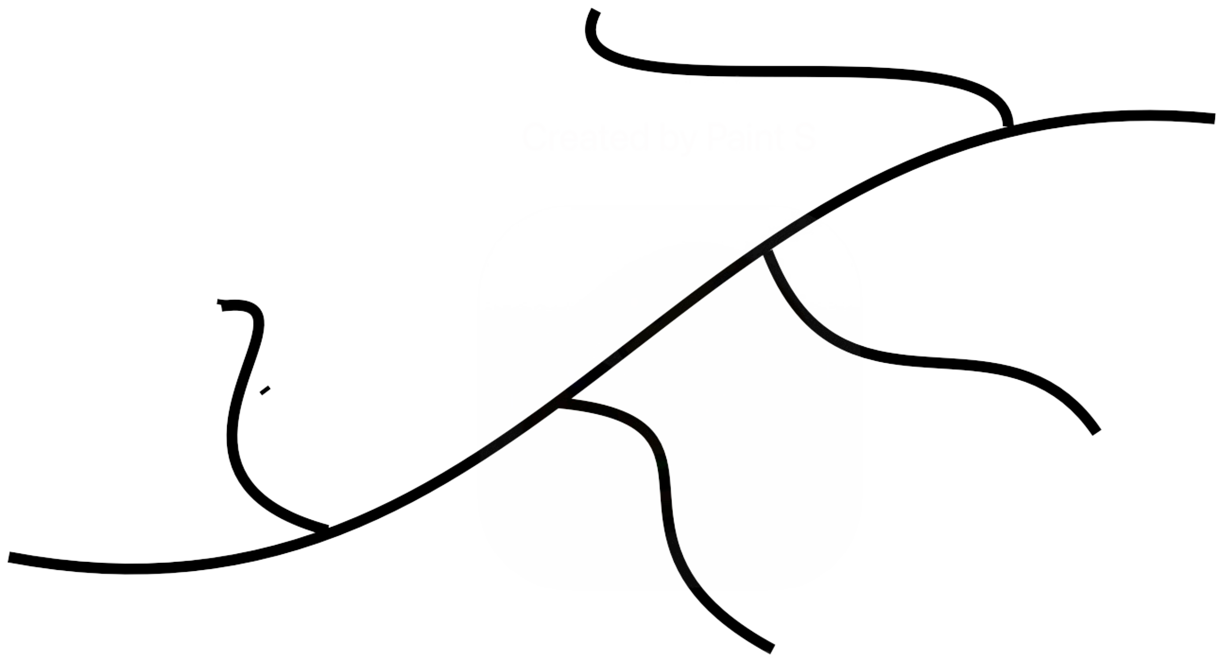
Counting combs

Conference honouring Tony Guttmann's 80th birthday, 2025
Joint work with Buks van Rensburg

Comb polymers

A comb polymer consists of a backbone, with t teeth attached to the backbone at vertices of degree 3. The backbone and the t teeth can all be modelled as self-avoiding walks that are mutually avoiding, except at the vertices of degree 3. Suppose that the teeth each have m_a edges. Suppose that there are m_b edges along the backbone, between adjacent vertices of degree 3, and between the first and last vertices of degree 3 and the end vertices of degree 1 of the backbone.



Comb polymers

Let the number of embeddings of a comb with fixed m_a, m_b and t be $g(m_a, m_b, t)$. The total number of edges in the comb is

$$n = m_a t + m_b(t + 1).$$

Some questions

1. Does the limit

$$\lim_{n\to\infty} n^{-1} \log g(m_a, m_b, t)$$

   exist, when at least one of m_a, m_b, t goes to infinity?

2. If so, how does the value of the limit depend on which, if any, of m_a, m_b, t is fixed?

3. When is the limit equal to the connective constant of the lattice, $\kappa = \lim_{n\to\infty} n^{-1} \log c_n$, where c_n is the number of n-edge self-avoiding walks?

Some previous results

1. When $m_a = m_b = m \to \infty$ with $t = 2$

$$\lim_{m\to\infty} \frac{1}{n} \log g(m, m, 2) = \kappa$$

   [Gaunt *et al J. Phys. A* **19** L811 (1986)]. Note that

$$n = (2t + 1)m = 5m.$$

2. There are Monte Carlo results suggesting that the limiting free energy is strictly less than κ when $t \to \infty$ with m_a and m_b fixed and small [Lipson *Macromolecules* **26** 203 (1993)].

We want to generalize the first and prove the second.

Behaviour when $m_a, m_b \to \infty$ with t fixed.

