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Knotting in stretched polygons

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Abstract

The knotting in a lattice polygon model of ring polymers is examined when a stretching force is applied to the polygon. By examining the incidence of cut-planes in the polygon, we prove a pattern theorem in the stretching regime for large applied forces. This theorem can be used to examine the incidence of entanglements such as knotting and writhing. In particular, we prove that for arbitrarily large positive, but finite, values of the stretching force, the probability that a stretched polygon is knotted approaches 1 as the length of the polygon increases. In the case of writhing, we prove that for stretched polygons of length n, and for every function $f(n) = o(\sqrt{n})$, the probability that the absolute value of the mean writhe is less than $f(n)$ approaches 0 as $n \to \infty$, for sufficiently large values of the applied stretching force.

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1. Introduction

Micro-manipulation techniques [10, 23] have made possible the probing and manipulation of single polymeric molecules to study their mechanical properties. For example, the effects of knotting on the mechanical properties of a linear polymer have been considered recently by Farago and co-workers [3]. These advanced laboratory techniques induce forces in single polymers, which may in turn affect the statistical and physical properties of the molecule, thus altering the incidence of topological and geometric quantities such as knotting and writhing.

A related situation is encountered when polymeric molecules are confined to a narrow pore or slit and interacting with the walls of the confining space [2, 21, 25]. These situations have been modeled by bead-spring models of polymers interacting with spheres or walls [20] and also numerically and rigorously using a self-avoiding walk model of a linear polymer in a slab [14, 15]. In these models there are attractive and repulsive forces between the polymer and the walls of the confining space, and several phases have been identified in the models, depending on the strength and nature of the forces.

Entanglements are an unavoidable feature in linear polymers in the scaling limit, even in confining spaces or when in an adsorbed state [26, 28]. The incidence of geometric and topological entanglements in polymeric molecules contributes to the free energy and may have an important effect on the thermodynamic properties of these molecules and on their mechanical properties [27]. Applied forces on a polymeric molecule may affect or influence the incidence of entanglements, with resulting consequences for the free energy and thermodynamic properties of the model.

In this paper we examine rigorously a self-avoiding walk model of a ring polymer pulled by a force, by subjecting a lattice polygon to an applied external force along the Z-direction of the lattice. This situation models a ring polymer, such as circular DNA, subject to a force in the presence of a topoisomerase which mediates strand passages which may change the knot type of the polymer.

We prove that this model has a limiting free energy $\mathcal{F}(f)$, and that the free energy is a non-decreasing and convex function of the applied force f. We next consider stretched polygons subject to an applied force, and we prove a pattern theorem for arbitrarily large positive values of the applied force f stretching the polygon. The method of proof relies on the incidence of *cut-planes* in the polygon (these are planes cutting the polygon into sub-walks with endpoints with minimum and maximum Z-coordinates). We prove that for large enough values of the force f there is a positive density of such cut-planes in the limit as the length of the polygons goes to infinity. This allows us to prove a pattern theorem in this model, which is presented in sections 3 and 4.

In section 5, some consequences of the pattern theorem are examined. In particular, we consider the incidence of knots in stretched polygons, and prove that for arbitrarily large positive but finite values of f a stretched polygon will be knotted with probability 1 in the limit as its length approaches infinity. We also consider writhe of stretched polygons, and we generalize a result for polygons to stretched polygons [13]: the absolute writhing of a stretched polygon of length n increases at least proportionally to $\sqrt{n}$ with probability 1, if the applied force is a pulling or stretching force.

2. Stretched polygons

Let p_n be the number of polygons of length n in the hypercubic lattice $\mathbb{Z}^d$, undirected and counted up to equivalence under translations. Similarly, let c_n be the number of self-avoiding walks of length n, undirected and counted up to equivalence under translations. It is known that the limits

$$\lim_{n\to\infty} c_n^{1/n} = \lim_{n\to\infty} p_n^{1/n} = \mu \tag{1}$$

exist [6, 8]. The limit of $p_n^{1/n}$ is taken only through even values of n, and in this paper we shall assume, without mentioning this again, that n is even and that limits such as the above are taken through the sequence of even numbers when we consider polygons. The number μ is the *growth constant* of self-avoiding walks.

Consider the d-dimensional hypercubic lattice $\mathbb{Z}^d$. If $x \in \mathbb{Z}^d$ is a vertex in $\mathbb{Z}^d$, then the coordinates of x are denoted by $(X(x), Y(x), \ldots, Z(x))$. The dth coordinate of x will always be denoted by $Z(x)$. The s-slab $\mathbb{L}_s \subset \mathbb{Z}^d$ is the set

$$\mathbb{L}_s = \{x \in \mathbb{Z}^d \mid 0 \leqslant Z(x) \leqslant s\}.$$

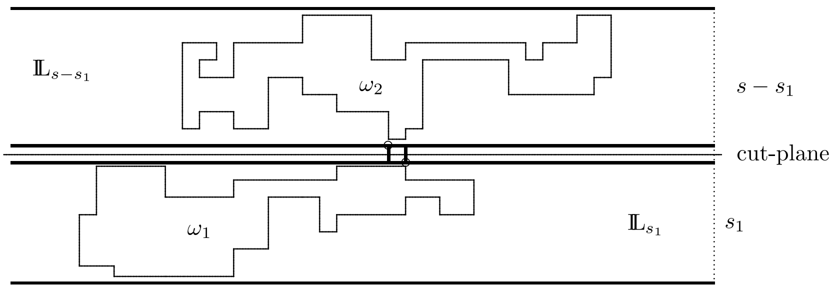

Figure 1. Concatenation of two stretched polygons ω_1 in $\mathbb{L}_{s_1}$ and ω_2 in $\mathbb{L}_{s-s_1}$. Translate $\mathbb{L}_{s-s_1}$ until its bottom bounding plane has Z-coordinate one more than the Z-coordinate of $\mathbb{L}_{s_1}$, as in figure 1. Next, rotate ω_2 (about the Z-axis) and translate it in $\mathbb{L}_{s-s_1}$ until its bottom edge is parallel and next neighbor to the top edge of ω_1 in $\mathbb{L}_{s_1}$. Finally, delete these top and bottom edges and replace them with two edges in the Z-direction to join the polygons into one single stretched polygon in $\mathbb{L}_{s+1}$. If the first stretched polygon had length n, and the second had length m, then the resulting polygon has length $n+m$. There are $p_n(s_1)$ choices for ω_1 and $p_m(s-s_1)/(d-1)$ choices for ω_2 (the factor $(d-1)$ arises from the rotations of ω_2 in $\mathbb{L}_{s-s_1}$). There are also $s+1$ choices for s_1 in $[0, s]$. Thus, the result is the inequality in equation (3). Observe that a cut-plane is created when two stretched polygons are concatenated in this way.

The planes $Z = 0$ and $Z = s$ are the *bottom* and *top bounding planes* of the slab $\mathbb{L}_s$, respectively. Walks and polygons confined to $\mathbb{L}_s$ are called *strained*, and this model was considered in [15, 26].

Consider $p_n(s)$, the number of lattice polygons of Z-span s, confined in the s-slab $\mathbb{L}_s$ with Z-span s, and counted up to equivalence under translations parallel to the bottom-bounding plane. The partition function of polygons in the *strained ensemble* is given by $Z_n^s(s) = p_n(s)$. The limiting free energy of this model is known to exist [15], and is defined by $\mathcal{F}_s(s) = \lim_{n\to\infty}\left[\log Z_n^s(s)\right]/n$.

An alternative ensemble is the *stressed ensemble*, defined by the introduction of a force of f on the bounding planes of the slab. The partition function of this model is

$$Z_n(f) = \sum_{s=0}^{n/2-1} p_n(s)\,\mathrm{e}^{fs} \tag{2}$$

where f is a *force* conjugate to the Z-span s. If $f > 0$, then the force is a pulling force, tending to stretch the polygon in the Z-direction: we refer to these polygons as *stretched polygons*. If $f < 0$, then the force tends to push the planes bounding the slab $\mathbb{L}_s$ together. This negative force regime appears difficult to treat rigorously, and not much will be said about it in this paper beyond proving that a limiting free energy exists (see theorem 2.1).

The *top vertex* of a stretched polygon is the lexicographic most vertex in the top-bounding plane. The *bottom vertex* of a stretched polygon is the lexicographic least vertex in the bottom bounding plane. The *top edge* of a stretched polygon is that edge in the top bounding plane incident with the top vertex and with lexicographic most midpoint. The top edge is always incident with the top vertex, and it is normal to the Z-direction. The *bottom edge* of a stretched polygon is that edge in the bottom bounding plane incident with the bottom vertex and with lexicographic least midpoint. The bottom edge is always incident with the bottom vertex, and it is normal to the Z-direction.

A *cut-plane* in a stretched polygon is a plane $Z = N + 1/2$ normal to the Z-direction where N is an integer and which cuts through the polygon in exactly two edges. A cut-plane is illustrated in figure 1.

