Lattice Path Counting: where Enumerative Combinatorics and Statistical Mechanics meet

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Genomics, Pattern Avoidance, and Statistical Mechanics

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Topic Outline

1. Counting
2. A Crash Course in Statistical Mechanics
3. Exact Counting
   - Lattice Paths and Generating Functions
   - Walks in a Triangle
   - Lattice Path Models of Polymers
   - Pulling Polymers off a Surface
4. Approximate Counting
   - Sampling of Simple Random Walks
   - Sampling of Self-Avoiding Walks
   - Applications

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- India: zero, decimal system
  1, 2, . . . , 9, 10, 11, . . .

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- Roman Empire:
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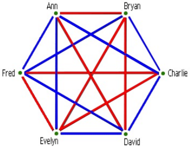

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    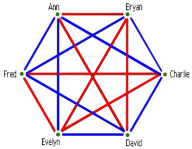

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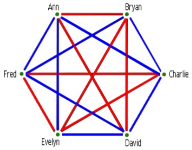

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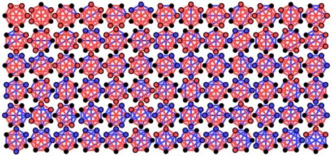

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    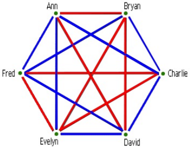

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    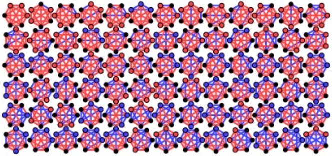

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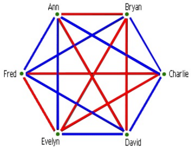

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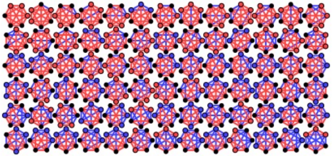

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- A third question
  - *Approximately* how many structures are there asymptotically?

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    - Example: N-step lattice paths on the square lattice starting at the origin. For simple random walks $c_n = 4^n$.

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can be rescaled when needed (permutations, permanents, ...)

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- c_n gets generalised to the *partition function*

$$Z_n(T) = \sum_{\phi\in\Omega_n} w_\phi(T) \qquad \text{so that } c_n = Z_n(T=\infty)$$

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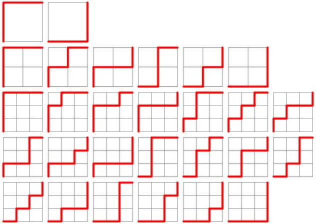

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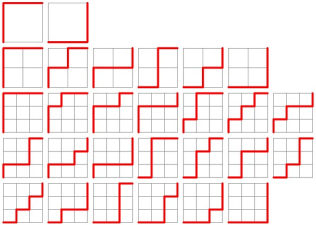

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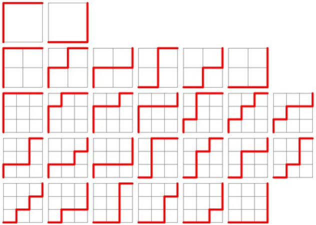

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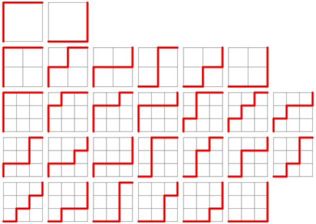

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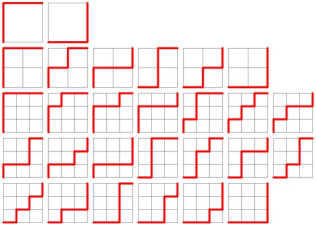

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$$Z(x) = \frac{1}{\sqrt{1-4x}}$$

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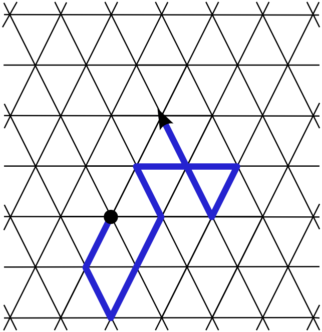
Walks on the Triangular Lattice



