# A brief review of results on the linking probability for 2-component links which span a lattice tube.

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Abstract : After a brief introduction to lattice models of ring polymers and their application to studying random knotting and linking, a review is given of recent results due to Atapour, Soteros, Ernst and Whittington [1] on the probability of topological and homological linking for 2-component links for which each component spans a lattice tube.

## 1 Lattice Models of Ring Polymers

Lattice models of polymers are well established as useful for modelling polymers in solution [2, 3]. For such models, a *polymer* is viewed simply as a large molecule made of repeated molecular units called *monomers*. The model is then used to answer questions about the average configurational properties of a polymer in solution. When compared to polymer experiments, such models have been shown to be both qualitatively (in the prediction of the existence of phase transitions) and quantitatively (in the prediction of critical exponent values) correct.

A standard lattice model for modelling ring polymer solutions is the *self-avoiding polygon (SAP) model* on the simple cubic lattice, $\mathbb{Z}^3$. This is a statistical mechanics model in which a polymer conformation is represented by a polygon composed of edges and vertices from the simple cubic lattice (see Figure 1 (a) for an example). The model has the advantages that: (i) the excluded volume property (the property that there is a volume around each monomer which excludes the entry of other monomers) is easily incorporated, (ii) there is substantial conformational freedom available, and (iii) combinatorial and asymptotic analysis is possible.

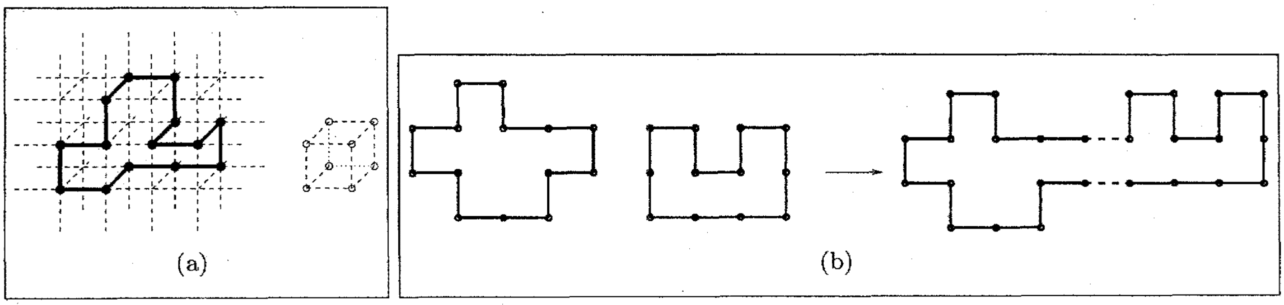

Figure 1: (a) A 14-edge SAP in $\mathbb{Z}^3$. (b) Concatentation of a 14-edge SAP to a 12-edge SAP.

One important application of this model has been to verifying the *Frisch-Wasserman Delbruck Conjecture* [4, 5] that sufficiently long ring polymers are knotted with high probability. This was proved to be true for SAPs in $\mathbb{Z}^3$ by Sumners and Whittington [6] and independently by Pippenger [7]. The proof of this relies first on standard *concatenation* arguments for SAPs. (See Figure 1 (b) for an example of the concatenation of two polygons.) For $p_n$, the number (up-to-translation) of $n$-edge SAPs in $\mathbb{Z}^3$, concatenation leads to

$$p_n p_m \leq 2p_{n+m} \leq 2(6)^{n+m},$$

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and, for $p_n(\phi)$, the number (up-to-translation) of $n$-edge unknotted SAPs in $\mathbb{Z}^3$, it leads to

$$p_n(\phi)p_m(\phi) \leq 2p_{n+m}(\phi) \leq 2p_{n+m}.$$

These inequalities lead to the existence of the following *exponential growth rates* for SAPs and unknotted SAPs, respectively: $\lim_{n\to\infty} \frac{1}{2n} \log p_{2n} \equiv \kappa$ and $\lim_{n\to\infty} \frac{1}{2n} \log p_{2n}(\phi) \equiv \kappa_0$. Then, by proving a *pattern theorem*, Sumners and Whittington [6] proved that $\kappa_o < \kappa$ and hence that the probability of knotting goes to one at an exponential rate, i.e. goes to one as $1 - e^{-(\kappa-\kappa_o)n+o(n)}$. This also means that all but exponentially few sufficiently long SAPs are knotted, hence proving the Frisch-Wasserman Delbruck conjecture.

Thus SAP models are useful for answering questions about the probability of knotting. What about their usefulness in studying the probability that two polymers are linked?

## 2 Random Linking of Pairs of SAPs

To use a lattice model to study the probability of topological linking (*i.e.* the probability of being non-splittable) for ring polymers, one must first specify some constraints on the polymers or the polymer solution. For example, if (as in the last section) one assumes that each polymer is isolated then clearly the probability of linking is zero. The next simplest case is to assume that at most two polymers can be "close" to each other. However, even in this case, further constraints are needed. For example, suppose the polymer conformations are represented by two SAPs placed arbitrarily on the simple cubic lattice. This results in an infinite number of configurations (up-to-translation) so that further restrictions are required just to define the probability of linking.

