KNOTTED LATTICE POLYGONS

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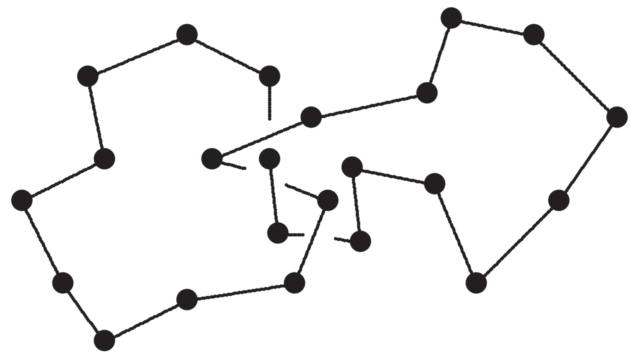
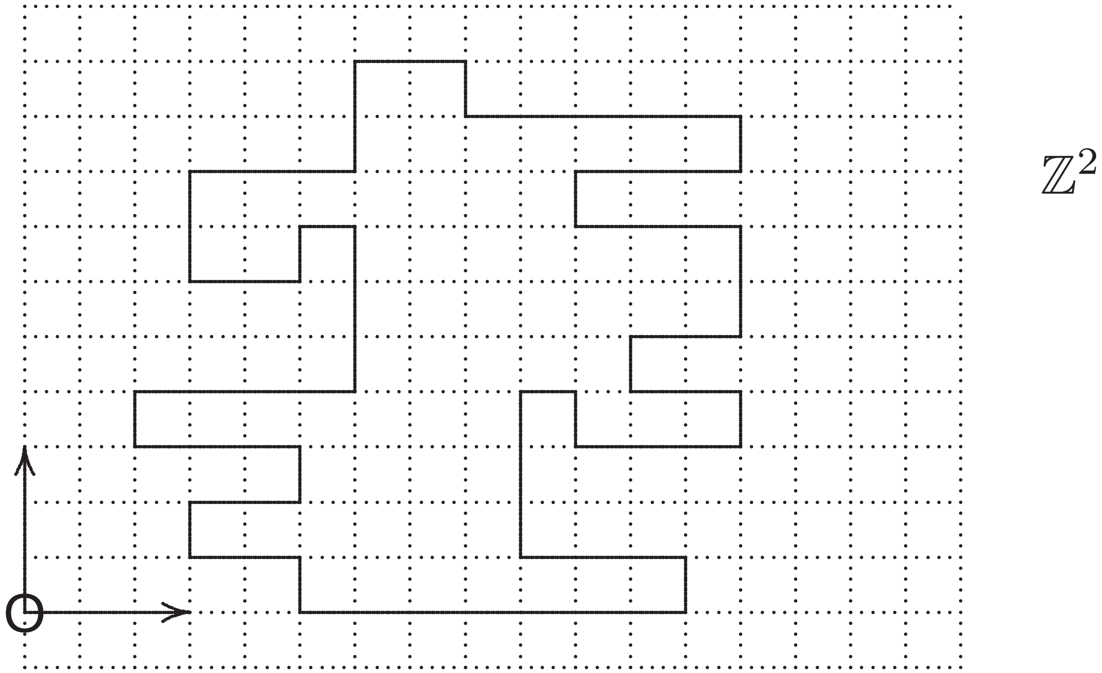
THE LATTICES AND TRAJECTORIES OF STU AND RAY

RING POLYMERS



- Ring polymer in a good solvent.
- Monomer activity t and Knot type K.
- Lattice models.

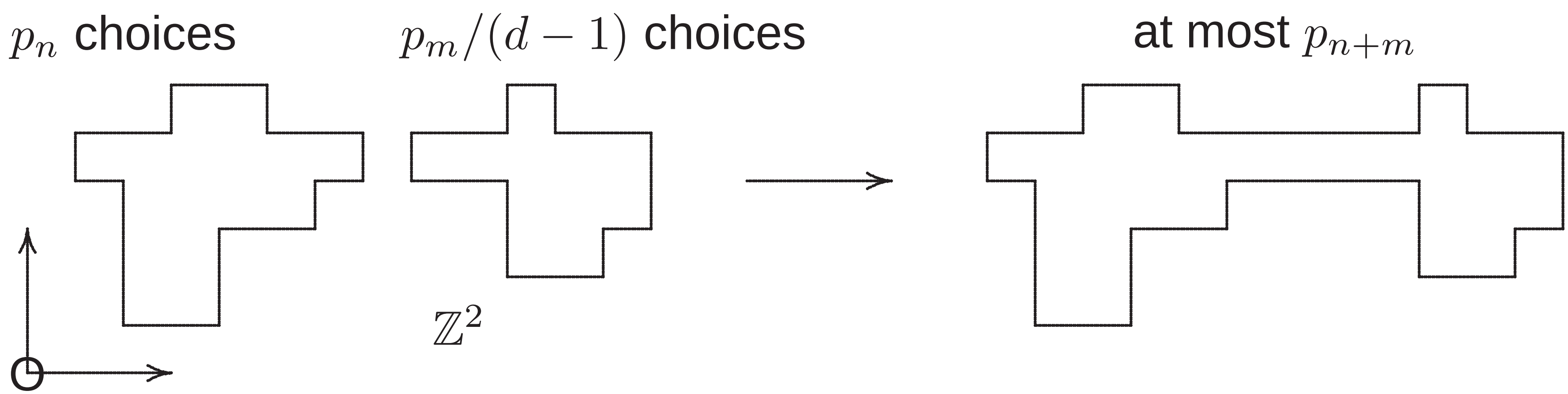
LATTICE MODEL OF A RING POLYMER



- Polygon in the (hyper)cubic lattice.
- Count polygons modulo translations:

$$p_n = \text{\# of polygons of length } n \text{ steps}$$

THE GROWTH CONSTANT



- $p_n p_m \leq (d-1) p_{n+m}$
- $\log \mu = \lim_{n\to\infty} \frac{1}{n} \log p_n.$ (GROWTH CONSTANT)
- $p_n \leq (d-1)\mu^n \qquad p_n = \mu^{n+o(n)}$

(Hammersley 1961)

ASYMPTOTIC GROWTH

In three dimensions:

$$\mu = 4.684043 \pm 0.000012 \qquad \text{(Clisby etal 2007)}$$

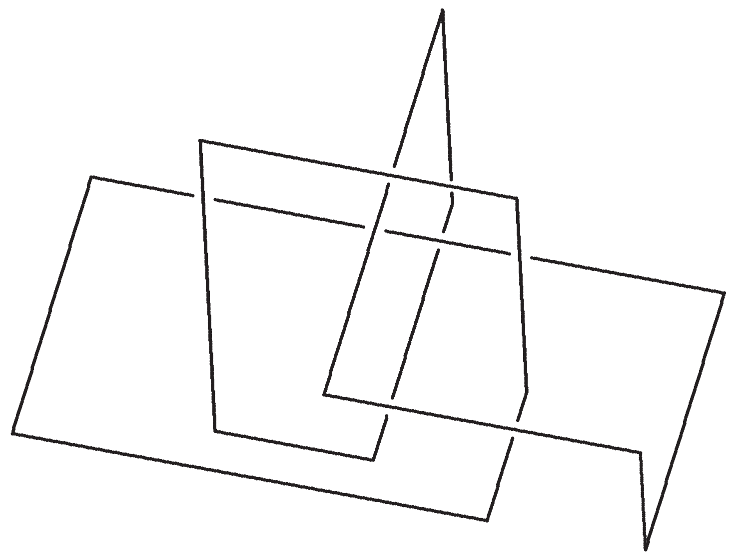
asymptotic behaviour of p_n...

$$p_n = A\, n^{\alpha-3} \mu^n \left(1 + B\, n^{-\Delta} + C\, n^{-1} + \ldots\right)$$

where

$$\begin{aligned} \alpha &= 0.237 \pm 0.005 \\ \Delta &= 0.56 \pm 0.03 \qquad \text{(Li, Madras, Sokal 1995)} \end{aligned}$$

KNOTTED POLYGONS



- $p_n(K)$ = number of polygons of length n, knottype K
- $\boxed{\log \mu_K = \limsup_{n\to\infty} \frac{1}{n} \log p_n(K).}$ (GROWTH CONSTANT)
- $p_n(K) \approx A_K n^{\alpha_K - 3} \mu_K^n$ where $\alpha_K = \alpha_\emptyset + N_K$.