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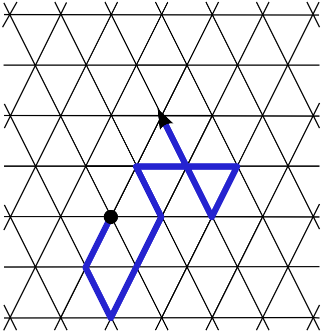

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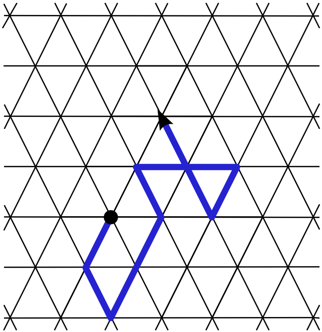
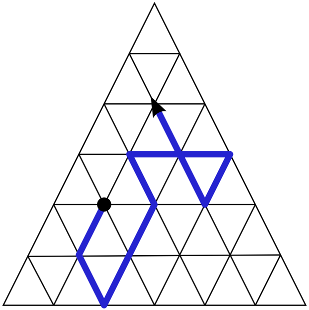


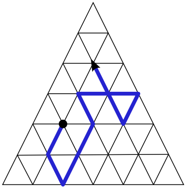
$$c_n = 6^n \,, \quad Z(x) = 1/(1-6x)$$

Walks in a Triangle



Restrict to a triangular domain

Counting Walks



Parameters

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- Number of steps n
- Starting point **a**
- End point **b**

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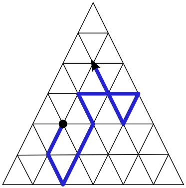

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Number of n-step walks from **a** to **b** within triangle of side-length L

$$c_{n,L}^{\mathbf{a},\mathbf{b}}$$

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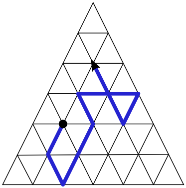

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$$c_{n,L}^{\mathbf{a},\mathbf{b}}$$

No general closed form known for $c_{n,L}^{\mathbf{a},\mathbf{b}}$ or associated generating function

$$Z_L^{\mathbf{a},\mathbf{b}}(t) = \sum_n c_{n,L}^{\mathbf{a},\mathbf{b}} t^n$$

A Special Case

Starting the walks in a corner of the triangle, we find

Theorem (Mortimer, Prellberg, 2015)

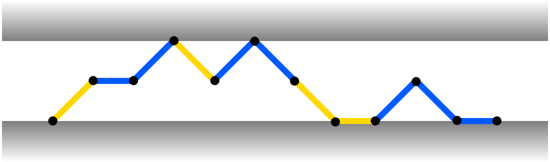
The generating function which counts n-step walks in a triangle of side-length L starting at a chosen corner with no restrictions on the endpoint is given by

$$\frac{(1-p^3)(1-p^{1+L})}{(1-p)(1-p^{3+L})}$$

where

$$p = \frac{1-2t-\sqrt{(1+2t)(1-6t)}}{4t}$$

Bi-Colored Motzkin Paths



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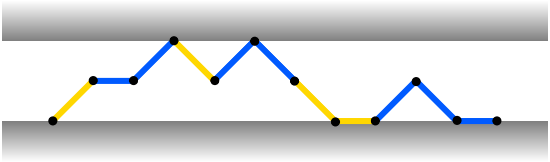
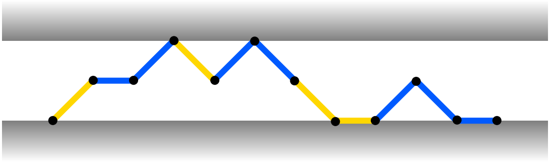


Corollary (Mortimer, Prellberg, 2015)

n-step walks starting in a corner of a triangle of odd side-length $L = 2H + 1$ with arbitrary endpoint are in one-to-one correspondence with bi-colored n-step Motzkin paths in a strip of height H.

Bi-Colored Motzkin Paths



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There is only a generating function proof, and no direct mapping is known.

