n be the number of n-edge polygons, defined up to translation (n must be even). Then

$$(p_{2m})_{m\geq 1} = 0, 3, 22, 207, 2412, 31754, 452640, 6840774, 108088232, 1768560270, \ldots$$

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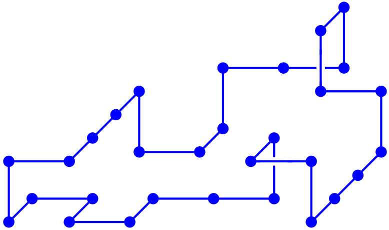

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(Known up to $n = 32$. [Clisby et al 2007])

Asymptotics of p_n

Theorem (Hammersley 1961)

There exists $\kappa = \log \mu$ such that

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The $e^{o(n)}$ is conjectured to follow a power law, so that

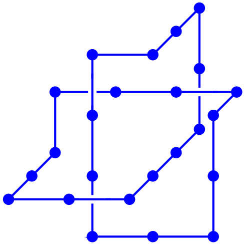
$$p_n \sim A n^{\alpha - 3} \mu^n$$

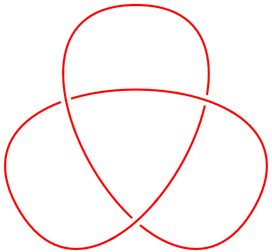
for some constants A and α. The exponent α is expected to be universal (the same for any 3-dimensional lattice), while A and μ are lattice-dependent. In 3D [Clisby & Dünweg 2016]

$$\alpha \approx 0.237209.$$

Knotted polygons

In three dimensions SAPs can be knotted:





Let $p_n(K)$ be the number of n-edge polygons of knot type K.

Knotted polygons cont'd

Theorem (Sumners & Whittington 1988)

There exists $\kappa_0 = \log \mu_0$ *such that*

$$p_n(0_1) = \exp\{\kappa_0 n + o(n)\} = e^{o(n)} \mu_0^n.$$

Moreover

$$\mu_0 < \mu.$$

That is, the probability of a random n-edge polygon being unknotted decays exponentially:

$$\mathbb{P}_n(0_1) = \frac{p_n(0_1)}{p_n} = e^{o(n)} \left(\frac{\mu_0}{\mu} \right)^n.$$

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But the decay is still slow [Janse van Rensburg 2008]:

$$\frac{\mu_0}{\mu} \approx 0.999996.$$

Knotted polygons cont'd

For $K \neq 0_1$ very little has been proved. It is straightforward to show that

$$\limsup_{n\to\infty} \frac{1}{n} \log p_n(K) \geq \kappa_0.$$

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But it is generally believed that

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and moreover

$$p_n(K) \sim A_K n^{\alpha-3+f(K)} \mu_0^n$$

where α is the same exponent as for all polygons, A_K is a constant and $f(K)$ is the number of prime knot factors in the knot decomposition of K.

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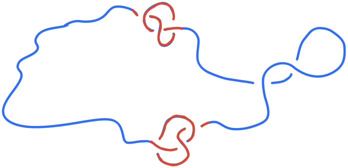
This is essentially because the "knotted parts" of a long polygon are expected to be small:

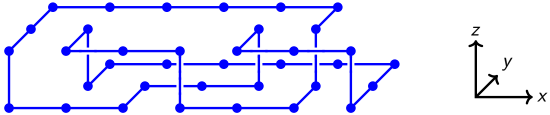


Polygons in lattice tubes

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

$$\mathbb{T}_{L,M} = \{(x, y, z) \,|\, 0 \leq y \leq L, 0 \leq z \leq M\}$$

and let $p_{\mathbb{T},n}$ be the number of SAPs in $\mathbb{T}$, defined up to translation in the x-direction only.



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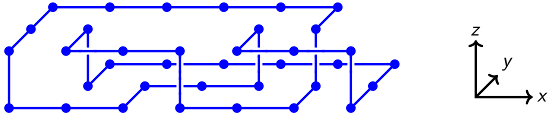

In $\mathbb{T}$, polygons are characterised by a finite transfer matrix $\Rightarrow$ growth rates, exponents, etc. can be computed exactly (in theory).

