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Knotted polygons with curvature in $\mathcal{Z}^3$

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Abstract. The knot probability of semiflexible polygons on the cubic lattice is investigated. The degree of stiffness of the polygon is mimicked by introducing a bending fugacity conjugate to the curvature of the polygon. By generalizing Kesten's pattern theorem to semiflexible walks, we show that for any finite value of the bending fugacity all except exponentially few sufficiently long polygons are knotted.

1. Introduction

The presence of knots in closed polymer chains is considered of interest in polymer physics, chemistry, molecular biology and knot theory, and knotting can have an important influence on a number of polymer properties. For instance, the effects of knots on the rheology of polymer networks were investigated by Edwards (1967, 1968), and de Gennes (1984) considered tight knots in polymers and the influence they can have on long-time memory effects in melts of crystallizable linear polymers. In addition, the presence of knots in closed circular DNA can give information about the mechanism of the action of enzymes acting on the DNA molecules (Wasserman and Cozzarelli 1986). In this context knots have been detected in circular DNA, their knot type identified by electron microscopy (Dean and Cozzarelli 1985) and the knot probability measured experimentally as a function of the degree of polymerization and the ionic strength (Shaw and Wang 1993).

A flexible ring polymer (such as closed circular DNA) can be modelled as an n-step self-avoiding polygon on a regular lattice, and the presence of knots in polygons (and in related models such as piecewise-linear closed curves in R^3) has been studied using Monte Carlo methods by a number of workers (Vologodskii *et al* 1974, Michels and Wiegel 1986, Janse van Rensburg and Whittington 1990, Koniaris and Muthukumar 1991, Deguchi and Tsurusaki 1993, 1994). Little is known rigorously, but it has been shown that sufficiently long polygons are knotted with probability one (Sumners and Whittington 1998, Pippenger 1989). These rigorous results have been successively extended to the more general case of graphs embedded in Z^3 (Soteros *et al* 1992) and to the problem of the entanglement complexity of self-avoiding walks (Janse van Rensburg *et al* 1992).

On the other hand, a large number of real polymer chains do not obey the simple statistics of flexible chains. These chains, called semiflexible or stiff, are in general characterized by having the correlation between the direction of the bonds not entirely vanishing. An important example of a stiff polymer is the DNA molecule in solution. Indeed due to the tight constraint of successive pairs of nuclei acids ('base pairs', or bp) by chemical and hydrogen bonds, the DNA has a thermal bending persistence length of about 150 bp (50 nm) (Darnell *et al* 1990, Hagerman 1988).

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A model of a semiflexible polymer chain was first introduced by Flory (1956) by assigning an energy loss for each consecutive pairs of parallel bonds in the chain. With this model Flory (1956) predicted a phase transition from an isotropic phase to an ordered state. Since then, variants of this model have been used in studying many other properties of polymer chains, such as crystallization (Flory 1982), glass transition (Gibbs and Di Marzio 1958), polymer melting (Bascle *et al* 1992) and protein folding (Doniach *et al* 1996).

In this paper we will focus on the topological properties of semiflexible polymers. In particular, we discuss the occurrence of knots in semiflexible ring polymers modelled by polygons in the cubic lattice weighted according to their curvature by a bending fugacity β. In particular, we will prove that for any finite value of the bending fugacity, sufficiently long polygons are knotted with probability one. The paper is arranged as follows. In section 2, after recalling some previous results on knotting probability, we introduce the notion of semiflexible self-avoiding walks by defining the curvature of a walk in Z^3 and its associated bending fugacity. A similar definition for semiflexible polygons is considered. The main result of the section is the proof that the limiting free energies of semiflexible walks and polygons exist and are equal, for any finite value of the bending fugacity β. In section 3 we generalize Kesten's pattern theorem to semiflexible walks and in section 4 we use this result to prove that the knot probability of semiflexible polygons goes to unity exponentially rapidly as the number of edges in the polygon goes to infinity, for any finite value of the bending fugacity β. Finally, in section 5 we summarize our results and we give some suggestions for future work.

2. Definitions and rigorous results on free energies

Let Z^3 be the simple cubic lattice whose vertices are the integer points in R^3, and with edges between vertices which are unit distance apart. An *n-step self-avoiding walk* is an ordered sequence of $n+1$ vertices such that the first vertex is the origin, neighbouring pairs of vertices in the sequence are unit distance apart and all vertices are distinct. We often use *walk* to mean self-avoiding walk. A walk and any translate of the walk form an equivalence class and we also use walk as a short-hand for *equivalence class of self-avoiding walks* when this is not likely to cause confusion.

An n-step self-avoiding circuit (n-SAC) is an $(n-1)$-step self-avoiding walk whose first and last vertices are unit distance apart, with the additional edge between these two vertices. Any cyclic permutation of an n-SAC is also an n-SAC, and so is the reverse permutation and all cyclic permutations of the reverse permutation. The resulting set of $2n$ n-SACs which originate from a given n-SAC can be regarded as a single geometrical object, which we call an n-step (self-avoiding) polygon. Two n-step polygons are equivalent if one is a translate of the other. For instance, $p_4 = 3$, $p_6 = 22$ and $p_8 = 207$. We also use the word polygon for an equivalence class of polygons, when no confusion is likely to arise.

Let p_n be the number of n-step polygons. Hammersley (1961) has shown that there exists a connective constant $\kappa > 0$ such that, in the large n limit,

$$p_n = \mathrm{e}^{\kappa n + o(n)} \tag{2.1}$$

and similar techniques, together with the use of a pattern theorem (Kesten 1963), have been used (Sumners and Whittington 1988, Pippenger 1989) to prove that the number p_n^0 of *unknotted* polygons behaves, in the large n limit, as

$$p_n^0 = \mathrm{e}^{\kappa_0 n + o(n)} \tag{2.2}$$

with $0 < \kappa_0 < \kappa$, so that the probability $P(n)$ that the polygon is a knot goes, as $n \to \infty$, to unity exponentially rapidly as

$$P(n) = 1 - p_n^0/p_n = 1 - \mathrm{e}^{-\alpha_0 n + o(n)} \tag{2.3}$$

for some positive constant $\alpha_0 = \kappa - \kappa_0$. One concludes that unknotted polygons amount to an exponentially small fraction of all polygons as n tends to infinity.