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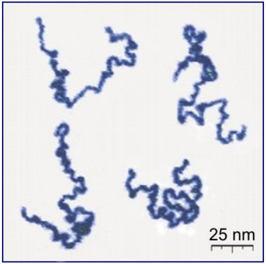

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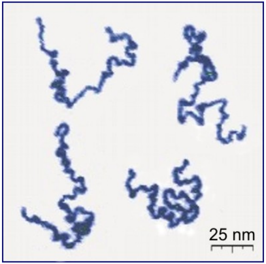

Lattice Paths

- Physical space $\rightarrow$ cubic lattice
- Ghost polymer $\rightarrow$ random walk

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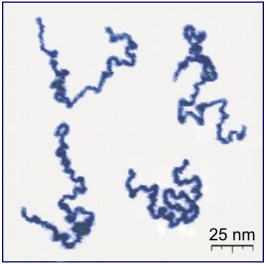

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Self-Avoiding Walks (SAW)

- Polymer with Excluded Volume $\rightarrow$ self-avoiding random walk

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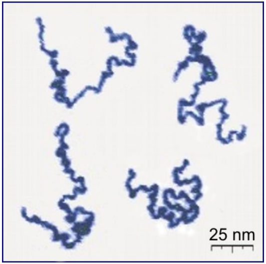

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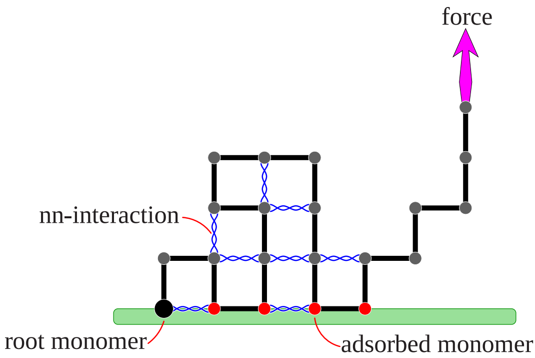
Interacting Self-Avoiding Walks (ISAW)

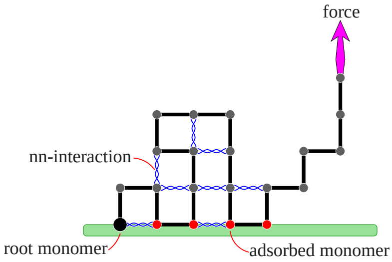
- Quality of solvent → interactions
- Model for the collapse of polymers

“Realistic” Lattice Models of Polymers



A self-avoiding walk lattice model of an interacting polymer tethered to a sticky surface under the influence of a pulling force

Counting and Density of States



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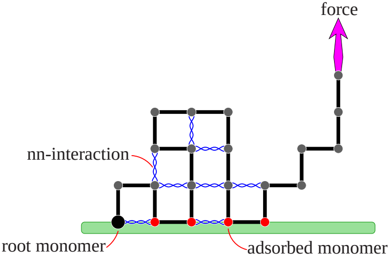

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- Physicists relate this to the Density of States and can extract from this lots of interesting thermodynamic information

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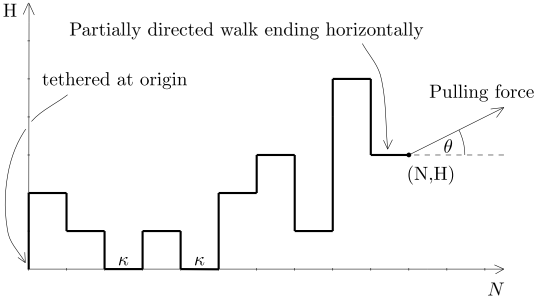
Pulling Polymers off a Surface

- A partially directed walk model of a polymer tethered to a sticky surface under the influence of a pulling force