Theorem (Soteros 1998)

There exist constants $A_{\mathbb{T}}$ and $\kappa_{\mathbb{T}} = \log \mu_{\mathbb{T}}$ such that

$$p_{\mathbb{T},n} \sim A_{\mathbb{T}} \mu_{\mathbb{T}}^n$$

$A_{\mathbb{T}}$ and $\mu_{\mathbb{T}}$ are algebraic numbers.

Knotted polygons in tubes

If $L, M > 0$ and $(L, M) \neq (1,1)$ then polygons in $\mathbb{T}$ can be knotted. (Only unknots in 1×1.)
Define $p_{\mathbb{T},n}(K)$ to count polygons of knot type K.

Similarly to $\mathbb{Z}^3$:

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There exists $\kappa_{\mathbb{T},0} = \log \mu_{\mathbb{T},0}$ *such that*

$$p_{\mathbb{T},n}(0_1) = \exp\{\kappa_{\mathbb{T},0} n + o(n)\} = e^{o(n)} \mu_{\mathbb{T},0}^n.$$

If $L, M > 0$ *and* $(L, M) \neq (1,1)$ *then*

$$\mu_{\mathbb{T},0} < \mu_{\mathbb{T}}.$$

That is, in a 3-dimensional tube other than 1×1, the probably of a polygon being unknotted decays exponentially.

Knotted polygons in tubes cont'd

As with $\mathbb{Z}^3$, it is easy to show that

$$\limsup_{n\to\infty} \frac{1}{n} \log p_{\mathbb{T},n}(K) \geq \kappa_{\mathbb{T},0}.$$

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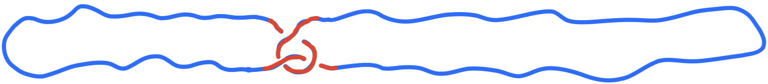

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Again expect that

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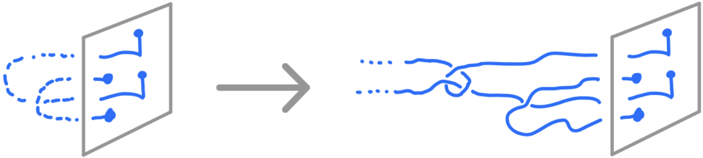
$B_{\mathbb{T}}$ and $\nu_{\mathbb{T}}$ are algebraic numbers.

Computing probabilities

Polygons in $\mathbb{T}$ are characterised by a finite transfer matrix, but polygons of fixed knot type (including unknots) are not. This is because the state depends on the previous entanglement of the "strands", and there are infinitely many possibilities:



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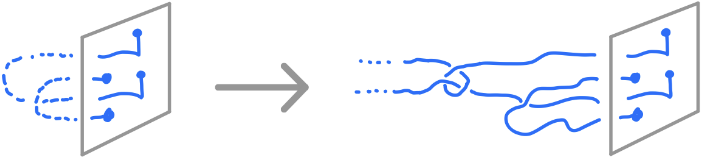

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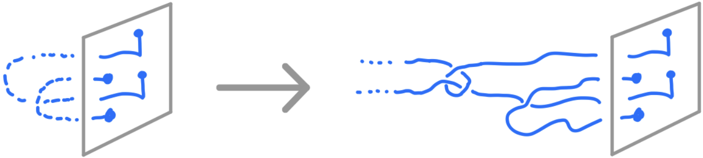

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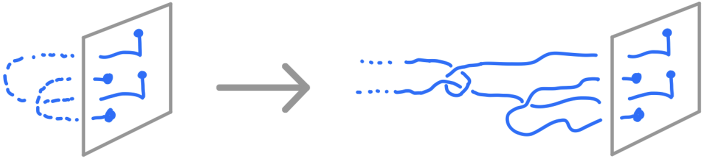

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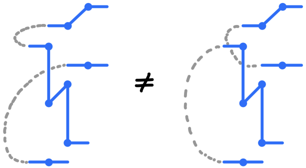
Must use Monte Carlo methods!

Transfer matrix Monte Carlo method

A 1-pattern is any configuration of vertices and (half)-edges between $x = k \pm \frac{1}{2}$ which can form part of a polygon, together with a pairing of the open half-edges on the left.