Two stretched polygons can be concatenated into a single stretched polygon as illustrated in figure 1. Consider two stretched polygons in slabs $\mathbb{L}_{s_1}$ and in $\mathbb{L}_{s-s_1}$. Translate the second slab until its bottom bounding plane has Z-coordinate one more than the Z-coordinate of the top bounding plane of the first slab, as in figure 1. Next, rotate (around the Z-axis) and translate the polygon in $\mathbb{L}_{s-s_1}$ until its bottom edge is parallel and next neighbor to the top edge of the polygon in $\mathbb{L}_{s_1}$. Finally, delete these top and bottom edges and replace them with two edges in the Z-direction to join the polygons into one single stretched polygon in $\mathbb{L}_{s+1}$. If the first stretched polygon had length n, and the second had length m, then the resulting polygon has length $n+m$. There are $p_n(s_1)$ choices for the polygon in the slab $\mathbb{L}_{s_1}$ and $p_m(s-s_1)/(d-1)$ choices for the polygon in the slab $\mathbb{L}_{s-s_1}$ (the factor $(d-1)$ arises from the rotations of the polygon in $\mathbb{L}_{s-s_1}$). There are also $s+1$ choices for s_1 in $[0, s]$. This construction shows that

$$\sum_{s_1=0}^{s} p_n(s_1)p_m(s-s_1) \leqslant (d-1)p_{n+m}(s+1). \tag{3}$$

If the inequality (3) is multiplied by e^{fs} and summed over s, then

$$Z_n(f)Z_m(f) \leqslant (d-1)\,\mathrm{e}^{-f}Z_{n+m}(f). \tag{4}$$

In other words, the function $[\mathrm{e}^f/(d-1)]Z_n(f)$ is a supermultiplicative function of n. In addition, observe that if $n \geqslant 4$ is even, then $Z_n(f)$ is bounded by

$$\max\left\{\mathrm{e}^f, \mathrm{e}^{(n/2)f}\right\} \leqslant Z_n(f) \leqslant \max\left\{\mathrm{e}^f, \mathrm{e}^{(n/2)f}\right\}p_n, \tag{5}$$

if $d = 2$, and

$$\max\left\{1, \mathrm{e}^{(n/2)f}\right\} \leqslant Z_n(f) \leqslant \max\left\{1, \mathrm{e}^{(n/2)f}\right\}p_n, \tag{6}$$

if $d > 2$, since there is at least one polygon of Z-span $(n/2)$ and also since there is at least one polygon of Z-span 1 in two dimensions and one polygon of Z-span zero if $d > 2$.

Theorem 2.1. *Let f be finite. Then the limiting free energy of stretched polygons is defined by*

$$\mathcal{F}(f) = \lim_{n\to\infty} \frac{1}{n}\log Z_n(f),$$

where the limit is taken through even values of n.

In addition, $Z_n(f) \leqslant (d-1)\,\mathrm{e}^{n\mathcal{F}(f)-f}$ and $\mathcal{F}(f)$ is convex in f and thus continuous and also differentiable almost everywhere. Finally, $f/2 \leqslant \mathcal{F}(f) \leqslant \log\mu + f/2$ if $f \geqslant 0$ while $0 \leqslant \mathcal{F}(f) \leqslant \log\mu$ if $f < 0$.

Proof. Existence of the limit and the bound on $Z_n(f)$ follow directly from equation (4) and from the bounds in equations (5) and (6) [11], after application of a basic theorem on subadditive functions, see [7, 11].

The Cauchy–Schwartz inequality gives

$$\begin{aligned} Z_n(f_1)Z_n(f_2) &= \sum_{s=0}^{n/2} p_n(s)\,\mathrm{e}^{f_1 s}\sum_{t=0}^{n/2} p_n(t)\,\mathrm{e}^{f_2 t} \\ &\geqslant \left(\sum_{s=0}^{n/2} p_n(s)\,\mathrm{e}^{[(f_1+f_2)/2]s}\right)^2 = (Z_n((f_1+f_2)/2))^2. \end{aligned}$$

Take logarithms of this, divide by n, and let $n \to \infty$. This shows that

$$\mathcal{F}(f_1) + \mathcal{F}(f_2) \geqslant 2\mathcal{F}((f_1+f_2)/2).$$

Thus $\mathcal{F}(f)$ is convex in f.

By equations (5) and (6), it follows that $0 \leqslant \mathcal{F}(f) \leqslant \log\mu$ if $f < 0$ and $f/2 \leqslant \mathcal{F}(f) \leqslant \log\mu + f/2$ if $f \geqslant 0$. This completes the proof. □

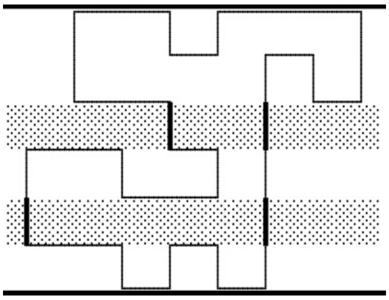

Figure 2. Cut-planes in this stretched polygon are indicated by the shaded strips. Pairs of cut-edges are in bold in the shaded strips.

3. Cut-planes

The concatenation in figure 1 creates two parallel edges oriented in the Z-direction. This construction can be reversed by deleting the two edges and filling in the resulting one-edge gaps in the sub-polygons. Two edges such as these are pairs of *cut-edges* in a polygon.

Generally, it is not necessary for the cut-edges to be adjacent in the lattice; two edges are a pair of cut-edges if they are parallel and also are the only pair of edges in a stretched polygon between two planes $Z = m$ and $Z = m + 1$, for some value of m. Examples of cut-edges in a polygon are given in figure 2.

In this section we consider the incidence of cut-edges and cut-planes in stretched polygons. In particular, we show that in the stretched regime ($f > 0$) for large enough values of f, almost all polygons will contain a positive density of cut-planes and cut-edges. This result proves that there are open spaces available in the polygon where one may insert a *pattern* (a sub-walk of a polygon), and makes possible the proof of a pattern theorem in section 4, provided that f is large and positive.

If two polygons A and B are concatenated to obtain a new polygon C as in figure 1, then A and B are the *components* of C. A and B will also be called *sub-polygons* in C. Concatenating two polygons as in figure 1 creates both a cut-plane and a pair of cut-edges in a polygon.

A *spanning walk* of length n and Z-span s is a self-avoiding walk in the slab $\mathbb{L}_s$ with endpoints in the planes $Z = 0$ and $Z = s$, respectively. Spanning walks between the vertices labeled by bullets in figure 3 occur between the top and bottom bounding planes of a slab containing a polygon. A *pair of spanning walks* is also illustrated in figure 4. In this case, two spanning walks of the slab are also mutually avoiding.

Cut-edges in a pair of spanning walks are two parallel edges which are also the only edges between two planes $Z = m$ and $Z = m + 1$, for some value of m. The pair of spanning walks in figure 4 has two pairs of cut-edges, each pair intersecting a *cut-plane*.

The two walks in a pair of spanning walks of a slab $\mathbb{L} - s$ are called its *components*. Observe that while the two components are self-avoiding, interactions amongst them are ignored. Any one or both components may be translated normal to the Z-direction.

3.1. Cut-planes and stretched polygons

Let $p_n(s; N)$ be the number of stretched polygons in $\mathbb{L}_s$ with exactly N cut-planes. If n is odd, or if $N > s$ or $N > n/2 - 1$, then $p_n(s; N) = 0$. Assume that n is always even. The partition function of stretched polygons of length n with $\lfloor bn \rfloor$ cut-planes is

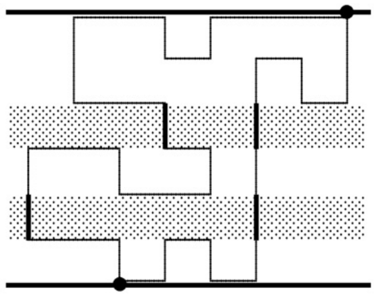

Figure 3. A stretched polygon in a slab can be decomposed into two spanning walks by cutting it in its lexicographic bottom vertex in the bottom bounding plane and in its lexicographic most vertex in its top-bounding plane. The resulting pair of spanning walks has coincident endpoints and has the same cut-planes as the original stretched polygon. In this figure the endpoints of the spanning walks are indicated by (•). Translating any one of the two components or both, normal to the *Z*-direction, will not destroy or create cut-planes.

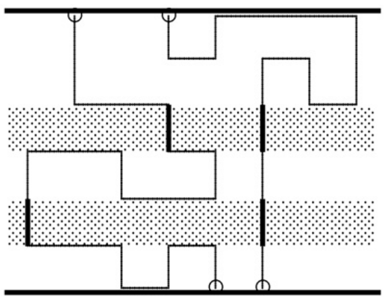

Figure 4. A pair of spanning walks in a slab with two cut-planes indicated by the shaded regions. Cut-edges in a polygon are indicated in bold in the shaded squares. Each walk in this pair is a spanning walk of the slab. The endpoints of the spanning walks are indicated by (○).

$$Z_n(f; \lfloor bn \rfloor) = \sum_{s=0}^{n/2-1} p_n(s; \lfloor bn \rfloor)\, \mathrm{e}^{fs}. \tag{7}$$

Define the limsup

$$\mu_b(f) = \limsup_{n\to\infty} [Z_n(f; \lfloor bn \rfloor)]^{1/n}, \tag{8}$$

and $\log \mu_b(f)$ may be interpreted as the limiting free energy of stretched polygons at force f with a density b of cut-planes. Naturally, $0 \leqslant b < 1/2$.

By concatenating two polygons as in figure 1, it follows that

$$Z_n(f; \lfloor b_1 n \rfloor) Z_m(f; \lfloor b_2 m \rfloor) \leqslant Z_{n+m}(f; \lfloor b_1 n \rfloor + \lfloor b_2 m \rfloor + 1).$$

If $b = b_1 = b_2$, then this shows that $Z_n(f; \lfloor bn \rfloor - 1)$ is a supermultiplicative function of n. More generally, one may check that $Z_n(f; \lfloor bn \rfloor - 1)$ satisfies assumption 3.1 in [12]. Thus, by lemmas 3.2, 3.3 and theorems 3.5 and 3.6, in [12], the following may be shown:

Theorem 3.1. *Let $b \in [0, 1/2)$ and let $Z_n(f; \lfloor bn \rfloor)$ be the partition function of stretched polygons of length n and with $\lfloor bn \rfloor$ cut-planes. Then, if $\mu_b(f)$ is defined as in equation (8), it follows that for all finite values f,*

(a)

$$\mu_b(f) = \lim_{n\to\infty} [Z_n(f; \lfloor bn \rfloor)]^{1/n};$$

(b) if $\delta_n/n \to b$ *as* $n \to \infty$*, where* $b \in [0, 1/2)$*, then*

$$\mu_b(f) = \lim_{n\to\infty} [Z_n(f; \delta_n)]^{1/n};$$

(c) $\mu_b(f)$ *is a concave function of* $b \in [0, 1/2)$*, and so is continuous in* $(0, 1/2)$ *and differentiable almost everywhere in* $(0, 1/2)$.