To define semiflexible walks (polygons) we need first to introduce the notion of curvature of a walk. A *right angle* is a vertex on the walk (or on the polygon) that is shared by two consecutive non-colinear edges. In an n-step self-avoiding walk there can be at most $n - 1$ right angles since the first and the last vertex are not shared by two edges. We write $w_n(c)$ and $p_n(c)$ for the numbers of self-avoiding walks and polygons with n edges and c right angles. The number c of right angles we call the *curvature* associated to the walk (polygon). By introducing the bending fugacity β conjugate to the curvature c, we define the partition function for semiflexible walks as

$$Z_n^w(\beta) = \sum_c w_n(c)\,\mathrm{e}^{\beta c} \tag{2.4}$$

and similarly for semiflexible polygons

$$Z_n^p(\beta) = \sum_c p_n(c)\,\mathrm{e}^{\beta c}. \tag{2.5}$$

Positive β values would correspond to walks with enhanced flexibility (the turns are favoured), whereas negative β values will weight straight walks. As β becomes more and more negative the walk becomes more and more stiff. The case $\beta = 0$ gives back the unweighted walk (polygon) problem. From now on the notion of semiflexible walks (and semiflexible polygons) will correspond to self-avoiding walks (polygons) with partition function (2.4) ((2.5)).

First, we prove the existence of the limiting free energy for semiflexible polygons.

2.1. Existence of the limiting free energy for polygons

Theorem 2.1. The limit

$$\lim_{n\to\infty} n^{-1} \log Z_n^p(\beta) \equiv \mathcal{F}^p(\beta) \tag{2.6}$$

exists for all $\beta \in R$.

Proof. The idea is to concatenate pairs of polygons, and establish that the partition function satisfies a generalized supermultiplicative inequality.

The top and bottom edges of a polygon are defined by a lexicographic ordering of the edges by the coordinates of their midpoints. The top edge is the one with lexicographically largest midpoint, and the bottom edge is the one with lexicographically smallest midpoint. Let $\mathcal{P}$ be a polygon in Z^3 with n edges and curvature $c - s$, and let $\mathcal{Q}$ be a polygon in Z^3 with m edges and curvature s. We call e_p the top edge of $\mathcal{P}$ and e_q the bottom edge of $\mathcal{Q}$. In order to concatenate $\mathcal{P}$ and $\mathcal{Q}$, we need to have e_p and e_q parallel. This implies that, once we have chosen $\mathcal{P}$ in $p_n(c-s)$ ways, we can choose $\mathcal{Q}$ in $p_m(s)/2$ ways. Now we can translate $\mathcal{Q}$ so that the midpoints of e_p and e_q differ by unity in their first coordinates (with all other coordinates identical, and e_q with the larger first coordinate). We concatenate $\mathcal{P}$ and $\mathcal{Q}$ by deleting e_p and e_q and by adding two new edges to join the endpoints of e_p and e_q. This gives a new polygon $\mathcal{P} \oplus \mathcal{Q}$. Observe that removal of an edge in any polygon can decrease the curvature by at most 2 units, and similarly addition of an edge to make a new polygon can increase the curvature by up to 2 units. Thus the curvature of $\mathcal{P} \oplus \mathcal{Q}$ can range from up to 4 less to up to 4 more than the sum of the curvature of $\mathcal{P}$ and $\mathcal{Q}$. Then $\mathcal{P} \oplus \mathcal{Q}$ has $n+m$ edges and curvature at least $c-4$ and at most $c+4$. Without loss of generality, we will assume from now on that $n \geqslant m$. Thus

$$\sum_s p_n(c-s)p_m(s) \leqslant 2\sum_{k=-4}^{4} p_{n+m}(c+k) \tag{2.7}$$

and the summation over s is over all those values of s which give a non-zero contribution to the sum. Multiply (2.7) by $e^{\beta c}$ and sum over c (remembering that we have $n \geqslant m$, and that $p_m(\ell) = 0$ if $\ell > m$) to obtain

$$\sum_{c=0}^{n}\sum_{s=0}^{c} p_n(c-s)p_m(s)\,e^{\beta(c-s)}\,e^{\beta s} \leqslant 2\sum_{k=-4}^{4}\sum_{c=0}^{n+m} p_{n+m}(c+k)\,e^{\beta(c+k)}\,e^{-\beta k} \tag{2.8}$$

which gives

$$\begin{aligned} Z_n^p(\beta)Z_m^p(\beta) \leqslant 2\{&e^{4\beta}Z_{n+m}^p(\beta) + \cdots + e^{\beta}Z_{n+m}^p(\beta) + Z_{n+m}^p(\beta) + e^{-\beta}(Z_{n+m}^p(\beta) - p_{n+m}(0)) \\ &+e^{-2\beta}(Z_{n+m}(\beta) - p_{n+m}(0) - p_{n+m}(1)) + \cdots\} \end{aligned} \tag{2.9}$$

thus

$$\begin{aligned} Z_n^p(\beta)Z_m^p(\beta) &\leqslant 2\Bigg[\Bigg(\sum_{j=-4}^{4} e^{j\beta}\Bigg)Z_{n+m}^p(\beta) - \Bigg(\sum_{j=1}^{4} e^{-j\beta}\Bigg)p_{n+m}(0) - \Bigg(\sum_{j=2}^{4} e^{-j\beta}\Bigg)p_{n+m}(1) \\ &\qquad -\Bigg(\sum_{j=3}^{4} e^{-j\beta}\Bigg)p_{n+m}(2) - e^{-4\beta}p_{n+m}(3)\Bigg] \\ &\leqslant 2\Bigg(\sum_{j=-4}^{4} e^{j\beta}\Bigg)Z_{n+m}^p(\beta) \end{aligned} \tag{2.10}$$

so that $\log Z_n^p(\beta)$ is a generalized superadditive sequence.