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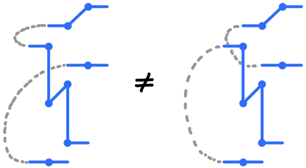

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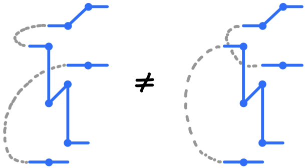

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Let $\mathbf{M}$ be the transfer matrix for internal 1-patterns, ie. $\mathbf{M}_{ij} = 1$ if i can be immediately followed by j and 0 otherwise. Since $\mathbf{M}$ is irreducible and aperiodic, it has a unique dominant eigenvalue $\lambda \in \mathbb{R}^{>0}$ with right eigenvector ζ.

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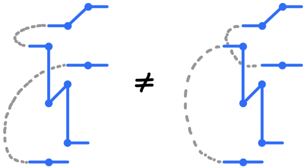

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Lemma (adapted from Alm & Janson 1990)

If i and j are internal 1-patterns such that j can follow i, let $p_{ij}^{\mathrm{sp}}(s)$ be the probability that an occurrence of i in a uniformly random polygon of span s is followed by j. Then as $s \to \infty$,

$$p_{ij}^{\mathrm{sp}}(s) \to p_{ij}^{\mathrm{sp}} = \lambda^{-1} \frac{\zeta_j}{\zeta_i}.$$

Transfer matrix Monte Carlo method cont'd

Can likewise define matrices **A** with rows indexed by $\mathcal{A}$ and columns indexed by $\mathcal{I}$, and **B** indexed by $\mathcal{I}$ and $\mathcal{B}$.

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We then use an algorithm for generating a polygon $\pi = \pi_0\pi_1 \cdots \pi_s$ uniformly at random. For $a \in \mathcal{A}$ and $i \in \mathcal{I}$, define

$$\mathcal{F}_{\text{start}}(a) = \{j \in \mathcal{I} : \mathbf{A}_{aj} = 1\} \quad \text{and} \quad \mathcal{F}_{\text{end}}(i) = \{b \in \mathcal{B} : \mathbf{B}_{ib} = 1\}$$

and then

$$t_1(a) = \sum_{j \in \mathcal{F}_{\text{start}}(a)} \zeta_j \quad \text{and} \quad t_s(i) = \frac{|\mathcal{F}_{\text{end}}(i)|}{\zeta_i}$$

1. Select π_0 uniformly at random from $\mathcal{S}$.
2. With probability $r_1(\pi_0)$ (see below) reject the sample and start from (1) again. Else select π_1 from $\mathcal{F}_{\text{start}}(\pi_0)$ with probability proportional to ζ_{π_1}.
3. For $k = 2, 3, \ldots, s-1$, choose π_k with probability $p^{\text{sp}}_{\pi_{k-1},\pi_k}$.
4. With probability $r_s(\pi_{s-1})$ (see below), reject the sample and start from (1) again. Otherwise select π_s uniformly from $\mathcal{F}_{\text{end}}(\pi_{s-1})$.

The rejection probabilities are chosen to make the sampling uniformly random:

$$r_1(\pi_0) = 1 - \frac{t_1(\pi_0)}{\max_{a \in \mathcal{S}}\{t_1(a)\}} \quad \text{and} \quad r_s(\pi_{s-1}) = 1 - \frac{t_s(\pi_{s-1})}{\max_{j \in \mathcal{I}}\{t_s(j)\}}$$

Computing probabilities cont'd

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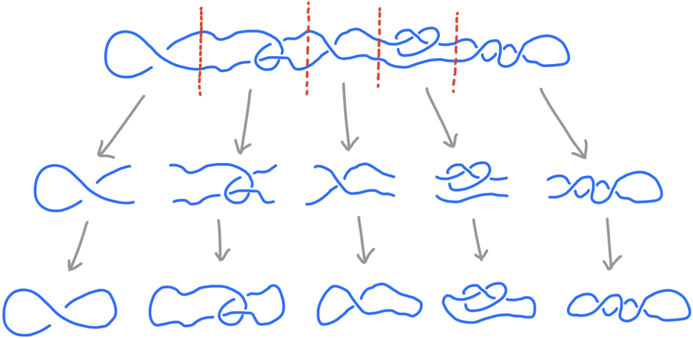

