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Stretched polygons in a lattice tube

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Abstract

We examine the topological entanglements of polygons confined to a lattice tube and under the influence of an external tensile force f. The existence of the limiting free energy for these so-called stretched polygons is proved and then, using transfer matrix arguments, a pattern theorem for stretched polygons is proved. Note that the tube constraint allows us to prove a pattern theorem for any arbitrary value of f, while without the tube constraint it has so far only been proved for large values of f. The stretched polygon pattern theorem is used first to show that the average span per edge of a randomly chosen n-edge stretched polygon approaches a positive value, non-decreasing in f, as $n \to \infty$. We then show that the knotting probability of an n-edge stretched polygon confined to a tube goes to one exponentially as $n \to \infty$. Thus as $n \to \infty$ when polygons are influenced by a force f, no matter its strength or direction, topological entanglements, as defined by knotting, occur with high probability.

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Introduction

The problem of knotting in ring polymers has been of interest for more than 40 years. For the model of self-avoiding polygons on a three-dimensional lattice it was proved in 1988 that all except exponentially few sufficiently long polygons are knotted [1, 2] and similar results were proved soon after for other models [3, 4]. The recent interest [5] in how polymers respond to a tensile force as applied, for instance, in atomic force microscopy, prompted interest in knotting under the influence of a force. For the lattice polygon model, consider a polygon with n edges subject to a tensile force f (measured in units of inverse length) so that the elastic energy is fs (dimensionless) where s is the span of the polygon in the direction in which the force is applied. There exists a value $f_0 > 0$ such that for any fixed force $f > f_0$ the probability of knotting goes to unity as n goes to infinity [6]. Note that f must be fixed before $n \to \infty$.

The general approach to proving these results is to prove a pattern theorem [7]. Roughly speaking, a pattern theorem ensures that any sequence of edges (i.e. a pattern) that can occur more than once in a polygon will occur at least once in all except exponentially few sufficiently long polygons. By a suitable choice of pattern the results about knotting follow easily [1]. We have pattern theorems for lattice polygons for zero force [1] and for sufficiently large forces [6]. (For self-avoiding walks a pattern theorem has been proved for all positive forces [8].)

If the polygon is confined to a right rectangular prism with infinite height (referred to herein as a tube) then for $f = 0$ a pattern theorem has been proved using transfer matrix methods [9]. This is possible because the confinement means that the problem is essentially one dimensional. In this paper, we prove a pattern theorem for polygons in a tube with a force applied along the long axis of the tube, for any value of the applied force. From this it follows that polygons confined to a tube, subject to any applied force f, are knotted with probability one in the $n \to \infty$ limit.

Stretched polygons in a tube

The three-dimensional integer lattice is defined to be the infinite graph embedded in $\mathbb{R}^3$ with vertex set $\mathbb{Z}^3$ and edge set $E(\mathbb{Z}^3) = \{\{u, v\} | u, v \in \mathbb{Z}^3, |u - v| = 1\}$, where $|u - v|$ is the Euclidean distance between u and v. The term *subgraph* of $\mathbb{Z}^3$ will refer to an embedding of a graph in $\mathbb{Z}^3$. An n-edge *self-avoiding polygon* (SAP) is an n-edge connected subgraph of $\mathbb{Z}^3$ with each vertex having degree 2. For SAPs, $n \geqslant 4$ and even and this will be assumed henceforth. We will also refer to a SAP as a polygon.

Given integers $N \geqslant 0$ and $M \geqslant 0$, we consider the tubular sublattice $T(N, M)$ of the simple cubic lattice induced by the vertex set $\{(x, y, z) \in \mathbb{Z}^3 | 0 \leqslant x \leqslant N, 0 \leqslant y \leqslant M, z \geqslant 0\}$. An n-edge SAP in $T(N, M)$ is defined to be an n-edge connected subgraph of $T(N, M)$ with each vertex having degree 2 and such that there is at least one vertex of the polygon in the plane $z = 0$. Define $\mathcal{P}_n(N, M)$ to be the set of n-edge SAPs in $T(N, M)$, $\mathcal{P}(N, M) = \cup_{n \geqslant 4} \mathcal{P}_n(N, M)$ and $p_n(N, M) = |\mathcal{P}_n(N, M)|$. Then, for $(N, M) \neq (0, 0)$, the following limit exists and satisfies [10]:

$$\log \mu_p(N, M) \equiv \kappa_p(N, M) \equiv \lim_{n \to \infty} n^{-1} \log p_n(N, M) = \sup_{n \geqslant 4} n^{-1} \log p_n(N, M) < \infty. \tag{1}$$

