Entanglement Complexity of Systems of Self-Avoiding Walks in Lattice Tubes

Conference on Knots and other Entanglements in Biopolymers: Topological and Geometrical Aspects of DNA, RNA and Protein Structures

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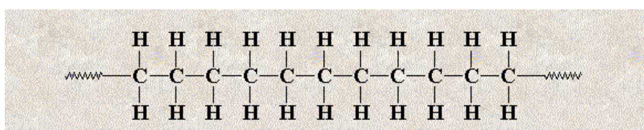
Talk Outline

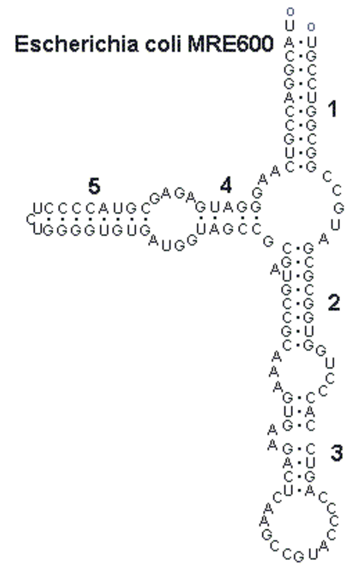
- Review of Lattice Models of Polymers
- Orlandini, Tesi and Whittington proposal for a “good” measure of entanglement complexity for dense polymer systems
- Results on what can be proved for this measure of the entanglement complexity for a system of self-avoiding walks in a tube (work with M. Atapour).

Introduction to Polymers

Polymer: Large molecule made of repeated molecular units called *monomers*; if there is more than one type of monomer *Copolymer*



homopolymer - polyethylene



copolymer - RNA

Fundamental Question of Interest: What properties of polymer solutions are primarily a result of the fact that a polymer is a very large molecule made up of repeated molecular units?

Modelling Polymers in Solution

ADVANTAGES of LATTICE MODELS:

excluded volume property is easily incorporated

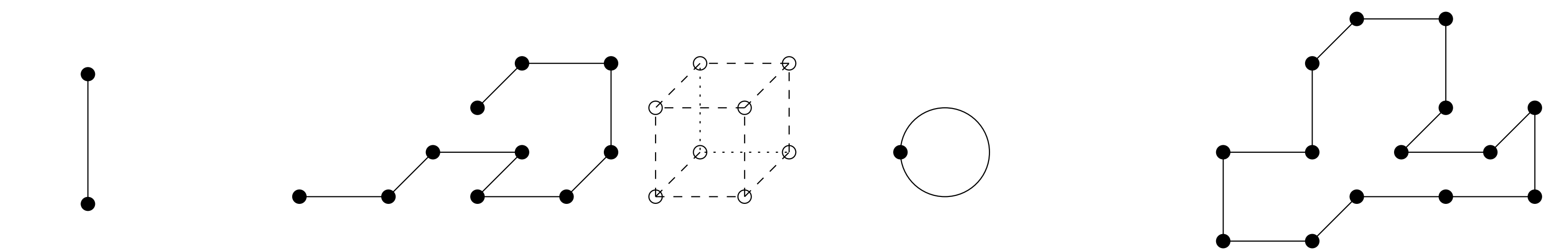
substantial conformational freedom available

combinatorial analysis possible

qualitative features of phase diagrams expected to be correct

values of critical exponents expected to be exact

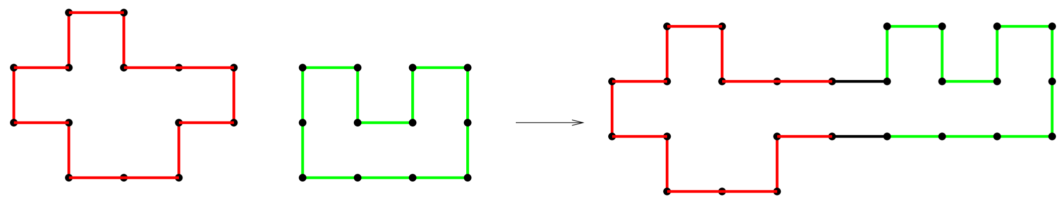
MODELS of LINEAR and RING POLYMERS:



LINE GRAPH — SELF–AVOIDING WALK — CIRCLE GRAPH — SELF–AVOIDING POLYGON

Properties of Self-avoiding Polygons (SAPs) in $\mathbb{Z}^d$

Standard Concatenation Argument



$$p_n p_m \leq (d-1)p_{n+m} \quad ; \; p_n \leq (2d)^n \Rightarrow \lim_{n\to\infty} \frac{1}{2n} \log p_{2n} \equiv \log \mu_d = \kappa_d$$

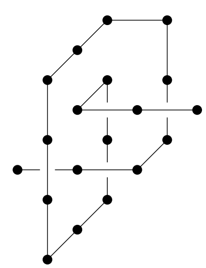
(Hammersley Proc.Camb.Phil.Soc. **58** (1961), 235–8)

$$p_n(\phi)p_m(\phi) \leq 2p_{n+m}(\phi) \quad ; \; p_n(\phi) \leq p_n \Rightarrow \lim_{n\to\infty} \frac{1}{2n} \log p_{2n}(\phi) \equiv \log \mu_0 = \kappa_0$$

(Sumners and Whittington JPA **21** (1988), 1689–94)

$$\kappa_o < \kappa_3 \quad \Rightarrow \textit{Prob. of Knotting} = 1 - \frac{p_n(\phi)}{p_n} = 1 - e^{-(\kappa-\kappa_o)n+o(n)}$$

Key ingredient: Pattern theorem (Kesten, 1963) used to prove that "tight trefoil" pattern occurs at least once in all but exponentially few sufficiently long SAPs.