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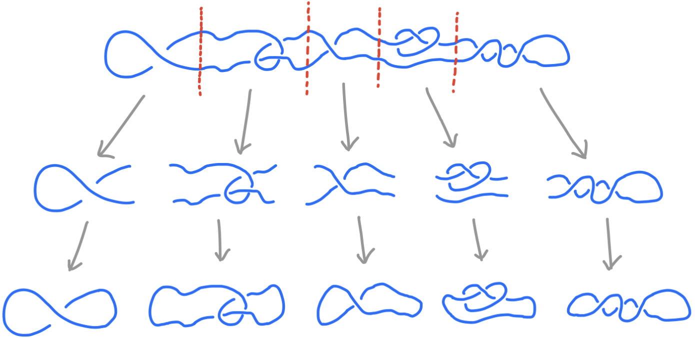

Then we compute the knot type of each, and the overall knot type is the connect-sum of the parts. Since long polygons have a positive density of 2-sections (guaranteed by pattern theorems), the pieces are almost always very small.

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Define

$$\mathbb{P}^{(\mathrm{sp})}_{\mathbb{T},s}(K) = \text{probability of knot-type } K \text{ among all knots of span } s \text{ in } \mathbb{T}$$

$$\mathbb{P}^{\mathrm{H}}_{\mathbb{T},s}(K) = \text{probability of knot-type } K \text{ among all Hamiltonian knots of span } s \text{ in } \mathbb{T}$$

$$\mathbb{P}^{*}_{\mathbb{T},s}(K) = \text{one of the above}$$

Results: Growth rates

Since $\mathbb{P}^*_{\mathbb{T},s}(0_1)$ decays exponentially, plot the log and take a linear best fit.

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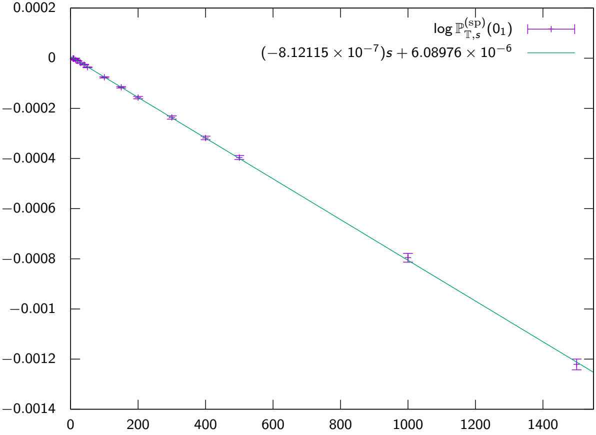
2×1 tube:



So

$$\chi_{\mathbb{T},0} - \chi_{\mathbb{T}} = -8.12115 \times 10^{-7} \quad \Rightarrow \quad \frac{\nu_{\mathbb{T},0}}{\nu_{\mathbb{T}}} = 0.99999919$$

Results: Growth rates

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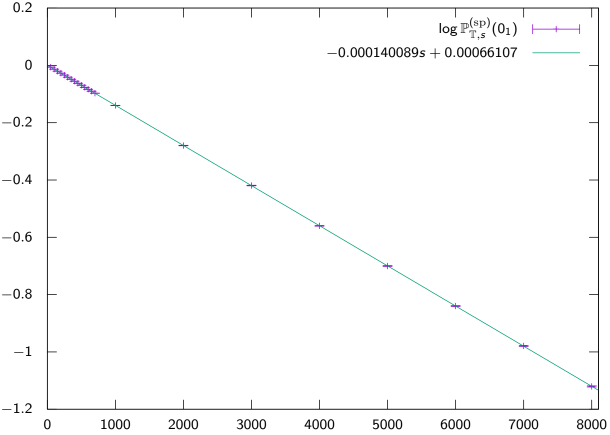
3×1 tube:



So

$$\chi_{\mathbb{T},0} - \chi_{\mathbb{T}} = -0.000140089 \quad \Rightarrow \quad \frac{\nu_{\mathbb{T},0}}{\nu_{\mathbb{T}}} = 0.99986$$