It is also necessary to prove that $\mu_b(f)$ is right continuous at $b = 0$. This is not immediate, and requires an examining of the relation between spanning walks and stretched polygons.

3.2. Cut-planes and spanning walks

In this section, pairs of spanning walks are related to stretched polygons with the goal of proving right continuity of $\mu_b(f)$ at $b = 0$.

Any stretched polygon may be decomposed into a pair of spanning walks with coincident endpoints by cutting the polygon in its lexicographic least vertex in the bottom bounding plane of the slab containing it and in its lexicographic most vertex in the top bounding plane of the slab containing it. This is illustrated in figure 3.

By cutting a stretched polygon into spanning walks in two vertices in the top and bottom bounding planes of the slab (as in figure 3), a pair of spanning walks of the slab $\mathbb{L}_s$ is obtained. The cut-planes and cut-edges of the pair of walks are preserved, even if the two components are translated with respect to one another. More generally, one may consider pairs of spanning walks (which may intersect each other), but which together have a given number of cut-planes. An example of such a pair is illustrated in figure 4.

Let $c_n^*(s; N)$ be the number of pairs of spanning walks of the slab $\mathbb{L}_s$, with exactly N cut-planes and total length n. The partition function of these pairs of spanning walks is defined by

$$Z_n^*(f; N) = \sum_{s=0}^{n/2} c_n^*(s; N)\, \mathrm{e}^{fs}. \tag{9}$$

By cutting a stretched polygon in its top and bottom planes into pairs of spanning walks, as illustrated in figure 3, one observes that $p_n(s; N) \leqslant c_n^*(s; N)$, or in terms of partition functions,

$$Z_n(f; N) \leqslant Z_n^*(f; N). \tag{10}$$

A component C in a pair of spanning walks of $\mathbb{L}_s$ is a self-avoiding walk with vertices $\{c_j\}_{j=0}^m$ and it is *X-unfolded* if the X-coordinates of the vertices satisfy $X(c_0) \leqslant X(c_j) < X(c_m)$ for $j = 0, 1, 2, \ldots, m-1$, where $(X(c), Y(c), \ldots, Z(c))$ are the Cartesian coordinates of the vertex c. The construction for unfolding a self-avoiding walk in a given direction is well understood [9] and it introduces a factor of $\mathrm{e}^{o(m)}$ for walks of length m. Each component of a pair of spanning walks can be unfolded: let $c_n^\dagger(s; N)$ be the number of such pairs of total length n with N cut-planes, then the result is

$$c_n^*(s; N) \leqslant \mathrm{e}^{o(n)} c_n^\dagger(s; N), \tag{11}$$

since unfolding, which involves the reflections of parts of the components through hyperplanes normal to the X-direction, does not create or destroy pairs of cut-edges. In terms of partition functions, the above becomes

$$Z_n^*(f; N) \leqslant \mathrm{e}^{o(n)} Z_n^\dagger(f; N), \tag{12}$$

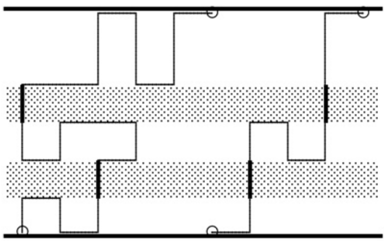

Figure 5. A pair of spanning walks with both components unfolded in a slab with two cut-planes indicated by the shaded regions. Cut-edges in a polygon are indicated in bold in the shaded squares. The endpoints of the spanning walks are indicated by ($\circ$).

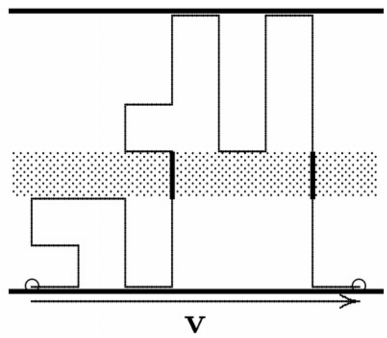

Figure 6. A loop of Z-span s in $\mathbb{L}_s$. A cut-plane is indicated by the shaded region. Cut-edges in a polygon are indicated in bold in the shaded squares. The endpoints of the loop are indicated by ($\circ$) and separated by the vector **v**.

where $Z_n^*(f; N)$ is the partition function of pairs of spanning walks of total length n and with N cut-planes, and $Z_n^\dagger(f; N)$ is the partition function of pairs of spanning walks with unfolded components of total length n and with N cut-planes. An example of a pair of spanning walks with unfolded components is given in figure 5.

A *loop* of Z-span s is a self-avoiding in $\mathbb{L}_s$ with both endpoints in the bottom bounding plane. Let $l_n(s; N)$ be the number of loops of length n, of span s with N cut-planes, and define $l_n(s; N; \mathbf{v})$ to be the number of loops of length n of span s with N cut-planes and with the vector $\mathbf{v}$ separating its two endpoints.

Observe that by reflecting one unfolded component in a pair of unfolded spanning walks, one may identify their endpoints to create a loop of the same total length. This in particular shows that

$$c_n^\dagger(s; N) \leqslant n l_n(s; N), \tag{13}$$

where the factor of n arises because a loop may be decomposed into spanning walks by cutting it in at most n points. In terms of partition functions, this becomes

$$Z_n^\dagger(f; N) \leqslant n L_n(f; N), \tag{14}$$

where $L_n(f; N) = \sum_{s\geqslant 0} l_n(s; N)\,\mathrm{e}^{fs}$ is the partition function of loops.

For a fixed value of f, let the partition function for loops with endpoints separated by $\mathbf{v}$ be $L_n(f; N; \mathbf{v})$. For given n and N, there is a vector $\mathbf{w}$ which maximizes $L_n(f; N; \mathbf{v})$: $L_n(f; N; \mathbf{v}) \leqslant L_n(f; N; \mathbf{w})$ for any vector $\mathbf{v}$. The vector $\mathbf{w}$ is the most popular value of $\mathbf{v}$. An example of such loops is illustrated in figure 6. Since the number of vectors $\mathbf{v}$ which can

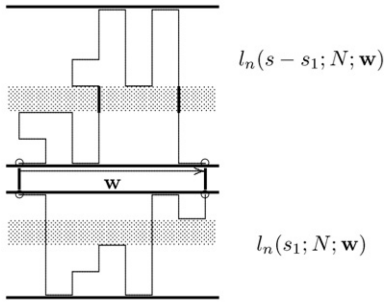

Figure 7. Concatenating two loops with the same vector separating their endpoints is done by inserting two new edges and creating one extra cut-plane. The endpoints of the loops are indicated by (○) and separated by the most popular value of the vector **v** separating the endpoints of the loops for given f. The result is a stretched polygon.

be between the endpoints of a loop is bounded by n^{d-1}, the result is that

$$L_n(f; N) = \sum_{\mathbf{v}} L_n(f; N; \mathbf{v}) \leqslant n^{d-1} \max_{\mathbf{v}} (L_n(f; N; \mathbf{v})) = n^{d-1} L_n(f; N; \mathbf{w}). \tag{15}$$

By turning one loop upside down, it can be concatenated with another loop with the same vector separating the endpoints as illustrated in figure 7. Since there are $l_n(s - s_1; N; \mathbf{w})$ choices for the top loop, and $l_n(s_1; N; \mathbf{w})$ choices for the bottom loop, the result is that

$$\sum_{s_1} l_n(s - s_1; N; \mathbf{w}) l_n(s_1; N; \mathbf{w}) \leqslant p_{2n+2}(s; 2N + 1). \tag{16}$$

Multiply this by e^{fs} and sum over s. The result is that

$$[L_n(f; N; \mathbf{w})]^2 \leqslant Z_{2n+2}(f; 2N + 1). \tag{17}$$

Comparison with equation (15) then shows that

$$[L_n(f; N)]^2 \leqslant n^{2d-2}[L_n(f; N; \mathbf{w})]^2 \leqslant n^{2d-2} Z_{2n+2}(f; 2N + 1). \tag{18}$$

By combining the inequalities in equations (12), (14) and (18), one obtains

$$[Z_n^*(f; N)]^2 \leqslant \mathrm{e}^{o(n)} n^{2d} Z_{2n+2}(f; 2N + 1). \tag{19}$$

By comparing this to equation (10) and by choosing $N = \lfloor bn \rfloor$, after taking logarithms, dividing by n and letting $n \to \infty$ and using the results in theorem 3.1, one obtains the following lemma.

Lemma 3.2. *Let f be fixed. Then*

$$\lim_{n\to\infty} \frac{1}{n} \log Z_n^*(f; \lfloor bn \rfloor) = \lim_{n\to\infty} \frac{1}{n} \log Z_n(f; \lfloor bn \rfloor).$$

In other words, pairs of spanning walks have the same limiting free energy as stretched polygons. In particular, if $b = 0$, then $Z_n^*(f; 0) = [\mu_0(f)]^{n+o(n)}$.

Similarly, for pairs of spanning walks and stretched polygons with any number of cut-planes,

$$\lim_{n\to\infty} \frac{1}{n} \log Z_n^*(f) = \lim_{n\to\infty} \frac{1}{n} \log Z_n(f).$$

This lemma can be used to prove that $\mu_b(f)$ is right continuous at $b = 0$.

Theorem 3.3. *For all finite values of f the function $\mu_b(f)$ is right continuous at $b = 0$:*

$$\lim_{b\to 0^+} \mu_b(f) = \mu_0(f).$$

Proof. Consider polygons of length n and $\lfloor bn\rfloor$ cut-planes counted by $p_n(s; \lfloor bn\rfloor)$. Cut these polygons in all their cut-planes into $\lfloor bn\rfloor + 1$ pairs of spanning walks (with no cut-planes) of lengths n_i and Z-spans s_i (where $\sum_i s_i = s - \lfloor bn\rfloor$ and $\sum_i n_i = n - 2\lfloor bn\rfloor$).

