II. PROBABILISTIC MODELS OF STATISTICAL PHYSICS

4. THE SELF-AVOIDING (random) WALK (SAW)

- Model of polymer geometry
- Very simple to define, poses notoriously difficult combinatorial problems
  (in fact, enumeration of SAWs is a good benchmark of computer performance)
- Dimension dependence:
  - $d > 4$: "mean field behavior", essentially the same as simple random walk (SRW) → (lace expansion techniques)
  - $d = 4$: —"— with logarithmic corrections, recent developments use "quantum field theory" inspired techniques
  - $d = 3$: mathematically "nothing" is known, no good conjectures (besides existence of critical exponents, existence of thermodynamical limit, ...)
  - $d = 2$: still mathematically "nothing" is known, but there are clear conjectures (values of critical exponents, description of scaling limit, ...) originating in theoretical physics (conformal field theory)

This lecture:

- combinatorics
- finite self-avoiding random walks
- thermodynamical limit of free energy

Finite simple random walks

$$W_N = \{ X : [\![0,N]\!] \to \mathbb{Z}^d \mid X(0) = \underline{0},\ \| X(t) - X(t-1) \| = 1 \quad \forall t = 1,2,\dots,N \}$$

= "the set of N step nearest neighbor walks on the hypercubic lattice in d dimensions, starting from the origin"

finite set : $\# W_N = (2d)^N$

__note__: N first steps of a simple random walk (SRW) are distributed according to the uniform measure on W_N.

Starting from $\underline{x} \in \mathbb{Z}^d$ instead of origin $\rightsquigarrow$ $\underline{x} + W_N$

Concatenation of walks $X \in W_N$, $X' \in W_M$ $\rightsquigarrow$ $X \boxplus X' \in W_{N+M}$

$$(X \boxplus X')(t) = \begin{cases} X(t) & \text{if } t \leq N \\ X(N) + X'(t-N) & \text{if } t > N \end{cases}$$

Inverse of concatenation is cutting, we can "identify"

$$W_{N+M} \cong W_N \times W_M$$

concatenation

cutting

Finite self-avoiding (random) walks

$$C_N = \{ X \in W_N \mid X \text{ injective} \}$$
$$= \{ X : [\![0,N]\!] \to \mathbb{Z}^d \mid X(0) = \underline{0}, \quad \|X(t) - X(t-1)\| = 1, \quad \forall t \neq s : \quad X(t) \neq X(s) \}$$

finite set : $\quad C_N \subset W_N \implies c_N := \# C_N \leq \# W_N$

Def: the N step self-avoiding (random) walk on $\mathbb{Z}^d$ from $\underline{0}$ is distributed according to the uniform probability measure on C_N.

(good model of polymer geometry)

Remark: $\quad$ (thermodynamical limit $N \to \infty$?)