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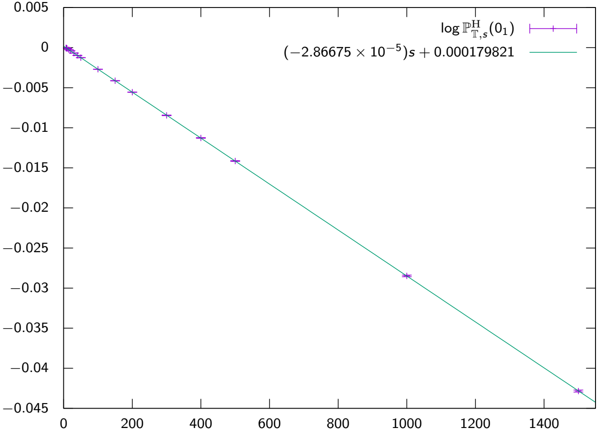
2×1 tube Hamiltonian:



So

$$\chi^{\mathrm{H}}_{\mathbb{T},0} - \chi^{\mathrm{H}}_{\mathbb{T}} = -2.86675 \times 10^{-5} \quad \Rightarrow \quad \frac{\nu^{\mathrm{H}}_{\mathbb{T},0}}{\nu^{\mathrm{H}}_{\mathbb{T}}} = 0.999971$$

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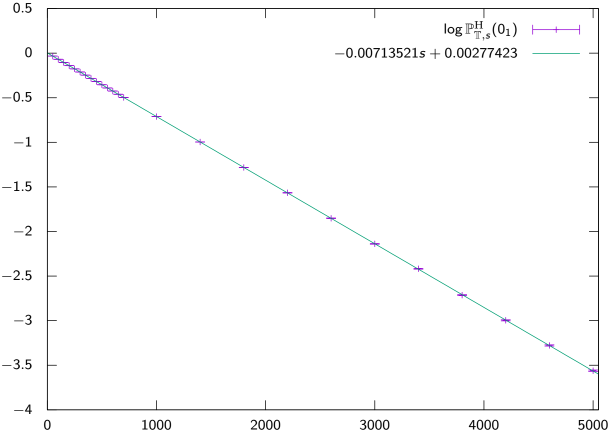

So

$$\chi^{\mathrm{H}}_{\mathbb{T},0} - \chi^{\mathrm{H}}_{\mathbb{T}} = -0.00713521 \quad \Rightarrow \quad \frac{\nu^{\mathrm{H}}_{\mathbb{T},0}}{\nu^{\mathrm{H}}_{\mathbb{T}}} = 0.99289$$

Results: Exponents

No evidence of logarithmic corrections: strongly suggests that

$$q_{\mathbb{T},s}(0_1) \sim B_{\mathbb{T},0}(\nu_{\mathbb{T},0})^s \quad \text{and} \quad q^{\mathrm{H}}_{\mathbb{T},s}(0_1) \sim B^{\mathrm{H}}_{\mathbb{T},0}(\nu^{\mathrm{H}}_{\mathbb{T},0})^s.$$

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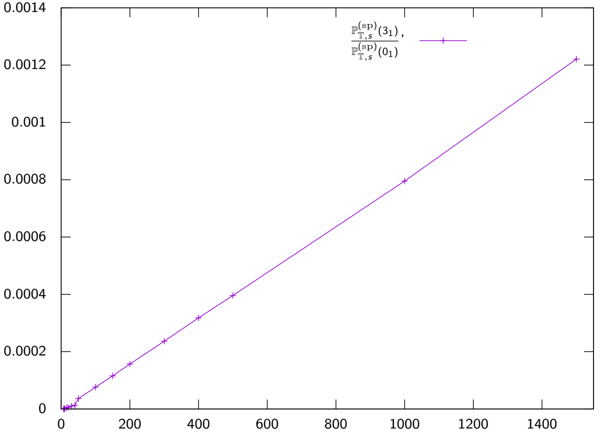