Since every polygon with $\lfloor bn\rfloor$ cut-planes may be decomposed in this way, this shows that

$$p_n(s; \lfloor bn\rfloor) \leqslant 2^{\lfloor bn\rfloor+1} \sum_{\{n_i\}} \sum_{\{s_i\}} \delta\left(n - 2\lfloor bn\rfloor - \sum_i n_i\right) \delta\left(s - \lfloor bn\rfloor - \sum_i s_i\right) \prod_{i=1}^{\lfloor bn\rfloor+1} c^*_{n_i}(s_i; 0),$$

and the sums over $\{n_i\}$ and $\{s_i\}$ are over all the possible values of n_i and s_i. The factor $2^{\lfloor bn\rfloor+1}$ arises by noting that there are two choices for connecting the two spanning walks in each pair back into the stretched polygon. Multiply this by e^{fs} and sum over s. This shows that

$$Z_n(f; \lfloor bn\rfloor) \leqslant 2^{\lfloor bn\rfloor+1} e^{\lfloor bn\rfloor f} \sum_{\{n_i\}} \delta\left(n - 2\lfloor bn\rfloor - \sum_i n_i\right) \prod_{i=1}^{\lfloor bn\rfloor+1} Z^*_{n_i}(f; 0).$$

The number of terms on the right-hand side of this inequality is at most $\binom{n/2}{\lfloor bn\rfloor}$ since the maximum Z-span of the polygon is at most $n/2$.

These arguments show that for $\{n_i\}$ which maximize the right-hand side,

$$Z_n(f; \lfloor bn\rfloor) \leqslant 2^{\lfloor bn\rfloor+1} e^{\lfloor bn\rfloor f} \binom{n/2}{\lfloor bn\rfloor} \prod_{i=0}^{\lfloor bn\rfloor} Z^*_{n_i}(f; 0). \tag{20}$$

Assume, without loss of generality, that $n_0 \geqslant n_1 \geqslant \cdots \geqslant n_{\lfloor bn\rfloor}$ for each value of n. Consider the limsups

$$\limsup_{n\to\infty} \frac{n_i}{n} = \alpha_i$$

and observe that $\alpha_0 \geqslant \alpha_1 \geqslant \alpha_2 \geqslant \cdots \geqslant 0$.

Then by theorem 3.1

$$\lim_{n\to\infty} \left[\prod_{i=0}^{\lfloor bn\rfloor} Z^*_{n_i}(f; 0)\right]^{1/n} = \lim_{n\to\infty} \left[Z^*_{n_0}(f; 0)\right]^{1/n} \cdot \lim_{n\to\infty} \left[\prod_{i=1}^{\lfloor bn\rfloor} Z^*_{n_i}(f; 0)\right]^{1/n}$$

and hence by lemma 3.2,

$$\lim_{n\to\infty} \left[\prod_{i=0}^{\lfloor bn\rfloor} Z^*_{n_i}(f; 0)\right]^{1/n} \leqslant [\mu_0(f)]^{\alpha_0} \lim_{n\to\infty} \left[\prod_{i=1}^{\lfloor bn\rfloor} Z^*_{n_i}(f; 0)\right]^{1/n}.$$

Inductively,

$$\lim_{n\to\infty} \left[\prod_{i=0}^{\lfloor bn\rfloor} Z^*_{n_i}(f; 0)\right]^{1/n} \leqslant [\mu_0(f)]^{\sum \alpha_i}.$$

Next, we note that partial sums of n_i are bounded: for each finite fixed N, $\sum_{i=0}^{N} n_i \leqslant n-2\lfloor bn\rfloor$, and hence $\sum \alpha_i \leqslant 1-2b$. Since $\mu_0(f) \geqslant 1$,[5] it follows that

$$\lim_{n\to\infty}\left[\prod_{i=0}^{\lfloor bn\rfloor} Z^*_{n_i}(f;0)\right]^{1/n} \leqslant [\mu_0(f)]^{\sum\alpha_i} \leqslant [\mu_0(f)]^{1-2b}.$$

Thus, by taking the $1/n$ power of equation (20),

$$\mu_b(f) \leqslant \frac{2^b\,\mathrm{e}^{bf}[\mu_0(f)]^{1-2b}}{b^b(1/2-b)^{1/2-b}\sqrt{2}}.$$

Take $b\to 0^+$ to see that

$$\lim_{b\to 0^+}\mu_b(f) \leqslant \mu_0(f).$$

However, since $\mu_b(f)$ is concave, $\mu_0(f) \leqslant \lim_{b\to 0^+}\mu_b(f)$. This completes the proof. □

One may extend the definition of $\mu_b(f)$ to the interval $[0,1/2]$ by defining $\lim_{b\to 1/2^-}\mu_b(f) = \mu_{1/2}(f)$. Then $\mu_b(f)$ is concave and continuous on the interval $[0,1/2]$.

3.3. $\mathcal{F}(f)$ and $\mu_b(f)$

$\mu_b(f)$ is closely related to $\mathcal{F}(f)$, the limiting free energy of stretched polygons. In particular, fix f and define b_n for each n by $Z_n(f;b_n) = \max_m Z_n(f;m)$. This implies that

$$Z_n(f;b_n) \leqslant Z_n(f) \leqslant \sum_{m=0}^{n/2} Z_n(f;m) \leqslant (n/2+1)Z_n(f;b_n). \tag{21}$$

This inequality gives the following lemma:

Lemma 3.4. *There exists a $b\in[0,1/2]$ for each fixed finite value of f, such that*

$$\mu_b(f) = \sup_{c\in[0,1/2]}\mu_c(f) = \mathrm{e}^{\mathcal{F}(f)}.$$

Proof. Take the power $1/n$ of equation (21), and let $n\to\infty$. By theorem 3.1(b) and theorem 2.1 this shows that

$$\lim_{n\to\infty}[Z_n(f;b_n)]^{1/n} = \mathrm{e}^{\mathcal{F}(f)}.$$

Moreover, if $\limsup_{n\to\infty}(b_n/n) = b$, then this shows that there exists a $b\in[0,1/2]$ such that

$$\sup_{c\in[0,1/2]}\mu_c(f) = \mu_b(f) = \mathrm{e}^{\mathcal{F}(f)}.$$

This completes the proof. □

The next theorem is the key idea underlying the construction of a pattern theorem for stretched polygons. It shows that the function $\mu_b(f)$ is strictly increasing at $b=0$, for sufficiently large values of f.

[5] This is obvious if $d\geqslant 3$. If $d=2$, we note that by bounding $Z_n(f,0)$ below by polygons in a slab of width three with no cut-planes,

$$Z_n(f,0) \geqslant p_{n-k}(3,0)\,\mathrm{e}^{3f}$$

where k is some positive constant. By taking the power $1/n$ and $n\to\infty$, this shows $\mu_0(f) = \lim_{n\to\infty}[Z_n(f,0)]^{1/n} \geqslant \lim_{n\to\infty}[p_{n-k}(3,0)]^{1/n} > 1$, since the number of polygons in a slab of width three grows exponentially in their lengths.

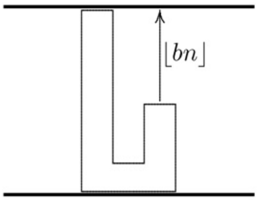

Figure 8. A polygon with $\lfloor bn \rfloor$ cut-planes has maximal span at most $(n - \lfloor bn \rfloor - c)/4$, where $c = 6$ in two dimensions. A slightly different conformation in three dimensions shows that $c = 4$ in three and higher dimensions.

Theorem 3.5. *There is an f_0 such that for all forces $f > f_0$ there exists a $b > 0$ such that $\mu_0(f) < \mu_b(f)$.*

Proof. Let $p_n(s; 0)$ be the number of stretched polygons of length n and Z-span s, and with 0 cut-planes. Such polygons have maximal span s at most $\lfloor (n-c)/4 \rfloor$ (see figure 8), where $c = 6$ in two dimensions, and $c = 4$ in three and higher dimensions. Thus, $Z_n(f; 0) \leqslant p_n \, e^{\lfloor (n-c)/4 \rfloor f}$ if $f \geqslant 0$, where p_n is the number of polygons of length n. Taking the power $1/n$ and letting $n \to \infty$ then shows that

$$\mu_0(f) \leqslant \mu \, e^{f/4},$$

where μ is defined in equation (1).

On the other hand, if a stretched polygon contains exactly $\lfloor bn \rfloor$ cut-planes, then $Z_n(f, \lfloor bn \rfloor) \geqslant e^{(\lfloor bn \rfloor + (n - 2\lfloor bn \rfloor - c)/4) f}$ since there are stretched polygons with total span $\lfloor bn \rfloor + (n - 2\lfloor bn \rfloor - c)/4$ and exactly $\lfloor bn \rfloor$ cut-planes (see figure 8). Taking the power $1/n$ and letting $n \to \infty$ then shows that

$$\mu_b(f) \geqslant e^{f/4 + bf/2}.$$

Comparing these results proves that $\mu_0(f) < \mu_b(f)$ provided that $e^{bf/2} > \mu$. This is so if $f > (2 \log \mu)/b$. Since $b \in (0, 1/2)$, for every $f > 4 \log \mu$ one can choose a $b \in (0, 1/2)$ to see that $\mu_0(f) < \mu_b(f)$, since $\mu_b(f)$ is right continuous at $b = 0$ and concave for $b \in [0, 1/2]$ by theorems 3.1 and 3.3.

Put $f_0 = 4 \log \mu$, then for any $f > f_0$ there is a $b > 0$ such that $\mu_0(f) < \mu_b(f)$. This completes the proof. □

By theorem 3.1(b), lemmas 3.4 and 3.2 we obtain the following:

Corollary 3.6. *There is a fixed f_0 such that for any fixed finite positive value of $f > f_0$ there exists a $b \in (0, 1/2]$ such that*

$$\lim_{n \to \infty} [Z_n^*(f; \lfloor bn \rfloor)]^{1/n} = \lim_{n \to \infty} [Z_n(f; \lfloor bn \rfloor)]^{1/n} = e^{\mathcal{F}(f)}.$$

In other words, the above is an equality for some value of $b > 0$.

The significance of this result is that it is in particular valid for large values of $f > f_0$.