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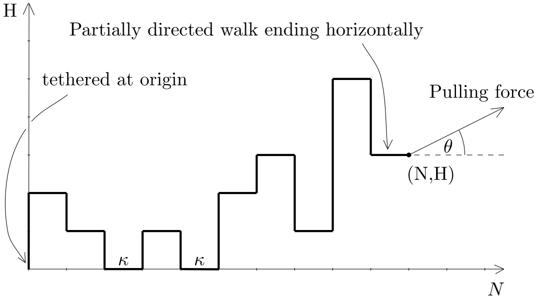
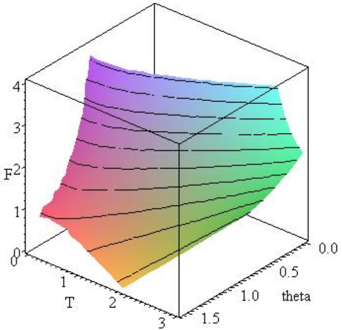
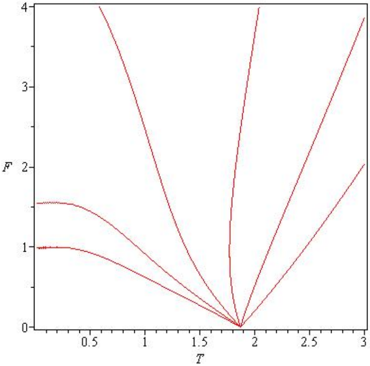


- This model is exactly solvable (Osborn, Prellberg, 2010)

Varying the Pulling Angle





- Thermal desorption at $T = 1/\log(1+\sqrt{2}/2) \approx 1.87$

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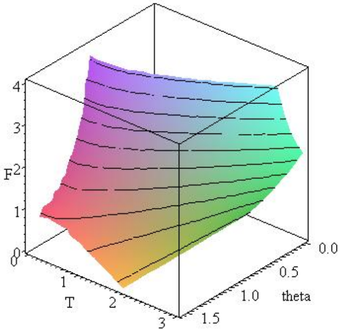

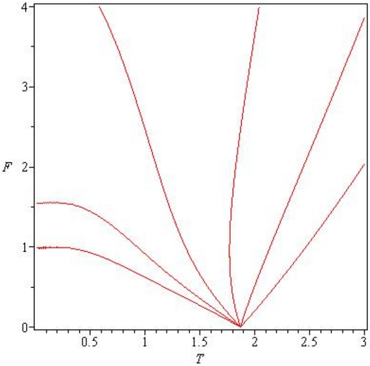

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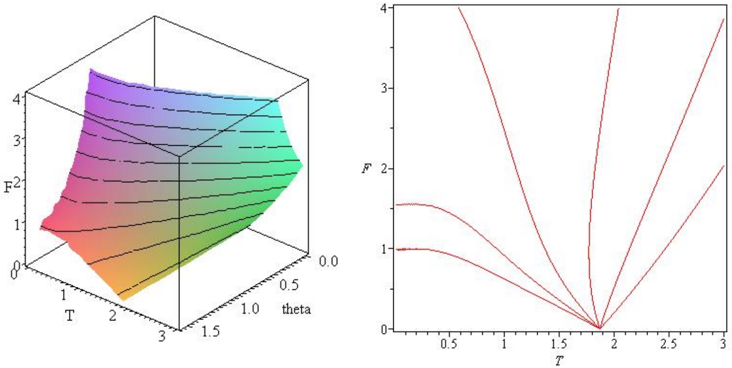

- Thermal desorption at $T = 1/\log(1+\sqrt{2}/2) \approx 1.87$
- Vertical pulling, $\theta = 90^o$ (left curve):
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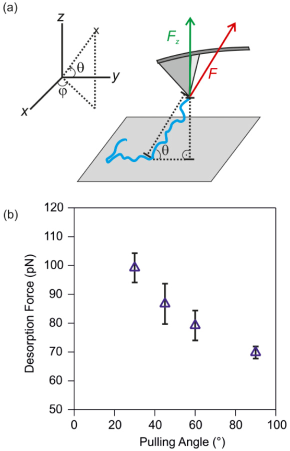
- Horizontal pulling, $\theta = 0^o$ (right curve):
  Increasing F disfavours desorption

Varying the Pulling Angle



REVIEW OF SCIENTIFIC INSTRUMENTS **88**, 033705 (2017)