Note that, since for $\beta \leqslant 0$ we have $Z_n^p(\beta) \leqslant \sum_{c=0}^{n} p_n(c) = p_n = e^{\kappa_3 n + o(n)}$,

$$Z_n^p(\beta) \leqslant e^{\kappa_3 n} \qquad \text{if } \beta \leqslant 0 \tag{2.11}$$

where $\kappa_3 < \infty$ is the connective constant of polygons† in Z^3, and

$$Z_n^p(\beta) \leqslant e^{(\kappa_3+\beta)n} \qquad \text{if } \beta > 0 \tag{2.12}$$

since, for $\beta > 0$, $Z_n^p(\beta) \leqslant e^{\beta n}\sum_{c=0}^{n} p_n(c) = e^{\beta n}p_n$. Thus $\lim_{n\to\infty} n^{-1}\log Z_n^p(\beta) = \mathcal{F}^p(\beta)$ exists and is finite for $\beta \in R$ (Hille 1948). □

2.2. Convexity and monotonicity

The convexity of the functions $F_n^p(\beta) = n^{-1}\log Z_n^p(\beta)$ follows from the Cauchy–Schwartz inequality, i.e.

$$\begin{aligned} Z_n^p(\beta_1)Z_n^p(\beta_2) &= \sum_{c=0}^{n} p_n(c)\,e^{\beta_1 c}\sum_{s=0}^{n} p_n(s)\,e^{\beta_2 s} \\ &\geqslant \Bigg(\sum_{c=0}^{n} p_n(c)\,e^{(\beta_1+\beta_2)/2c}\Bigg)^2 \end{aligned}$$

† The connective constant of polygons is defined to be the limit $\lim_{n\to\infty}(1/n)\log p_n = \kappa_d$ in d dimensions (Hammersley 1957, 1961). The connective constant of self-avoiding walks is defined by replacing p_n by w_n (the number of self-avoiding walks of n steps) and it is equal to κ_d (Hammersley 1957, 1961).

$$= \left(Z_n^p \left(\frac{\beta_1 + \beta_2}{2} \right) \right)^2 \tag{2.13}$$

which implies that

$$\frac{1}{n} \log Z_n^p \left(\frac{\beta_1 + \beta_2}{2} \right) \leqslant \frac{1}{2} \left(\frac{1}{n} \log Z_n^p(\beta_1) + \frac{1}{n} \log Z_n^p(\beta_2) \right) \tag{2.14}$$

i.e. that $F_n^p(\beta)$ is a convex function of β. Since $\mathcal{F}^p(\beta)$ is the limit of a sequence of convex functions, it is convex in $\beta \in (-\infty, \infty)$. It is therefore continuous in $\beta \in (-\infty, +\infty)$, and differentiable almost everywhere (Hardy *et al* 1952).

2.3. Bounds on $\mathcal{F}^p(\beta)$

We use the bounds on the partition function $Z_n^p(\beta)$ in order to obtain bounds on the free energy. If $\beta = 0$, then $Z_n^p(0) = p_n$, and by the definition of the free energy we obtain

$$\mathcal{F}^p(0) = \kappa_3. \tag{2.15}$$

Moreover, from equation (2.11) and (2.12) we obtain

$$\mathcal{F}^p(\beta) \leqslant k_3 + \beta \qquad \text{for } \beta > 0 \tag{2.16}$$

and

$$\mathcal{F}^p(\beta) \leqslant \kappa_3 \qquad \text{for } \beta < 0. \tag{2.17}$$

We next prove the main result of the section.

2.4. The limiting free energies of semiflexible walks and polygons are equal

The idea is to find an upper and a lower bound for $Z_n^w(\beta)$ that involve the partition function for polygons modulo some factors that become irrelevant in the thermodynamic limit. The lower bound is easy to find and the result can be stated as follows.

Lemma 2.2. The partition functions for polygons and walks are related by the inequality

$$2n Z_n^p(\beta) \leqslant \left(\sum_{k=-2}^{0} \mathrm{e}^{-\beta k} \right) Z_{n-1}^w(\beta). \tag{2.18}$$

Proof. By deleting any of the n edges in a polygon with n edges and curvature c, we obtain a $n-1$-step walk with curvature $c' \in \{c-2, c-1, c\}$. Thus,

$$2n p_n(c) \leqslant \sum_{k=-2}^{0} w_{n-1}(c+k) \tag{2.19}$$

where the factor of 2 comes from the two possible ways in which we can choose the origin of the resulting walk. Multiplying equation (2.19) by $\mathrm{e}^{\beta c}$ and summing over the curvature c we obtain the result. □

The inequality in the opposite direction is more complicated to obtain. The idea is to unfold a walk, show that walks and unfolded walks have the same exponential behaviour and then construct a subset of polygons by a suitable concatenation of unfolded walks. In order to do that we need some subsidiary lemmas about unfolded walks. We write (x_i, y_i, z_i), $i = 0, \ldots, n$, for the coordinates of vertex i in an n-step self-avoiding walk. A self-avoiding walk is *x-unfolded* if $x_0 < x_i < x_n$, $i = 1, \ldots, n-1$. Similarly, we define a walk to be *(x, z)-unfolded* if $x_0 \leqslant x_i$ and $z_0 < z_i$, $\forall i > 0$, and $x_n > x_i$ and $z_n \geqslant z_i$, $\forall i < n$. We write $w_n^\dagger(c)$ $(w_n^\ddagger(c))$ for the number of x-unfolded ((x, z)-unfolded) n-step walks with c right angles, and define the partition function

$$Z_n^\dagger(\beta) = \sum_c w_n^\dagger(c)\,\mathrm{e}^{\beta c} \tag{2.20}$$

with a similar definition for $Z_n^\ddagger(\beta)$.