4. Events in stretched polygons

In this section the discussion will be limited to stretched polygons with a force $f > f_0$, where f_0 is defined in theorem 3.5. In these circumstances, corollary 3.6 is applicable, and a class of

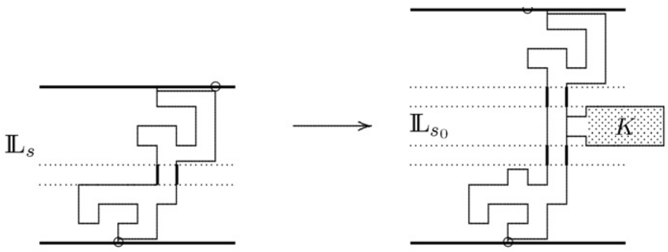

Figure 9. A schematic diagram illustrating the pasting of an arbitrary polygon into a stretched polygon at a cut-plane. In this example, a polygon K of span s_0 in a slab $\mathbb{L}_{s_0}$ is translated and then concatenated at the cut-plane into a stretched polygon, increasing the Z-span of the stretched polygon by $s_0 + 1$.

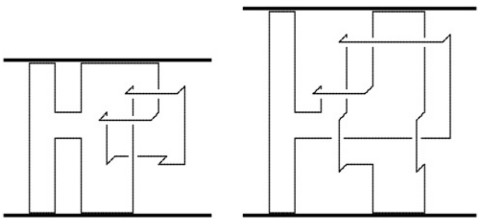

Figure 10. Possible conformations of the polygon K in figure 9. In (a), K is a knotted polygon, while (b) is an unknotted polygon. These events do not have cut-planes and are irreducible.

stretched polygons with a positive density of cut-planes determines the limiting free energy in the model.

The basic construction in this section is illustrated in figure 9: a polygon K is translated to a cut-plane of a stretched polygon. The stretched polygon is decomposed by deleting the pair of cut-edges in the cut-plane and its components are moved apart to create space for inserting K, possibly rotated by 90° about the Z-axis to line up edges which must be concatenated. K is inserted by concatenating it to a sequence of edges in the Z-direction along one of the lines which contained the original cut-edges.

When the polygon K is concatenated into a stretched polygon in this way, it maintains all its edges, save one, and it is called an *event*. An event in a stretched polygon is irreducible if it does not contain any cut-edges of the stretched polygon. The events in figure 10 are irreducible. Observe that if the cut-edges in a cut-plane of a polygon are deleted, that the irreducible event K will not be affected, it will still occur in one of the resulting pairs of spanning walks. Observe that an event may occur any number of times in a stretched polygon. We assume in what follows that all events are irreducible.

Let P be an arbitrary self-avoiding walk. P *occurs* in a polygon K of Z-span s_0 if P can be translated to become identical with a sub-walk in K see figure 11. In this case, P is called a *pattern*. Observe that if a pattern can occur three times in a polygon, then it can potentially occur any number of times; such patterns are called *proper*, and all patterns will be assumed to be proper.

The first result is a proof that the class of stretched polygons in which a given event K never occurs is an exponentially small subclass of stretched polygons, for $f > f_0$.

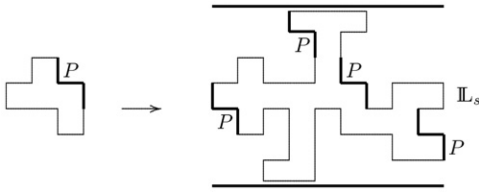

Figure 11. Occurrences of a pattern P in a stretched polygon. The pattern P on the left side is a sub-walk of a polygon and it occurs in the stretched polygon on the right.

Define $p_n(s; \lfloor bn \rfloor, NK)$ to be the number of polygons of length n and Z-span s, with $\lfloor bn \rfloor$ cut-planes and with N occurrences of the (irreducible) event K. Define the partition function of this class of polygons by $Z_n(f; \lfloor bn \rfloor, NK)$.

Using the same arguments leading to theorem 3.1 (see [12]), define the limits

$$\mu_b(\overline{K}, f) = \lim_{n\to\infty} [Z_n(f; \lfloor bn \rfloor, 0K)]^{1/n} = \lim_{n\to\infty} [Z_n(f; \delta_n, 0K)]^{1/n}, \tag{22}$$

where $\delta_n/n \to b$ as $n \to \infty$. Then $\mu_b(\overline{K}, f)$ may be shown to be concave for $b \in [0, 1/2)$ and thus continuous in $(0, 1/2)$. One may also show that $\mu_b(\overline{K}, f)$ is right continuous at $b = 0$ by using the arguments leading to theorem 3.3. In addition, exactly as in theorem 3.5 and corollary 3.6, there exists a $b > 0$ such that $\mu_0(\overline{K}, f) < \mu_b(\overline{K}, f)$ if $f > f_0$.

Lemma 4.1. *Suppose $f > f_0$ and K is the event that a given polygon occurs. Then for any $b \in (0, 1/2)$ it is the case that*

$$\mu_b(\overline{K}, f) = \lim_{n\to\infty} [Z_n(f; \lfloor bn \rfloor, 0K)]^{1/n} < e^{\mathcal{F}(f)}.$$

Moveover, $\mu_b(\overline{K}, f)$ is concave on $[0, 1/2)$ and right continuous at $b = 0$.

Proof. Suppose that K is the (irreducible) event that a polygon of length k and Z-span s_0 occurs.

Concavity and right continuity at $b = 0$ follow from arguments similar to theorem 3.3. It remains to show that $\mu_b(\overline{K}, f) = \lim_{n\to\infty} [Z_n(f; \lfloor bn \rfloor, 0K)]^{1/n} < e^{\mathcal{F}(f)}$.

Consider polygons counted by $p_n(s; \lfloor bn \rfloor, 0K)$. If A is such a polygon of length n, then it has $\lfloor bn \rfloor$ cut-planes. Let $0 < \delta < b$, and choose $\lfloor \delta n \rfloor$ cut-planes. Perform the construction in figure 9 at each of the chosen cut-planes. This increases the length of A by $k\lfloor \delta n \rfloor$ (for some fixed k) and increases the Z-span by $(s_0 + 1)\lfloor \delta n \rfloor$. The number of cut-planes is also increased by $\lfloor \delta n \rfloor$. Thus

$$\binom{\lfloor bn \rfloor}{\lfloor \delta n \rfloor} p_n(s; \lfloor bn \rfloor, 0K) \leqslant p_{n+k\lfloor \delta n \rfloor}(s + (s_0+1)\lfloor \delta n \rfloor; \lfloor bn \rfloor + \lfloor \delta n \rfloor, \lfloor \delta n \rfloor K).$$

Multiply this by e^{fs} and sum over s:

$$\binom{\lfloor bn \rfloor}{\lfloor \delta n \rfloor} Z_n(f; \lfloor bn \rfloor, 0K) \leqslant e^{-(s_0+1)\lfloor \delta n \rfloor f} Z_{n+k\lfloor \delta n \rfloor}(f; \lfloor bn \rfloor + \lfloor \delta n \rfloor, \lfloor \delta n \rfloor K).$$

Take the power $1/n$ and the limit of the left-hand side as $n \to \infty$. The partition function on the right-hand side is bounded above in the limit by the partition function of all stretched polygons, and so the result is that

$$\left[\frac{b^b\, e^{(s_0+1)\delta f}\, e^{k\delta \mathcal{F}(f)}}{\delta^\delta (b-\delta)^{b-\delta}}\right] \lim_{n\to\infty} [Z_n(f; \lfloor bn \rfloor, 0K)]^{1/n} \leqslant e^{\mathcal{F}(f)}$$

after terms have been rearranged. If the value of b is fixed at a value bigger than zero, then for small enough values of $\delta > 0$ the factor in square brackets above is strictly larger than 1. This proves the lemma. □

Since $\mu_0(\overline{K}, f) < \mu_b(\overline{K}, f)$ if $f > f_0$ and $\mu_b(\overline{K}, f)$ is right continuous at $b = 0$, lemma 4.1 is true for any $b \in [0, 1/2)$ if $f > f_0$. Define $\mu_{1/2}(\overline{K}, f) = \lim_{b\to 1/2^-} \mu_b(\overline{K}, f)$. Since $Z_n(f; n/2 - 1; 0K) = \mathrm{e}^{f(n/2-1)}$, it also follows that $\mu_{1/2}(\overline{K}, f) \leqslant \mathrm{e}^{f/2} < \mathrm{e}^{\mathcal{F}(f)}$ since by theorem 2.1 $\mathcal{F}(f) > f/2$ if $f > 0$. Thus, $\mu_b(\overline{K}, f)$ is continuous on the interval $[0, 1/2]$ and bounded away from $\mathrm{e}^{\mathcal{F}(f)}$ if $f > f_0$. In these circumstances $\mu_b(\overline{K}, f)$ is uniformly bounded away from $\mathrm{e}^{\mathcal{F}(f)}$ for $b \in [0, 1/2]$. We state this in corollary 4.2.

Corollary 4.2. *Suppose that $f > f_0$. Then for any $b \in [0, 1/2)$ it is the case that*

$$\mu_b(\overline{K}, f) = \lim_{n\to\infty} [Z_n(f; \lfloor bn \rfloor, 0K)]^{1/n} < \mathrm{e}^{\mathcal{F}(f)}.$$

In addition $\mu_b(\overline{K}, f)$ is uniformly bounded away from $\mathrm{e}^{\mathcal{F}(f)}$; there exists an $\epsilon > 0$ independent of b such that for any $b \in [0, 1/2]$,

$$\mu_b(\overline{K}, f) = \lim_{n\to\infty} [Z_n(f; \lfloor bn \rfloor, 0K)]^{1/n} \leqslant \mathrm{e}^{\mathcal{F}(f)}(1 - \epsilon).$$

The result of lemma 4.1 and corollary 4.2 is that the exponential growth rate of $Z_n(f; 0K)$ is strictly less than $\mathrm{e}^{\mathcal{F}(f)}$, provided that $f > f_0$.