Pulling angle-dependent force microscopy

L. Grebíková, H. Gojzewski, B. D. Kieviet,[a)] M. Klein Gunnewiek, and G. J. Vancso[b)]
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(Received 22 November 2016; accepted 28 February 2017; published online 20 March 2017)

In this paper, we describe a method allowing one to perform three-dimensional displacement control in force spectroscopy by atomic force microscopy (AFM). Traditionally, AFM force curves are measured in the normal direction of the contacted surface. The method described can be employed to address not only the magnitude of the measured force but also its direction. We demonstrate the technique using a case study of angle-dependent desorption of a single poly(2-hydroxyethyl methacrylate) (PHEMA) chain from a planar silica surface in an aqueous solution. The chains were end-grafted from the AFM tip in high dilution, enabling single macromolecule pull experiments. Our experiments give evidence of angular dependence of the desorption force of single polymer chains and illustrate the added value of introducing force direction control in AFM. *Published by AIP Publishing.* [http://dx.doi.org/10.1063/1.4978452]

IV. CONCLUSIONS

We describe in this study the design and implementation of performing directional force spectroscopy experiments by AFM. By modifying the built-in functions of a standard AFM instrument, we were able to control the cantilever trajectory. This approach has been demonstrated by a case study on the angle-dependent desorption of an end-grafted polymer chain. The polymer response to the external force exerted at various pulling angles with respect to the substrate has been addressed. By employing this technique in single molecule force spectroscopy experiments, we obtained experimental evidence for theoretically predicted enhancement of polymer adhesion while decreasing the pulling angle with respect to planar substrate surfaces.[18,33]

Outline

1. Counting
2. A Crash Course in Statistical Mechanics
3. Exact Counting
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   - Walks in a Triangle
   - Lattice Path Models of Polymers
   - Pulling Polymers off a Surface
4. Approximate Counting
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   - Applications

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Simple Random Walk in One Dimension

Galton Board

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Galton Board

- Start at origin and go to left or right with equal probability (fair coin-toss)
- 2^n possible random walks with n steps
- Endpoint position follows binomial distribution
- Trajectories are directed lattice paths

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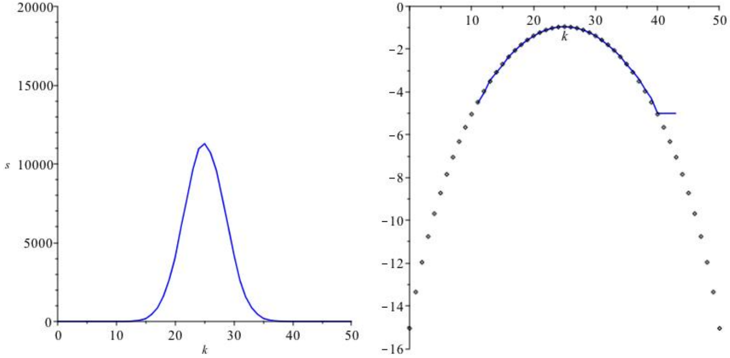
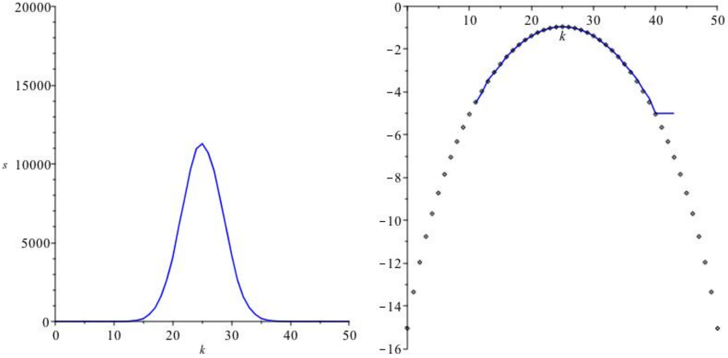
Model of a directed polymer in two dimensions

Simple Sampling



Simple sampling of simple random walk for $n = 50$ steps. For each simulation, 100000 samples were generated.