  (Orlandini et.al. 1996)

GROWTH CONSTANTS OF KNOTTED POLYGONS

- THEOREM: $\mu_\emptyset \le \mu_K < \mu$

  (Sumners and Whittington 1988, Pippenger 1989, Soteros et.al 1992)

- Numerically (JvR + Whittington 1990+2000)

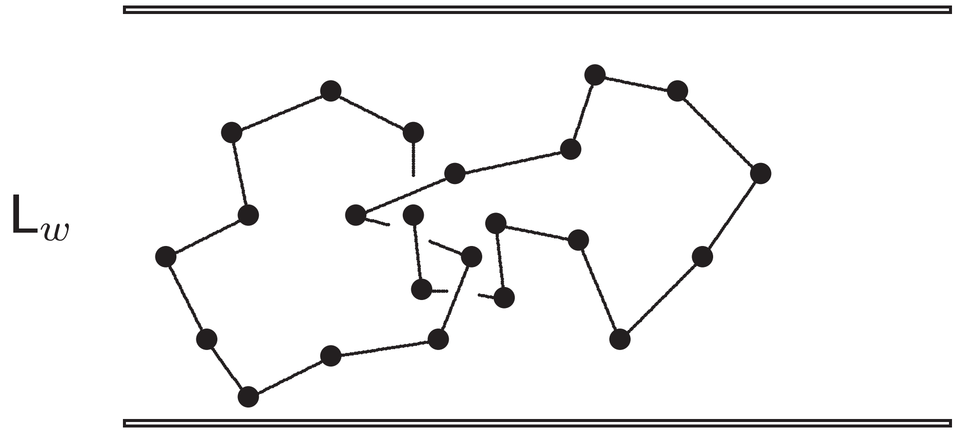
$$\log \mu - \log \mu_\emptyset = (4.15 \pm 0.32) \times 10^{-6}$$

- In other words

$$\begin{aligned} \mu &= 4.6838ab\ldots \\ \mu_\emptyset &= 4.6838ac\ldots \end{aligned}$$

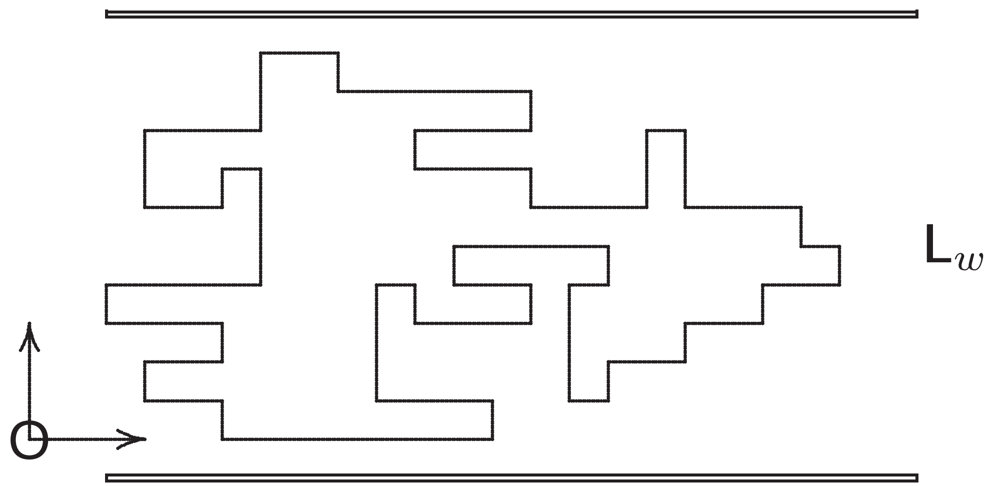
- Current computer technology may now be good enough to explicitly extend series in three dimensions and to verify these MC estimates?

A RING POLYMER IN A CONFINED SPACE



- Monomer activity t, and knot type K.
- What is the equilibrium length?
- Are there forces on the confining planes?

LATTICE POLYGONS IN A SLAB

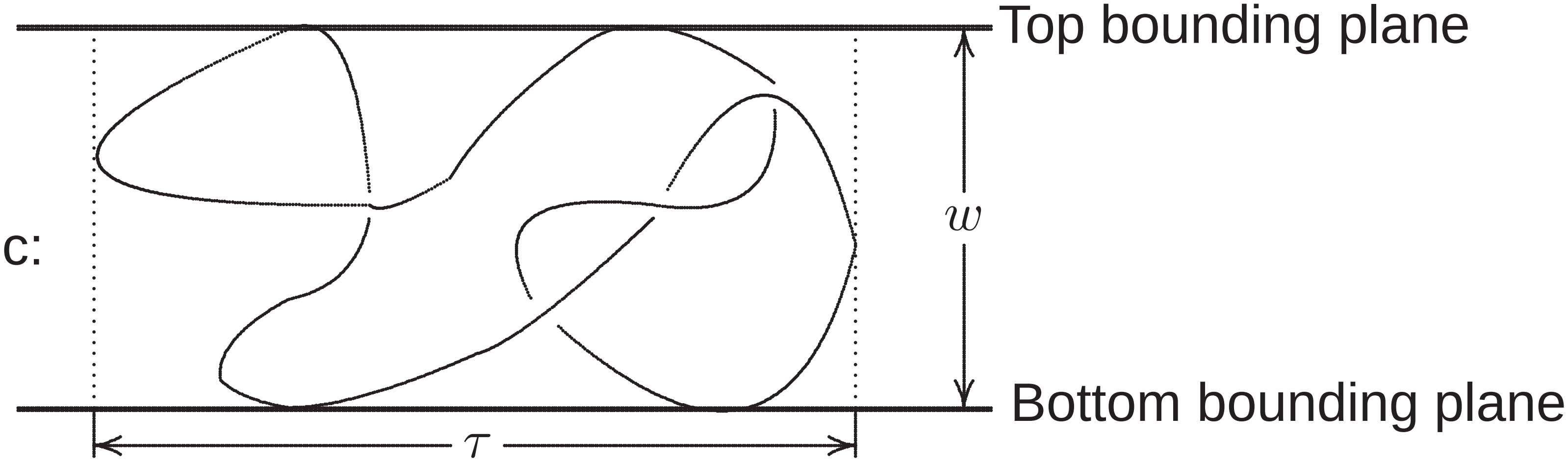


- A lattice polygon in a slab in $\mathbb{Z}^3$.
- This is the embedding of a circle - the knot type is defined.
- Questions:
  - Growth Constant and Free Energy?
  - Equilibrium length?
  - Metric Properties?