Good Measures of Knot Complexity

Results extended in several directions ... **Soteros, Sumners and Whittington** (1992 MathProcCambPhilSoc 111 75)

Good Measures of Knot Complexity: Function $F : \mathcal{K} \to [0, \infty)$ s.t.

(i) $F(\phi) = 0$

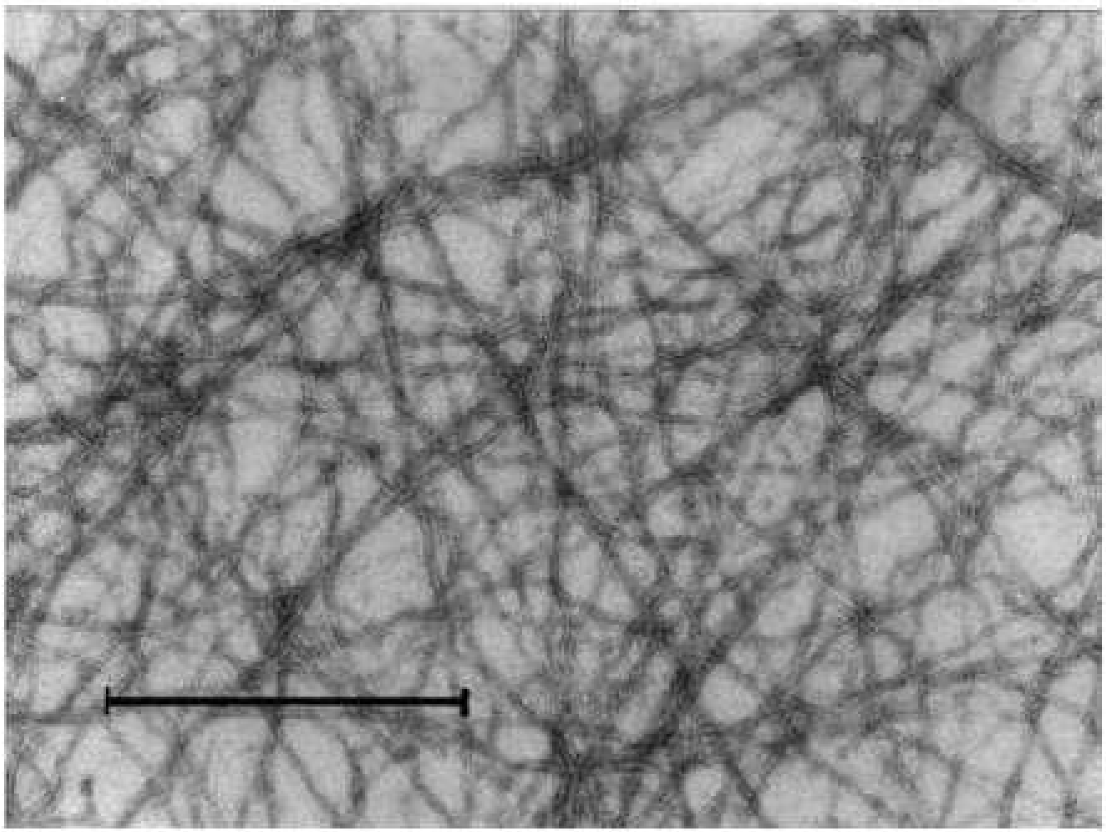
(ii) $\exists K \in \mathcal{K}$ s.t. $F(nK\#L) \geq nF(K) > 0 \; \forall L \in \mathcal{K}$ (i.e. roughly additive w.r.t. knot product)

Then Sumners & Whittington (1988) $\Rightarrow$

If F is a good measure of knot complexity, let K be a knot which satisfies part (ii) above. Then, there exists $n_K, A_k > 0$ s.t. $\forall n > n_K$ all but exponentially few n-SAPs have F-complexity exceeding $A_K n$.

Examples of **Good Measures:** Crossing number, number of prime factors, genus, bridge number minus one, span of any non-trivial Laurent knot polynomial, log(order), unknotting number, minor index, braid index minus one.

For Dense Polymer Solutions or Polymer Melts, What is a "Good" Measure of Entanglement Complexity?



