

Polygons in restricted geometries subjected to infinite forces

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Abstract

We consider self-avoiding polygons in a restricted geometry, namely an infinite $L \times M$ tube in \mathbb{Z}^3 . These polygons are subjected to a force f , parallel to the infinite axis of the tube. When $f > 0$ the force stretches the polygons, while when $f < 0$ the force is compressive. We obtain and prove the asymptotic form of the free energy in both limits $f \rightarrow \pm\infty$. We conjecture that the $f \rightarrow -\infty$ asymptote is the same as the limiting free energy of “Hamiltonian” polygons, polygons which visit every vertex in a $L \times M \times N$ box. We investigate such polygons, and in particular use a transfer-matrix methodology to establish that the conjecture is true for some small tube sizes.

Dedicated to Anthony J. Guttmann on the occasion of his 70th birthday.

1 Introduction

Since the advent of single molecule experiments using, for example, atomic force microscopy, there has been much interest in modelling polymers subject to a tensile force (see for example [3, 4, 6, 12, 16, 18, 29]). Models range from random walk in \mathbb{R}^3 to lattice models and they have been studied both numerically and using combinatorial or probabilistic analysis. Recent advances on the theoretical side, include a proof for the self-avoiding walk (SAW) lattice model of linear polymers that there is a phase transition between a free and a ballistic phase at a critical force, f_c , corresponding to when the force, $f = f_c = 0$ [4]. Most recently, for the square lattice, conjectures based on Schramm-Loewner evolution have been used to predict the form of the partition function and associated critical exponents [6].

From the beginning, one particular area of focus has been on the effect of topological constraints [12] and, for example, how the knotting probability in ring polymers depends on the force [29]. For a lattice model of this, self-avoiding polygons on the simple cubic lattice are the standard model. For this case, Janse van Rensburg et al [29] found that for sufficiently large fixed forces, all but exponentially few sufficiently large polygons are knotted. It is believed that this should hold for any force f , but this has yet to be proved. By restricting the polygons to lie in a lattice tube however, Atapour et al [3] proved that for any fixed force (either stretching or compressing), all but exponentially few sufficiently large polygons are knotted. The proof was based on transfer-matrix theory and pattern theorem arguments. In this paper, we explore the Atapour et al model further by investigating the asymptotes as the force goes to either plus or minus infinity. We establish the existence of the asymptotes and their form. Furthermore, we determine a subset of polygons whose free energy becomes dominant in the limit as the force goes to negative infinity. One subset of these polygons are those which correspond to undirected Hamiltonian circuits (called *Hamiltonian* polygons); using arguments adapted from [10] we establish for this subset

that the limiting free energy exists, and we review the result from [10] that all but exponentially few sufficiently large Hamiltonian polygons are knotted. From transfer-matrix calculations, we also explore whether Hamiltonian polygons dominate as the force goes to negative infinity. We establish that they do dominate for small tube sizes, and conjecture that this holds for all tube sizes. If this conjecture holds then, for example, for any force $f \in [-\infty, \infty)$, all but exponentially few sufficiently large polygons will be knotted.

The tube models studied here also have potential applications to the study of single DNA molecules in nanochannels [8, 22, 23], DNA under confinement [1, 21], or protein configurations [19]. As discussed in [8], DNA under high tensile forces $f \gg 0$ behaves similarly to DNA confined to a nanochannel. For this comparison, typically the DNA length is fixed and either force is increased or channel-size is decreased. In this paper, we prove for a lattice model of a nanochannel, that, regardless of the tube size (including all of \mathbb{Z}^3), the order of the limits of polymer length (n) going to infinity and force (f) going to infinity can be interchanged, to yield the same asymptotic limit for the free energy. In the $f \ll 0$ regime, polymers are compressed and behaviour can be comparable to polymers in semi-dilute solution [8], tightly packed polymers, or collapsed polymers. Again in typical experiments, polymer length is fixed and one is interested in configurational properties as compression is increased. Here, we provide evidence that again the order of the limits can be interchanged and that maximally compressed polymers can be modelled by Hamiltonian polygons.

To obtain these results, we use exact enumeration and transfer-matrix methods to study self-avoiding polygons, building on the numerous contributions of A. J. Guttmann to this area. For example, in [11, 13], Guttmann and collaborators developed transfer matrix methods for efficient exact enumeration to, amongst other things, obtain bounds on growth constants and study the critical exponents for polygons on the square lattice. In the recent paper [6], related approaches are used to study compressed walks, bridges and polygons. Here we follow in a similar vein but explore compressed and stretched three-dimensional polygons embedded in an essentially one-dimensional lattice subset and we use transfer-matrix theory and exact enumeration/generation methods to obtain relationships between free energies and growth constants.

The paper is structured as follows. First the details of the Atapour et al model are reviewed, highlighting known upper and lower bounds for the free energy as a function of the force f . Next we establish the asymptotic forms for the free energy, first as $f \rightarrow \infty$ and next as $f \rightarrow -\infty$. Finally we prove results about Hamiltonian polygons and use transfer matrix arguments for small tube sizes to validate our conjecture that they dominate the free energy as the force goes to minus infinity.

