Polymers, polygons and pattern theorems

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Joint work with:

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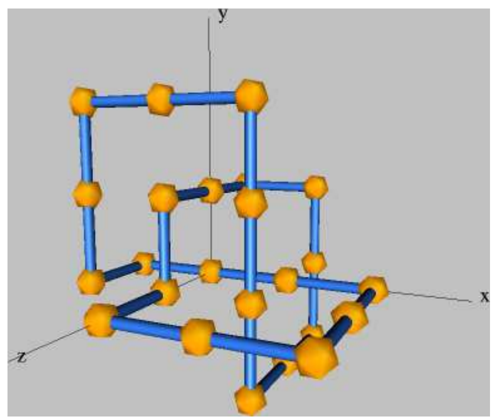
Modelling ring polymers on a lattice

Lattice polygons



Counting polygons on Z^3

We can count polygons with n edges up to translation.

$$p_4 = 3 \quad p_6 = 22 \quad p_8 = 207$$

Large n behaviour

Classic result due to John Hammersley:

$$\log 3 \le \lim_{n\to\infty} n^{-1} \log p_n = \kappa \le \log 5$$

Counting unknotted polygons on Z^3

If we write p_n^o for the number of *unknotted* polygons with n edges then

$$p_4^o = 3$$

$$p_6^o = 22$$

and in fact $p_n^o = p_n$ if $n < 24$ (Diao).

Unknotted polygons and pattern theorems

$$\lim_{n \to \infty} n^{-1} \log p_n^o = \kappa_o$$

and

$$\kappa_o < \kappa$$

which establishes the FWD conjecture for this model.

Unknotted polygons and pattern theorems

$$\lim_{n\to\infty} n^{-1} \log p_n^o = \kappa_o$$

and

$$\kappa_o < \kappa$$

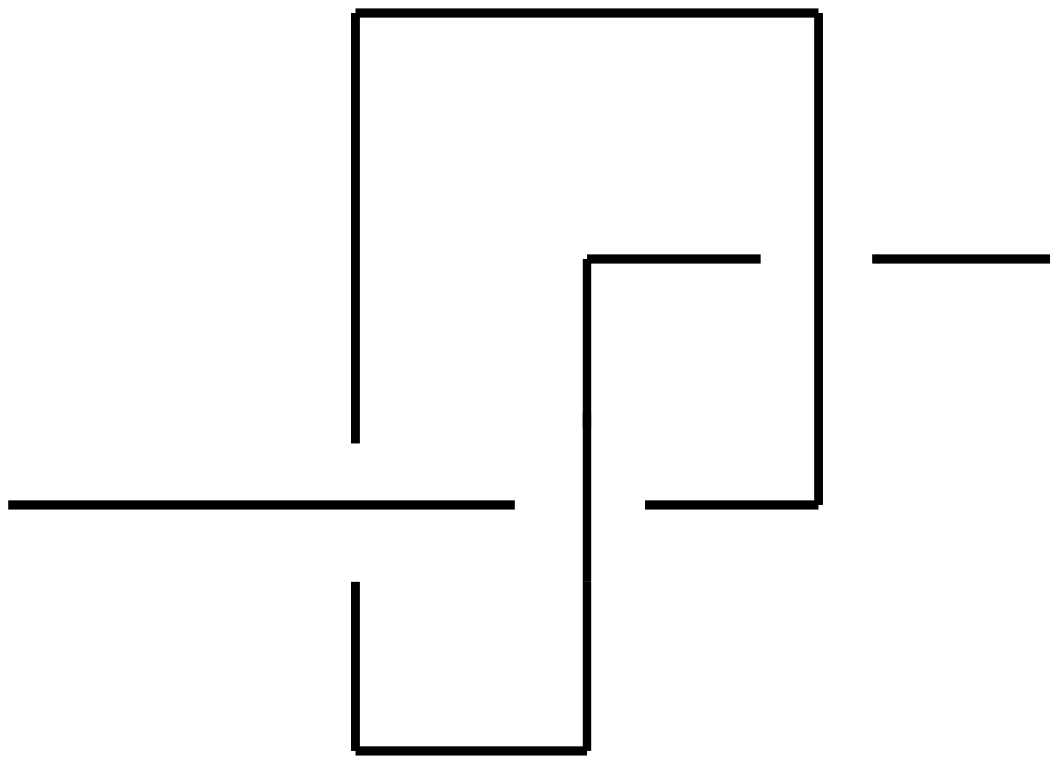
Idea of proof:

1. no antiknots

2. knotted ball pairs

3. Kesten's pattern theorem

A tight trefoil pattern P_{3_1}



Open question: Find good bounds on $\kappa - \kappa_O$

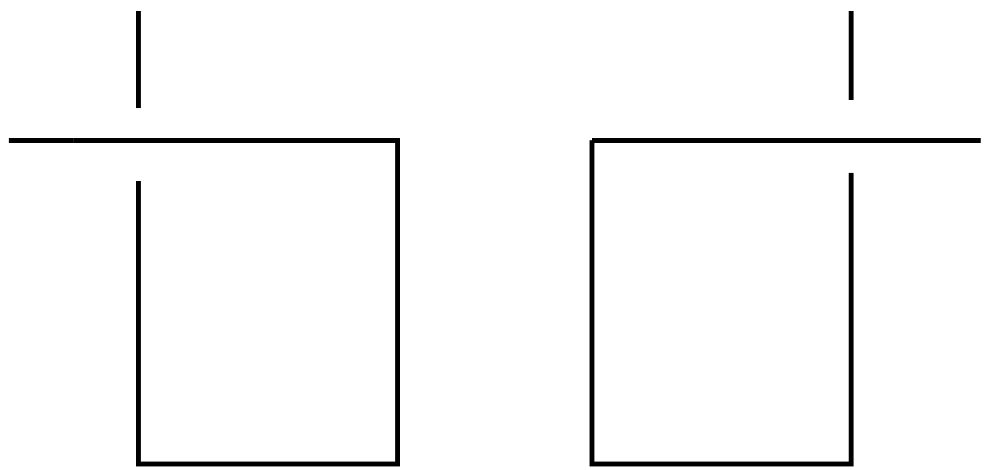
Writhe

Construct two mirror image patterns that contribute $\pm\omega$ independently with equal probability. The total writhe is given by

$$Wr = Wr_{external} + \sum_k Wr_k$$

where $Wr_k = \pm\omega$ comes from the kth pattern. If the writhe is zero the external writhe must be cancelled by the sum of the pattern writhes. This has probability at most $1/\sqrt{\epsilon n}$ for some $\epsilon > 0$.

Patterns contributing writhe



positive writhe　　negative writhe

Writhe

A pattern theorem plus coin tossing establishes that there exists an $A > 0$ such that

$$\langle |Wr| \rangle_n \geq An^{1/2}$$

for sufficiently large n.

Open question: Is this also true for unknotted polygons?