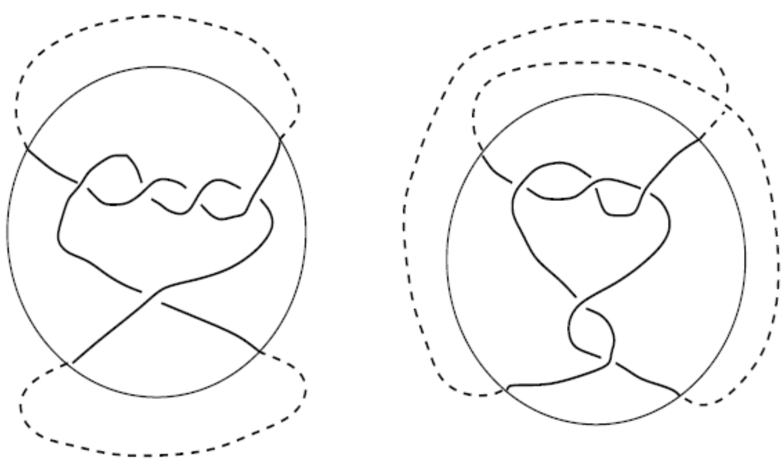
Electron micrograph of a 0.4 mg/ml actin solution polymerized in vitro. Bar = 1 μm. (Gotter *et al* arXiv:cond-mat/9611097 v1 20 Nov 1995.)

Orlandini, Tesi and Whittington 2000 - characterize entanglement by "linking number" for a tube or cube from solution.

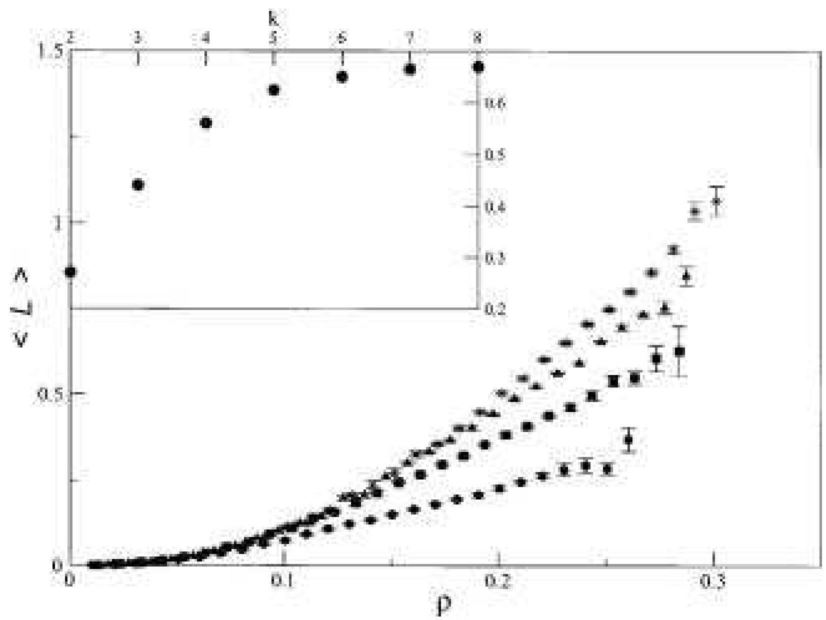
Orlandini et al (2000) Measure for Entanglement Complexity in Dense Systems

Proposal: Take a random cube (or tube) from n-edge system composed of c chains. Assume endpts are in the cube boundary and no edges in the boundary. For each pair (i, j) of chains, join up the two ends of each chain by an arc outside the cube and compute linking number $Lk(i, j) = \frac{1}{2}\sum_m \sigma_m$.

Entanglement Measure: $EC = \sum_{i=1}^{k-1}\sum_{j>i} |Lk(i, j)|$



Regular Projections of Two Chains



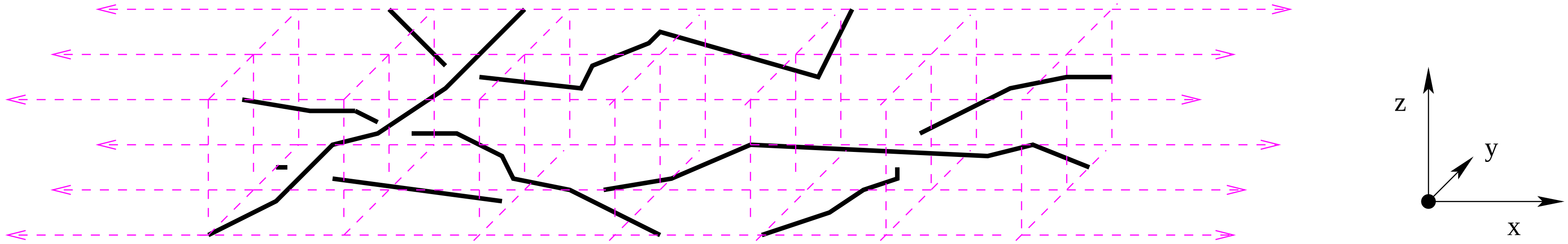
Density dependence of $\langle EC \rangle$ for cube size 10

(Orlandini *et al* JPA **33** (2000) L181-L186.)

(Orlandini and Whittington JCP **121** (2004) 12094–9.)

What Can Be Proved About This Entanglement Measure?

SSAWs in $\infty \times N \times M$ Tube



Define: A *System of Self-avoiding Walks* (SSAW) of size n, span s and with c components in an (N, M)-tube is a finite subgraph of the tube with n-edges and c connected components s.t.