POLYGONS IN A SLAB $\mathbf{L}_w$

Polygons in L_w

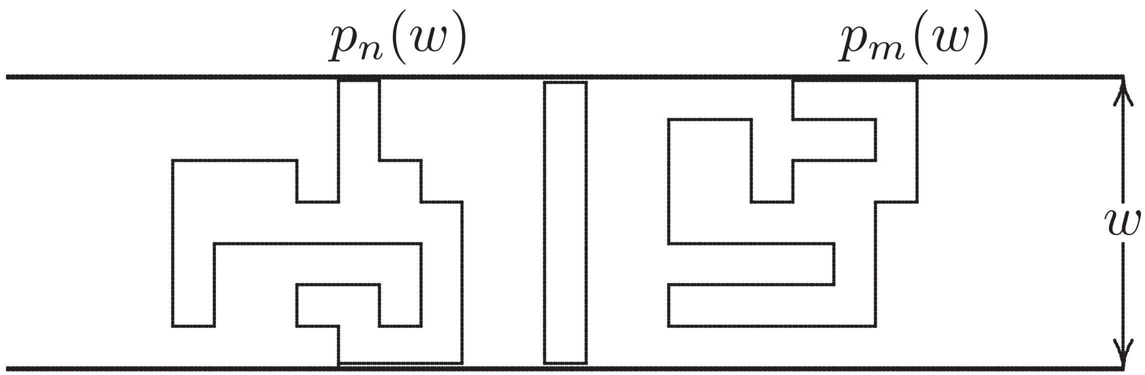
Schematic:



- $p_n(w) =$ (number of polygons in slab of length n) $\approx C_w n^{\alpha_w - 3} \mu_w^n$
- $\boxed{\log \mu_w = \lim_{n\to\infty} \frac{1}{n} \log p_n(w).}$ (GROWTH CONSTANT)

(Soteros and Whittington 1991,1992)

CONCATENATING POLYGONS IN A SLAB



- Concatenate:

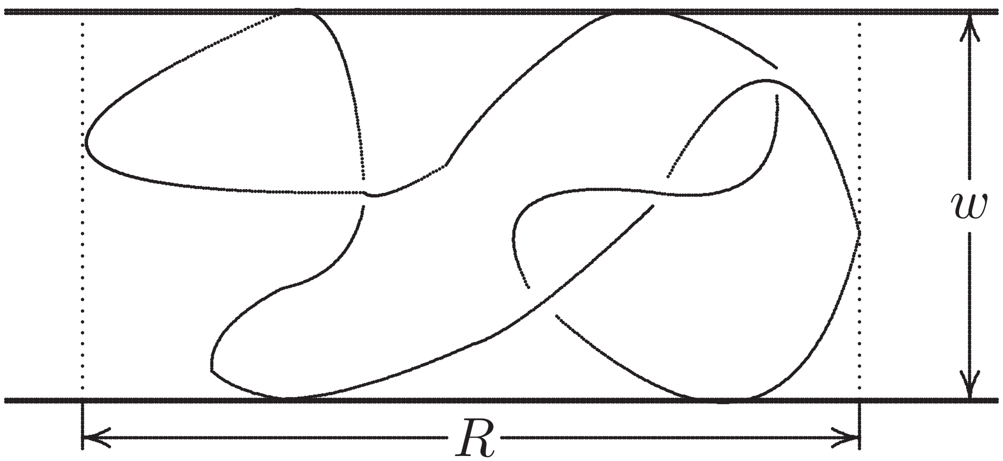
$$p_n(w) p_m(w) \leq p_{n+m+2(w+1)}(w)$$

(2 dimensions, harder in higher dimensions).

- Thus $\lim_{n\to\infty}[p_n(w)]^{1/n} = \mu_w$

- In three and more dimensions, μ_w is the same as for walks in a slab.

SCALING AND FREE ENERGY



$R \sim n^{\nu}$

- Two Length Scales: R and w.

$$\mathcal{F}_w = n^{-1} F(R/w) = w^{-1/\nu} F_1(n^{\nu}/w)$$

- Since $\mathcal{F}_w = \log \mu_w$:

$$\mu_w \approx \mu\, e^{-C w^{-1/\nu}} \approx \mu\,(1 - C w^{-1/\nu}).$$

GROWTH CONSTANTS IN A SLAB L$_w$

- THEOREM: $\lim_{w\to\infty} \mu_w = \mu$ and $\mu_w \approx \mu\,(1 - Cw^{-1/\nu})$.

  (JvR, Orlandini, Whittington 2006).

- Generating function:

$$g_w(t) = \sum_{n\geq 0} p_n(w) t^n \sim |\log(\mu_w t)|^{2-\alpha_w}$$

- This gives the rate $g_w(t) \to g_\infty(t)$ as $w \to \infty$:

$$g_w(t) \approx g_\infty(t)\left(1 - C|\log(\mu_w t)|^{2-\alpha_w}\right)$$

EXPECTED LENGTH OF POLYGONS

- At $t = 1/\mu$:

$$\langle n \rangle_w = t \frac{d}{dt} \log g_w(t) \Big|_{t=1/\mu} \approx C_1 + \frac{C(2-\alpha_w)|\log(\mu_w/\mu)|^{1-\alpha_w}}{1 - C|\log(\mu_w/\mu)|^{2-\alpha_w}}$$

- Noting that $\mu_w/\mu \approx (1 - Cw^{-1/\nu})$ gives:

$$\langle n \rangle_w \approx C_1 + C_2 w^{-(1-\alpha_w)/\nu} + \ldots$$

to leading order.

- This gives the dependence of the mean length of a polygon confined to the slab L_w on w.

- Knotted Polygons: assume that

$$\alpha_{K,w} = \alpha_{\emptyset,w} + N_K$$

EXPECTED LENGTH OF KNOTTED POLYGONS

- One expects that

$$\alpha_{\emptyset,w} \approx 1/2, \qquad \nu \approx 0.58$$

so that $\alpha_{\emptyset,w}/\nu \approx 0.85$.

- Substituting these values show

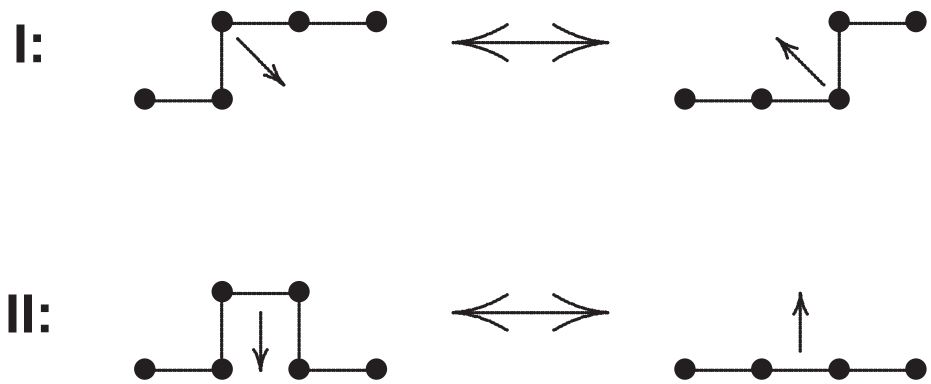
$$\langle n \rangle_{K,w} = \begin{cases} C_1 + O(w^{-(1-\alpha_{\emptyset,w})/\nu}) = C_1 + O(w^{-0.85}) & \text{for unknots} \\ C_2 + O(w^{\alpha_{\emptyset,w}/\nu}) = C_2 + O(w^{0.85}) & \text{for prime knots} \\ C_3 + O(w^{1/\nu}) = C_3 + O(w^{1.70}) & \text{for compound knots} \end{cases}$$

at $t = 1/\mu$.

Can this be tested?

SIMULATING KNOTTED POLYGONS IN A SLAB

The BFACF algorithm: This Monte Carlo algorithm samples along a Markov Chain in the state space of polygons using elementary moves:



THE BFACF ALGORITHM I

The transition probability matrix in a Metropolis style implementation is given by

$$\text{Pr}(\omega \to \omega') = \begin{cases} 1, & \text{if } |\omega| \geq |\omega'|; \\ \frac{|\omega'|^{q-1}}{|\omega|^{q-1}} \min\{1, t^2\}, & \text{otherwise,} \end{cases}$$

where q is a parameter of the algorithm.

- Choose an edge.
- Move the edge perpendicular in one of $2(d-1)$ directions.
- Determine if this is a move of type I or type II
- Accept/Reject this proposed move with probability Pr.

THE BFACF ALGORITHM II

The stationary distribution is

$$\Pi_L(\omega) = \left[\frac{|\omega|^q t^{|\omega|}}{\Phi}\right] \chi_L(\omega)$$

in an ergodicity class L.

THEOREM: The ergodicity classes of the BFACF algorithm, when applied to unrooted lattice polygons in the cubic lattice, are the knot types of the polygons. (JvR + Whittington 1991)

IMPLEMENTATION: Start at a polygon of knot type K, and sample along a Markov Chain in the state space of polygons of knot type K by implementing the elementary moves.