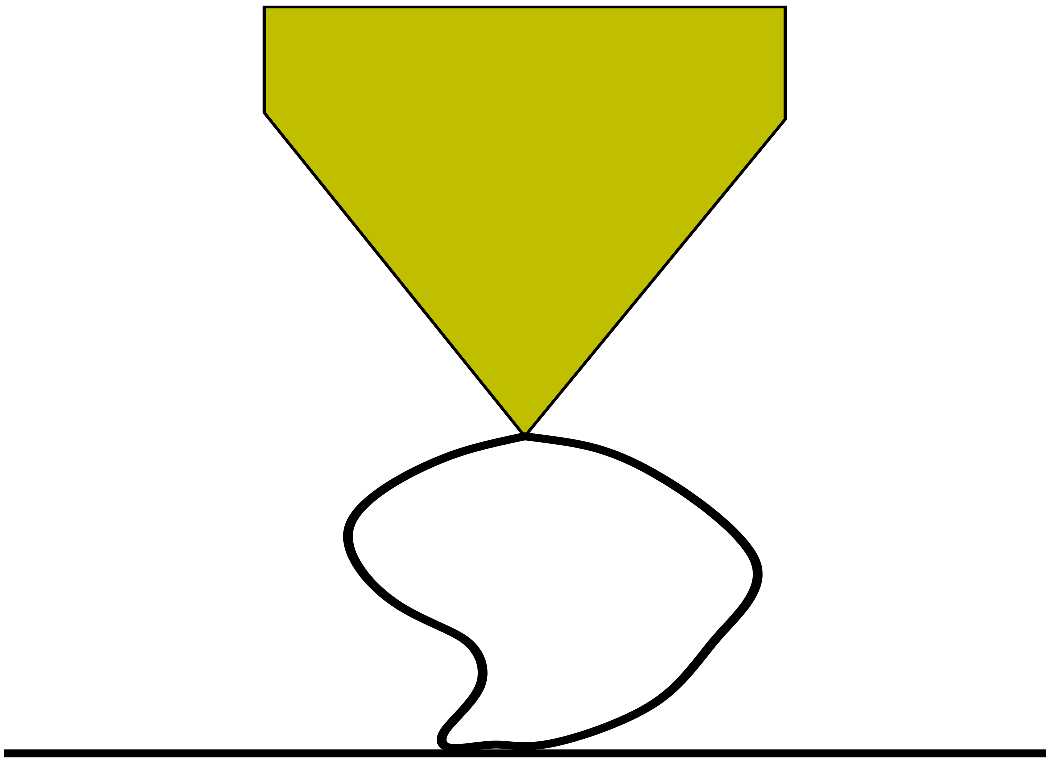
Polygons with a tensile force in the z-direction

Suppose that $p_n(s)$ is the number of n-edge polygons with span s in the z-direction. The polygons are not equally weighted but have partition function