Theorem 4.3. *Suppose that $f > f_0$. Then*

$$\lim_{n\to\infty} [Z_n(f; 0K)]^{1/n} < \mathrm{e}^{\mathcal{F}(f)}.$$

Proof. Observe that

$$Z_n(f; 0K) = \sum_{m=0}^{n/2} Z_n(f; m; 0K).$$

For fixed values of f and any value of n, there exists a δ_n such that $Z_n(f; m; 0K) \leqslant Z_n(f; \delta_n; 0K)$ for any value of m. Hence

$$Z_n(f; \delta_n, 0K) \leqslant Z_n(f; 0K) \leqslant (n/2 + 1) Z_n(f; \delta_n, 0K). \tag{23}$$

By corollary 4.2 there exists an $\epsilon > 0$ such that if $f > 0$, then

$$\limsup_{n\to\infty} [Z_n(f; \delta_n; 0K)]^{1/n} \leqslant \mathrm{e}^{\mathcal{F}(f)}(1 - \epsilon).$$

In other words, from equation (23), if $f > f_0$ then

$$\lim_{n\to\infty} [Z_n(f; 0K)]^{1/n} = \limsup_{n\to\infty} [Z_n(f; \delta_n; 0K)]^{1/n} \leqslant \mathrm{e}^{\mathcal{F}(f)}(1 - \epsilon).$$

This proves the theorem. □

This theorem shows that, for values of $f > f_0$, the partition function of the class of stretched polygons in which a given event K does not occur is exponentially small compared to the partition function of all stretched polygons. In particular, events such as those illustrated in figure 10 will occur at least once in almost all sufficiently long stretched polygons. This result may be strengthened to show that almost all sufficiently long stretched polygons contain a positive density of a given event K, in a sense which will be explained below.

One may now repeat the set of constructions in section 3 leading to lemma 3.2 to see that if $Z_n^*(f, 0K)$ is the partition function of pairs of spanning walks of total length n not containing the event K, then if K is an irreducible event, one obtains the following.

Corollary 4.4. *Suppose that* $f > f_0$. *Then*

$$\lim_{n\to\infty}[Z_n^*(f;0K)]^{1/n} = \lim_{n\to\infty}[Z_n(f;0K)]^{1/n} < \mathrm{e}^{\mathcal{F}(f)}.$$

A set of $N-1$ cut-planes cuts a polygon of length n into N pairs of spanning walks of *almost equal length* if the combined length of each pair of spanning walks is at least $\lfloor (n-2N+2)/N\rfloor$ and at most $\lceil (n-2N+2)/N\rceil$.

Define $p_n^{\ddagger}(s;\lfloor bn\rfloor, NK)$ to be the number of stretched polygons, with at most N occurrences of the event K, of length n and Z-span s, and with *at least* $\lfloor bn\rfloor$ cut-planes of which a subset consisting of exactly $\lfloor bn\rfloor$ cut-planes cuts each polygon into $\lfloor bn\rfloor - 1$ pairs of spanning walks of almost equal total lengths. The partition function of this set is denoted by $Z_n^{\ddagger}(f;\lfloor bn\rfloor, NK)$.

Theorem 4.5. *Suppose that* $f > f_0$. *Let* K *be an event which may occur in a stretched polygon. Then for any* $0 < b < 1/2$ *there is a* $\rho_0 > 0$ *such that*

$$\limsup_{n\to\infty}\left[Z_n^{\ddagger}(f;\lfloor bn\rfloor,\lfloor \rho n\rfloor K)\right]^{1/n} < \mathrm{e}^{\mathcal{F}(f)}$$

uniformly for $b \in (0, 1/2)$ *and for* $0 \leqslant \rho \leqslant \rho_0$.

Proof. For fixed values of $b > 0$ and $\rho \geqslant 0$, consider stretched polygons with $\lfloor bn\rfloor$ cut-planes which cut the polygons into almost equal length pairs of spanning walks, and with exactly $\lfloor \rho n\rfloor$ occurrences of the event K, counted by $p_n^{\ddagger}(s;\lfloor bn\rfloor,\lfloor \rho n\rfloor K)$. Since the events are assumed to be irreducible, cutting the stretched polygon in the cut-planes will not destroy any event K.

These stretched polygons have $\lfloor bn\rfloor$ cut-planes cutting them into $m = \lfloor bn\rfloor + 1$ pairs of spanning walks of almost equal total length (at least $\lfloor n/m\rfloor$). Let $\rho > 0$ be small and fix $\epsilon > 0$ also small.

By theorem 4.3 and corollary 4.4 there is an N_0 such that for all $n \geqslant N_0$,

$$Z_n^*(f;0K) \leqslant [\mathrm{e}^{\mathcal{F}(f)}(1-\epsilon)]^n,$$

if $\epsilon > 0$ was fixed small enough, but independent of b and ρ.

In addition, by lemma 3.2 there exists an N_1 such that for $n \geqslant N_1$,

$$Z_n^*(f) \leqslant [\mathrm{e}^{\mathcal{F}(f)}(1+\epsilon)]^n,$$

for the same value of $\epsilon > 0$ fixed above.

Each stretched polygon counted by $p_n^{\ddagger}(s;\lfloor bn\rfloor,\lfloor \rho n\rfloor K)$ may be considered to be an ordered sequence of m pairs of spanning walks of almost equal length, separated by $\lfloor bn\rfloor$ cut-planes, and in which at most $\lfloor \rho n\rfloor$ of these pairs of spanning walks the event K may occur at least once.

The $\lfloor bn\rfloor + 1$ pairs of spanning walks defined by the cut-planes may be reordered by excising any pair between its cut-planes and inserting it back at any other cut-plane (and where any intersections between the components of the pair are now ignored). This does not change the overall Z-span or length. Use this construction to reorder the pairs in sequence such that the first j may each contain the event K, and the remaining $\lfloor bn\rfloor + 1 - j$ do not contain K. If there were j pairs of spanning walks which contain K, then at most $\binom{\lfloor bn\rfloor+1}{j}$ polygons may be reordered onto the same structure.

This construction reorders each polygon into two parts: a first part which is a pair of spanning walks of total length at most $j(\lfloor n/m\rfloor + 2)$ which contains copies of K and of length q_1 at least $j\lfloor n/m\rfloor$ and span s_1. The remaining part is a pair of spanning walks of length q_2 at least $(m-j)\lfloor n/m\rfloor$ and at most $(m-j)(\lfloor n/m\rfloor + 2)$ and span s_2, where $s_1 + s_2 = s - 1$, and these walks may not contain the event K. In addition $q_1 + q_2 = n$ and $j \leqslant \lfloor \rho n\rfloor$.

The number of conformations of pairs of walks which may contain the event K and of length q_1 and span s_1 is at most $p^*_{q_1}(s_1)$, and the number of pairs of walks of length q_2 and span s_2 which do not contain copies of K is $p^*_{q_2}(s_2, 0K)$. This shows that

$$p^\ddagger_n(s; \lfloor bn\rfloor, \lfloor \rho n\rfloor K) \leqslant \sum_{j=0}^{\lfloor \rho n\rfloor} \binom{m}{j} \sum_{\{q_i\}} \sum_{\{s_i\}} [p^*_{q_1}(s_1)][p^*_{q_2}(s_2, 0K)]\delta\left(s - 1 - \sum_k s_k\right),$$

where the sum over q_i is constrained and depends on j, as above. Multiply by e^{fs} and sum over s. This shows that

$$Z^\ddagger_n(f; \lfloor bn\rfloor, \lfloor \rho n\rfloor K) \leqslant e^f \sum_{j=0}^{\lfloor \rho n\rfloor} \binom{m}{j} \sum_{\{q_i\}} \big[Z^*_{q_1}(f)\big]\big[Z^*_{q_2}(f; 0K))\big]. \tag{24}$$

Since $Z^*_{q_1}(f)$ and $Z^*_{q_2}(f; 0K)$ both increase exponentially with q_1 and q_2, for small values of ρ, the terms on the right-hand side are dominated by the $j = \lfloor \rho n\rfloor$ term. For this value of j, if n is taken large enough that $q_i \geqslant \min\{N_0, N_1\}$, this term is smaller than

$$e^f \binom{m}{\lfloor \rho n\rfloor} \sum_{\{q_i\}} [e^{\mathcal{F}(f)}(1+\epsilon)]^{q_1}[e^{\mathcal{F}(f)}(1-\epsilon)]^{q_2},$$

where we recall that q_1 is between $\lfloor \rho n\rfloor \lfloor n/m\rfloor$ and $\lfloor \rho n\rfloor(\lfloor n/m\rfloor + 2)$ and q_2 is between $(m - \lfloor \rho n\rfloor)\lfloor n/m\rfloor$ and $(m - \lfloor \rho n\rfloor)(\lfloor n/m\rfloor + 2)$, and where $m = \lfloor bn\rfloor + 1$ and $q_1 + q_2 = n$.