ENTROPIC EXPONENTS FOR KNOTS

- The Number of lattice knots: $p_n(K) \approx A_K n^{\alpha_K - 3} \mu_K^n$
- BFACF can be used to estimate A_K, α_K and μ_K.
-

$$\begin{aligned} \mu(\emptyset) &= 4.6852 \\ \mu(3_1) &= 4.6832 \\ \mu(3_1 \# 3_1) &= 4.6800 \end{aligned}$$

- Test α_K by computing

$$\rho(K_1, K_2) = \frac{\alpha_{K_1} + 1}{\alpha_{K_2} + 1}$$

- $\rho(K_1, K_2) = 1$ consistent with $\alpha_{K_1} = \alpha_{K_2}$.
- $\rho(K_1, \emptyset) = 1.75$ consistent with $\alpha_{K_1} = \alpha_\emptyset + 1$.
- $\rho(K_1, 3_1) = 1.44$ consistent with $\alpha_{K_1} = \alpha_{3_1} + 1$.

THE ENTROPIC EXPONENT

- The BFACF algorithm gives

$$\begin{aligned} \rho(3_1,\emptyset) &= 1.69 \pm 0.11 \\ \rho(4_1,\emptyset) &= 1.67 \pm 0.11 \\ \rho(6_2,\emptyset) &= 1.75 \pm 0.05 \end{aligned}$$

consistent with $\alpha(K) = \alpha(\emptyset) + 1$.

- Other examples

$$\begin{aligned} \rho(3_1,4_1) &= 1.01 \pm 0.11 \\ \rho(3_1\#3_1,3_1\#4_1) &= 0.93 \pm 0.07 \\ \rho(3_1\#3_1,3_1) &= 1.25 \pm 0.16 \end{aligned}$$

consistent with $\alpha(K) = \alpha_\emptyset + N_K$.

- These data strongly support the notion that

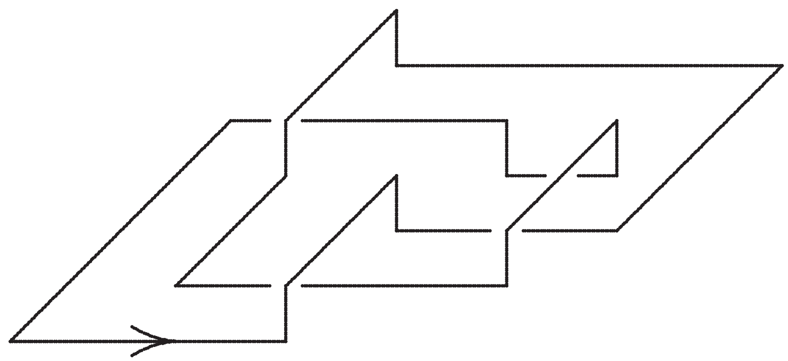
$$\alpha_K = \alpha_\emptyset + N_K$$

where N_K is the number of prime components in the knot.

- The Amplitude A_K is also independent of the knot type (Orlandini, Tesi, JvR, Whittington 1996).

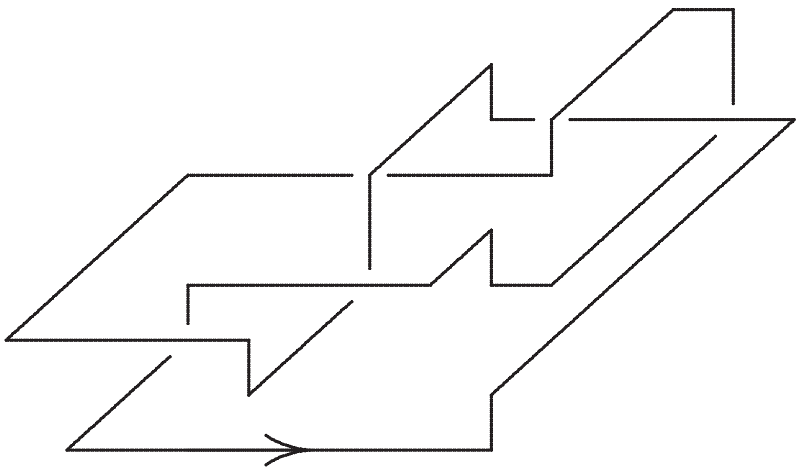
THE BFACF ALGORITHM IN A SLAB

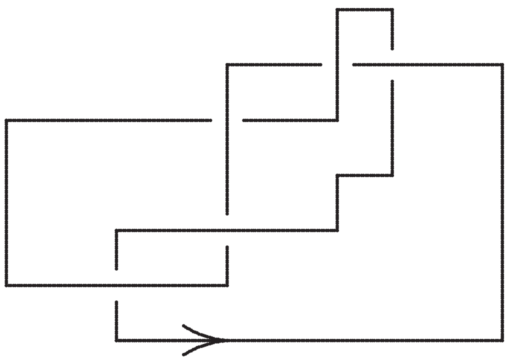
THEOREM: The ergodicity classes of the BFACF algorithms, when applied to unrooted lattice polygons confined to the slab L_w with $w > 1$, are the knot types of the polygons. (JvR 2006)



OUTLINE OF PROOF I

Lattice regular projection of a lattice knot:



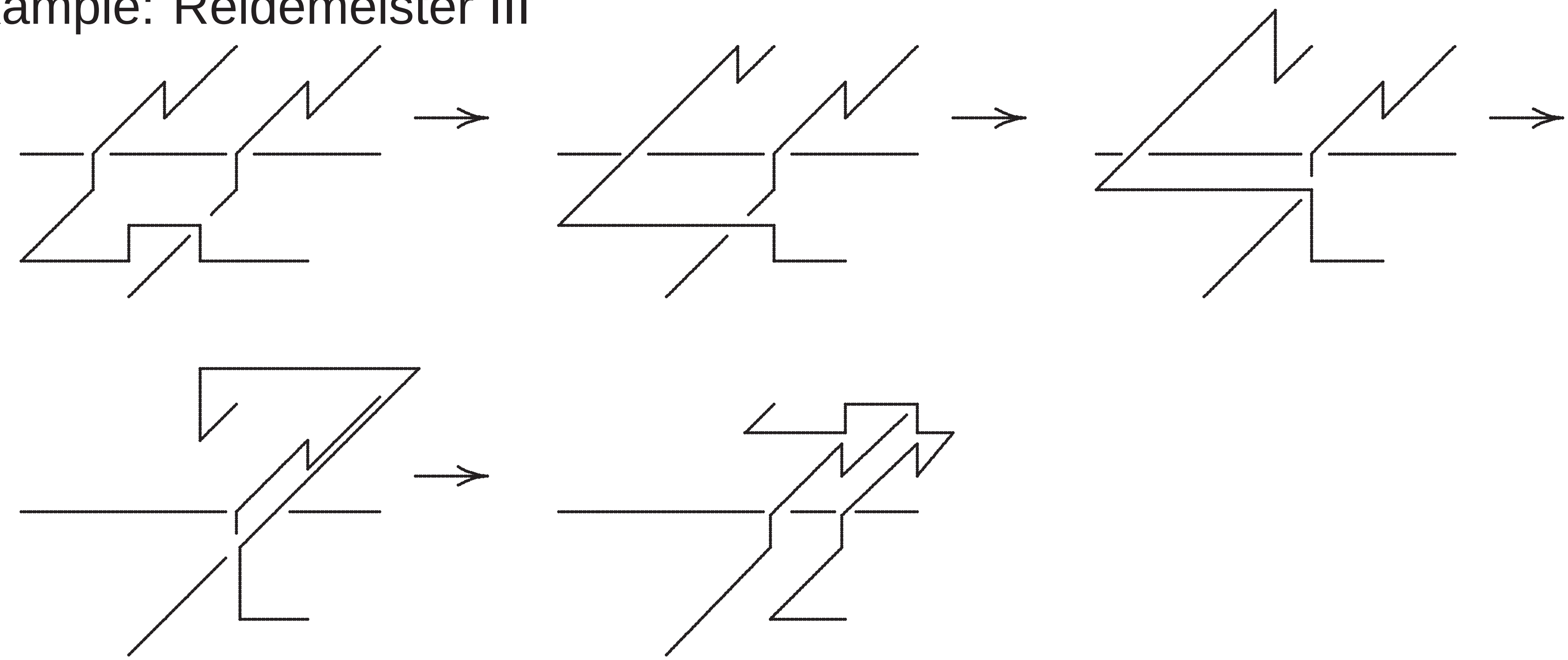


THEOREM: By applying elementary moves in the BFACF algorithm, a lattice knot can be transformed into a lattice knot with a regular lattice projection in the bottom bounding plane of L_w.