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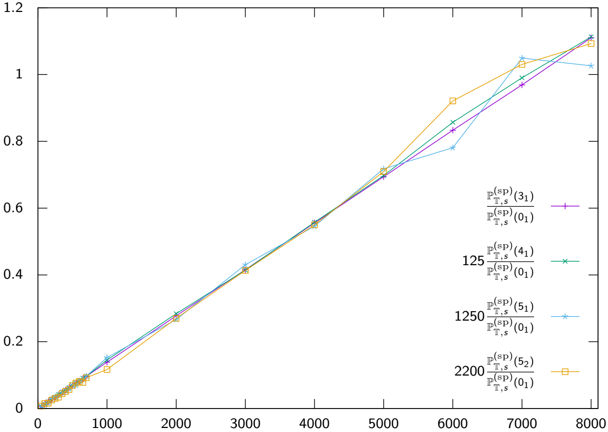

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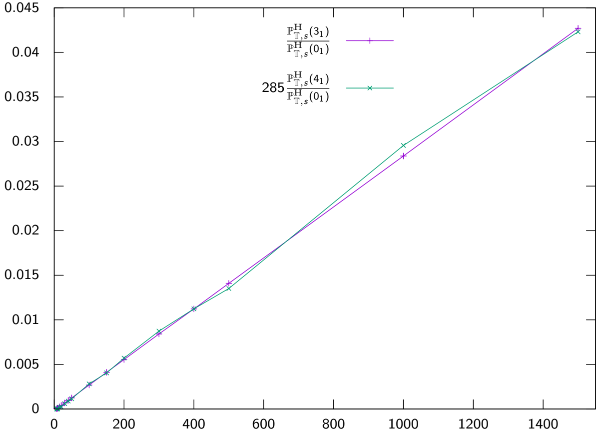

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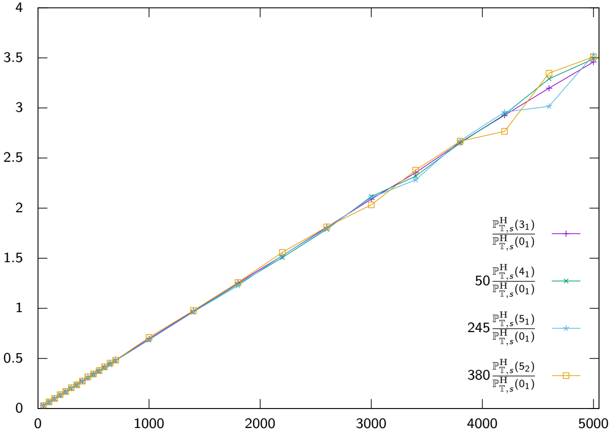

Results: Exponents cont'd

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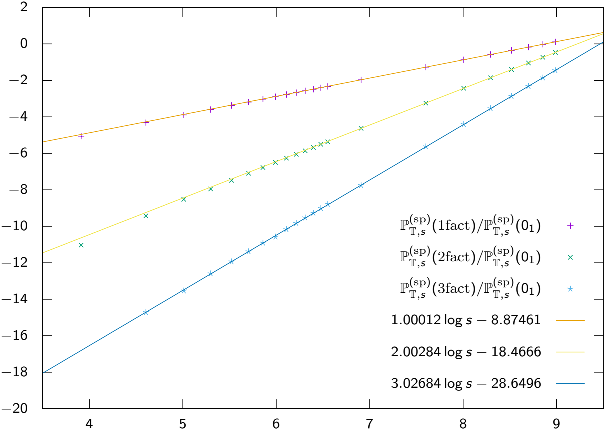

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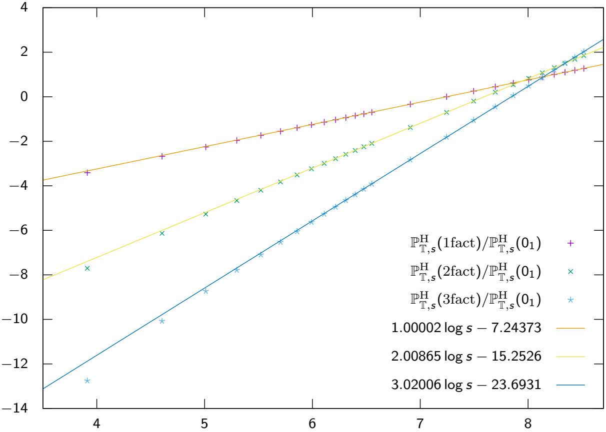