One natural restriction is to assume that the two polygons are confined to a bounded region $\mathcal{B}$ in $\mathbb{Z}^3$. Orlandini *et al* [8] considered the case that $\mathcal{B}$ is a cube of sidelength $D$, and studied linking of pairs of $n$-edge SAPs in $\mathcal{B}$, with $n \leq D$ and $D = e^{o(n)}$. They proved that the number of pairs which are splittable has the same exponential growth rate (as $n \to \infty$) as the number which are not splittable. Hence, unlike the situation for knottedness, topologically unlinked pairs are NOT exponentially rare.

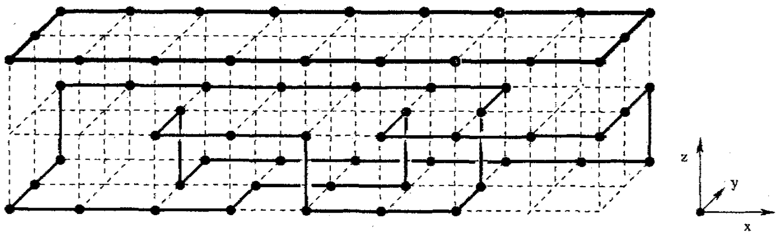
Tesi *et al* [9] extended these results to "tubes". That is for fixed $N$ and $M$, they considered a subset of the simple cubic lattice given by $T(D,N,M) = \{(x,y,z) \in \mathbb{Z}^3 | 0 \leq x \leq D, 0 \leq y \leq N, 0 \leq z \leq M\}$ and studied linking of pairs of $n$-edge SAPs in $T(D,N,M)$ with $n \leq D$ and $D = e^{o(n)}$. In this case, it is again proved that the number of pairs which are splittable has the same exponential growth rate (as $n \to \infty$) as the number which are not splittable.

This left open the question: "What restrictions are sufficient to establish that all but exponentially few sufficiently long pairs of SAPs are topologically linked?"

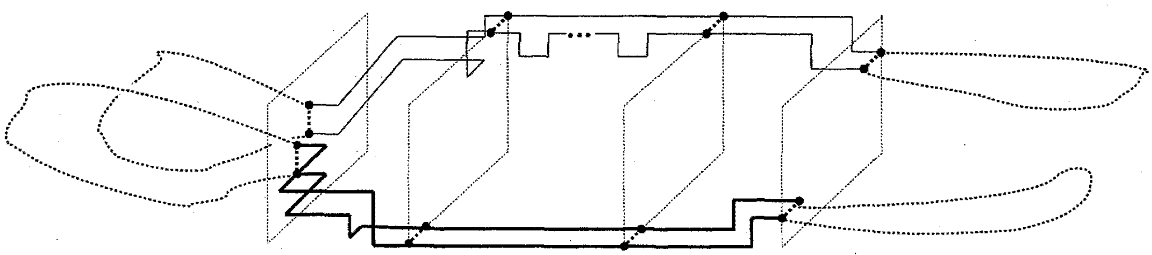
## 3 Random Linking of Pairs of SAPs which Span a Lattice Tube

One answer to this question was obtained recently by Atapour *et al* [1] by restricting the two SAPs to the lattice tube $T(N,M) = \{(x,y,z) \in \mathbb{Z}^3 | 0 \leq y \leq N, 0 \leq z \leq M\}$, and by considering $q_n(N,M)$, the number of pairs, $(\omega_1, \omega_2)$, of mutually avoiding SAPs in $T(N,M)$ (up to translation) such that $\omega_1$ and $\omega_2$ together have a total of $n$-edges and such that they each have the same left-most and right-most planes (see Figure 2 (a) for an example). Such a pair of SAPs is referred to as an $n$-edge 2SAP and the distance between the left-most and right-most planes of the 2SAP is referred to as its *span*.

It is proved that that there exists $c > 0$ and $b > 0$ such that any $n$-edge 2SAP $G$ can be *concatenated* (see Figure 2 (b)) to any $m$-edge 2SAP $H$ to create a new $(n+m+c)$-edge 2SAP




(a)



(b)