OUTLINE OF PROOF II

THEOREM: By applying elementary moves from the BFACF algorithm to a lattice knot in L_w with a regular lattice knot projection, Reidemeister moves can be performed on the knot projection, provided that $w > 1$.

Example: Reidemeister III



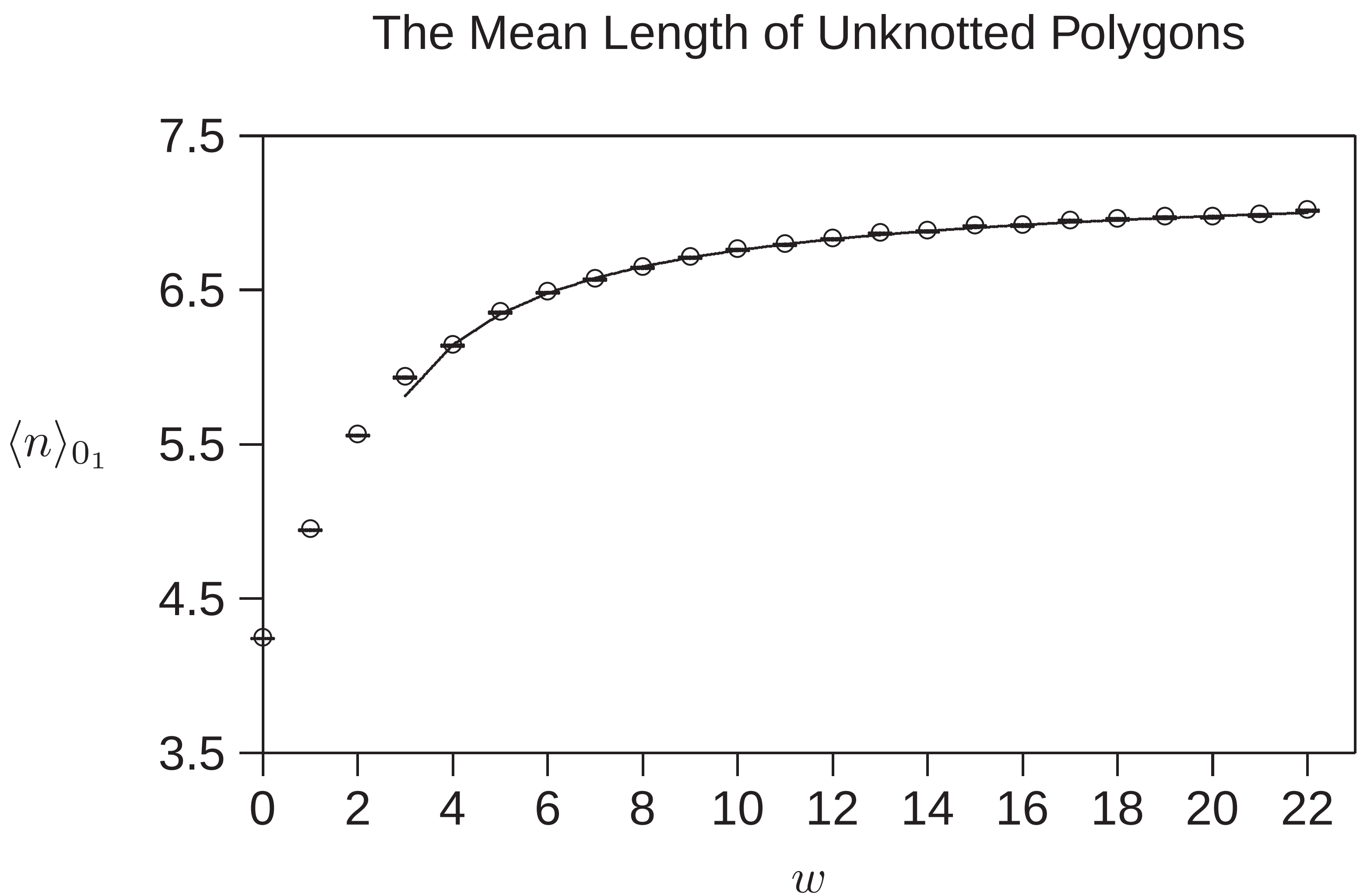
OUTLINE OF PROOF III

- Two lattice knots with equivalent lattice knot projection in the bottom bounding plane of L_w can be made identical by application of elementary moves from the BFACF algorithm.

- The BFACF algorithm can now be used to sample polygons of knot types K in slabs L_w ($2 \leq w \leq 22$).

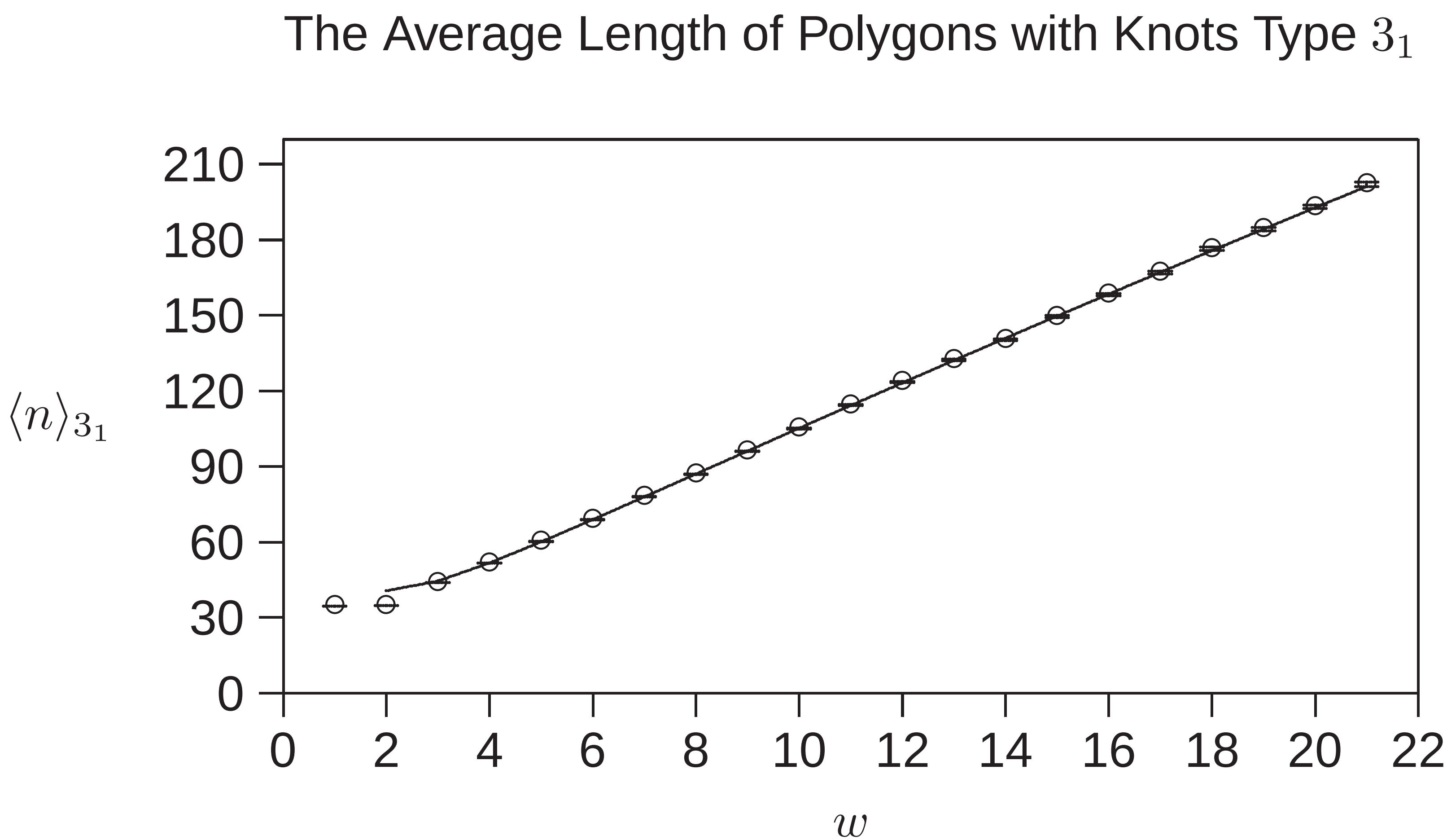
- Expectations for $\langle n \rangle_w$:
  - Approach a constant if $K = \emptyset$;
  - Divergent and Concave of w if K is prime;
  - Divergent and Convex of w if K is compound.