Given a SAP $\omega \in \mathcal{P}_n(N, M)$, its *span* is defined to be the maximum z-coordinate over all the z-coordinates of the vertices in ω and is denoted by $s(\omega)$. Given $m \geqslant 0$, we investigate polygons of span m which are confined to a tube. We assume that a force f parallel to the z-axis, perpendicular to and incident on the plane $z = m$ is applied to a single ring polymer modelled by a SAP. Figure 1 illustrates an example of such a scenario.

The partition function of this model is defined to be

$$Z_n(N, M; f) = \sum_{m=0}^{(n/2)-1} p_n(N, M; m)\, \mathrm{e}^{fm}, \tag{2}$$

where $p_n(N, M; m)$ denotes the number of n-edge SAPs with span m in $\mathcal{P}_n(N, M)$. If $f > 0$ then the force is a tensile force, tending to stretch the polygon in the z-direction and the polygons influenced by this force are called *stretched polygons* [6]. On the other hand, if $f < 0$, then the force tends to push the planes $z = 0$ and $z = m$ together. Here, for convenience, regardless of the sign of f we call the polygons under the influence of f stretched polygons.

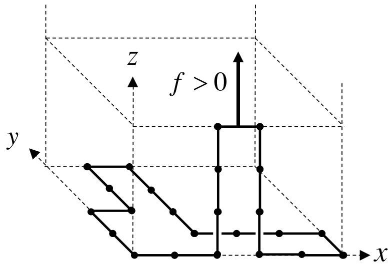


Figure 1. Example of a polygon confined to a tube and subject to a force f.

Let W_n be a random n-edge stretched polygon with probability mass function (pmf) given by

$$\mathbb{P}(W_n = \omega) = \frac{e^{fs(\omega)}}{Z_n(N, M; f)}, \qquad \text{for all} \quad \omega \in \mathcal{P}_n(N, M). \tag{3}$$

One goal here is to investigate the behaviour of the expected value of $s(W_n)$ as a function of f. To do this, we first prove some results about the asymptotic behaviour of the partition function.

As discussed in [10, section 4], for polygons in $T(N, M)$ there exist non-negative values c_T and t_T, $c_T \geqslant 2t_T$, such that concatenating an n_1-edge polygon with span m_1 to an n_2-edge polygon with span $(m - m_1)$ results in an $(n_1 + n_2 + c_T)$-edge polygon with span $(m + t_T)$. Therefore, the following inequality holds

$$\sum_{m_1=0}^{\frac{n_1}{2}-1} p_{n_1}(N, M; m_1) p_{n_2}(N, M; m - m_1) \leqslant p_{n_1+n_2+c_T}(N, M; m + t_T). \tag{4}$$

Multiplying both sides of this inequality by e^{fm} and summing over m gives rise to

$$Z_{n_1}(N, M; f) Z_{n_2}(N, M; f) \leqslant e^{-ft_T} Z_{n_1+n_2+c_T}(N, M; f), \tag{5}$$

where we have used the facts that $c_T \geqslant 2t_T$, $n_1/2 - 1 < m$ and $n_1 \geqslant 2m_1$. Furthermore, using equation (1)

$$\max\{1, e^{f(n-1)/2}\} \leqslant Z_n(N, M; f) = \sum_{m=0}^{\frac{n}{2}-1} p_n(N, M; m) e^{fm} \leqslant \max\{1, e^{f(n-1)/2}\} (\mu_p(N, M))^n. \tag{6}$$

We next use these facts to establish the existence and other properties of the limiting free energy for the model. Note that the series of results presented next follow *mutatis mutandis* from the arguments given in [6, theorem 2.1] for polygons in $\mathbb{Z}^3$ without the tube constraint.