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$$\lim_{\substack{m_a, m_b \to \infty \\ m_a = o(m_b)}} n^{-1} \log g(m_a, m_b, t) = \kappa, \quad 2 \le t < \infty$$

$$\lim_{\substack{m_a, m_b \to \infty \\ m_b = o(m_a)}} n^{-1} \log g(m_a, m_b, t) = \kappa, \quad 2 \le t < \infty$$

$$\lim_{m \to \infty} \frac{1}{(2t+1)m} \log g(m, m, t) = \kappa, \quad 2 \le t < \infty$$

$t \to \infty$ after $m_a, m_b \to \infty$

In each of these three cases, we have the same result if $t \to \infty$ after the limit $m_a, m_b \to \infty$ is taken.

Behaviour when $m_a \to \infty$ with m_b and t fixed, the star limit

$$\lim_{m_a \to \infty} n^{-1} \log g(m_a, m_b, t) = \kappa, \quad 1 \leq m_b < \infty, 2 \leq t < \infty$$

Behaviour when $m_b \to \infty$ with m_a and t fixed, the SAW limit

$$\lim_{m_b \to \infty} n^{-1} \log g(m_a, m_b, t) = \kappa, \quad 1 \leq m_a < \infty, 2 \leq t < \infty$$

Behaviour when $t \to \infty$ with m_a, m_b fixed.

Existence of the limit when $t \to \infty$ with m_a, m_b fixed

The limit

$$\lim_{t\to\infty} n^{-1} \log g(m_a, m_b, t) \equiv \zeta(m_a, m_b)$$

exists for all $1 \leq m_a, m_b < \infty$. This can be proved by a concatenation argument.

$t \to \infty$ with m_a, m_b fixed

Is $\zeta(m_a, m_b) < \kappa$?

The idea is to construct an upper bound on $\zeta(m_a, m_b)$ and compare with a lower bound on κ.

We have three approaches to constructing these upper bounds.

A pattern theorem argument shows that $\zeta(m_a, m_b) < \kappa$ for $m_a = 1$, $1 \leq m_b < \infty$ for the square and simple cubic lattices.

A second approach to constructing an upper bound on $\zeta(m_a, m_b)$ is to consider a backbone with attached teeth where the teeth can mutually intersect, and can intersect the backbone. For a lattice with coordination number q, we have the bound

$$g(m_a, m_b, t) \leq c_{m_b(t+1)} \left(\frac{(q-2)}{q} c_{m_a} \right)^t,$$

giving

$$\zeta(m_a, m_b) \leq \kappa + \frac{\log((q-2)/q) + \log c_{m_a} - m_a \kappa}{m_a + m_b}.$$

We need lower bounds on κ and values of c_{m_a}.

Examples

- Square lattice: $\zeta(m_a, m_b) < \kappa_2$ if $m_a = 1, 2, 3$ and $1 \leq m_b < \infty$.

- Simple cubic lattice: $\zeta(1, m_b) < \kappa_3$ for all $1 \leq m_b < \infty$.

- Hexagonal lattice: $\zeta(m_a, m_b) < \kappa_H$ if $1 \leq m_a \leq 15$ and $1 \leq m_b < \infty$.

Concatenating 3-stars, etc.

Another approach is to construct a super-set of combs by concatenating small graphs, such as 3-stars. This gives useful bounds for small m_a, m_b, especially for the square lattice, but means that we can't say anything for all finite m_b.

For instance, for the square lattice:

$$\zeta(m_a, m_b) < \kappa_2, \quad \text{when} \quad 2 \leq m_a, m_b \leq 6$$

Extension to brushes

All of these techniques can be extended to give partial answers for the case of brushes, where the branch points along the backbone have vertex degree greater than 3. We shall write f for the vertex degree of the branch points so that the number of teeth at each branch point is $f-2$.

An upper bound for brushes

$$b_f(m_a, m_b, t) \le c_{(t+1)m_b} \binom{q-2}{f-2}^t \left(\frac{c_{m_a}}{q}\right)^{(f-2)t}$$

For the square lattice with 2 teeth at each branch point ($f = 4$) we have

$$\zeta_4(m_a, m_b) \le \kappa_2 + \frac{2\log(c_{m_a}/4) - 2m_a\kappa_2}{2m_a + m_b}$$

Generally speaking, the results for brushes are somewhat stronger than the results for combs. For instance, for square lattice brushes with 2 teeth at each branch point

$$\zeta_4(m_a, m_b) < \kappa_2 \quad \text{when} \quad 1 \leq m_a \leq 23, 1 \leq m_b < \infty.$$

Open question

Although we have made some progress, this leaves open the question:

Is $\zeta(m_a, m_b) < \kappa$ for all $1 \leq m_a, m_b < \infty$?