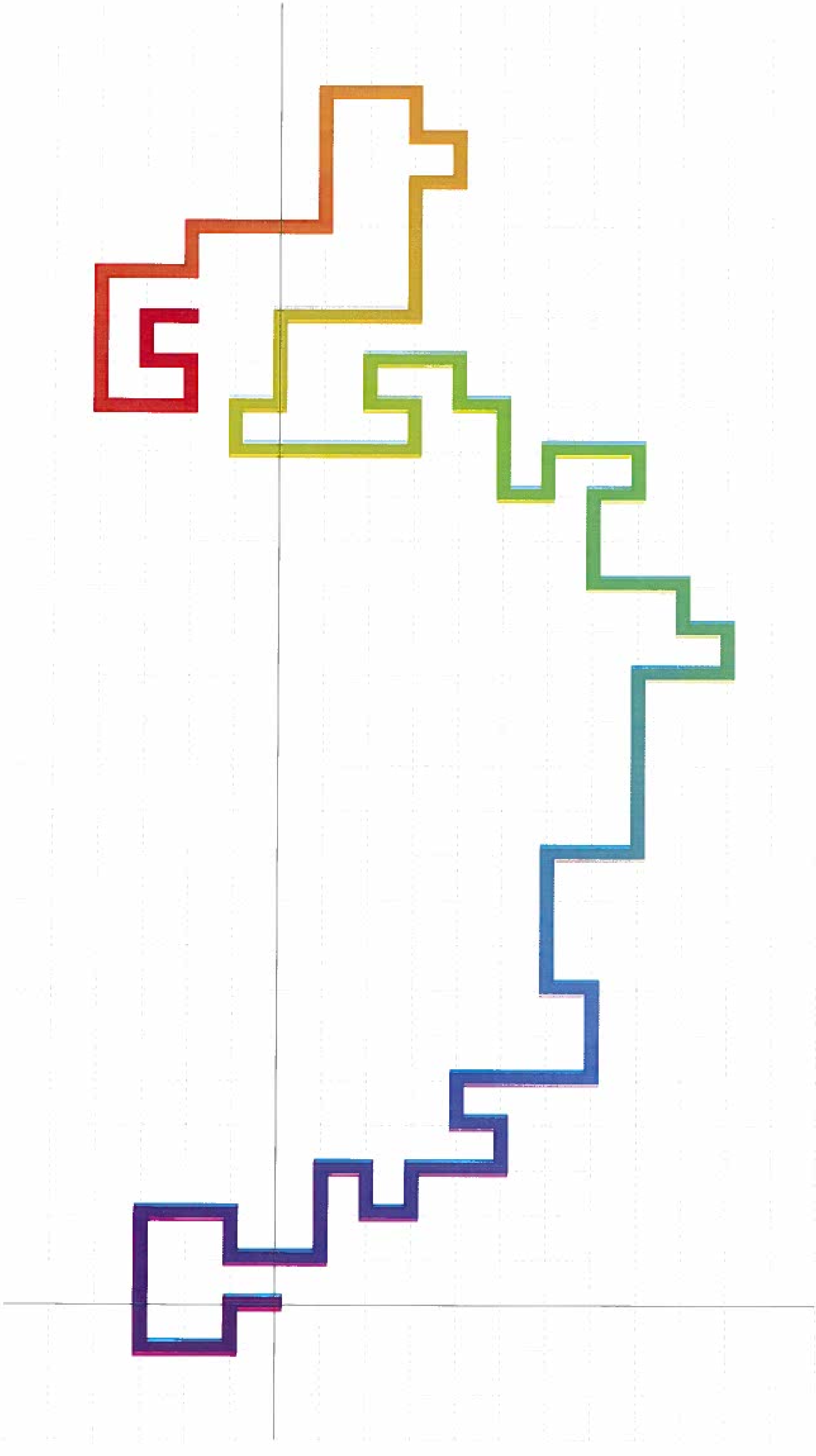
- For simple random walk, the measures of N step walks are "consistent" : the measure on smaller number of steps is obtained as a marginal (projecting out the last steps) from longer walks.
  For self-avoiding walks, the measures are not "consistent" $\rightsquigarrow$ no "obvious" definition of infinite self-avoiding walk. (See Exercises)
- We would like to define the thermodynamical limit $N \to \infty$ as follows. Embed

$$C_1 \hookrightarrow C_2 \hookrightarrow \dots \hookrightarrow C_N \hookrightarrow \dots \hookrightarrow (\mathbb{Z}^d)^{\mathbb{N}}$$
$$= \{ \text{functions } \mathbb{N} \to \mathbb{Z}^d \}$$

and equip $(\mathbb{Z}^d)^{\mathbb{N}}$ with a reasonable topology, and show weak convergence

$$\underset{\text{"N step SAW"}}{\nu_N} \xrightarrow[N \to \infty]{w} \underset{\text{"infinite SAW"}}{\nu_\infty}.$$

Unfortunately, the existence of the weak limit remains an open problem in $d=2$ and $d=3$.



Thermodynamical limit of free energy

obvious bounds for $c_N = \# \mathcal{C}_N$

$$d^N \le c_N \le 2d \cdot (2d-1)^N \implies (c_N)_{N\in\mathbb{N}}$$ grows exponentially

if all steps in positive coordinate axis directions

first step

other steps can't retrace the previous

Next we claim there is a well defined exponential growth speed for c_N, $c_N \sim \mu^N$ (i.e. $\frac{\log(c_N)}{N\log(\mu)} \to 1$)

Physically this means that the polymer free energy has a thermodynamical limit:

- energy of all possible polymer shapes the same, e.g. $H(X) = 0 \quad \forall X \in \mathcal{C}_N$.
- partition function $Z_N = \sum_{X\in\mathcal{C}_N} \underbrace{e^{-\beta H(X)}}_{=1} = c_N$
- free energy
$$F_N = \frac{-1}{\beta}\log(Z_N)$$ "purely entropic"
- free energy per unit (i.e. per monomer)
$$f_N = \frac{-1}{\beta N}\log(Z_N) \longrightarrow -\frac{\log(\mu)}{\beta} \quad \text{if } c_N \sim \mu^N$$