UNKNOTTED POLYGONS



$$\langle n \rangle_{0_1} \approx C_1 + C_2 w^{-0.85} + \dots \qquad [C_1 = 7.248 \pm 0.007].$$

TREFOILS



$\langle n \rangle_{3_1} \approx C_1 + C_2 w^{0.85} + \ldots \qquad [C_1 = -11.45 \pm 0.04].$

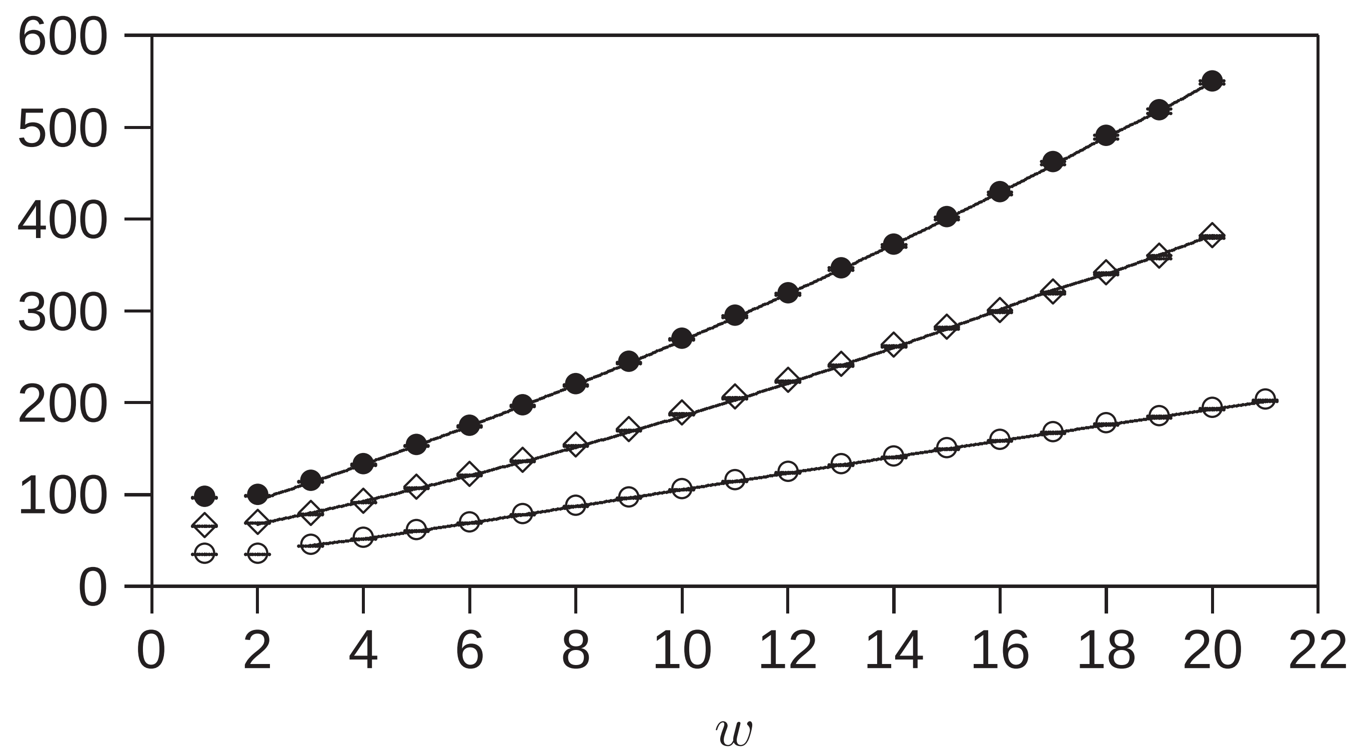
COMPOUNDED TREFOILS

Average Lengths of Compounded Trefoils

$\langle n \rangle_{3_1^+ \# 3_1^+ \# 3_1^+}$ (•)

$\langle n \rangle_{3_1^+ \# 3_1^+}$ (◇)

$\langle n \rangle_{3_1^+}$ (○)



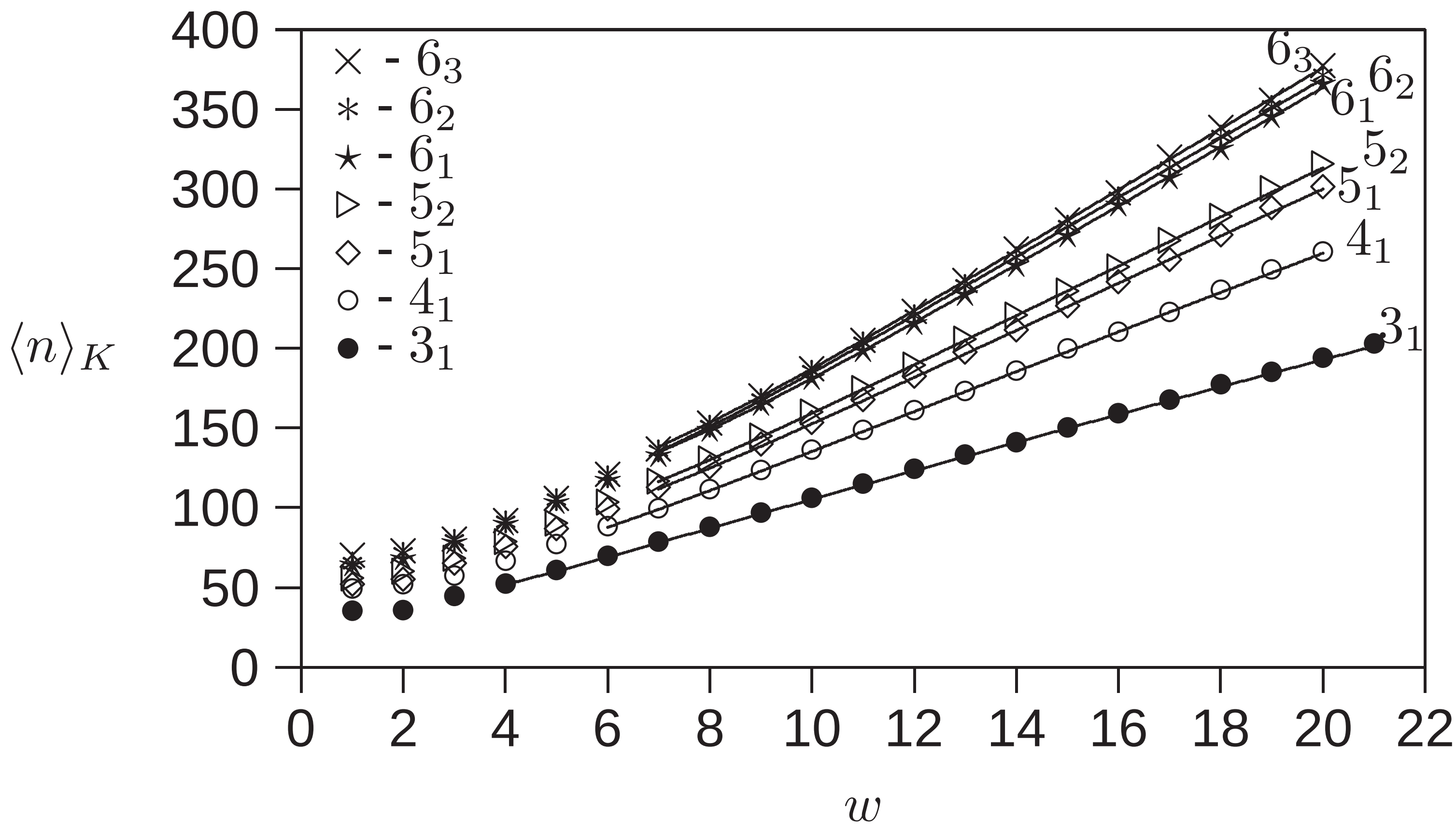
Data fitted by:

$\langle n \rangle_{3_1} = C_1 + C_2 w^{0.85} + \ldots$ for trefoils

$\langle n \rangle_K = C_1 + C_2 w^{1.70} + \ldots$ when K is compound

OTHER PRIME KNOTS

Average Lengths of Polygons of Non-Trivial Knot Types



$$\langle n \rangle_K \approx C_1 + C_2 w^{0.85} + \ldots$$

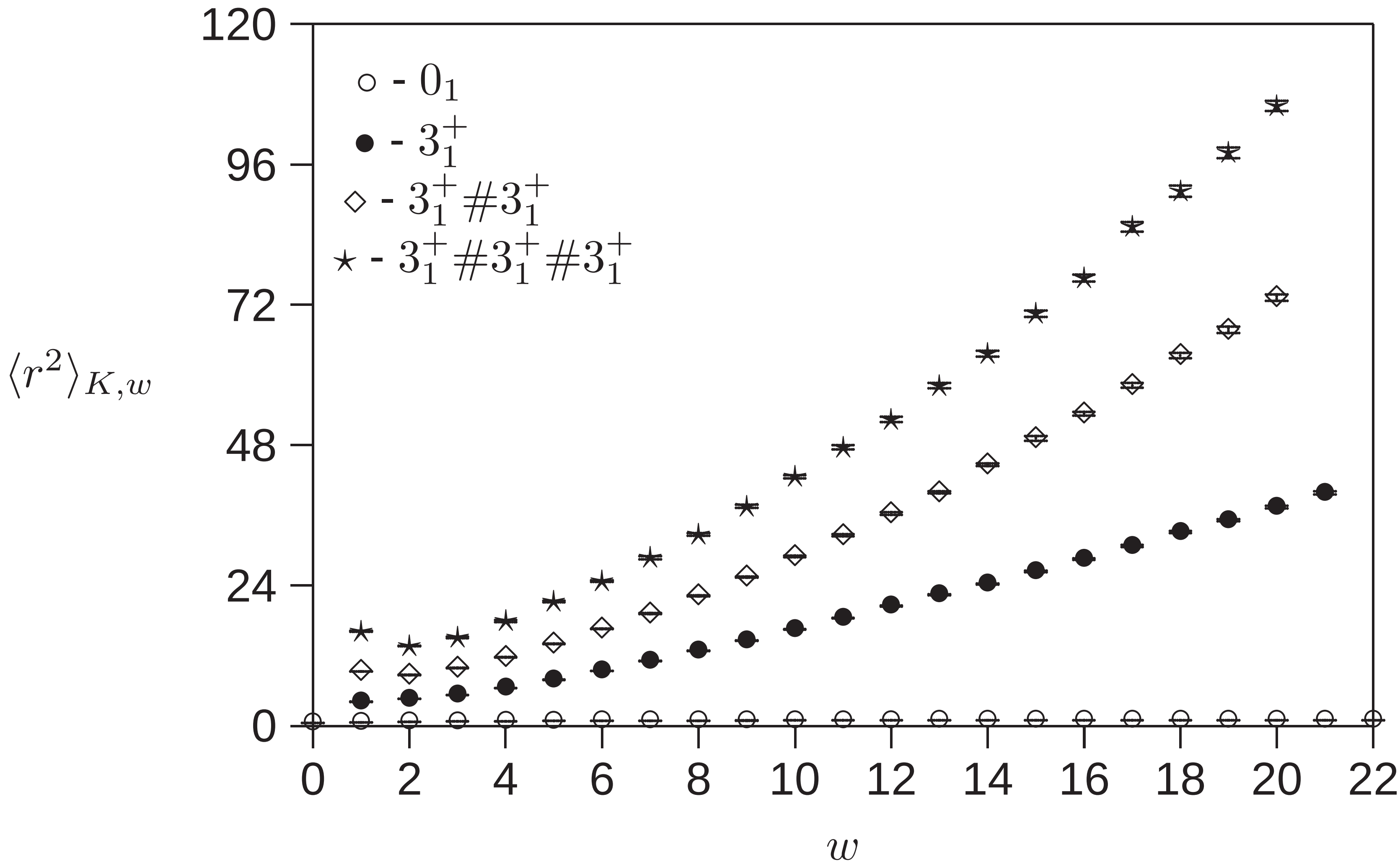
METRIC PROPERTIES

Metric properties in this ensemble: $p_n(r^2, w)$ is the number of polygons of length n in L$_w$ with square radius of gyration r^2.

$$\langle r^2 \rangle_w = \frac{\sum_{n,r^2} r^2 p_n(r^2, w) t^n}{\sum_{n,r^2} p_n(r^2, w) t^n}$$

The mean square radius of gyration increases with w at $t = 1/\mu$.

MEAN SQUARE RADIUS OF GYRATION



AMPLITUDE RATIO

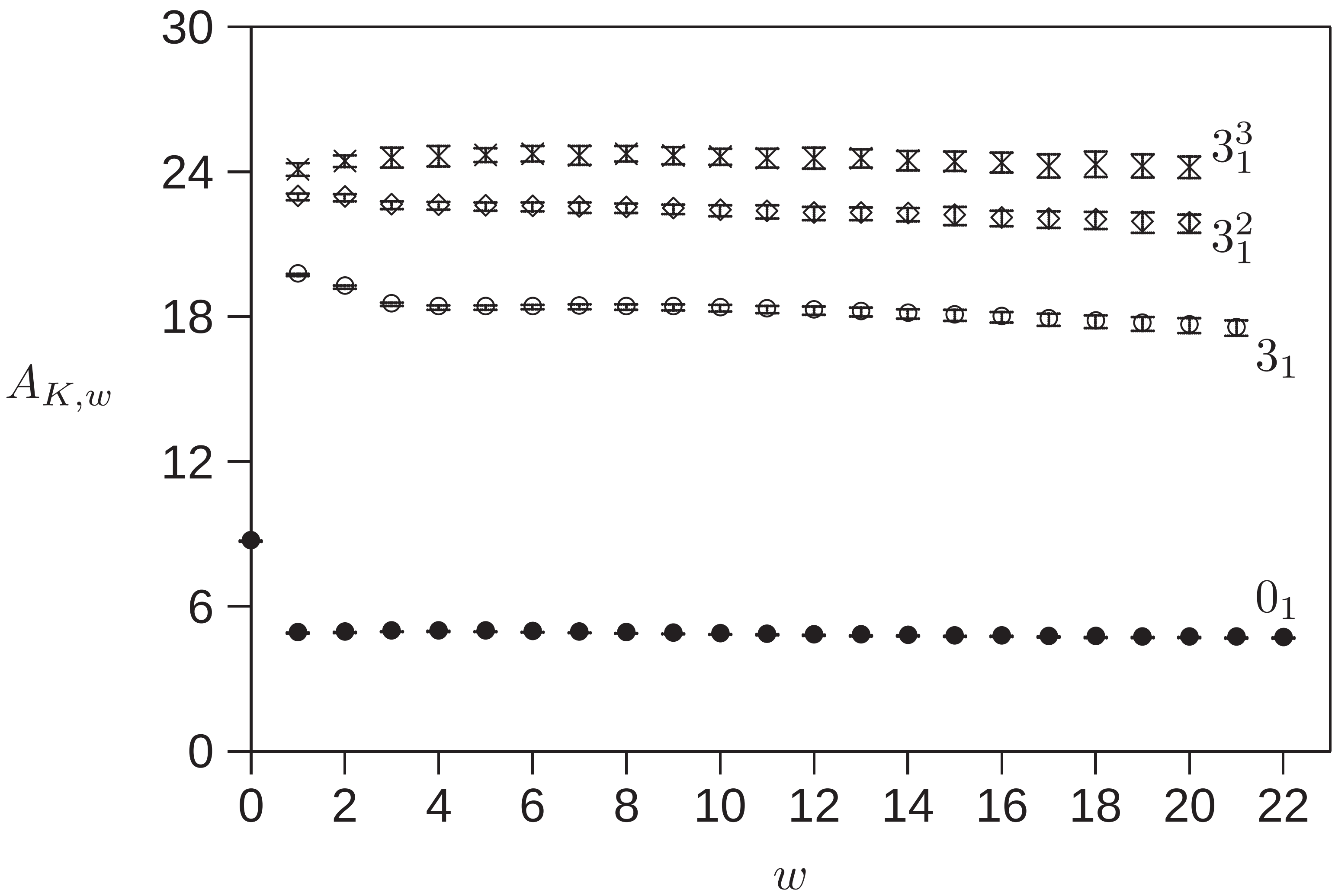
Define $\langle S_{xy} \rangle_w$ to be the mean span in the XY-plane.