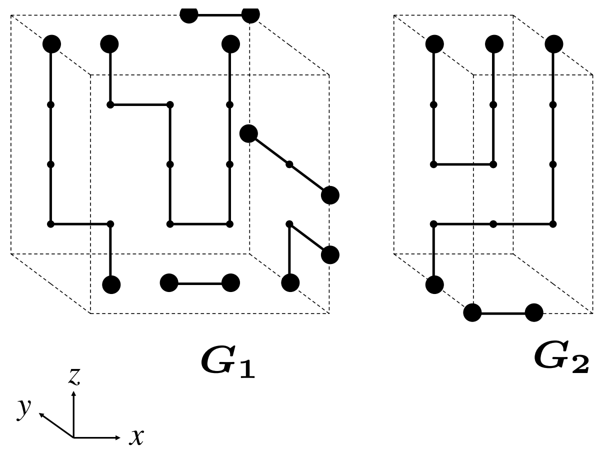
(i) each connected component is an undirected SAW (USAW) with its endpts in a tube wall (e.g. $y = 0$, $y = N$, $z = 0$ or $z = M$) and no degree two vertices in any wall of the tube

(ii) for each integer $m \in [0, s]$, there is at least one vertex of the SSAW in the plane $x = m$ and no vertices in $x = m$, $\forall m \notin [0, s]$.

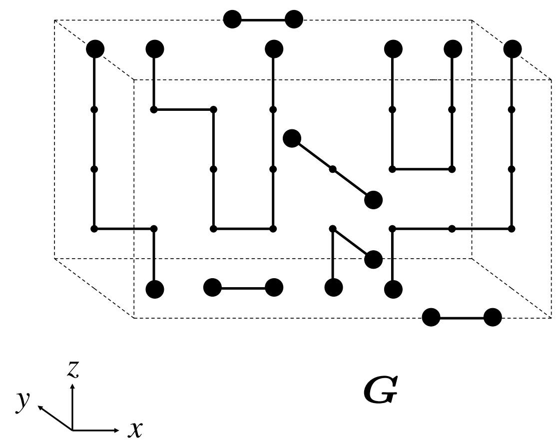
$\boldsymbol{q_s(N, M; n, c)}$ - # of $\boldsymbol{n}$-edge, span $\boldsymbol{s}$, $\boldsymbol{c}$-component SSAWs in $\boldsymbol{(N, M)}$-tube (up to $\boldsymbol{x}$-translation)

Note: $\boldsymbol{c = \frac{1}{2}} \times$ (# of degree one vertices in SSAW)

Concatenation of SSAWs:



Two SSAWs G_1 ($s_1 = 4, n_1 = 19, c_1 = 6$) and G_2 ($s_2 = 2, n_2 = 12, c_2 = 3$) in $T(2,4)$.



SSAW G ($s = 7, n = 31, c = 9$), the concatenation of G_1 and G_2.

Concatenation gives

$q_{s_1}(N, M; n_1, c_1) q_{s_2}(N, M; n_2, c_2) \le q_{s_1+s_2+1}(N, M; n_1 + n_2, c_1 + c_2)$

$\Rightarrow$ (via standard arguments, c.f. Janse van Rensburg 2000)

the existence of the limiting free energy:

$$F(N, M; x, y) = \lim_{s \to \infty} \frac{1}{s} \log Z_s(N, M; x, y)$$

where

$$Z_s(N, M; x, y) = \sum_{n,c} q_s(N, M; n, c) x^n y^c.$$

$$F(N,M;x,y) = \lim_{s\to\infty} \frac{1}{s} \log Z_s(N,M;x,y); \qquad Z_s(N,M;x,y) = \sum_{n,c} q_s(N,M;n,c) x^n y^c.$$

Plus $F(N,M;x,y)$ is

(i) a convex function of $\log x$ (for fixed y) and of $\log y$ (for fixed x);

(ii) its right and left derivatives in x (for fixed y) and in y (for fixed x) exist everywhere in $(0,\infty)$;

(iii) it is differentiable almost everywhere, and when the derivative exists the order of the limit and derivative can be interchanged.

$\Rightarrow$

For r.v. X with state space span s SSAWs and $\boxed{\mathbb{P}(X=G) = \frac{x^{n(G)} y^{c(G)}}{Z_s(N,M;x,y)}}$

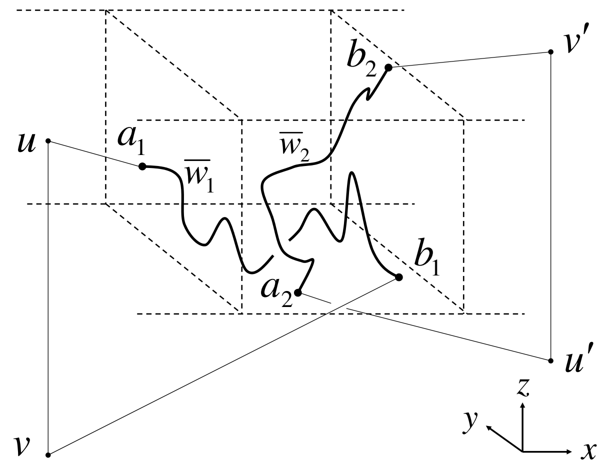
$\lim_{s\to\infty} \frac{\mathbb{E}[n(X)]}{s}$ exists a.e. and is non-decreasing in x, i.e.

For fixed (x,y), the avg. edge-density $\frac{\mathbb{E}[n(X)]}{sNM}$ goes to $\rho_e(x,y)$ as $s\to\infty$, and $\uparrow$ as $x\uparrow$.