We need the following frequently useful lemma

Lemma (Subadditive limit lemma) If $(a_n)_{n\in\mathbb{N}}$ is a subadditive sequence of real numbers, i.e. $a_{n+m} \le a_n + a_m \quad \forall n,m\in\mathbb{N}$, then $\lim_{n\to\infty} \frac{1}{n} a_n$ exists and equals $\phi = \inf_{n\in\mathbb{N}} \left(\frac{a_n}{n}\right) \in [-\infty, \infty)$

<u>Proof</u>: If $\phi' > \phi$, then we can choose a n_0 s.t. $\frac{a_{n_0}}{n_0} \le \phi'$. For general $n \in \mathbb{N}$ use division algorithm to write $n = m \cdot n_0 + r$ with $0 \le r < n_0$.

Then $\frac{a_n}{n} = \frac{a_{mn_0+r}}{n} \le \frac{m\, a_{n_0} + a_r}{n} \le \frac{a_{n_0}}{n_0} + \frac{a_r}{n} \xrightarrow[n\to\infty]{} \frac{a_{n_0}}{n_0} \le \phi'$.

Thus $\limsup \frac{a_n}{n} \le \phi$. But clearly $\liminf \frac{a_n}{n} \ge \inf \frac{a_n}{n} = \phi$. $\square$

Now observe that "cutting" a walk of $N+M$ steps to two walks of N and M steps preserves self-avoidance property, so

$$\mathcal{C}_{N+M} \xrightarrow[\text{"cut"}]{} \mathcal{C}_N \times \mathcal{C}_M \quad \text{is injective}$$

and consequently $c_{N+M} \le c_N c_M$.

Thus $a_n = \log(c_n)$ defines a subadditive sequence. We get:

<u>Proposition</u> The limit $\phi = \lim_{N\to\infty} \frac{\log(c_N)}{N}$ exists, i.e. $c_N \sim \mu^N$ where $\mu = e^\phi$. Moreover $c_N \ge \mu^N$ $\forall N$.

<u>Exercise</u> Use this to get explicit numerical bounds on c_N and μ.

<u>Remark</u> $\mu = \lim_{N\to\infty} (c_N^{1/N})$ is called the connective constant of the lattice $\mathbb{Z}^d$.

we have: $d \le \mu \le (2d-1)$

Asymptotics of the number of self-avoiding walks

We have shown so far that $c_N = \mu^{N + o(N)}$.

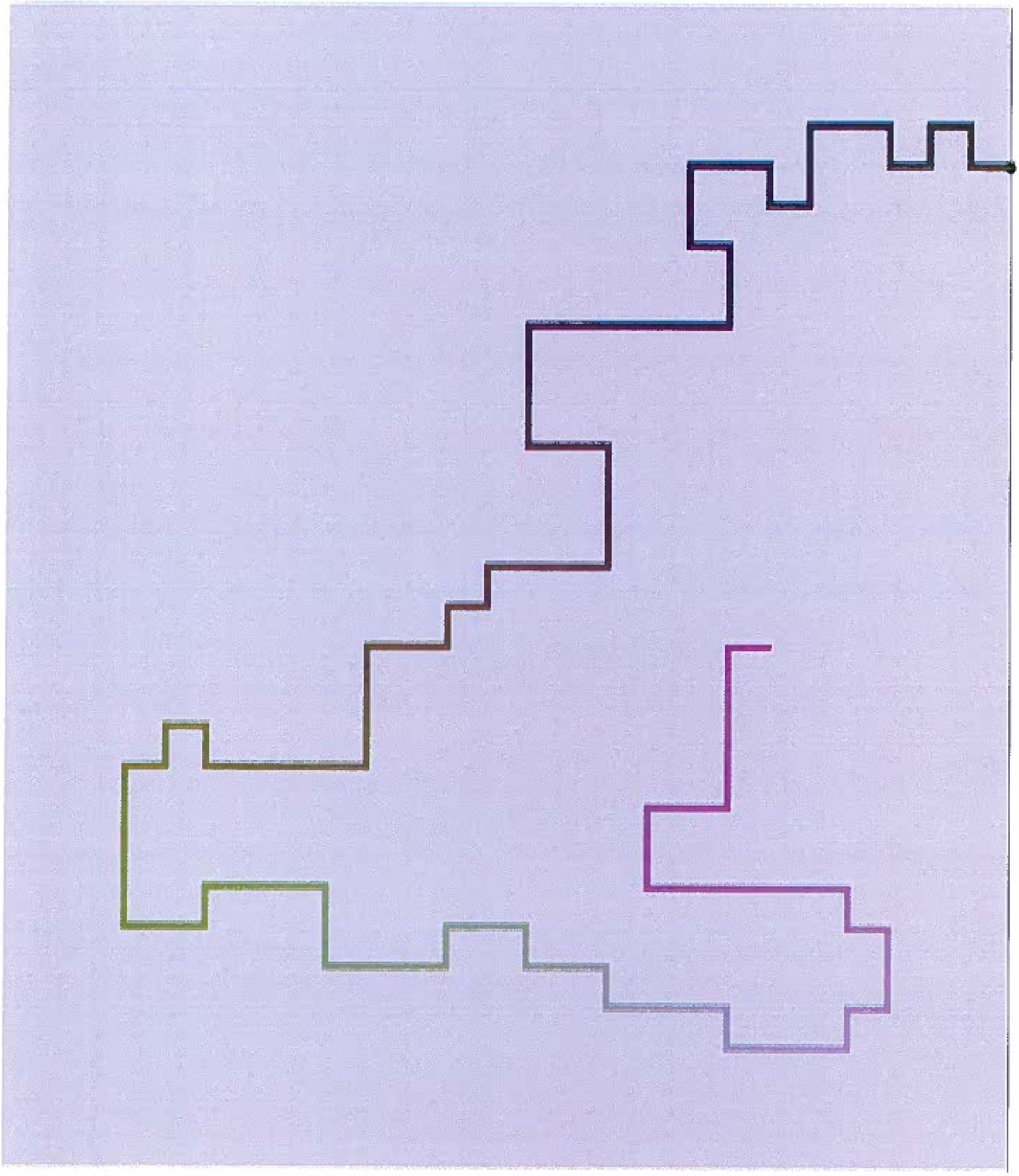
We will show $c_N = \mu^{N + \mathcal{O}(\sqrt{N})}$, which is the best rigorous result in $d=2$, and not far from the best in $d=3$.