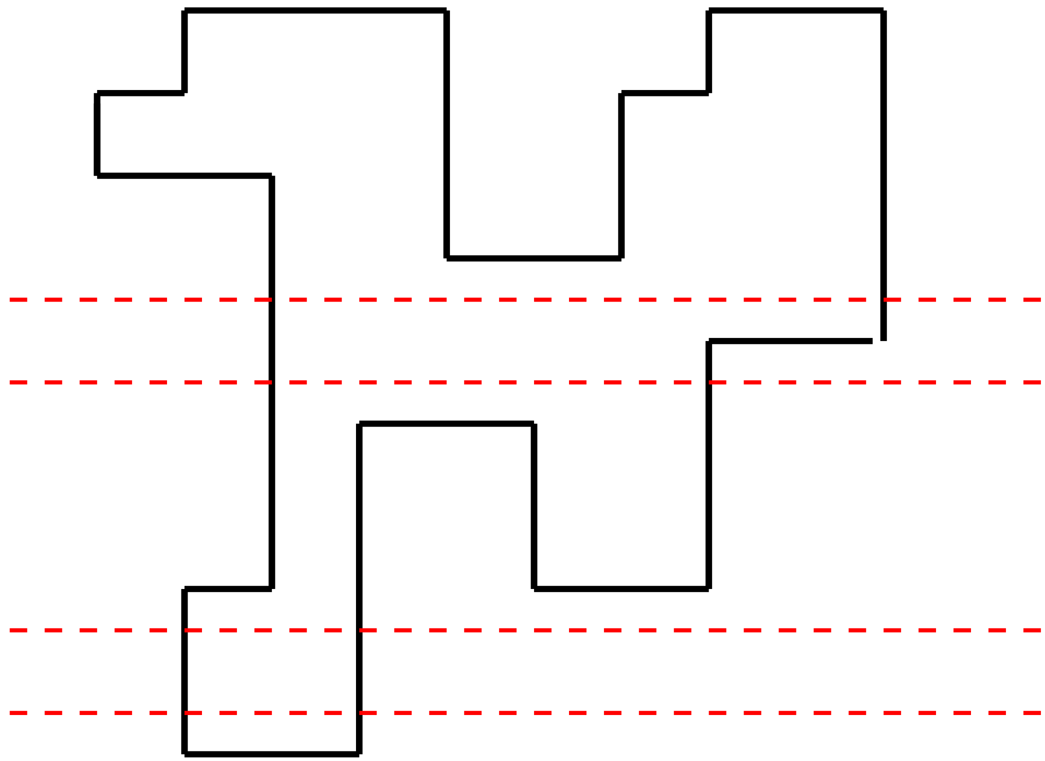
$$Z_n(y) = \sum_s p_n(s) y^s$$

where $y = \exp[\bar{f}/kT] = \exp(f)$. If $f > 0$ then $y > 1$ and polygons with larger spans have larger weights.

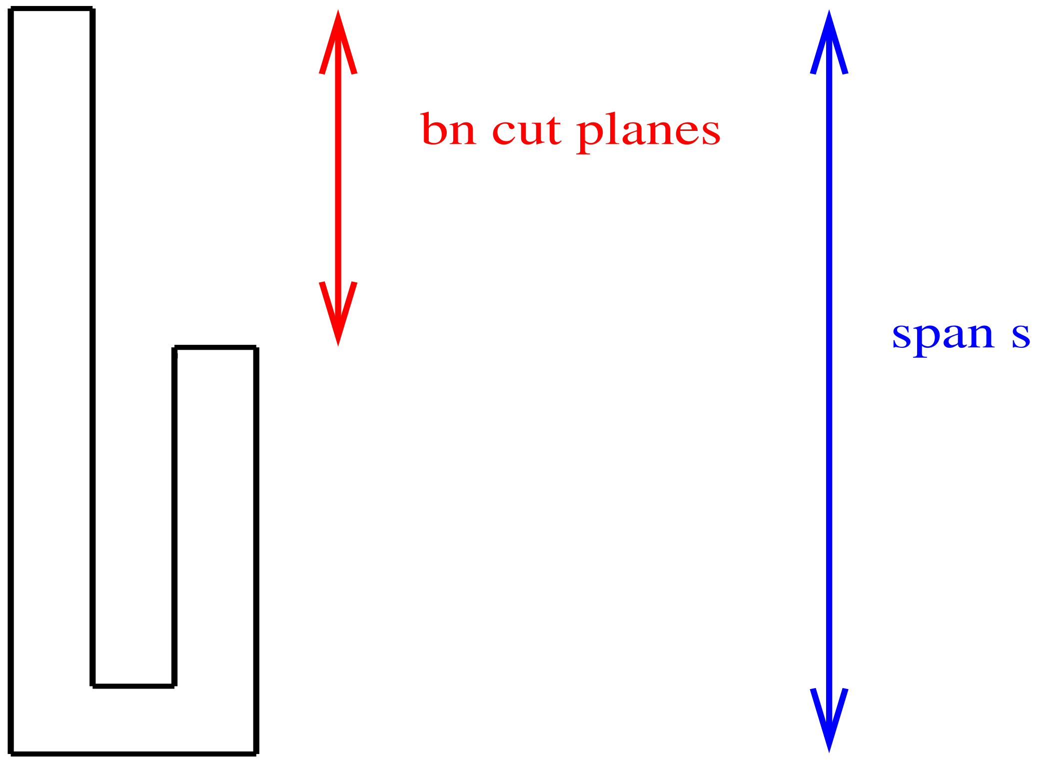
What's the experiment?