Lemma 2.3. We have

$$Z_n^w(\beta) \leqslant \mathrm{e}^{O(\sqrt{n})}\left(\sum_{k=0}^{2} \mathrm{e}^{-\beta k}\right) Z_{n+2}^\dagger(\beta) \leqslant \mathrm{e}^{O(\sqrt{n})}\,\mathrm{e}^{-\beta}\left(\sum_{k=0}^{2} \mathrm{e}^{-\beta k}\right) Z_{n+3}^\ddagger(\beta). \tag{2.21}$$

Proof. To relate $w_n(c)$ to $w_n^\dagger(c)$ we make use of an unfolding transformation along the x-direction (Hammersley and Welsh 1962). For a particular walk in $w_n(c)$ let $x_{\min} = \min_i\{x_i\}$ and $x_{\max} = \max_i\{x_i\}$. Let p_1 be the smallest integer such that $x_{p_1} = x_{\min}$ and let p_2 be the largest integer such that $x_{p_2} = x_{\max}$. Now reflect the vertices $i = 0, 1, \ldots, p_1 - 1$ with respect to the plane $x = x_{\min}$ and the vertices $i = p_2 + 1, \ldots, n$ with respect to the plane $x = x_{\max}$. Note that the transformation does not change the number of right angles. By repeated application of these reflections we eventually obtain, apart from the trivial translation, a walk having $p_1 = 0$, $p_2 = n$ and c right angles. Finally, to obtain an x-unfolded walk two edges must be added at the extremities, one of coordinates $x_0 - 1, x_0$ and the other of coordinates $x_n, x_n + 1$. The x-unfolded walk obtained will have $n+2$ steps and $c + k$ right angles with $k \in \{0, 1, 2\}$. In general, the same walk in $w_{n+2}^\dagger(c + k)$ can be obtained from different members of $w_n(c)$ but Hammersley and Welsh (1962) have shown that there exists a constant b such that at most $\mathrm{e}^{b\sqrt{n}}$ different members of $w_n(c)$ can lead to the same member of $w_{n+2}^\dagger(c + k)$. We then have

$$w_n(c) \leqslant \sum_{k=0}^{2} w_{n+2}^\dagger(c + k)\,\mathrm{e}^{O(\sqrt{n})}. \tag{2.22}$$

The unfolding procedure is similarly performed along the z-direction to obtain from an x-unfolded walk a walk unfolded in the (x, z) directions. Moreover, since a bond is added at the vertex x_0 along z, this will create an additional right angle. In terms of configurations we then have

$$w_n^\dagger(c) \leqslant w_{n+1}^\ddagger(c + 1)\,\mathrm{e}^{O(\sqrt{n})}. \tag{2.23}$$

By multiplying equations (2.22) and (2.23) by $\mathrm{e}^{\beta c}$ and summing over c we have respectively

$$Z_n^w(\beta) \leqslant \sum_c \sum_{k=0}^{2} w_{n+2}^\dagger(c + k)\,\mathrm{e}^{O(\sqrt{n})}\,\mathrm{e}^{\beta(c+k)}\,\mathrm{e}^{-\beta k} \tag{2.24}$$

and

$$Z_n^\dagger(\beta) \leqslant \sum_c w_{n+1}^\ddagger(c + 1)\,\mathrm{e}^{O(\sqrt{n})}\,\mathrm{e}^{\beta(c+1)}\,\mathrm{e}^{-\beta}. \tag{2.25}$$

Since

$$\sum_c \sum_{k=0}^{2} w^{\dagger}_{n+2}(c+k)\,\mathrm{e}^{\beta(c+k)}\,\mathrm{e}^{-\beta k} = Z^{\dagger}_{n+2}(\beta)\left(\sum_{k=0}^{2}\mathrm{e}^{-\beta k}\right) - \mathrm{e}^{-\beta} w^{\dagger}_{n+2}(0) \tag{2.26}$$

$$-\mathrm{e}^{-2\beta}(w^{\dagger}_{n+2}(0) + w^{\dagger}_{n+2}(1))$$

$$\leqslant Z^{\dagger}_{n+2}(\beta)\left(\sum_{k=0}^{2}\mathrm{e}^{-\beta k}\right) \tag{2.27}$$

we obtain the first inequality of the lemma. The second inequality is then obtained in a similar way. □

We next concatenate (x, z)-unfolded walks to form polygons.

Lemma 2.4. We have

$$Z^p_{4n}(\beta) \geqslant \frac{(Z^{\ddagger}_n(\beta))^4}{16n^8}. \tag{2.28}$$

Proof. The set of n-step (x, z)-unfolded walks can be divided into N_s subsets according to the value of the *height* $h = z_n - z_0$ of the walk. There are no more than n such subsets (i.e. $N_s \leqslant n$), which we call $W^{\ddagger}_n(h), h = 1, \ldots, n$, where h is the height of the members of the subset. Let the number of members of $W^{\ddagger}_n(h)$, which have c right angles, be $w^{\ddagger}_n(c, h)$ and define the partition function $Z^{\ddagger}_n(\beta, h) = \sum_c w^{\ddagger}_n(c, h)\,\mathrm{e}^{\beta c}$.

For a given value of β, let $h_o = h_o(\beta)$ be the smallest integer such that $Z^{\ddagger}_n(\beta, h_o) \geqslant Z^{\ddagger}_n(\beta, h)$ for all h. In other words h_o identifies the 'most popular class'. Since the most popular class must contain at least a fraction $1/N_s$ of (x, z)-unfolded walks, we have the estimate

$$Z^{\ddagger}_n(\beta, h_o) \geqslant \frac{Z^{\ddagger}_n(\beta)}{N_s} \geqslant \frac{Z^{\ddagger}_n(\beta)}{n}.$$

We define an *n-loop* as an n-step self-avoiding walk such that $x_0 \leqslant x_i \leqslant x_n, \forall i$ and $z_0 = z_n < z_i, \forall i \neq 0, n$. Let the number of n-loops with c right angles be $l_n(c)$, with corresponding partition function $Z^l_n(\beta) = \sum_c l_n(c)\,\mathrm{e}^{\beta c}$. Concatenating a member of $W^{\ddagger}_n(h_o)$, with a second (not necessarily different) member, reflected in the plane $x = x_n$, gives a loop with $2n$ edges, so that

$$l_{2n}(c) \geqslant \sum_{c_1} w^{\ddagger}_n(c_1, h_o) w^{\ddagger}_n(c - c_1, h_o). \tag{2.29}$$

Hence

$$Z^l_{2n}(\beta) \geqslant Z^{\ddagger}_n(\beta, h_o)^2 \geqslant \left(\frac{Z^{\ddagger}_n(\beta)}{n}\right)^2. \tag{2.30}$$

In a similar way one can split loops into classes, according to the x and y coordinates of the first and the last vertex (giving at most n^2 possible classes), and concatenate in pairs to form polygons, giving the inequality

$$Z^p_{2n}(\beta) \geqslant \left(\frac{Z^l_n(\beta)}{n^2}\right)^2. \tag{2.31}$$

Lemma 2.4 then follows immediately. □

Now we can state the main result of the section.