- The Amplitude Ratio $A_{K,w}$ is the dimensionless quantity

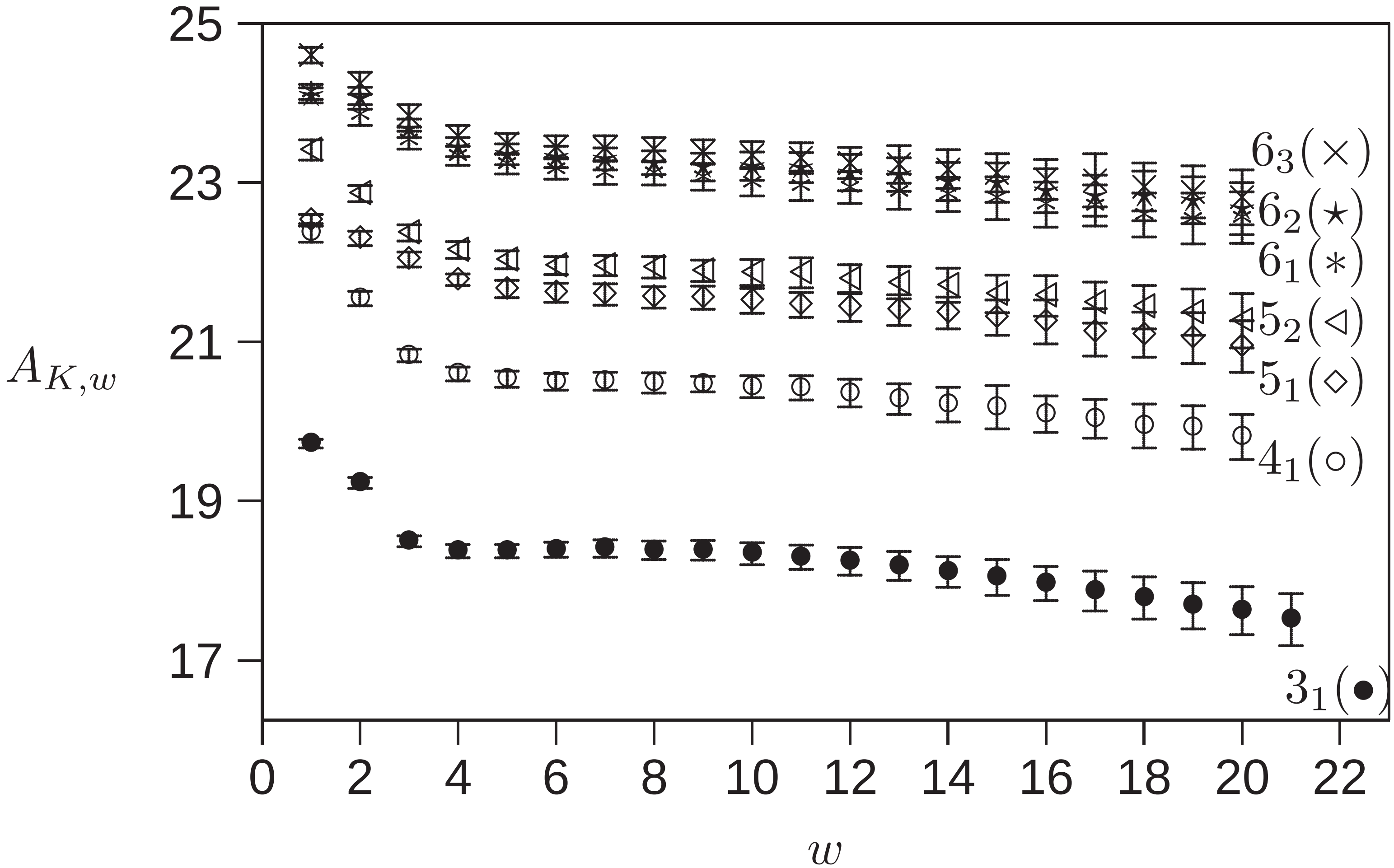
$$\boxed{A_{K,w} = \frac{\langle S_{xy} \rangle_w^2}{\langle r^2 \rangle_w}}$$

- For small w the polygon is spread out in the XY-plane.
- For large w the polygon will not interact with the slab.
- A knotted polygon is ”swollen” for small w, thus a larger amplitude ratio.

AMPLITUDE RATIOS FOR TREFOILS



AMPLITUDE RATIOS FOR OTHER KNOTS



AMPLITUDE RATIOS

Three phases:

1) Small w: Declining $A_{K,w}$.

Very strong interaction between knot and the slab.

2) Intermediate w: Constant $A_{K,w}$.

Strong interaction between knot and the slab.

3) Large w: Slowly declining $A_{K,w}$.

Weak interaction between the knot and the slab.

AVERAGE AMPLITUDES

Knot	$A_{K,4}$	$A_{K,10}$	$\langle A_{K,w} \rangle$
0_1	$4.952(21)$	$4.834(19)$	4.90
3_1	$18.499(69)$	$18.343(138)$	18.38
4_1	$20.599(85)$	$20.438(141)$	20.51
5_1	$21.781(71)$	$21.519(155)$	21.61
5_2	$22.156(106)$	$21.872(161)$	21.97
6_1	$23.342(119)$	$23.003(171)$	23.15
6_2	$23.446(122)$	$23.209(176)$	23.30
6_3	$23.589(128)$	$23.352(164)$	23.45
$3_1^+ \# 3_1^+$	$22.588(156)$	$23.377(230)$	22.50
$3_1^+ \# 3_1^-$	$22.565(149)$	$22.368(232)$	22.50
$3_1^+ \# 3_1^+ \# 3_1^+$	$24.645(429)$	$24.619(223)$	24.68

- Averages for $w \in [4, 10]$ (constant regime).
- Increasing with Crossing Number - the knot is more swollen.

CONCLUSIONS

- Scaling arguments can predict the mean length of a knotted polygon in a slab at activity $t = 1/\mu_\emptyset$.
- The BFACF algorithm can be used to sample polygons of fixed knot type in a slab.
- The Unknot does not interact with the slab as $w \to \infty$.
- Knotted polygons do interact with the slab as $w \to \infty$.
- Prime knots interact differently with the slab, compared to compound knots.
- Knots are swollen in the XY-plane in narrow slabs.