$\lim_{s\to\infty} \frac{\mathbb{E}[c(X)]}{s}$ exists a.e. and is non-decreasing in y, i.e.

For fixed (x,y), the avg. walk-density goes to $\rho_w(x,y)$ as $s\to\infty$, and $\uparrow$ as $y\uparrow$.

Entanglement Complexity of SSAWs in $\infty \times N \times M$ Tube



A two-component link K_{12} is associated to a pair of USAWs $(\bar{w}_1, \bar{w}_2)$.

The following result has been proved (c.f. Atapour, PhD thesis):

Corollary 1 *Given an n-edge SSAW G, let $w_1, \ldots w_c$ be the sequence of USAWs in G. Let $\bar{G}$ be the SSAW associated to G as prescribed in Lemma 6.2.1. For any $1 \leq i < j \leq k$, there exists a two-component polygonal link $K_{ij} = (K_i, K_j)$ corresponding to the pair of USAWs (w_i, w_j) such that when it is projected into the xy-plane those edges of K_{ij} which lie outside B_G will create no crossing with the edges inside B_G and at most one crossing, involving both polygons K_i and K_j, amongst themselves.*

The $Entanglement\ Complexity$, $EC(G)$, of any SSAW G is now defined as follows:

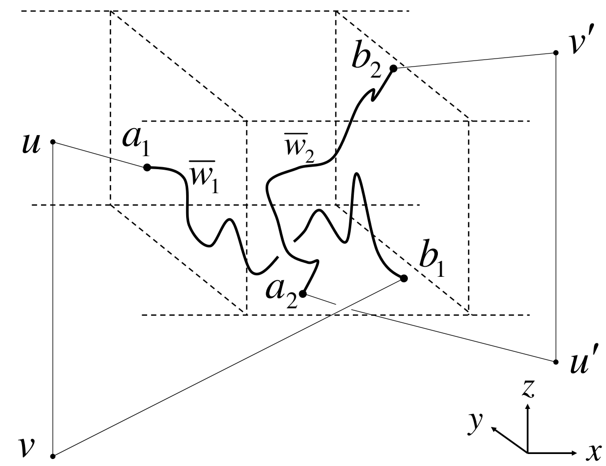
$$EC(G) = \sum_{i=1}^{c-1} \sum_{j=i+1}^{c} |Lk(K_{ij})|, \qquad (1)$$

where $Lk(K_{ij})$ is the linking number of K_{ij}.

Upper Bound on EC of SSAWs: Since one can bound the number of crossings associated with an edge of the SSAW by a constant (dependent only on N and M), the EC-complexity can be bounded above by a linear function of n or s:

(i) Given a pair of SAWs, we can extend their endpts (by adding at most a(N,M) edges) so that the new endpoints are "away" from the tube.

(ii) For any $\epsilon > 0$, there exists a "push-off" of the walk pair which has a regular projection in the (x, y)-plane such that the (x, y) coordinates of walk vertices are within ϵ of their values in the regular projection. The endpoints will be on the boundary of the projection.



$$\Rightarrow EC = \sum_{i=1}^{c-1} \sum_{j>i} |Lk(i,j)| \leq \sum_{i=1}^{c} \sum_{m=1}^{n_i} C(i,m) + \sum_{i=1}^{c} ex(i)$$

n_i := number of edges in the ith SAW

$C(i, m)$:= the number of edges crossed by the mth edge of the ith SAW $\leq$ the number of edges E in a $3 \times (N + 2) \times M$ slice of the lattice

$ex(i)$:= the number of walk pairs involving the ith walk which could result in an extra crossing $\leq$ the number of walks (other than the ith) which have vertices in a slice of the tube determined by the location of the endpts of the ith walk $\leq$ number of vertices in that tube slice $\leq (N + 2)(M + 1)n_i$

$$\Rightarrow EC = \sum_{i=1}^{c-1} \sum_{j>i} |Lk(i,j)| \leq d(N,M)n \leq dd(N,M)s$$

A Lower Bound for EC of SSAWs in Tubes

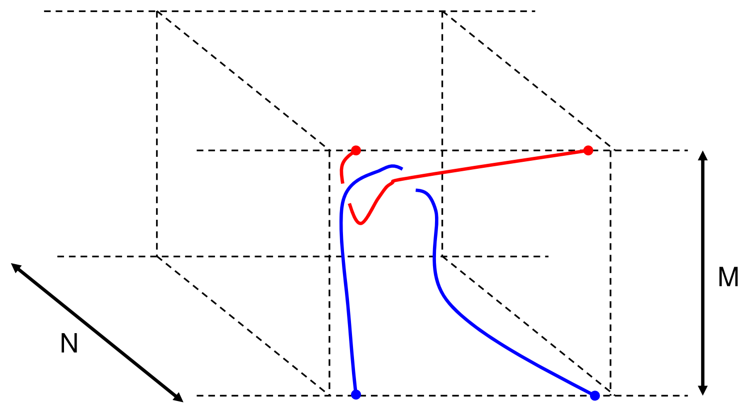
$q_s(N, M; n, c; < m, P)$ - # of n-edge, span s, c-component SSAWs in (N, M)-tube (up to x-translation) which contain less than m translates of pattern P