Theorem 2.5. The limiting free energy for semiflexible walks

$$\mathcal{F}^w(\beta) = \lim_{n\to\infty} n^{-1} \log Z_n^w(\beta) \tag{2.32}$$

exists and it is equal to the one for semiflexible polygons, that is

$$\mathcal{F}^w(\beta) = \mathcal{F}^p(\beta) \qquad \forall\beta \in R. \tag{2.33}$$

Proof. From lemmas 2.2–2.4 we have

$$\begin{aligned} 2nZ_n^p(\beta) &\leqslant \left(\sum_{k=-2}^{0} \mathrm{e}^{-\beta k}\right) Z_{n-1}^w(\beta) \\ &\leqslant \mathrm{e}^{O(\sqrt{n})}\,\mathrm{e}^{-\beta}\left(\sum_{k=0}^{2} \mathrm{e}^{-\beta k}\right)\left(\sum_{k=-2}^{0} \mathrm{e}^{-\beta k}\right) Z_{n+2}^{\ddagger}(\beta) \\ &\leqslant \mathrm{e}^{O(\sqrt{n-1})}\,\mathrm{e}^{-\beta}\left(\sum_{k=0}^{2} \mathrm{e}^{-\beta k}\right)\left(\sum_{k=-2}^{0} \mathrm{e}^{-\beta k}\right) 2(n+2)^2 (Z_{4(n+2)}^p(\beta))^{1/4}. \end{aligned} \tag{2.34}$$

By taking logarithms in (2.3) and (2.34), dividing by n and letting n tend to infinity, the theorem follows immediately. □

Note that from inequality (2.34) we have also that the limiting free energies of x-unfolded and (x, z)-unfolded walks exist and are all equal to the limiting free energy of walks, namely

$$\lim_{n\to\infty} n^{-1} \log Z_n^{\dagger}(\beta) = \lim_{n\to\infty} n^{-1} \log Z_n^{\ddagger}(\beta) = \mathcal{F}^w(\beta) \qquad \forall\beta \in R. \tag{2.35}$$

3. Pattern theorem for semiflexible walks

In this section we state and prove a pattern theorem for walks with curvature, similar to Kesten's pattern theorem for self-avoiding walks (Kesten 1963). The proof that we shall give is closely related to an unpublished proof of Kesten's theorem due to Hammersley and recently used to prove a similar result for open ribbons (Janse van Rensburg *et al* 1996). We begin by defining a *factorization* of an x-unfolded walk. The x-unfolded walk has a *cutting plane* if there is a vertex x_k with $0 < k < n$ such that $x_j < x_k < x_i$ for all $j = 0, \ldots, k-1$ and $i = k+1, \ldots, n$. The cutting plane is the plane $x = x_k$. If an x-unfolded walk has no cutting planes, then it is a *prime walk*. Let q_n be the number of n-step prime walks and $q_n(c)$ the number of n-step prime walks with c right angles. Clearly $\sum_c q_n(c) = q_n$. We define the partition function for prime walks and its generating function as follows:

$$Q_n(\beta) = \sum_{c\geqslant 0} q_n(c)\,\mathrm{e}^{\beta c} \tag{3.1}$$

$$\mathcal{Q}(x, \beta) = \sum_{n>0} Q_n(\beta) x^n. \tag{3.2}$$

Similarly we can define a generating function $\mathcal{W}^{\dagger}(x, \beta)$ for x-unfolded walks. The idea is now to relate the two generating functions by using a generalized renewal equation. Indeed, by factorization at the first available cutting plane we obtain the generalized renewal equation

$$w_n^{\dagger}(c) = q_n(c) + \sum_{c_1\geqslant 0}^{c} \sum_{m}^{n-1} q_m(c - c_1) w_{n-m}^{\dagger}(c_1) \tag{3.3}$$

which can be rewritten in terms of the generating functions as

$$\mathcal{W}^{\dagger}(x,\beta) = \frac{\mathcal{Q}(x,\beta)}{1-\mathcal{Q}(x,\beta)}. \tag{3.4}$$

In order to show for which values of $x = x(\beta)$ $\mathcal{W}^{\dagger}(x,\beta)$ diverges we need the generating function for the walks with weighted curvature, namely

$$\mathcal{W}(x,\beta) = \sum_{n>0} Z_n^w(\beta) x^n. \tag{3.5}$$

From theorem 2.5, we know that $\mathcal{W}(x,\beta)$ diverges at $x = x(\beta) = \mathrm{e}^{-\mathcal{F}^w(\beta)}$ and we can use such a result to get the asymptotic behaviour of $\mathcal{W}^{\dagger}(x,\beta)$. In order to do that we introduce another special subset of walks, the *bridges*. We define a n-step walk to be a *bridge* if $x_0 < x_i, \forall i > 0$, and $x_i \leqslant x_n, \forall i < n$. Let $b_n(c)$ be the number of n-steps bridges (up to translation) with c right angles. The partition function and the generating function follows as