Letting $a_n = \log\left(e^{ft_T} Z_{n-c_T}(N, M; f)\right)$, equation (5) implies that $\{a_n\}$ is a super-additive sequence. Therefore, standard arguments (see [11–14]) together with the final bound from equation (6) show that the limiting free energy, $\mathcal{F}(N, M; f)$, exists and satisfies

$$\mathcal{F}(N, M; f) \equiv \lim_{n\to\infty} n^{-1} \log Z_n(N, M; f) = \sup_{n\geqslant 4} n^{-1} a_n < \infty. \tag{7}$$

Equation (6) leads to bounds on the free energy: for $f \geqslant 0$

$$f/2 \leqslant \mathcal{F}(N, M; f) \leqslant \log \mu_p(N, M) + f/2, \tag{8}$$

while for $f < 0$

$$0 \leqslant \mathcal{F}(N, M; f) \leqslant \log \mu_p(N, M). \tag{9}$$

The Cauchy–Schwartz inequality gives immediately that the function $Z_n(N, M; f)$ is a log-convex function of f. Hence $F_n(N, M; f) = n^{-1} \log Z_n(N, M; f)$ is convex in f and equation (7) gives that (see [14, 15]) $\mathcal{F}(N, M; f)$ is also convex in f. Furthermore [14, 15], $\mathcal{F}(N, M; f)$ is continuous and differentiable almost everywhere (a.e.) with a non-decreasing derivative in f such that a.e.:

$$\lim_{n\to\infty} (\mathrm{d}F_n(N, M; f)/\mathrm{d}f) = \mathrm{d}\mathcal{F}(N, M; f)/\mathrm{d}f. \tag{10}$$

Thus

$$\begin{aligned} n\frac{\mathrm{d}}{\mathrm{d}f} F_n(N, M; f) &= \frac{\mathrm{d}}{\mathrm{d}f}\big[\log Z_n(N, M; f)\big] \\ &= \frac{\sum_{m=0}^{(n/2)-1} m p_n(N, M; m)\mathrm{e}^{fm}}{Z_n(N, M; f)} \\ &= \mathbb{E}_f(s(W_n)) \end{aligned} \tag{11}$$

is non-decreasing in f, where the expected value is with respect to the pmf of equation (3). Furthermore, by equation (10), the following limit exists a.e. and is non-decreasing in f:

$$\lim_{n\to\infty} \frac{\mathbb{E}_f(s(W_n))}{n} = \lim_{n\to\infty} \frac{\mathrm{d}}{\mathrm{d}f} F_n(N, M; f). \tag{12}$$

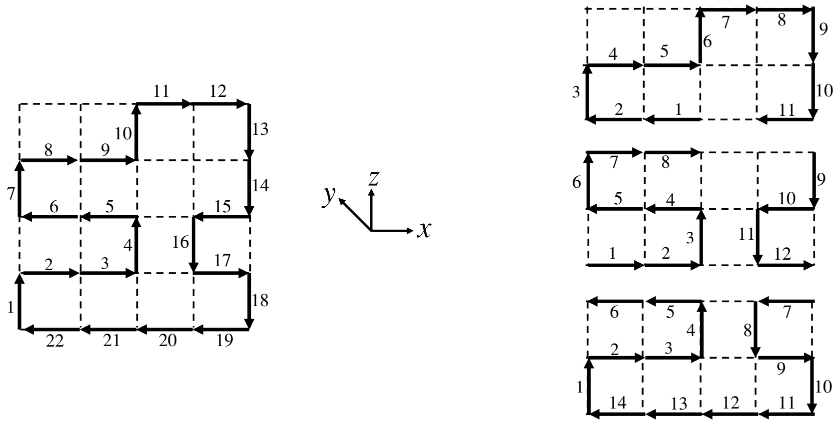
Pattern theorem

In this section, the transfer matrix arguments used by Soteros [9] to prove a pattern theorem for SAPs in a tube with $f = 0$ are generalized to prove a pattern theorem for stretched polygons subject to an arbitrary fixed force f.

Given any integers $k \geqslant 0$ and $i \geqslant 1$ we define the *ith k-tube* to be the sublattice of the (N, M)-tube induced by the vertex set $\{(x, y, z) \in \mathbb{Z}^3 | 0 \leqslant x \leqslant N, 0 \leqslant y \leqslant M, i - 1 \leqslant z \leqslant i - 1 + k\}$. Given a polygon $G \in \mathcal{P}(N, M)$ with span m and given integers k and i such that $0 \leqslant k \leqslant m$ and $1 \leqslant i \leqslant m - k + 1$, G's *configuration* in the ith k-tube consists of this sublattice plus G's edges in it with a specific relative ordering assigned to them (see, for example, figure 2). The specific relative ordering comes from a specified order on the edges of G which is defined as follows (see also [9]). Let v_b and $e_b = \{v_b, v\}$ be respectively the bottom vertex and edge of G (see [9] for standard definitions of bottom vertex and edge). A direction is assigned to e_b by directing the edge to go from v_b to v. This naturally induces an ordering on G starting with edge e_b as the first edge and ordering the other edges following the direction induced by that of e_b. For convenience, G's *configuration* in the ith k-tube is referred to as the *SAP configuration* with span k (*k-config* for short) of G which *occurs* at the ith subsection of G.