A Pattern Theorem would allow us to compare:

$$F(N, M; x, y; \epsilon, P) = \lim_{s \to \infty} \frac{1}{s} \log Z_s(N, M; x, y; \epsilon, P);$$
$$Z_s(N, M; x, y; \epsilon, P) = \sum_{n,c} q_s(N, M; n, c; < \epsilon s, P) x^n y^c.$$

to

$$F(N, M; x, y) = \lim_{s \to \infty} \frac{1}{s} \log Z_s(N, M; x, y);$$
$$Z_s(N, M; x, y) = \sum_{n,c} q_s(N, M; n, c) x^n y^c.$$



If $F(N, M; x, y; \epsilon, P) < F(N, M; x, y)$ then

$\Rightarrow$ All but exponentially few sufficiently wide span s "weighted" SSAWs contain at least ϵs translates of P.

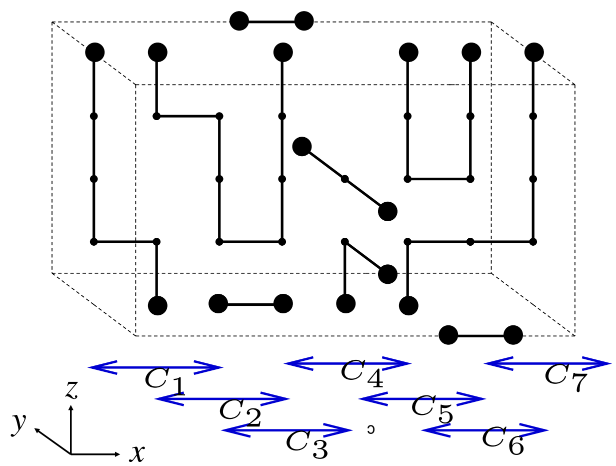
Since P cannot occur more than ϵs times in an SSAW with $EC \leq \epsilon s \Rightarrow$

(i) All but exponentially few sufficiently wide SSAWs have entanglement measure $EC > \epsilon s$, i.e. EC grows at least linearly in the span.

(ii) The probability that a span s SSAW has EC greater than ϵs goes to 1 as $s \to \infty$

HENCE A PATTERN THEOREM IS NEEDED - TRANSFER MATRIX WILL BE USED

Transfer Matrix for SSAWs: Given $k \geq 2$, an SSAW is a sequence of overlapping k-configs.

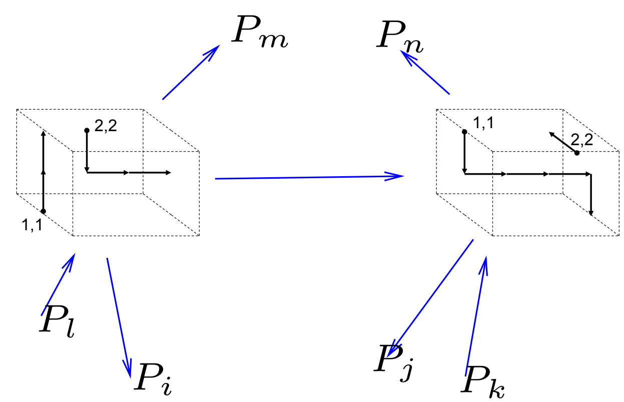


$\mathcal{S}_k$: set of all possible SSAW k-configs

$\mathcal{S}_{k,o}$: subset of $\mathcal{S}_k$ that are *start* k-configs

$\mathcal{S}_{k,f}$: subset of $\mathcal{S}_k$ that are *end* k-configs

$\mathcal{G}_k = (V, A)$:
graph with vertex set $V = \mathcal{S}_k = \{P_1, P_2, \ldots\}$
and arc $(P_i, P_j) \in A$ iff $P_i P_j$ is in $\mathcal{S}_{k+1}$.

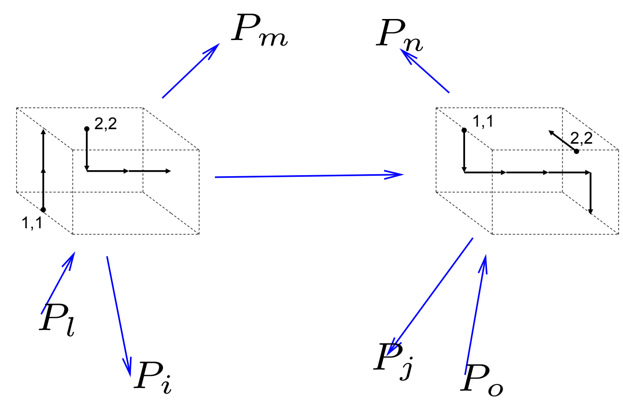


Any walk on $\mathcal{G}_k$ starting
in $\mathcal{S}_{k,o}$ and ending in $\mathcal{S}_{k,f}$ corresponds to an SSAW.

Transfer Matrix for SSAWS: Given $k \geq 2$ and $\mathcal{G}_k$

$\mathcal{G}_k = (V, A)$:
graph with vertex set $V = \mathcal{S}_k = \{P_1, P_2, \ldots\}$
and arc $(P_i, P_j) \in A$ iff $P_i P_j$ is in $\mathcal{S}_{k+1}$.