Take the power $1/n$ of this. Since terms in equation (24) above are dominated by the $j = \lfloor \rho n\rfloor$ term, for small enough values of $\rho > 0$, it follows that if $n \to \infty$, then

$$\limsup_{n\to\infty} \big[Z^\ddagger_n(f; \lfloor bn\rfloor, \lfloor \rho n\rfloor K)\big]^{1/n} \leqslant \left[\frac{e^{\mathcal{F}(f)} b^b}{\rho^\rho (b-\rho)^{b-\rho}}\right] \left(\frac{1+\epsilon}{1-\epsilon}\right)^{\rho/b} (1-\epsilon)\,. \tag{25}$$

Finally, observe that there is a ρ_0 such that the factor

$$\left[\frac{b^b}{\rho^\rho (b-\rho)^{b-\rho}}\right] \left(\frac{1+\epsilon}{1-\epsilon}\right)^{\rho/b} (1-\epsilon) = \left[\left[\frac{1}{(\rho/b)^{\rho/b}(1-\rho/b)^{1-\rho/b}}\right]^b \left(\frac{1+\epsilon}{1-\epsilon}\right)^{\rho/b}\right] (1-\epsilon)$$

is strictly smaller than 1 if $0 < \rho < \rho_0 \leqslant b$, since the factor in square brackets approaches 1 as $\rho \to 0^+$. Thus, for any $b \in (0, 1/2]$ one may take ρ small enough so this factor becomes less than (say) $(1 - \epsilon/2)$ for a fixed value of ϵ. This proves the theorem. □

This result gives the following theorem:

Theorem 4.6. *Suppose that $f > f_0$ and that K is an event which may occur in stretched polygons. Then there exists a $\rho_0 > 0$ such that for all* $0 \leqslant \rho \leqslant \rho_0$

$$\limsup_{n\to\infty} [Z_n(f; \lfloor \rho n\rfloor K)]^{1/n} < e^{\mathcal{F}(f)}.$$

Proof. Consider stretched polygons in the partition function $Z_n(f; \lfloor \rho n\rfloor K)$. By concatenating $N + 1$ such polygons as in figure 1, a stretched polygon of length $n(N + 1) + 2N$ with N cut-planes cutting it into sub-polygons of length n is obtained, and in which the event K occurs at most $\lfloor \rho n\rfloor(N + 1)$ times. This shows in particular that

$$[Z_n(f; \lfloor \rho n\rfloor)]^{N+1} \leqslant Z^\ddagger_{n(N+1)+2N}(f; N; \lfloor \rho n\rfloor(N+1)K).$$

Take the power $1/(n(N + 1) + 2N)$ of this, and let $N \to \infty$:

$$\begin{aligned}[Z_n(f; \lfloor \rho n\rfloor)]^{\frac{1}{n+2}} &\leqslant \limsup_{N\to\infty} \big[Z^\ddagger_{n(N+1)+2N}(f; N; \lfloor \rho n\rfloor(N+1)K)\big]^{\frac{1}{n(N+1)+2N}} \\ &\leqslant \limsup_{m\to\infty} \big[Z^\ddagger_m(f; \delta_{m,n}, \lfloor \rho m\rfloor K)\big]^{\frac{1}{m}},\end{aligned}$$

where $\delta_{m,n} = \lfloor (m-n)/(n+2) \rfloor$ and where we note that $\lfloor \rho n \rfloor (N+1) = \lfloor \rho n \rfloor ((m-n)/(n+2)+1) \leqslant \lfloor \rho m \rfloor$ if $m = n(N+1)+2N$.

By theorem 4.5, for any given fixed n, there is an $\epsilon > 0$ (independent of n if ϵ is small enough) and a $\rho_0 > 0$ (dependent on n) such that for all $0 \leqslant \rho \leqslant \rho_0$,

$$\limsup_{m\to\infty} \left[Z_m^{\ddagger}(f; \delta_{m,n}, \lfloor \rho m \rfloor K) \right]^{\frac{1}{m}} \leqslant (1-\epsilon)\, \mathrm{e}^{\mathcal{F}(f)}.$$

Thus, there is an $\epsilon > 0$ and a $\rho_0 > 0$ such that for all $0 \leqslant \rho \leqslant \rho_0$,

$$[Z_n(f; \lfloor \rho n \rfloor)]^{\frac{1}{n+2}} \leqslant (1-\epsilon)\, \mathrm{e}^{\mathcal{F}(f)}.$$

Next, choose n large enough, and ρ_0 small enough, such that

$$\limsup_{m\to\infty} [Z_m(f; \lfloor \rho \rfloor K)]^{1/m} < (1+\epsilon)[Z_n(f; \lfloor \rho n \rfloor)]^{\frac{1}{n+2}},$$

for the value of ϵ above (which is independent of n). This shows that

$$\limsup_{m\to\infty} [Z_m(f; \lfloor \rho \rfloor K)]^{1/m} < (1-\epsilon^2)\, \mathrm{e}^{\mathcal{F}(f)}$$

for $0 \leqslant \rho \leqslant \rho_0$, for some $\rho_0 > 0$. This completes the proof. □

Observe that theorem 4.6 states that if K is an event and $f > f_0$, then K will occur with a positive density in almost all polygons of length n, and with positive density with probability 1 as if $n \to \infty$. The occurrence of K is in the sense illustrated in figure 9.

This result may strengthened as follows: we say that a self-avoiding walk L is a *stretched pattern* if there exists a stretched polygon which contains L as a sub-walk. We say that a stretched pattern L occurs in a stretched polygon P if P contains a sub-walk which is a translate of L: that is, L is identical to a sub-walk in P. P contains Lm times if m copies of L can be translated onto m distinct sub-walks of P. Define $Z_n(f; mL)$ to be the partition function of stretched polygons of length n at force f which contains exactly m copies of a stretched pattern L. Then one may repeat the arguments starting in lemma 4.1 by inserting stretched polygons containing a given stretched pattern L at cut-planes to prove that any given stretched pattern will occur with positive density with probability 1 in stretched polygons if $f > f_0$ as $n \to \infty$. We make this precise as follows:

Theorem 4.7. *Let $f > f_0$ and let L be a stretched pattern. Then there exists a $\rho_0 > 0$ such that for all $0 \leqslant \rho \leqslant \rho_0$*

$$\limsup_{n\to\infty} [Z_n(f; \lfloor \rho n \rfloor L)]^{1/n} < \mathrm{e}^{\mathcal{F}(f)}.$$

In particular, for sufficiently small values of $\epsilon > 0$ and $\rho_0 > 0$ there exists an N_0 such that for all $n \geqslant N_0$ and for all $\rho \in [0, \rho_0]$

$$[Z_n(f; \lfloor \rho n \rfloor L)]^{1/n} \leqslant \mathrm{e}^{\mathcal{F}(f)}(1-\epsilon).$$

5. Applications

In this section, we confine the model to three dimensions and consider the implications of the pattern theorem for knotting and writhing of a stretched polygon given large positive (pulling or stretching) forces.

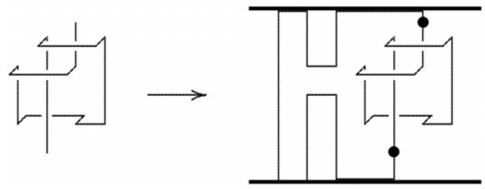

Figure 12. A stretched pattern occurring in a stretched polygon as the sub-walk with endpoints denoted by the bullets. This will be an irreducible event in a stretched polygon.

5.1. Knotting probability

Consider the event in figure 12 or equivalently the event in figure 10(a). If this event occurs in a stretched polygon, then the knot type of the polygon is a connected sum with at least one non-trivial factor, and so it is not trivial. Let K denote this event and suppose that $Z_n(f; \lfloor \rho n \rfloor K)$ is the partition function of stretched polygons of length n which contain the event exactly $\lfloor \rho n \rfloor$ times, for some $\rho > 0$. From theorem 4.6 we obtain the following lemma.

Lemma 5.1. *There exists a* $\rho_0 > 0$ *such that for all* $0 \leqslant \rho < \rho_0$ *and for* $f > f_0$

$$\lim_{n\to\infty} \frac{Z_n(f; \lfloor \rho n \rfloor K)}{Z_n(f)} = 0$$

where K is the event that a knotted polygon occurs as given in figure 12.

Proof. Let K be any event. Then by theorem 4.6 there exists a $\rho_0 > 0$ such that for any $0 \leqslant \rho \leqslant \rho_0$, and all n large enough (say $n \geqslant N$),

$$Z_n(f; \lfloor \rho n \rfloor K) \leqslant \mathrm{e}^{n\mathcal{F}(f)}(1-\epsilon)^n,$$

provided that $f > f_0$. Since $Z_n(f) = \mathrm{e}^{n\mathcal{F}(f)+o(n)}$, the lemma follows. □

Lemma 5.1 implies that the Frisch–Wasserman–Delbrück conjecture is true for stretched polygons of arbitrarily large but finite f, where $f > f_0$ [1, 4]. This can be made precise by defining $Z_n(f; \emptyset)$ to be the partition function of all stretched polygons at force f with knot type the unknot $\emptyset$. Clearly, for any finite value of n,

$$Z_n(f; \emptyset) \leqslant \sum_{m=0}^{\lfloor \rho n \rfloor} Z_n(f; mK), \tag{26}$$

where K is for example the event in figure 12.

Choose $\rho_0 > 0$ as in lemma 5.1. The probability that a stretched polygon of length n is a non-trivial knot is given by

$$\Pr(f; n) = \frac{Z_n(f) - Z_n(f; \emptyset)}{Z_n(f)}. \tag{27}$$

By equation (26) if follows that

$$\Pr(f; n) \geqslant \frac{Z_n(f) - \sum_{m=0}^{\lfloor \rho n \rfloor} Z_n(f; mK)}{Z_n(f)}. \tag{28}$$

Thus, by taking $n \to \infty$, and choosing $\rho > 0$ and $\rho < \rho_0$, if follows from lemma 5.1 that

$$\lim_{n\to\infty} \Pr(f; n) \geqslant 1 - \lim_{n\to\infty} \frac{\sum_{m=0}^{\lfloor \rho n \rfloor} Z_n(f; mK)}{Z_n(f)} = 1 \tag{29}$$

or $\lim_{n\to\infty} \Pr(f; n) = 1$, for any $f > f_0$. This result gives the following theorem.