Hence the k-config at the ith subsection of G is defined not just by the edges of G in the ith k-tube but also by their relative ordering, according to the assigned order on the edges in G. Any two k-configs are considered *equivalent* if they have the same set of occupied vertices and edges (up to z-translation) and have the same relative ordering on their edges. Any k-config that occurs at the first, $i = 1$, (last, $i = s(G) - k + 1$) subsection of some polygon $G \in \mathcal{P}(N, M)$ is referred to as a *start* (*end*) k-config. Any k-config that occurs at the ith subsection, $2 \leqslant i \leqslant s(G) - k$, of some polygon $G \in \mathcal{P}(N, M)$ with $s(G) \geqslant k + 2$ is referred to as a *proper* k-config.

Given $k \geqslant 2$, let $\Pi(k)$, $\Pi_1(k)$ and $\Pi_2(k)$ be the sets of distinct k-configs corresponding to the proper, start and end k-configs respectively such that each k-config is considered to be a



(*a*) (*b*)

Figure 2. (*a*) An example of a 22-edge oriented polygon with span 4 in $T(4, 0)$. The first edge is e_b, the bottom edge of the polygon. (*b*) The associated SAP configurations with span 2 (2-configs). The number beside an edge indicates its relative order.

configuration on the first k-tube of $T(N, M)$. Define a digraph $D_k = (V_k, A_k)$ as follows: let the k-configs in $\Pi(k) \cup \Pi_1(k) \cup \Pi_2(k)$ be the vertices of the digraph, i.e.

$$V_k = \Pi(k) \cup \Pi_1(k) \cup \Pi_2(k) = \{P_1, P_2, \dots, P_{|V_k|}\}. \tag{13}$$

An arc from P_i to P_j belongs to A_k if and only if the configuration of the k-config P_i on the second $(k-1)$-tube is equivalent to the configuration of the k-config P_j on the first $(k-1)$-tube.

It can be shown that $\Pi(k)$, $\Pi_1(k)$ and $\Pi_2(k)$ and their corresponding digraph D_k satisfy the following: given $r \geqslant 2$, consider a walk, $P_{i_1}, P_{i_2}, P_{i_3}, \dots, P_{i_{r-1}}, P_{i_r}$, on the digraph with length $r-1$ where $P_{i_1} \in \Pi_1(k)$, $P_{i_r} \in \Pi_2(k)$ and, for $r \geqslant 3$, $P_{i_j} \in \Pi(k)$ for $2 \leqslant j \leqslant r-1$ (this is also called a sequence of *correctly connected* k-configs). D_k has the property that every such walk defines a span $r+k-1$ polygon $G \in \mathcal{P}(N, M)$ starting (ending) with the config P_{i_1} (P_{i_r}) and in which, for $r \geqslant 3$, config P_{i_j} occurs at the jth subsection, for $j = 2, \dots, r-1$. Moreover, any span $r+k-1$ SAP $G \in \mathcal{P}(N, M)$ starting with config P_{i_1} and ending with config P_{i_r} corresponds to a walk of length $r-1$ on D_k as above.

Using this digraph we can define a transfer matrix as follows. First, since each k-config is contained in a finite subgraph of the lattice (namely the first k-tube) and there is only a finite number of ways to assign a relative ordering to its edges, there is a finite number of such configs. Hence, let

$$\Pi(k) = \{P_1, P_2, \dots, P_{|\Pi(k)|}\}, \qquad \Pi_1(k) = \left\{P'_1, P'_2, \dots, P'_{|\Pi_1(k)|}\right\},$$
$$\Pi_2(k) = \left\{P''_1, P''_2, \dots, P''_{|\Pi_2(k)|}\right\}. \tag{14}$$