Any walk on $\mathcal{G}_k$ starting
in $\mathcal{S}_{k,o}$ and ending in $\mathcal{S}_{k,f}$ corresponds to an SSAW.



Simplest Transfer Matrix: $T = (T_{i,j})$

$$T_{i,j} = \begin{cases} 1\ , & (P_i, P_j) \in A \\ 0\ , & \text{otherwise} \end{cases} .$$

$\Rightarrow$

$(T^r)_{i,j} = \#$ of $(k+r)$-configs starting with P_i & ending with P_j.

If $P_i \in \mathcal{S}_{k,o}$ and $P_j \in \mathcal{S}_{k,f}$, then they are SSAWs.

More General Transfer Matrix for SSAWS:

Recall: X a r.v. with state space all span s SSAWs.

$$\mathbb{P}(X=G) = \frac{x^{n(G)}y^{c(G)}}{Z_s(N,M;x,y)}$$

$n(G)$- # of edges of G ; $c(G)$- # of walks in G (i.e. # of connected components)

Grand Canonial Partition function:

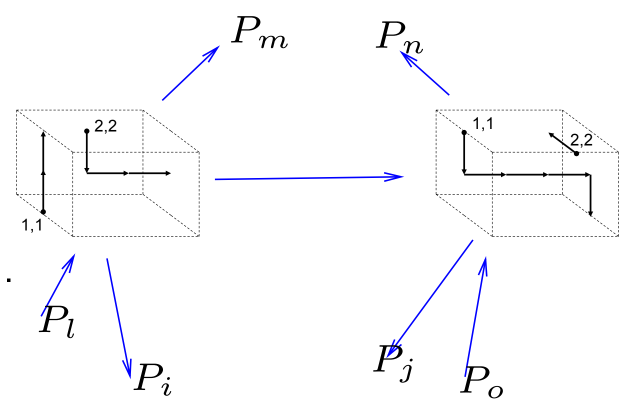
$$Q(x,y,z) = \sum_{s,n,c} q_s(N,M;n,c)x^n y^c z^s = \sum_s Z_s(N,M;x,y)z^s.$$

$-\log R_Q(x,y) =$
$F(N,M;x,y) = \lim_{s\to\infty} s^{-1}\log Z_s(N,M;x,y)$

Given $k \geq 2$ and $\mathcal{G}_k$

General Transfer Matrix: $T = (T_{i,j})$

$$T_{i,j} = \begin{cases} z^{s(P_i,P_j)}x^{n(P_i,P_j)}y^{c(P_i,P_j)}, & (P_i,P_j)\in A \\ 0, & \text{otherwise} \end{cases}.$$



$\Rightarrow$

$$Q(x,y,z) = \sum_{r=0}^{\infty} \sum_{\{i:P_i\in\mathcal{S}_{k,o}\}} \sum_{\{j:P_j\in\mathcal{S}_{k,f}\}} (T^r)_{i,j} = \frac{f(x,y,z)}{\det(I-T)}.$$

where $f(x,y,z)$ is analytic.

Consequences of the Transfer Matrix Representation

$q_s(N, M; n, c; \bar{P})$ - # of n-edge, span s, c-component SSAWs in (N, M)-tube (up to x-translation) which DO NOT contain pattern P

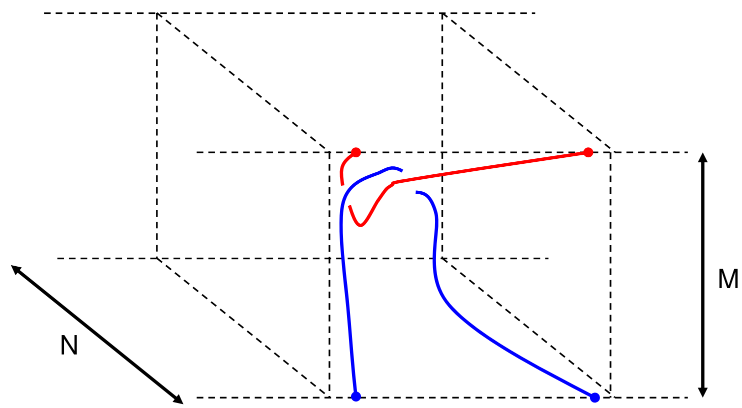
$$Z_s(N, M; x, y; \bar{P}) = \sum_{n,c} q_s(N, M; n, c; \bar{P}) x^n y^c.$$

The transfer matrix and Perron-Frobenius Theory $\Rightarrow$

$$F(N, M; x, y; \bar{P}) = \lim_{s \to \infty} \frac{1}{s} \log Z_s(N, M; x, y; \bar{P})$$

is strictly less than

$$F(N, M; x, y) = \lim_{s \to \infty} \frac{1}{s} \log Z_s(N, M; x, y)$$



Moreover, for any non-negative integer valued *additive functional* ψ defined for SSAWs, there exists $\gamma_{\psi,x,y} > 0$ (can be determined from the eigenvalues and eigenvectors of T) such that as $s \to \infty$

$$\mathbb{E}[\psi(X)] = (\gamma_{\psi,x,y})s + O(1)$$

HENCE:

For the edge count: $\mathbb{E}[n(X)] = (\gamma_{e,x,y})s + O(1)$

For the walk count: $\mathbb{E}[c(X)] = (\gamma_{w,x,y})s + O(1)$

For $n_P(X)$- # of translates of P occurring in X: $\mathbb{E}[n_P(X)] = (\gamma_{P,x,y})s + O(1)$

For $n_\times(X)$- # of crossings in a regular projection of X: $\mathbb{E}[n_\times(X)] = (\gamma_{\times,x,y})s + O(1)$

For the Entanglement Complexity Measure EC:

$$\boxed{(\gamma_{P,x,y})s + O(1) \ \leq\ \mathbb{E}[EC(X)] \ \leq\ (\gamma_{\times,x,y})s + d'(N,M)s + O(1)}$$

$$\Rightarrow$$

EC IS A GOOD MEASURE OF ENTANGLEMENT COMPLEXITY

Future Work

For the Entanglement Complexity Measure EC:

$$(\gamma_{P,x,y})s + O(1) \ \leq \ \mathbb{E}[EC(X)] \ \leq \ (\gamma_{\times,x,y})s + d'(N,M)s + O(1)$$

How do the γ's change with (x, y)? i.e. How does avg. $EC(X)$ change as the edge-density and the walk-density change?

For fixed limiting edge-density:

$$f(N, M; \alpha) \equiv \lim_{s\to\infty} s^{-1} \log q_s(N, M; \lfloor \alpha s \rfloor),$$

where $q_s(N, M; \lfloor \alpha s \rfloor)$ is the $\#$ of span s, $\lfloor \alpha s \rfloor$-edge SSAWs (up-to x-translation). What do these results mean for EC?

What happens as N and M change?

What about other measures of Entanglement Complexity?

Stretching a Polygon in an (N, M)-Tube

$p_n(N, M; s)$: # of n-edge, span s SAPs in (N, M)-tube

$$\hat{Z}_n(N, M; x) = \sum_s p_n(N, M; s) e^{fs} \quad ,$$

where $x = e^f$

Standard concatenation argument for SAPs in a tube $\Rightarrow$

$$\hat{F}(N, M; x) = \lim_{n \to \infty} n^{-1} \log \hat{Z}_n(N, M; x)$$

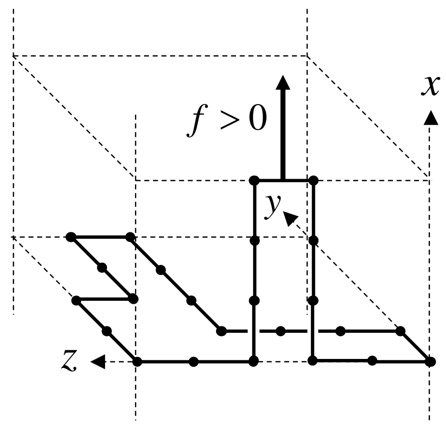
exists.

For r.v. X with state space n-edge SAPs,

$$\mathbb{P}(X = \omega) = \frac{x^s}{\hat{Z}_n(N, M; x)} = \frac{e^{fs}}{\hat{Z}_n(N, M; e^f)}$$

Transfer matrix arguments $\Rightarrow$

$\mathbb{E}[s(X)] = \frac{1}{\rho_e(f)} n + O(1)$
and is non-decreasing in f.



A SAP under the influence of a fixed force $f > 0$; note that the tube is rotated 90 degrees counter-clockwise.

Knot Complexity of Stretched Polygons in a Tube

$p_n(N, M; s; \bar{P})$: # of n-edge, span s SAPs in (N, M)-tube which do NOT contain pattern P

$$\hat{Z}_n(N, M; x; \bar{P}) = \sum_s p_n(N, M; s; \bar{P}) e^{fs} \quad ,$$

where $x = e^f$

A concatenation argument for SAPs in a tube $\Rightarrow$

$$\hat{F}(N, M; x; \bar{P}) = \lim_{n \to \infty} n^{-1} \log \hat{Z}_n(N, M; x; \bar{P})$$

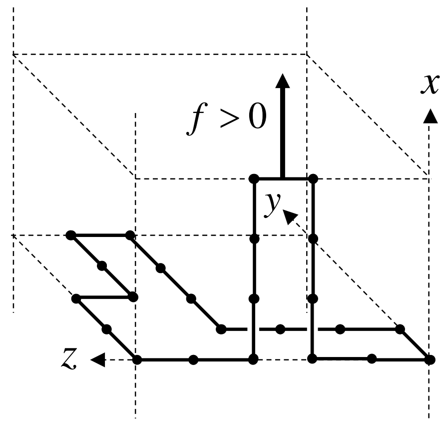
exists.

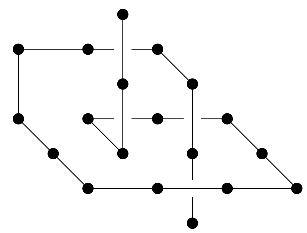
Transfer-matrix arguments $\Rightarrow$

$$\hat{F}(N, M; x; \bar{P}) < \hat{F}(N, M; x)$$

$$\mathbb{E}[n_P(X)] = (\gamma_{P,f})n + O(1)$$

For any f, all sufficiently long n-edge SAPs under the influence of the force f contain at least $\gamma_{P,f}\, n$ trefoils in their knot decomposition.





Part of a tight trefoil pattern for the tube.