Cut planes and a pattern theorem

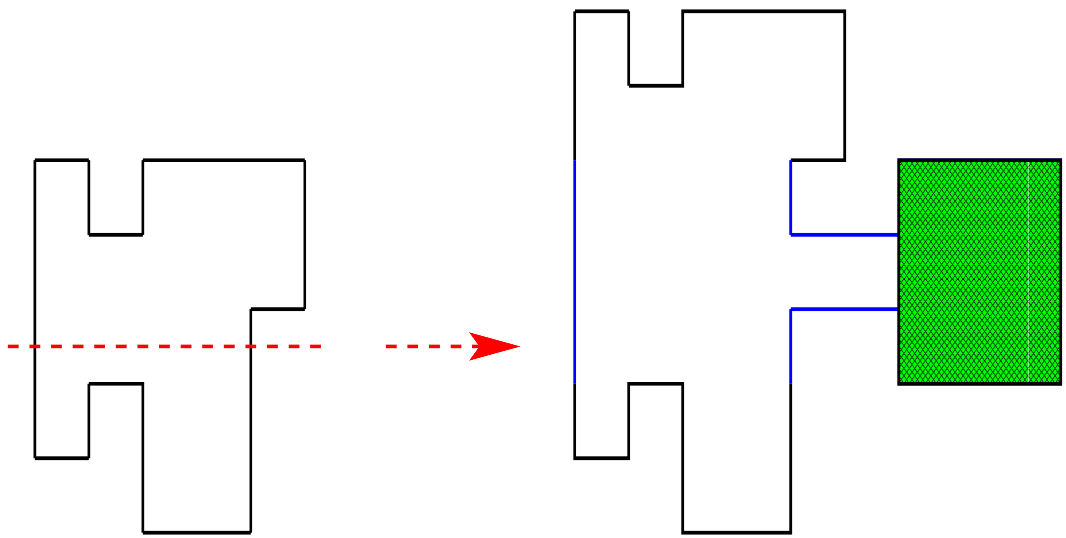


Span of a stretched polygon



For sufficiently large forces polygons have a positive density of cut planes.

Inserting a pattern



If the polygon has at least bn cut planes then we can insert an patterns ($a < b$) in at least $\binom{bn}{an}$ ways.

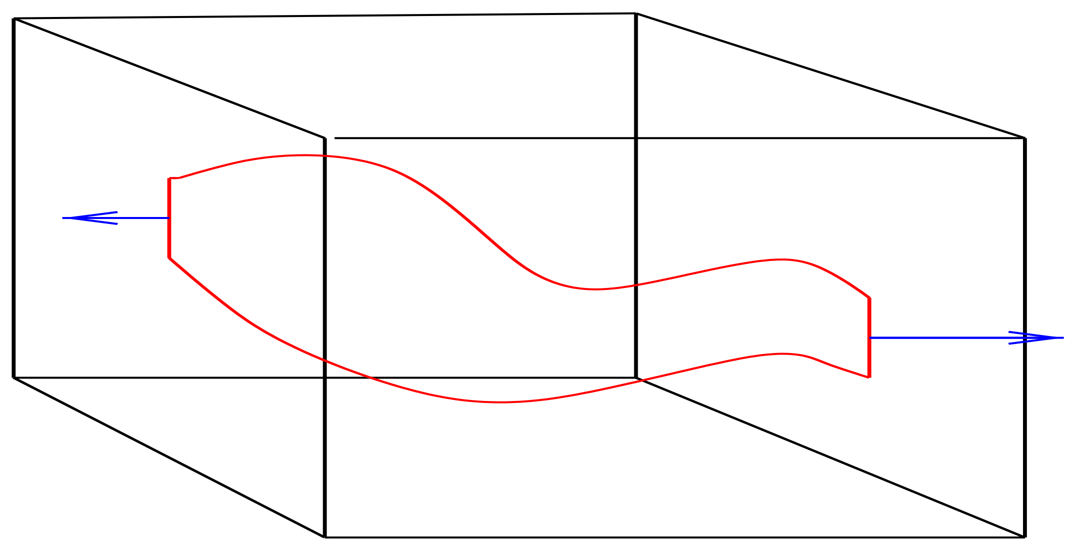
This is enough to prove that polygons not containing the pattern are exponentially rare and that all except exponentially few polygons contain the pattern a positive density of times.

Then choose the pattern to be knotted to show that almost all polygons subject to a sufficiently large tensile force are knotted.

Can we say anything about small forces?

We can do something for the special case of a polygon confined to a prism.

The prism is infinite in the direction in which the force is applied (say the z-direction) but finite in the other two coordinate directions.



Now we can prove a pattern theorem for any extensional force and so show that polygons in a prism are knotted for any such force.