As discussed above, a walk in the digraph which starts with a start config, ends with an end config and otherwise only traverses proper configs leads to a polygon in $\mathcal{P}(N, M)$. The goal is to define a transfer matrix so that each such walk gets weighted by $x^n e^{fm}$, where n is the number of edges and m is the span of the resulting polygon, and the weight is calculated using the configs traversed in the walk. Given $k \geqslant 2$, the span of the polygon is obtained simply by adding $k-1$ to the number of configs traversed in the walk. However, because subsequent configs in the walk correspond to overlapping configs in the polygon, edges must be counted more carefully so as to avoid overcounting. To do this properly, for both start and proper configs traversed, only edges in the first 1-tube of the config are considered while for an end config, all the edges in the config are counted. That is, for any $1 \leqslant i \leqslant |\Pi(k)|$ ($1 \leqslant i \leqslant |\Pi_1(k)|$), define e_i (e_i') to be the number of edges of P_i (P_i') within the first 1-tube but not in the plane $z = 1$ and, for any $1 \leqslant i \leqslant |\Pi_2(k)|$, define e_i'' to be the total number of edges in P_i''. This allows for the definition of the $|\Pi(k)| \times |\Pi(k)|$ *transfer matrix* $G(x) = (g_{i,j}(x))$ as follows:

$$g_{i,j}(x) = \begin{cases} x^{e_i} & \text{if} \quad (P_i, P_j) \in A_k,\ P_i, P_j \in \Pi(k) \\ 0 & \text{otherwise.} \end{cases} \tag{15}$$

Define also the $|\Pi_1(k)| \times |\Pi(k)|$ matrix $B(x) = (u_{i,j}(x))$ as follows:

$$u_{i,j}(x) = \begin{cases} x^{e_i'} & \text{if} \quad (P_i', P_j) \in A_k,\ P_i' \in \Pi_1(k),\ P_j \in \Pi(k) \\ 0 & \text{otherwise.} \end{cases} \tag{16}$$

Similarly define the $|\Pi(k)| \times |\Pi_2(k)|$ matrix $C(x) = (v_{i,j}(x))$ as follows:

$$v_{i,j}(x) = \begin{cases} x^{e_i''} & \text{if} \quad (P_i, P_j'') \in A_k,\ P_i \in \Pi(k),\ P_j'' \in \Pi_2(k) \\ 0 & \text{otherwise.} \end{cases} \tag{17}$$

Given any $x > 0$, it can be shown using concatenation that for any pair of proper configs $P_i, P_j \in \Pi(k)$ there exists an integer m such that $(G(x)^m)_{i,j} > 0$. To see this, start with a polygon in $\mathcal{P}(N, M)$ in which proper config P_i occurs and concatenate it to a polygon in $\mathcal{P}(N, M)$ in which proper config P_j occurs. This yields a polygon in $\mathcal{P}(N, M)$ in which P_i occurs at some subsection and config P_j occurs at a later subsection. From this one obtains a sequence of m correctly connected configs starting with config P_i and ending in config P_j. Thus for any $x > 0$, $G(x)$ is an irreducible matrix and since at least one diagonal entry of $G(x)$ can be shown to be non-zero, $G(x)$ is also an aperiodic matrix.

Given $x > 0, r \geqslant 2$, consider a sequence of r correctly connected k-configs of the form $P_{i_1}', P_{i_2}, P_{i_3}, \ldots, P_{i_{r-1}}, P_{i_r}''$, such that $u_{i_1,i_2}(x) \neq 0$, $v_{i_{r-1},i_r}(x) \neq 0$, and, for $r \geqslant 3$, $g_{i_j,i_{j+1}}(x) \neq 0$ for $2 \leqslant j \leqslant r-2$. This sequence defines a span $r + k - 1$ cluster, G, starting (ending) with config P_{i_1}' (P_{i_r}'') and in which, for $r \geqslant 3$, proper config P_{i_j} occurs at the jth subsection, for $j = 2, \ldots, r-1$. The weight associated with this polygon in $(B(x)G(x)^{r-2}C(x))_{i_1,i_r}$ is $x^{e_{i_1}' + e_{i_r}'' + \sum_{j=2}^{r-1} e_{i_j}} = x^{e(G)}$, where $e(G)$ is the total number of edges in G and if $r = 2$ the last sum in the exponent is zero. Hence the weight associated with this polygon in $\mathrm{e}^{f(k+1)}(B(x)[\mathrm{e}^f G(x)]^{r-2}C(x))_{i_1,i_r}$ is $x^{e(G)}\mathrm{e}^{fs(G)}$.