Physically, one expects much more precise asymptotics:

<u>Conjecture</u> There exists $A > 0$, $\gamma \ge 1$, such that

$$c_N = \mu^N \cdot N^{\gamma - 1} \cdot (A + o(1))$$

γ is a critical exponent, physically the most relevant quantity here.



With the conjectured asymptotics one could e.g. derive:

<u>Exercise</u> Assuming γ exists, we have, for two independent self-avoiding random walks of length N,

$$\mathbb{P}\left[\text{the two walks don't intersect except at origin}\right] \sim N^{1-\gamma}$$

(In particular, the "non-universal" constants A, μ don't appear in this asymptotic of intersection probability)

Our main goal is:

<u>Theorem</u> (The Hammersley–Welsh bound)
For any $\varepsilon > 0$ there exists $C > 0$ such that for all $N \in \mathbb{N}$

$$\mu^N \leq c_N \leq \mu^N \cdot e^{(\pi\sqrt{\frac{2}{3}}+\varepsilon)\sqrt{N}}$$

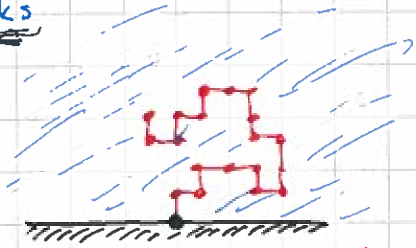
To work towards this, we introduce different versions of self-avoiding walks.

Half-space self-avoiding walks and bridges

π_1 takes the first component of the d-dim vector

$$\mathcal{H}_N = \{ X \in \mathcal{C}_N \mid \pi_1 X(t) > 0 \quad \forall t = 1, 2, \ldots, N \}$$

$=$ "N step self-avoiding <u>half-space walks</u>"



an example of a half-space walk ($d=2$)

Again finite set

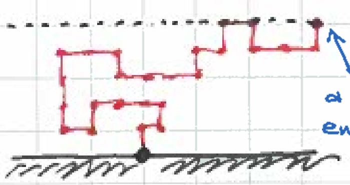
$$\mathcal{H}_N \subset \mathcal{C}_N \subset \mathcal{W}_N$$

Half-space walks are also physically relevant: "polymer attached to a membrane"

Turns out to be clever to first look at a subset

$$\mathcal{B}_N = \{ X \in \mathcal{H}_N \mid \pi_1 X(t) \leq \pi_1 X(N) \quad \forall t \}$$

$=$ "N step self-avoiding <u>bridges</u>"