Simple Sampling



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How can we tweak the algorithm to reach the tails?

Pruned and Enriched Sampling

- Smart idea: change sampling rate to achieve uniform sampling

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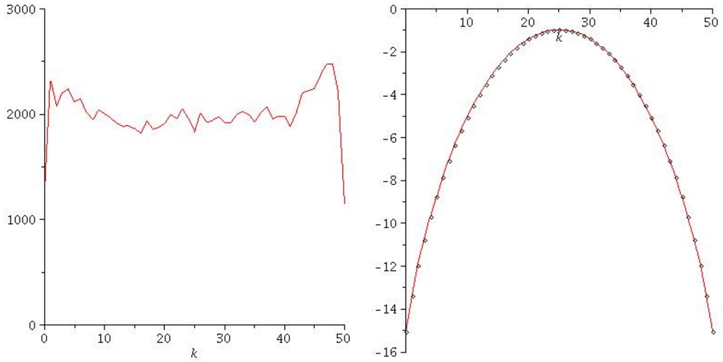
Pruning and Enrichment Strategy

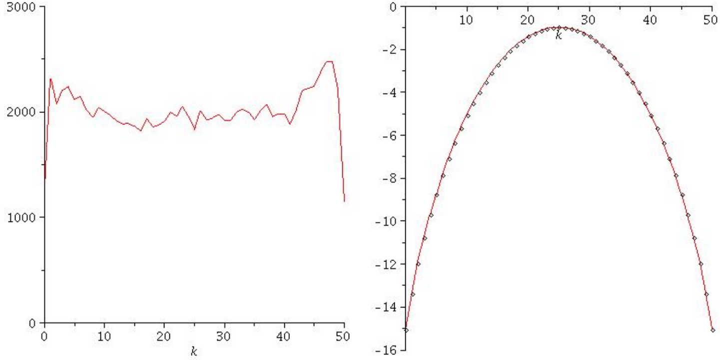
- **Pruning** If sampling rate is too large, remove the configuration probabilistically
- **Enrichment** If sampling rate is too small, make several copies of the configuration and continue growing each

Pruned and Enriched Sampling



- Uniform sampling with genuinely blind algorithm

Pruned and Enriched Sampling



- Uniform sampling with genuinely blind algorithm

Can be applied to a large class of growth processes

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Simple Sampling of Self-Avoiding Walk

Consider Self-Avoiding Walks (SAW) on the square lattice $\mathbb{Z}^2$

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Generating SAW with simple sampling is very inefficient

- There are 4^n n-step random walks, but only about 2.638^n n-step SAW
- The probability of successfully generating an n-step SAW decreases exponentially fast

This is called exponential attrition

Algorithm Development

- Rosenbluth Method (Rosenbluth, Rosenbluth, 1956): Only take steps that avoid intersections

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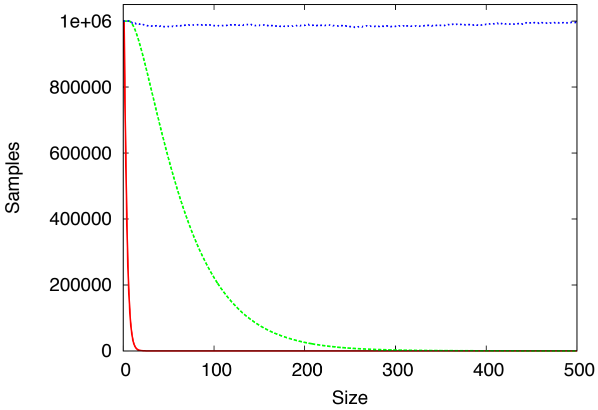
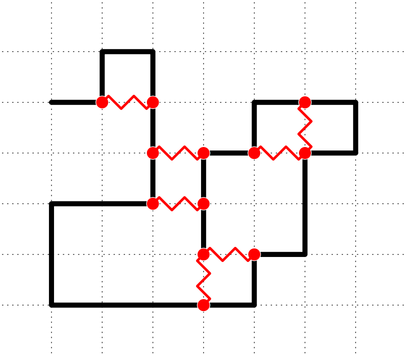
  Only take steps that avoid intersections
- PERM (Grassberger, 1997):
  Add Pruning and Enrichment to Rosenbluth Method
- FlatPERM (Prellberg, Krawczyk, 2004):
  Add Uniform Sampling Strategy to PERM