$$B_n(\beta) = \sum_{c\geqslant 0} b_n(c)\,\mathrm{e}^{\beta c} \tag{3.6}$$

$$\mathcal{B}(x,\beta) = \sum_{n>0} B_n(\beta) x^n. \tag{3.7}$$

It is easy to show that $\mathcal{B}(x,\beta)$ and $\mathcal{W}^{\dagger}(x,\beta)$ have the same asymptotic behaviour. Indeed, from the inequality $w_n^{\dagger}(c) \leqslant b_n(c), \forall c$ (the x-unfolded walks are a subset of bridges), it follows $\mathcal{W}^{\dagger}(x,\beta) \leqslant \mathcal{B}(x,\beta)$. Moreover, one can obtain an $(n+1)$-step x-unfolded walk by adding a step to the rightmost vertex of an n-step bridge. Since this procedure can produce at most a new right angle, we have $b_n(c) = \sum_{k=0}^{1} w_{n+1}^{\dagger}(c+k)$. By multiplying by the Boltzmann factor $\mathrm{e}^{\beta c}$ and summing over c, we obtain $B_n(\beta) \leqslant Z_{n+1}^{\dagger}(\beta)(1+\mathrm{e}^{-\beta})$, and in terms of the generating functions we have the reversed inequality $\mathcal{B}(x,\beta) \leqslant (1+\mathrm{e}^{-\beta})\mathcal{W}^{\dagger}(x,\beta)$.

Given that $\mathcal{B}(x,\beta)$ and $\mathcal{W}^{\dagger}(x,\beta)$ have the same asymptotic behaviour it remains to relate $\mathcal{B}(x,\beta)$ to the generating function for the walks. This is achieved in the following lemma.

Lemma 3.1. We have

$$\mathcal{W}(x,\beta) \leqslant \frac{\mathrm{e}^{2\mathcal{B}(x,\beta)/x}}{x}. \tag{3.8}$$

Proof. The proof is very similar to the proof of corollary 3.1.8 in Madras and Slade (1993, p 61). Here we give a sketch of this proof without entering into the details (which can be found in the above-mentioned reference) but stressing the differences we encounter between the present case and the case for unweighted walks discussed in Madras and Slade.

Bridges are a particular subclass of half-space walks, that is walks for which $x_0 < x_i, \forall i > 0$. Each self-avoiding walk can be split into two half-space walks (see Madras and Slade 1993, p 60) and this process does not affect the number of right angles. This procedure leads to the following inequality

$$w_n(c) \leqslant \sum_{r=0}^{c}\sum_{m=1}^{n} h_{n-m}(c-r) h_{m+1}(k) \tag{3.9}$$

where $h_n(c)$ is the number of n-step half-space walks with c right angles. Moreover, each half-space walk can be decomposed into a finite sequence of bridges where the ith bridge is characterized by a span A_i (for a definition of a span of a walk see Madras and Slade), length m_i and number of right angles c_i. In addition, the following constraints hold: $A_1 > A_2 > A_3 > \cdots > A_k > 0$ and $\sum_i^k m_i = n$. Since each time we break the half-space walk we loose a right angle, we control this variable by adding at the end of each bridge of the decomposition, an edge perpendicular to the last edge of the bridge. In this way we have

$$h_n(c) \leqslant \sum \prod_{i=1}^{k} b_{m_i+1,A_i}(\tilde{c}_i) \tag{3.10}$$

where the sum is over all integers $k \geqslant 1$, all integers $A_1 > A_2 > A_3 > \cdots > A_k > 0$, and all integers m_i such that $\sum_i^k m_i = n$. In addition, we have the constraint $\sum_{i=1}^k \tilde{c}_i = c$. From (3.10), following Madras and Slade (1993, p 62), we obtain

$$\begin{aligned} \sum_{n\geqslant 1}\sum_{c\geqslant 0} h_n(c)\,\mathrm{e}^{\beta c}x^n &\leqslant \prod_{A=1}^{\infty}\left(1+\sum_{c=0}^{\infty}\sum_{m=1}^{\infty} b_{m+1,A}(c)\,\mathrm{e}^{\beta c}x^m\right) \\ &\leqslant \exp\left(\sum_{A=1}^{\infty}\sum_{m=1}^{\infty}\left(\sum_{c=0}^{m} b_{m+1,A}(c)\,\mathrm{e}^{\beta c}\right)x^m\right) \\ &= \exp\left(\sum_{A=1}^{\infty}\sum_{m=1}^{\infty} B_{m+1,A}(\beta)x^m\right) \\ &= \exp\left(\frac{\mathcal{B}(x,\beta)}{x}\right). \end{aligned} \tag{3.11}$$

This inequality combined with equation (3.9) gives

$$\begin{aligned} \sum_{n\geqslant 1}\sum_{c\geqslant 0} w_n(c)\,\mathrm{e}^{\beta c}x^n &\leqslant \sum_{n\geqslant 1}\sum_{c\geqslant 0}\sum_{r=0}^{c}\sum_{m=1}^{n} h_{n-m}(c-r)\,\mathrm{e}^{\beta(c-r)}x^{n-m}\,\frac{h_{m+1}(r)\,\mathrm{e}^{\beta r}x^{m+1}}{x} \\ &= \frac{1}{x}\left(\sum_{n\geqslant 1}\sum_{c\geqslant 0} h_n(c)\,\mathrm{e}^{\beta c}x^n\right)^2 \end{aligned} \tag{3.12}$$

which gives the desired result. □

Since $\mathcal{W}(x,\beta)$ diverges at $x = x(\beta) = \mathrm{e}^{-\mathcal{F}^w(\beta)}$, $\mathcal{B}(x,\beta)$ also diverges at $\mathrm{e}^{-\mathcal{F}^w(\beta)}$ (lemma 3.1), and hence $\mathcal{W}^\dagger(x,\beta)$ diverges at $\mathrm{e}^{-\mathcal{F}^w(\beta)}$.