Also, given $r \geqslant 2$, any polygon with span $r+k-1$ in $\mathcal{P}(N, M)$ starting with config P_{i_1}' and ending with config P_{i_r}'' can be decomposed into a sequence of r configs as above. Thus for any fixed real f and fixed integer $k \geqslant 2$, the generating function $Q(x, f) = \sum_{n \geqslant 4} Z_n(N, M; f)x^n$ satisfies the following:

$$Q(x, f) = Q_1(x, f) + Q_2(x, f), \qquad \text{where} \tag{18}$$

$$Q_2(x, f) = \mathrm{e}^{f(k+1)} \sum_{h=0}^{\infty} \sum_{i=1}^{\Pi_1(k)} \sum_{j=1}^{\Pi_2(k)} (B(x)[\mathrm{e}^f G(x)]^h C(x))_{i,j}, \tag{19}$$

and $Q_1(x, f) = \sum_{n=4}^{h(k)} \sum_{m \leqslant k} p_n(N, M; m)\, \mathrm{e}^{fm} x^n$ is the analytic (since it is a finite sum) contribution to $Q(x, f)$ due to SAPs with span at most k. Given a fixed f, using standard results from linear algebra and Perron–Frobenius Theory [18], there exists $x_0(f) > 0$ such that for all $|x| < x_0(f)$

$$Q_2(x, f) = \frac{1}{\det(I - \mathrm{e}^f G(x))} \sum_{i=1}^{\Pi_1(k)} \sum_{j=1}^{\Pi_2(k)} \sum_{o=1}^{\Pi(k)} \sum_{l=1}^{\Pi(k)} u_{i,l}(x) \det(I - \mathrm{e}^f G(x); o, l) v_{o,j}(x), \tag{20}$$

where $(A; o, l)$ represents the matrix obtained by removing the lth row and oth column from a given matrix A. The large n properties of $Z_n(N, M; f)$ can be determined from the non-analyticities of $Q(x, f)$ which are the same as those of $Q_2(x, f)$. As presented below, these can be determined from the matrix $e^f G(x)$.

The transfer matrix $G(x)$ is essentially the same as the transfer matrix defined in [9]. Hence the proof of the pattern theorem in [9, theorem 6.1], which is based on Perron–Frobenius theory [18] and arguments the same as those used in [16, lemma 9 and theorem 3], applies again here with only minor modifications to accommodate replacing $G(x)$ by $e^f G(x)$ (see also [17] for further generalizations of this argument). This results in the following pattern theorem for stretched polygons.

Theorem 1. *For any integer $k \geqslant 2$, any proper k-config $P \in \Pi(k)$ and any real fixed force f, there exist non-negative values β_f and $x_0(f)$ such that*

$$Q(x, f) \to \beta_f (x_0(f) - x)^{-1} \qquad \text{as} \quad x \to x_0(f) \tag{21}$$

and

$$Z_n(N, M; f) = \beta_f (x_0(f))^{-n-1} + o((x_0(f))^{-n}) \qquad \text{as} \quad n \to \infty, \tag{22}$$

with $x_0(f)$ the unique non-negative value of x such that e^{-f} is an eigenvalue of $G(x)$. Moreover, there exist non-negative values $\bar{x}_0(f) > x_0(f)$ and $\bar{\alpha}_f$ such that

$$Z_n(N, M; \bar{P}, f) = \bar{\alpha}_f (\bar{x}_0(f))^{-n} + o((\bar{x}_0(f))^{-n}) \qquad \text{as} \quad n \to \infty, \tag{23}$$

where $Z_n(N, M; \bar{P}, f) = \sum_m p_n(N, M; \bar{P}, m) e^{fm}$ with $p_n(N, M; \bar{P}, m)$ the number of span m SAPs in $\mathcal{P}_n(N, M)$ in which P never occurs.

Similarly the proof of [16, theorem 9] can be modified in a straightforward manner to prove the following result for stretched polygons.

Theorem 2. *Given any f, then there exists $\gamma_f > 0$ such that as $n \to \infty$*

$$\mathbb{E}_f(s(W_n)) = \gamma_f n + O(1), \tag{24}$$

where W_n has pmf given by equation (3). Thus the following limit exists everywhere and (by equation (12)) is non-decreasing in f

$$\lim_{n\to\infty} \frac{1}{n} \mathbb{E}_f(s(W_n)) = \gamma_f. \tag{25}$$

Entanglement complexity of stretched polygons

Having the pattern theorem for stretched polygons in a tube, we can now discuss their knotting probability. In particular, we can take P to be a tight trefoil pattern (e.g. the pattern shown in figure 3) in $T(N, M)$ and prove that the knotting probability goes to one as $n \to \infty$ for any arbitrary value of f.