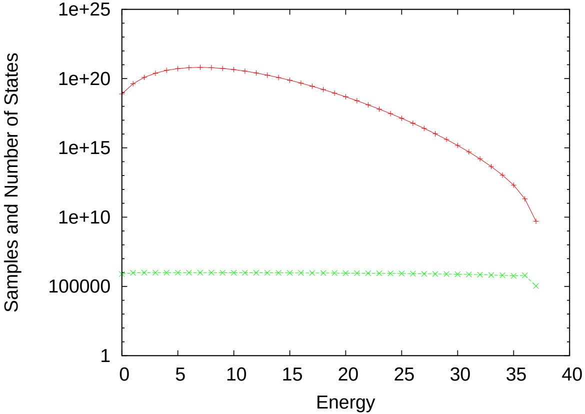
Attrition for Simple Sampling, Rosenbluth Sampling, and PERM

Interacting Self-Avoiding Walks

Consider sampling with respect to an extra parameter, for example the number of nearest-neighbour contacts



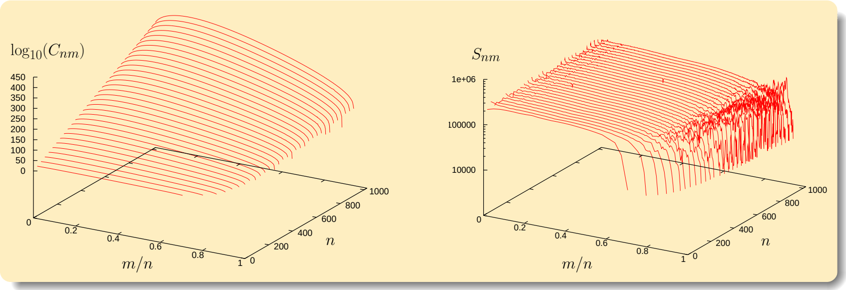
An interacting self-avoiding walk on the square lattice with $n = 26$ steps and $m = 7$ contacts.



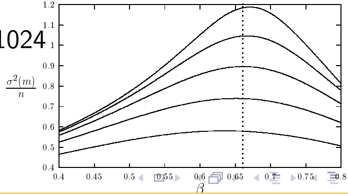
Generated samples and estimated number of states for ISAW with 50 steps estimated from 10^6 flatPERM tours.

ISAW simulations

Prellberg, Krawczyk, 2004



- Square lattice ISAW up to $n = 1024$
- One simulation suffices
- 400 orders of magnitude



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A Pure Mathematics Application

"On the cogrowth of Thompson's F group"
Rechnitzer, Elder, Wong (2012)

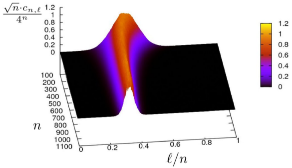


Figure 3: A plot of the normalised distribution of the number of words $c_{n,\ell}$ of length n and geodesic length ℓ in Thompson's group F. Notice that the peak position is quite stable, indicating that the mean geodesic length grows roughly linearly with word length.

We will proceed along a similar line but using a more powerful random sampling method based on flat-histogram ideas used in the FlatPERM algorithm [18, 19]. Each sample word is grown in a similar manner to simple sampling — append one generator at a time chosen uniformly at random. The weight of a word of n symbols is simply 1, so that the total weight of all possible words at any given length is just 4^n. As the word grows we keep track of its geodesic length. We now deviate from simple sampling by "pruning" and "enriching" the words.

The mean geodesic length of the amenable groups studied grow sublinearly, while those of $\mathbb{Z} \wr F_2$ and Thompson's group are observed to grow linearly. Using simple sampling we estimate that the mean geodesic length of Thompson's group does indeed grow linearly and that the rate of escape is 0.27 ± 0.01.