A *pattern* is any fixed finite self-avoiding walk, and a *prime pattern* is any finite prime walk. Consider a prime pattern P and the set of n-step walks with c right angles, not containing P. We write $w_n(c;\bar{P})$, $b_n(c;\bar{P})$, $w_n^\dagger(c;\bar{P})$ and $q_n(c;\bar{P})$ for the numbers of walks, bridges, x-unfolded walks and prime walks, respectively, with n steps and c right angles, not containing the prime pattern P. Similarly, we write $\mathcal{W}(x,\beta;\bar{P})$, $\mathcal{B}(x,\beta;\bar{P})$, $\mathcal{W}^\dagger(x,\beta;\bar{P})$ and $\mathcal{Q}(x,\beta;\bar{P})$ for the corresponding generating functions. For the class of walks that do not contain the pattern P we then define the partition function $Z_n^w(\beta;\bar{P})$ in analogy with $Z_n^w(\beta)$. A simple concatenation argument gives the following result.

Lemma 3.2. The limit

$$\lim_{n\to\infty} n^{-1}\log Z_n^w(\beta;\bar{P}) \equiv \mathcal{F}^w(\beta;\bar{P}) \tag{3.13}$$

exists for all $\beta \in R$.

Proof. Since by concatenating two walks we will create at most one right angle, we have

$$\sum_{c_1 \geqslant 0} w_n(c - c_1; \bar{P}) w_m(c_1; \bar{P}) \geqslant \sum_{k=0}^{1} w_{m+n}(c + k; \bar{P}). \tag{3.14}$$

Indeed, the sense of the inequality allows us to reject configurations obtained by concatenation that do contain the pattern P. By multiplying by $e^{\beta c}$ and summing over c, we have

$$\sum_{c \geqslant 0} \sum_{c_1} w_n(c - c_1; \bar{P}) \, e^{\beta(c - c_1)} w_m(c_1; \bar{P}) \, e^{\beta c_1} \geqslant \sum_{c \geqslant 0} \sum_{k=0}^{1} w_{n+m}(c + k; \bar{P}) \, e^{\beta c} \tag{3.15}$$

$$\geqslant \sum_{c \geqslant 0} w_{n+m}(c; \bar{P}) \, e^{\beta c} \tag{3.16}$$

hence

$$Z_n^w(\beta; \bar{P}) Z_m^w(\beta; \bar{P}) \geqslant Z_{n+m}^w(\beta; \bar{P}). \tag{3.17}$$

Since $Z_n^w(\beta; \bar{P}) \leqslant Z_n^w(\beta), \forall \beta \in R$, the limit $\lim_{n \to \infty} n^{-1} \log Z_n^p(\beta; \bar{P}) = \lim_{n \to \infty} F_n^w(\beta; \bar{P}) = \mathcal{F}^w(\beta; \bar{P})$ exists and is finite for all $\beta \in R$. Moreover, $\mathcal{F}^w(\beta; \bar{P}) \leqslant \mathcal{F}^w(\beta)$. □

The result of the lemma implies that $\mathcal{W}(x, \beta; \bar{P})$ diverges at $x = x(\beta) = e^{-\mathcal{F}^w(\beta; \bar{P})}$ where $\mathcal{F}^w(\beta; \bar{P}) \leqslant \mathcal{F}^w(\beta)$. On the other hand, by using the same arguments as in lemma 3.1 we have

$$\mathcal{W}(x, \beta; \bar{P}) \leqslant \frac{e^{2\mathcal{B}(x, \beta; \bar{P})/x}}{x} \tag{3.18}$$

so $\mathcal{B}(x, \beta; \bar{P})$ also diverges at $x = x(\beta) = e^{-\mathcal{F}^w(\beta; \bar{P})}$, and converges for all $x < x(\beta) = e^{-\mathcal{F}^w(\beta; \bar{P})}$ given that $\mathcal{B}(x, \beta; \bar{P}) \leqslant \mathcal{W}(x, \beta; \bar{P}), \forall x \geqslant 0$. Since $\mathcal{B}(x, \beta; \bar{P})$ and $\mathcal{W}^\dagger(x, \beta; \bar{P})$ have the same asymptotic behaviour (by an argument exactly similar to that given above for $\mathcal{B}(x, \beta)$ and $\mathcal{W}^\dagger(x, \beta)$), then also $\mathcal{W}^\dagger(x, \beta; \bar{P})$ diverges at $x = x(\beta) = e^{-\mathcal{F}^w(\beta; \bar{P})}$, and converges for all $x < x(\beta) = e^{-\mathcal{F}^w(\beta; \bar{P})}$. It remains to show that $\mathcal{W}^\dagger(x = e^{-\mathcal{F}^w(\beta)}, \beta; \bar{P})$ is finite; this result would imply that $e^{-\mathcal{F}^w(\beta)} < e^{-\mathcal{F}^w(\beta; \bar{P})}$. Since $q_m(c, \bar{P}) < q_m(c)$ for at least one value of m (the obvious case being when the prime walk is the prime pattern P made by m edges) we have for the generating function

$$\begin{aligned} \mathcal{Q}(e^{-\mathcal{F}^w(\beta)}, \beta; \bar{P}) &= Q_m(\beta; \bar{P})(e^{-\mathcal{F}^w(\beta)})^m + \sum_{n \neq m} Q_n(\beta; \bar{P}) \, e^{-\mathcal{F}^w(\beta) n} < Q_m(\beta)(e^{-\mathcal{F}^w(\beta)})^m \\ &\quad + \sum_{n \neq m} Q_n(\beta) \, e^{-\mathcal{F}^w(\beta) n} \\ &= \mathcal{Q}(e^{-\mathcal{F}^w(\beta)}, \beta). \end{aligned} \tag{3.19}$$

On the other hand, $\mathcal{W}^\dagger(e^{-\mathcal{F}^w(\beta)}, \beta)$ diverges and from equation (3.4) this implies $\mathcal{Q}(e^{-\mathcal{F}^w(\beta)}, \beta) = 1$. From inequality (3.19) we then have $\mathcal{Q}(e^{-\mathcal{F}^w(\beta)}, \beta; \bar{P}) < 1$. This implies, using an equation analogous to (3.4), that $\mathcal{W}^\dagger(x = e^{-\mathcal{F}^w(\beta)}, \beta; \bar{P})$ is finite. Hence $e^{-\mathcal{F}^w(\beta)} < e^{-\mathcal{F}^w(\beta; \bar{P})}$. This is the key result of the section which we state as follows.