Denote $b_N = \# \mathcal{B}_N$, $h_N = \# \mathcal{H}_N$. Then

$$\mathcal{B}_N \subset \mathcal{H}_N \subset \mathcal{C}_N$$

$$\underset{\substack{\uparrow \\ \text{all but first step} \\ \text{can be in arbitrary} \\ \text{positive coord. axis direction}}}{d^{N-1}} \leq b_N \leq h_N \leq c_N \leq \underset{\substack{\uparrow \\ \text{shown before}}}{2d \cdot (2d-1)^N}$$

For bridges, cutting / concatenation gives the opposite inequality compared to self-avoiding walks:

- the concatenation of bridges $X \in \mathcal{B}_N$, $X' \in \mathcal{B}_M$ is a new bridge $X \boxplus X' \in \mathcal{B}_{N+M}$

$$\boxplus : \mathcal{B}_N \times \mathcal{B}_M \longrightarrow \mathcal{B}_{N+M} \quad \text{injective}$$

$$\Longrightarrow \quad b_N \, b_M \leq b_{N+M}$$

(compare with $c_{N+M} \leq c_N c_M$)

Thus $(b_N)_{N \in \mathbb{N}}$ is super-multiplicative, and $a_n = -\log(b_n)$ is again subadditive and we get

<u>Proposition</u> The limit $\lim_{N \to \infty} \frac{\log(b_N)}{N} = \phi_{\text{bridge}}$ exists, and

$$b_N \sim \underbrace{\mu_{\text{bridge}}}_{= e^{\phi_{\text{bridge}}}}{}^{N} \quad \text{and} \quad b_N \leq \mu_{\text{bridge}}^N \quad \forall N.$$

Thus for we have

$$\mu_{\text{bridge}}^N \sim b_N \leq h_N \leq c_N \sim \mu^N$$

so in particular $\mu_{\text{bridge}} \leq \mu$. We will show

- $\mu_{\text{bridge}} = \mu$
- "reverse inequalities" can be written with $e^{\Theta(\sqrt{N})}$ loss.

<u>Exercise</u> Use this to find numerical lower bounds on the number of bridges and connective constant μ.

We first bound the number of half-space walks from above by the number of bridges (with some loss...).

Denote p'_N the number of ways to partition the integer N to distinct integers :

$$p'_N = \#\left\{ (n_1, \dots, n_k) \;\middle|\; k \in \mathbb{N},\quad n_1 > n_2 > \dots > n_k \geq 1,\quad n_1 + \dots + n_k = N \right\}$$

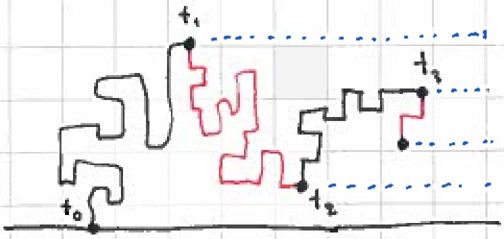
<u>Lemma</u> We have $h_N \leq p'_N \cdot b_N$.

<u>Proof</u> The idea is to decompose a half-space walk X to upwards and downwards going bridges.

Define
$$t_0 = 0,$$
$$t_1 = \max\left\{ t > t_0 \;\middle|\; \pi_1 X(t) = \max_{s > t_0} \pi_1 X(s) \right\}$$
$$t_2 = \max\left\{ t > t_1 \;\middle|\; \pi_1 X(t) = \min_{s > t_1} \pi_1 X(s) \right\}$$
$$t_3 = \max\left\{ t > t_2 \;\middle|\; \pi_1 X(t) = \max_{s > t_2} \pi_1 X(s) \right\}$$
$$\vdots$$

t_0 } upwards
t_1 } downwards
t_2 } upwards
t_3 } ...
$\vdots$

until $t_k = N$ for some k.



Then $X|_{[\![t_{j-1}, t_j]\!]}$ is essentially a bridge (translated, and if j is even, reflected in the first coordinate).

The entire walk can be recovered from the bridges defined by $X|_{[\![t_{j-1}, t_j]\!]}$

Denote $a_j = \left| \pi_1 X(t_j) - \pi_1 X(t_{j-1}) \right|$ the "span" of the bridge.

By construction $a_1 > a_2 > \dots > a_k > 0$.

Let $h_N[a_1, \dots, a_k]$ be the number of $X \in \mathcal{H}_N$ with these spans.

In particular $h_N[a_1] = b_N[a_1]$ is the number of bridges with span a_1.