Let

$$Z_n^\circ(N, M; f) = \sum_{m=0}^{n/2-1} p_n^\circ(N, M; m)\, e^{fm}, \tag{26}$$

where $p_n^\circ(N, M; m)$ is the number of unknotted n-edge SAPs with span m in $T(N, M)$. Concatenating two unknotted polygons results in an unknotted polygon, so the proof of

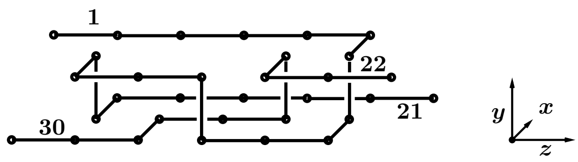


Figure 3. A tight trefoil 6-config in $T(2, 1)$ such that its occurrence in any polygon guarantees that the polygon is knotted.

equation (7) can be modified in a straightforward fashion to show the existence of the limiting free energy for unknotted stretched polygons:

$$\mathcal{F}^o(N, M; f) \equiv \lim_{n\to\infty} n^{-1} \log Z_n^o(N, M; f). \tag{27}$$

For the tight trefoil proper SAP 6-config P, as shown in figure 3, an n-edge unknotted polygon cannot contain P. Hence

$$p_n^\circ(N, M; m) \leqslant p_n(N, M; \bar{P}, m). \tag{28}$$

Multiplying both sides by e^{fm} and summing over m gives

$$Z_n^o(N, M; f) \leqslant Z_n(N, M; \bar{P}, f). \tag{29}$$

Taking logarithms, multiplying both sides by n^{-1} and letting $n \to \infty$ gives

$$\mathcal{F}^o(N, M; f) \leqslant \mathcal{F}(N, M; \bar{P}, f) < \mathcal{F}(N, M; f), \tag{30}$$

where the final inequality comes from the pattern theorem for stretched polygons, theorem 1.

Thus the probability that a stretched polygon is knotted satisfies

$$\frac{Z_n(N, M; f) - Z_n^o(N, M; f)}{Z_n(N, M; f)} = 1 - \frac{Z_n^o(N, M; f)}{Z_n(N, M; f)} = 1 - e^{-(\mathcal{F}(N,M;f)-\mathcal{F}^o(N,M;f))n+o(n)}, \tag{31}$$

which goes to one exponentially as $n \to \infty$.

The proof of [16, theorem 7] (see also [17]) can also be modified in a straightforward manner to give the following result for the density of proper 6-config P in stretched polygons.

Theorem 3. *Given $T(N, M)$ with $N \geqslant 2$ and $M \geqslant 1$ and any f, there exists $\delta_f > 0$ such that as $n \to \infty$*

$$\mathbb{E}_f(n_P(W_n)) = \delta_f n + O(1), \tag{32}$$

where W_n has pmf given by equation (3) and $n_P(W_n)$ is the number of 6-configs in W_n which are equivalent to P. Thus the following limit exists

$$\lim_{n\to\infty} \frac{1}{n}\mathbb{E}_f(n_P(W_n)) = \delta_f. \tag{33}$$

Therefore, most random stretched polygons have a non-zero density of trefoils in their knot decomposition.

Discussion

We proved a pattern theorem for polygons confined to a tube in $\mathbb{Z}^3$ and subject to a force and we used this to show that trefoils occur with high probability in the knot decomposition of large confined polygons for any value of the applied force. The same approach can be used for any other knot type (provided that the cross section of the tube is large enough to admit the knot) and the approach can be extended to show that each knot type occurs a positive density of times for sufficiently large confined polygons for any value of the force. This implies that the polygons have a high degree of topological entanglement complexity. We also use the convexity of the limiting free energy and transfer matrix arguments to prove that the expected span per edge of large confined polygons approaches a positive value which is non-decreasing in the applied force f.

The same approach can be applied to investigate the topological entanglement complexity of loops (graphs with two vertices of degree 1 in the plane $z = 0$ and all other vertices of degree 2) confined to a tube. The results are essentially identical to those for polygons.

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