Theorem 5.2. *Suppose that f is an arbitrarily large but finite force such that $f > f_0$. Then the probability that a stretched polygon of length n is the unknot approaches 0 at an exponential rate with increasing n. In other words, the limiting free energy of stretched polygons is completely determined by knotted polygons.*

One may prove a somewhat stronger result than this. Suppose that f is finite and $f > f_0$. Denote the expected number of times that the event K in figure 12 occurs in stretched polygons of length n by $\langle nK\rangle_f$. Then

$$\begin{aligned}\frac{\langle nK\rangle_f}{n} &= \frac{\sum_{m\geqslant 0} mZ_n(f;mK)}{nZ_n(f)}\\ &\geqslant \frac{\sum_{m\geqslant\lfloor\rho n\rfloor} mZ_n(f;mK)}{nZ_n(f)}\\ &\geqslant \frac{\lfloor\rho n\rfloor}{n}\left(\frac{\sum_{m\geqslant\lfloor\rho n\rfloor} Z_n(f;mK)}{Z_n(f)}\right),\end{aligned} \tag{30}$$

where we choose $0 < \rho < \rho_0$, with ρ_0 defined in lemma 5.1. Take $n \to \infty$ in the last equation. This shows that

$$\liminf_{n\to\infty}\left(\frac{\langle nK\rangle_f}{n}\right) \geqslant \rho > 0 \tag{31}$$

for some value of ρ. In other words, given $0 < \epsilon < \rho$ there exists an N, large but finite, such that

$$\langle nK\rangle_f \geqslant (\rho-\epsilon)n \tag{32}$$

for all $n > N$. If ϵ is chosen small enough, then this shows that the event K occurs at least $(\rho-\epsilon)n$ times in almost all polygons of length n. In other words, the knot type of almost all polygons of length $n > N$ has a factor K^m, where $m \geqslant (\rho-\epsilon)n$, for any finite value of f such that $f > f_0$, where ρ depends on f but is strictly bounded away from zero.

5.2. Writhing in stretched polygons

In this section, we generalize the results on the writhe of polygons obtained in [13]. In particular, we show that for arbitrarily large values of the force f, the absolute value of the writhe of a stretched polygon of length n grows faster than $o(\sqrt{n})$.

Let α be any piecewise linear and continuous curve in three space. A projection of α into a plane with normal unit vector ξ may in general have crossings where the projected arcs of α intersect other arcs transversely. The projection is regular if all singular points in the projection are transverse crossings. The projection is turned into an oriented knot projection by orienting the projected curve and by indicating which arc in the projection overpasses at crossings. This is usually done by removing a small arc from the underpassing projected arc. The crossing then has the appearance of one of the two cases indicated in figure 13. The sign of a crossing is determined by a right-hand rule: take the overpassing arc into the right hand; if the fingers curl around this arc in the direction of the arrow on the underpassing arc, then the crossing is said to be positive or right handed. Otherwise it is negative or left handed.

The writhe of a simple closed curve α is defined as the sum of signed crossings averaged over all directions ξ [5]. For lattice polygons in the cubic lattice the writhe can be computed from the Lacher–Sumners theorem [18]: the writhe of a lattice polygon in the cubic lattice is the average of the linking numbers of the polygon with its push-offs into four non-antipodal octants.

Figure 13. Signed crossings in a projection are determined by a right-hand rule: take the overpassing arc in your right hand with thumb in the direction of the arrow. If the fingers curl underneath the overpassing arc in the direction of the underpassing arc, then the crossing is positive.

Figure 14. Two stretched polygons with positive and negative writhe. The polygon marked A has $W(A) = +1/2$, and the polygons marked B has $W(B) = -1/2$.

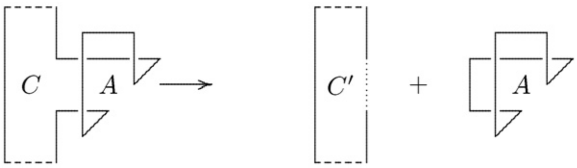

Figure 15. Cutting A from a stretched polygon.

The Lacher–Sumners theorem allows the explicit computations of the writhe of the polygons in figure 14. The polygon marked by A has writhe $W(A) = +1/2$, and the polygon marked B has write $W(B) = -1/2$. Both A and B may occur as events in a stretched polygon. In particular, theorem 4.7 applies in this case, and the stretched patterns which are sub-walks in the stretched polygons in figure 14 will occur with positive density in almost all stretched polygons with $f > f_0$.

The polygons in figure 14 may be cut from stretched polygon as illustrated for A in figure 15. This construction will change the writhe of the polygon; suppose C is a polygon containing the stretched pattern marked by A in figure 14, then this pattern may be cut from C as illustrated in figure 15 to obtain a polygon C' and a small polygon containing A. One can check that

$$W(C) = W(C') + W(A), \tag{33}$$

see, for example, lemma 5.50 in [12]. With this result, it can now be proven that for any finite value of f such that $f > f_0$, the expected value of the writhe should increase at least as fast as $C\sqrt{n}$ for sufficiently large values of n, where n is the length of the stretched polygon, and for some non-zero constant C.

Let $Z_n(f; \geqslant\lfloor\rho n\rfloor)$ be the partition function of stretched polygons of length n containing at least $\lfloor\rho n\rfloor$ occurrences of the stretched patterns A or B in figure 14.

If $f > f_0$, then by theorem 4.7 there exists a ρ_0 such that for all $\rho \in [0, \rho_0)$ and for all $n > N_0$, where N_0 is a finite integer,

$$Z_n(f; \lfloor\rho n\rfloor L) \leqslant \mathrm{e}^{n\mathcal{F}(f)}\,\mathrm{e}^{-k_f n}, \tag{34}$$

where $k_f > 0$ is dependent on f. Thus, there exists a σ (say $\sigma = \rho_0/2$) such that

$$Z_n(f; \leqslant \lfloor \sigma n \rfloor L) \leqslant \mathrm{e}^{n\mathcal{F}(f)}\, \mathrm{e}^{-k_f n} \tag{35}$$

for some constant $k_f > 0$ and for sufficiently large values of n.

In other words, the probability $P_n(f)$ that a stretched polygon contains at least $\lfloor \sigma n \rfloor$ occurrences of the stretched patterns A or B is greater or equal to $(Z_n(f) - Z_n(f; \leqslant \lfloor \sigma n \rfloor L))/Z_n(f)$ or

$$P_n(f) \geqslant 1 - \frac{\mathrm{e}^{n\mathcal{F}(f)}\, \mathrm{e}^{-k_f n}}{Z_n(f)}. \tag{36}$$

The distribution of A or B in L is binomial along any polygon C which contains A and B at least $\lfloor \sigma n \rfloor$ times. The probability that B occurs exactly k times amongst the $\lfloor \sigma n \rfloor$ occurrences of A and B is less than $1/\lfloor \sigma n \rfloor$.

The writhe of C is composed of two terms as shown in equation (33). The first term is obtained by truncating the $\lfloor \sigma n \rfloor$ occurrences of A and B as in figure 15, and the second term is due to the contributions A and B make to the writhe.

Suppose that the absolute value of the writhe of C is less than $g(n)$, where $g(n)$ is some function of n. Then the contribution to the writhe of C of the occurrences of A and B is one of at most $\lceil g(n) \rceil + 1$ different values. In other words,

$$\mathrm{Prob}\,(|W(C)| < g(n)) \leqslant P_n(f) \frac{\lceil g(n) \rceil + 1}{\sqrt{\lfloor \sigma n \rfloor}} + (1 - P_n(f)) R_n, \tag{37}$$

where we noted that contribution of A and B is at most $(\lceil g(n) \rceil + 1)/\sqrt{\lfloor \sigma n \rfloor}$, and where $P_n(f)$ is the probability that C will contain at least $\lfloor \sigma n \rfloor$ occurrences of A and B at force f. But $P_n(f)$, we say above, is at least $1 - \mathrm{e}^{n\mathcal{F}(f)}\, \mathrm{e}^{-k_f n}/Z_n(f)$, and since $Z_n(f) = \mathrm{e}^{n\mathcal{F}(f) + o(n)}$, it follows that $P_n(f) \to 1$ as $n \to \infty$. Thus, if $g(n) = o(\sqrt{n})$, then $\mathrm{Prob}\,(|W(C)| < g(n)) \to 0$ as $n \to \infty$. This gives the following theorem:

Theorem 5.3. *Let C be a stretched polygon at force f with $f > f_0$. Then for every function $g(n) = o(\sqrt{n})$, the probability that the absolute value of the mean writhe of C is less than $g(n)$ approaches 0 as $n \to \infty$.*

6. Conclusions

In this paper, we examined entanglements in stretched polygons in the cubic lattice. The key result is a pattern theorem for stretched polygons. The method of proof of this theorem is based on the results in section 3 that cut-planes and pairs of cut-edges occur with positive density in that class of polygons which makes the dominating contribution to the limiting free energy in this model. The cut-planes cut the polygons into independent sub-polygons separated by cut-planes. This is reminiscent of the Pincus argument [22] which describes scaling in stretched polymers in the intermediate force regime by cutting the polymer into independent 'Pincus-balls' which are composed of unperturbed pieces of the polymer.

The pattern theorem is stated explicitly in theorems 4.6 and 4.7, and it implies that for sufficiently large positive (or stretching) values of the applied force a given pattern will occur with positive density in almost all stretched polygons of length n, except in an exponentially small class. The condition $f > f_0$ in corollary 3.6 implies that this pattern theorem is only valid for sufficiently large stretching values of the force. There exists a pattern theorem for $f = 0$ [16], but a proof that a pattern theorem is valid for all finite f remains an open problem.

The pattern theorem for stretching forces in particular implies that in the strong stretching regime ($f \gg 0$) entanglements as defined by knotting and writhing persist in the limit as

$n \to \infty$. This result follows from theorem 5.2, which states that the probability of knotting in stretched polygons approaches unity as the length increases to infinity.

The results of lemma 5.1 imply that any stretched polygon will be badly knotted in the limit as $n \to \infty$. Since any knotted stretched pattern as in figure 12 will occur with positive density, stretched polygons with a prime knot type will be exponentially rare: the knot type will almost always contain a positive density of components of knot type 3_1. This implies that the spans of the Jones and Alexander polynomials, the crossing numbers, the unknotting numbers and other measures of knot complexity will increase on average at least linearly with the length of the stretched polygon, for any large fixed positive value of the force $f > gf_0$ [24].

For negative f (the compressive regime) the methods in this paper break down, and the existence of a pattern theorem remains an open question.

Finally, the pattern theorem in this paper also has implications for geometric quantities such as the writhe of the polygon. In section 5.3 we generalize a result of [13] to stretched polygons with sufficiently large applied force: for every function $g(n) = o(\sqrt{n})$, the probability that the absolute value of the mean writhe of the stretched polygon is less than $g(n)$ approaches 0 as $n \to \infty$.

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