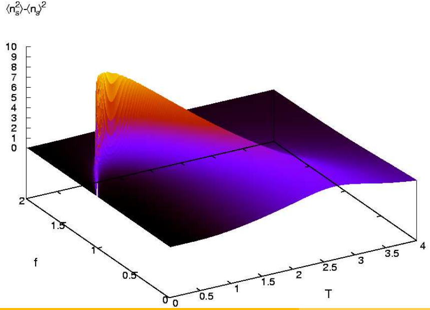
Indication that Thompson's F group is not amenable[1]

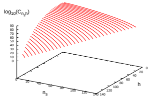
[1] does not have a finitely-additive left-invariant probability measure

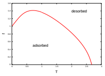
2-Dimensional Density of States

Krawczyk, Owczarek, Prellberg (2004)

- Force-induced desorption of adsorbed polymers
  - Relevance: optical tweezers, AFM; related to DNA unzipping
- 3-dim polymer in a half space, one simulation, up to $n = 256$

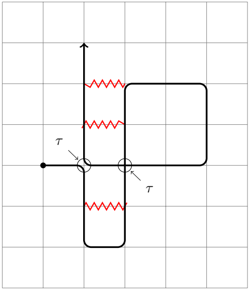


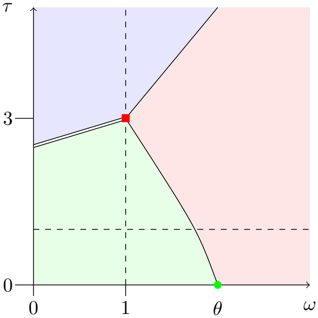




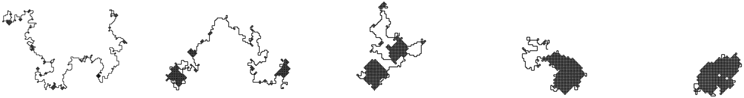
Lattice polymers with two competing interactions

Bedini, Owczarek, Prellberg (2014)



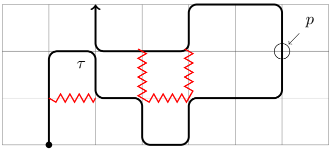


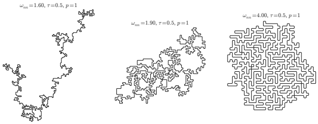
$\omega = 0.5$, increasing τ:

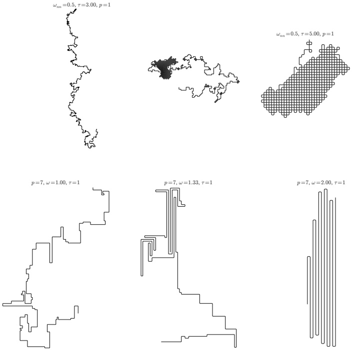


Self-attracting polymers in two dimensions with three low-temperature phases

Bedini, Owczarek, Prellberg (2017)

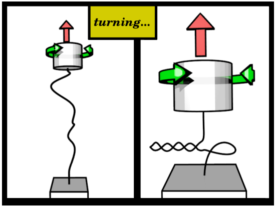


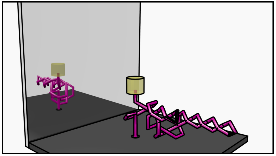


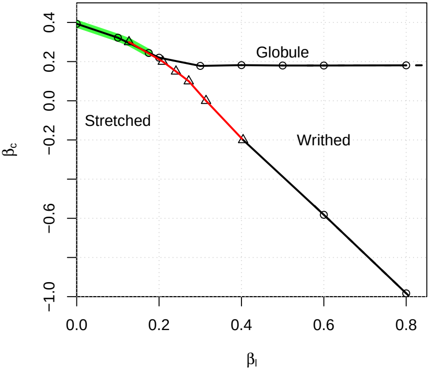


Supercoiling in a lattice polymer

Dagrosa, Owczarek, Prellberg (2017)







A big THANK YOU to all co-authors

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