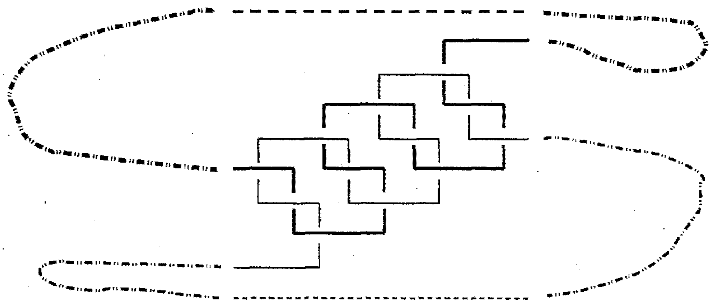
Figure 2: (a) 60-edge 2SAP in $T(2,2)$ with span 8. (b) Concatenation of two 2SAPs. One 2SAP is indicated by the dashed-line pair of polygons on the left and the other is the dashed-line pair of polygons on the right. The solid connecting lines in between represent the edges added to concatenate the two 2SAPs.

having span equal to $span(G)+span(H)+b$. This leads to the inequality $q_n(N,M)q_m(N,M) \leq q_{n+m+c}(N,M)$, and this combined with an upper bound on $q_{n+m+c}(N,M)$ establishes the existence of the *exponential growth rate for 2SAPs*: $\kappa^{(2)}(N,M) = \lim_{n\to\infty} \frac{1}{n} \log q_n(N,M)$.

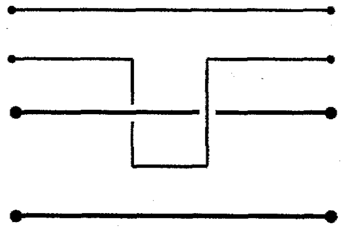
The concatenation process (CONCAT) defined as in Figure 2 (b), combined with a (CAPOFF) procedure given in Atapour *et al* [1] is then used to establish a pattern theorem for 2SAPs. Specifically a "Pattern Insertion" strategy based on [10] (see also [11, 12] ) was employed to establish the *2SAP Pattern Theorem*: Given any proper 2SAP pattern $P$ in $T(N,M)$, there exists an $\epsilon_P > 0$ such that the probability that an $n$-edge 2SAP contains at least $\lfloor \epsilon_P n \rfloor$ copies of the pattern $P$ approaches one exponentially fast as $n$ goes to infinity.

Next, using the theory of tangles, it is proved that the occurrence in a 2SAP of the proper 2SAP pattern $P_T$ whose projection is shown in Figure 3 (a) (the pattern is the central dashed and solid lines) ensures that the 2SAP is topologically linked. Hence by the 2SAP pattern theorem, for $M+N \geq 4$ (to ensure that $P_T$ can occur), all but exponentially few sufficiently large 2SAPs in $T(N,M)$ are topologically linked. Furthermore, the probability that an $n$-edge 2SAP is topologically linked goes to 1 exponentially fast.

Finally, using the proper 2SAP pattern $P_L$ (see Figure 3 (b)) plus a "coin-tossing" argument, it is established that the linking number $Lk$ of an $n$-edge 2SAP $G_n$ satisfies $\lim_{n\to\infty} \mathbb{P}(|Lk(G_n)| \geq f(n)) = 1$ for any function $f(n) = o(\sqrt{n})$. Hence the probability of a non zero linking number for an $n$-edge 2SAP approaches one as $n$ goes to infinity, which implies that the probability of homological linking also goes to 1 (as $n \to \infty$). Finally, it is established that, due to the tube constraint, the linking number of an $n$-edge 2SAP grows at most linearly in $n$.



(a)




(b) Pattern $P_L$.

Figure 3: (a) Projection (central dashed and solid lines only) of a proper 2SAP pattern, $P_T$, which guarantees topological linking. (b) Projection of the proper 2SAP pattern $P_L$.

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## References

[1] M. Atapour, C. E. Soteros, C. Ernst and S. G. Whittington, J. Knot Theory and its Ramifications (in press)

[2] C. Vanderzande, Lattice Models of Polymers (Cambridge University Press; Cambridge, England) (2004).

[3] E. Orlandini and S. G. Whittington, Reviews of Modern Physics **79** (2007) 611-642.

[4] H. L. Frisch and E. Wasserman, J. Am Chem Soc. **83** (1961) 3789-3795.

[5] M. Delbruck, Proc. Symp. on Appl. Math.**14** (1962) 55-63.

[6] D. W. Sumners and S. G. Whittington, J. Phys. A: Math. Gen. **21** (1988) 1689-1694.

[7] N. Pippenger, Discrete Applied Math. **25** (1989) 273-278.

[8] E. Orlandini, E. J. Janse van Rensburg, M. C. Tesi and S. G. Whittington, J. Phys. A: Math. Gen. **27** (1994) 335-345.

[9] M. C. Tesi, E. J. Janse van Rensburg, E. Orlandini and S. G. Whittington, IMA Vol. in Math. and its Appl. **103** (1998) 135-157.

[10] N. Madras, Annals of Combinatorics **3** (1999) 357-384.

[11] C. E. Soteros, Journal of Physics: Conference Series **42** (2006) 258–267.

[12] M. Atapour, Topological Entanglement Complexity of Systems of Polygons and Walks in Tubes (PhD thesis, University of Saskatchewan) (2008)