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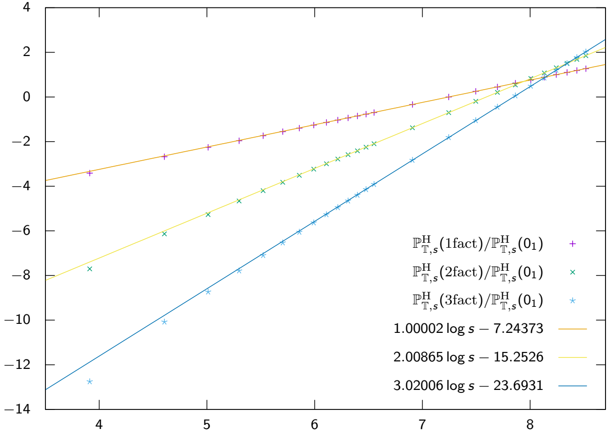

Altogether, strongly implies

$$q_{\mathbb{T},s}(K) \sim B_{\mathbb{T},K} s^{f(K)} (\nu_{\mathbb{T},0})^s \quad \text{and} \quad q^{\mathrm{H}}_{\mathbb{T},s}(K) \sim B^{\mathrm{H}}_{\mathbb{T},K} s^{f(K)} (\nu^{\mathrm{H}}_{\mathbb{T},0})^s.$$

Results: Probability maxima

$\mathbb{P}^*_{\mathbb{T},s}(K)$ decays exponentially for any fixed knot type K or set of knot types. But if $K \neq 0_1$ then $\mathbb{P}^*_{\mathbb{T},s}(K)$ initially increases, reaches some maximum, then decreases to 0.

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If

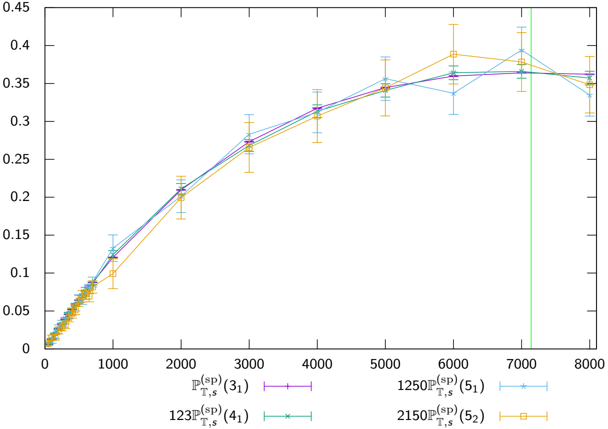
$$\mathbb{P}^*_{\mathbb{T},s}(K) \sim C^*_{\mathbb{T},K} s^{f(K)} \left(\frac{\nu^*_{\mathbb{T},0}}{\nu^*_{\mathbb{T}}} \right)^s$$

then the maximum should be at roughly

$$s^* \approx M^*_{\mathbb{T}}(K) = \frac{f(K)}{\chi^*_{\mathbb{T}} - \chi^*_{\mathbb{T},0}} = \begin{cases} (1.23 \times 10^6) f(K) & 2 \times 1 \text{ tube} \\ 7140 f(K) & 3 \times 1 \text{ tube} \\ 34900 f(K) & 2 \times 1 \text{ tube Hamiltonian} \\ 1400 f(K) & 3 \times 1 \text{ tube Hamiltonian} \end{cases}$$

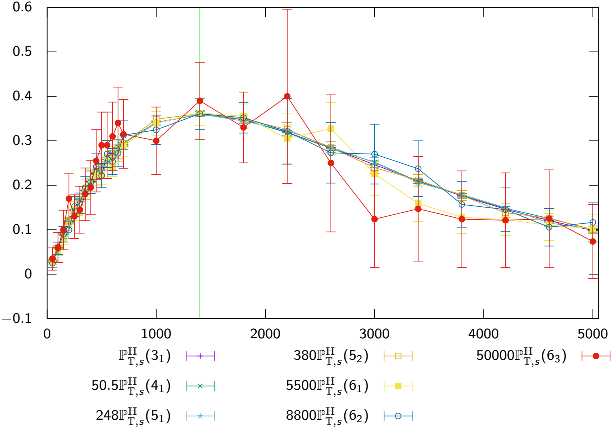
Results: Probability maxima cont'd

Prime knots in the 3×1 tube:



Results: Probability maxima cont'd

Prime Hamiltonian knots in the 3×1 tube:



Results: Probability maxima cont'd

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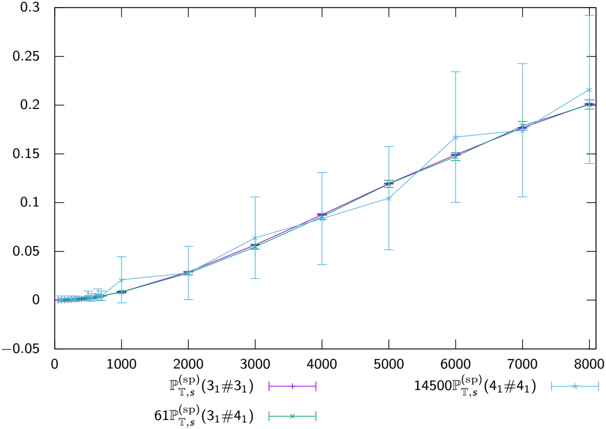

Results: Probability maxima cont'd

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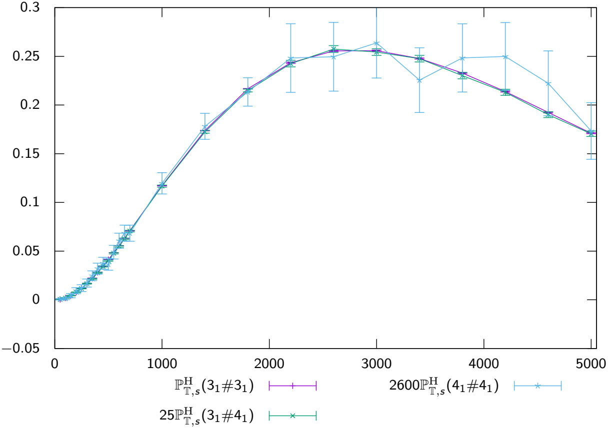

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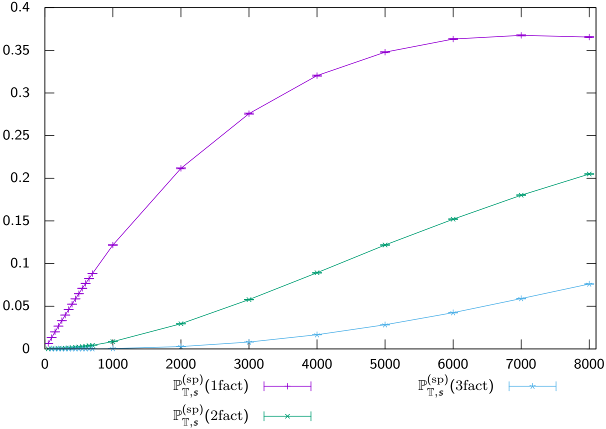

Results: Probability maxima cont'd

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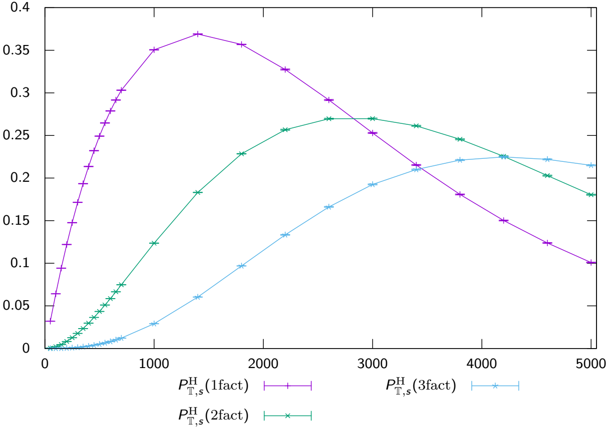

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NRB, Eng & Soteros
Knotting statistics for polygons in lattice tubes
J. Phys. A: Math. Theor. **52** (2019), 144003.

Thank you!