Theorem 3.3. Semiflexible self-avoiding walks that do not contain the prime pattern P at least once have a free energy $\mathcal{F}^w(\beta; \bar{P})$ that is strictly less than the free energy $\mathcal{F}^w(\beta)$ of the set of all semiflexible self-avoiding walks. That is,

$$\mathcal{F}^w(\beta; \bar{P}) < \mathcal{F}^w(\beta) \qquad \forall \beta \in R. \tag{3.20}$$

The next theorem is the corresponding result for the polygons.

Theorem 3.4. Defining $\mathcal{F}^p(\beta; \bar{P}) \equiv \lim_{n\to\infty} \sup(1/n) \ln Z_n^p(\beta; \bar{P})$ we have

$$\mathcal{F}^p(\beta; \bar{P}) \leqslant \mathcal{F}^w(\beta; \bar{P}) < \mathcal{F}^w(\beta) = \mathcal{F}^p(\beta) \qquad \forall\beta \in R. \tag{3.21}$$

Proof. If an edge of a n-edge polygon with curvature c is deleted, the corresponding graph is a self-avoiding walk with $(n-1)$ edges and curvature $c' \in \{c-2, c-1, c\}$. Moreover, deleting an edge cannot create a pattern so that $2np_n(c; \bar{P}) \leqslant \sum_{k=-2}^{0} w_{n-1}(c+k; \bar{P})$. Multiplying both terms by $e^{\beta c}$ and summing over c we have

$$2nZ_n^p(\beta; \bar{P}) \leqslant Z_{n-1}^w(\beta; \bar{P})(1 + e^{\beta} + e^{2\beta}). \tag{3.22}$$

Taking logarithms, dividing by n and letting $n \to \infty$, by using (3.20) and (2.33), we obtain (3.21). □

4. Knots in semiflexible polygons

In this section we shall be concerned with knots in polygons with weighted curvature. The main result will be an extension of theorem 1 in Sumners and Whittington (1988) on the probability for a polygon to be knotted. Indeed we prove that, as n goes to infinity, the probability that the polygon weighted by curvature is knotted goes to unity exponentially rapidly for all finite values of the curvature parameter β. We first prove a preliminary lemma.

Lemma 4.1. Let $p_n^o(c)$ the subclass of unknotted polygons with n edges and c right angles. Let $Z_n^{p^o}(\beta) = \sum_c p_n^o(c)\, e^{\beta c}$ be the partition function for the corresponding model in which the curvature of unknotted polygons is weighted by the bending fugacity β. The limit

$$\lim_{n\to\infty} \frac{1}{n} \ln Z_n^{p^o}(\beta) = \mathcal{F}^o(\beta) \tag{4.1}$$

exists $\forall\beta \in R$.

Proof. The proof, based on concatenation of a pair of unknotted polygons, is similar to that of theorem 2.1. □

We now come to the main theorem of this section.

Theorem 4.2. For any finite value of the bending fugacity β, unknotted self-avoiding polygons are exponentially rare in the set of all polygons. That is,

$$\alpha(\beta) = \mathcal{F}^p(\beta) - \mathcal{F}^o(\beta) > 0 \qquad \forall\beta < \infty. \tag{4.2}$$

Proof. We take

$$T = \{i, i, j, k, k, -j, -j, -k, -i, -k, -k, j, j, k, k, -j, i, i\} \tag{4.3}$$

where i, j, k are unit vectors in the coordinate directions and T stands for trefoil. The sequence of edges is a *knotted arc* (see Sumners and Whittington (1998) for the technical definition of knotted arc), and its presence in a polygon ensures that the polygon will be knotted. Replacing P by T in theorem 3.4 we have $\mathcal{F}^p(\beta; \bar{T}) < \mathcal{F}^p(\beta), \forall\beta \in R$. On the other hand, the subset of unknotted semiflexible polygons with n-edges is a subset of the corresponding semiflexible polygons which do not contain the pattern T defined above. We then have $\mathcal{F}^o(\beta) \leqslant \mathcal{F}^p(\beta; \bar{T}) < \mathcal{F}^p(\beta), \forall\beta \in R$. □

If we introduce the knotting probability as

$$P_n(\beta) = 1 - \frac{Z_n^{p^o}(\beta)}{Z_n^p(\beta)} \tag{4.4}$$

then theorem 4.2 implies that for large n

$$P_n(\beta) = 1 - \exp(-\alpha(\beta)n + o(n)) \tag{4.5}$$

i.e. the probability that a semiflexible polygons is knotted goes to one as n goes to infinity for any *finite* value of the bending parameter β.

5. Discussion

By proving a pattern theorem for weighted (by curvature) walks, we have shown rigorously that, for semiflexible polygons in Z^3, the knot probability goes to unity exponentially rapidly as the size of the polygon increases, for any finite value of the bending fugacity β. Specialized to the less obvious case $\beta < 0$, this result means that no matter how stiff the n-edges polygon is (finite stiffness however), if n is sufficiently big the polygon will be knotted with probability one. This is an interesting result if one considers the experimental evidence of the presence of knots in long and stiff polymers in solution such as DNA. Notice that in the limit $\beta \to -\infty$ the polygon will have the minimal number of bends ($c = 4$) and no knots can occur in this configuration. In this sense the point $\beta = -\infty$ is singular for the function $\alpha(\beta)$. A similar approach based on the density functions of right angles should allow a more precise study of the function $\alpha(\beta)$.

The arguments in theorem 3.3 could be extended to show that every pattern occurs at positive density with high probability and $\forall\beta$ finite. This should allow the proof results about entanglement complexity following the arguments used in Soteros *et al* (1992) for unweighted self-avoiding walks.

The results obtained in this paper are all asymptotic in nature. In particular, they say little about knotting in semiflexible polygons for small values of n. It would then be very interesting to tackle the finite n problem by numerical approaches, such as Monte Carlo simulations.

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