Note that figures 1 and 3 as well as an extended abstract of the $f \rightarrow -\infty$ asymptote arguments also appear in [5].

2 The model

For non-negative integers L, M , let $\mathbb{T}_{L,M} \equiv \mathbb{T} \subset \mathbb{Z}^3$ be the semi-infinite $L \times M$ tube on the cubic lattice defined by

$$\mathbb{T} = \{(x, y, z) \in \mathbb{Z}^3 : x \geq 0, 0 \leq y \leq L, 0 \leq z \leq M\}.$$

Define $\mathcal{P}_{\mathbb{T}}$ to be the set of self-avoiding polygons in \mathbb{T} which occupy at least one vertex in the plane $x = 0$, and let $\mathcal{P}_{\mathbb{T},n}$ be the subset of $\mathcal{P}_{\mathbb{T}}$ comprising polygons with n edges. Then let $p_{\mathbb{T},n} = |\mathcal{P}_{\mathbb{T},n}|$. See Figure 1 for a polygon in the 2×1 tube.

Remark. Throughout the rest of this paper, the symbol n will only be used to denote the number of edges in polygons. We will thus always assume that n is even. This includes limits and, for example, $\lim_{n \rightarrow \infty}$

Note that $|\mathcal{P}_{\mathbb{T},n}| = p_{\mathbb{T},n} = Z_{\mathbb{T},n}(0) \leq Wp_n$, where p_n is the number of n -edge self-avoiding polygons in \mathbb{Z}^3 counted up to translation. It has been proved that [25, 26],

$$\mathcal{F}_{\mathbb{T}}(0) = \lim_{n \rightarrow \infty} n^{-1} \log p_{\mathbb{T},n} < \lim_{n \rightarrow \infty} n^{-1} \log p_n = \lim_{n \rightarrow \infty} n^{-1} \log c_n \equiv \kappa \equiv \log \mu, \quad (4)$$

where c_n is the number of n -step self-avoiding walks (SAWs) in \mathbb{Z}^3 starting at the origin and κ is their connective constant.

The bounds in (1) lead to the following bounds on the free energy:

$$\begin{aligned} \max\{f/2, (f/W) + \limsup_{n \rightarrow \infty} n^{-1} \log p_{\mathbb{T},n}(s_{\min}(n))\} &\leq \mathcal{F}_{\mathbb{T}}(f) \\ &\leq \max\{f/W, f/2\} + \mathcal{F}_{\mathbb{T}}(0). \end{aligned}$$

For the lower bound, one set of polygons which have minimum span are the Hamiltonian polygons. We define the number of Hamiltonian polygons, $p_{\mathbb{T},n}^{\text{H}}$, to be the number of n -edge, for $n = W(s+1)$, span- s polygons in $\mathcal{P}_{\mathbb{T},n}$ which occupy every vertex in an $L \times M \times s$ subtube of \mathbb{T} . In [10], the following limit is proved to exist and we have:

$$\kappa_{\mathbb{T}}^{\text{H}} \equiv \lim_{s \rightarrow \infty} \frac{1}{(s+1)W} \log p_{\mathbb{T},(s+1)W}^{\text{H}} \leq \limsup_{n \rightarrow \infty} n^{-1} \log p_{\mathbb{T},n}(s_{\min}(n)).$$

Thus another set of bounds for the free energy is given by:

$$\max\{f/2, (f/W) + \kappa_{\mathbb{T}}^{\text{H}}\} \leq \mathcal{F}_{\mathbb{T}}(f) \leq \max\{f/W, f/2\} + \mathcal{F}_{\mathbb{T}}(0). \quad (5)$$

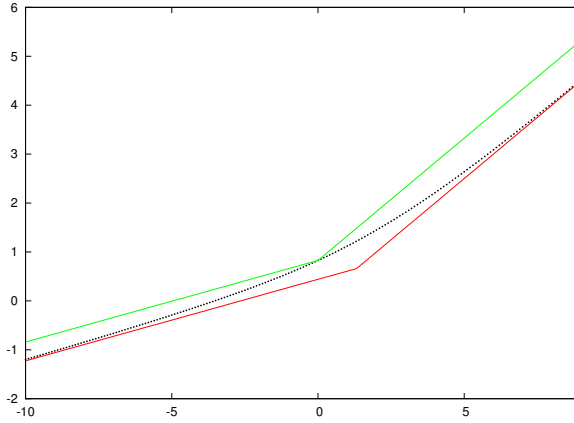
For small tube sizes, $\mathcal{F}_{\mathbb{T}}(f)$, $f \in (-\infty, \infty)$, and $\kappa_{\mathbb{T}}^{\text{H}}$ have been obtained from numerical calculations of the eigenvalues of appropriate transfer matrices [10]; the resulting free energy and bounds associated with (5) are shown in Figure 2 (more details about these calculations will be given in Section 4). These graphs strongly suggest that the free energy is asymptotic to the lower bound as f goes to $\pm\infty$. In the next section we explore this proposition, and prove that it is indeed the case for $f \rightarrow \infty$. We also establish the form for the asymptote as $f \rightarrow -\infty$ and provide further evidence, for small tube sizes, that it corresponds to the lower bound in (5).

3 $f \rightarrow \pm\infty$ asymptotes

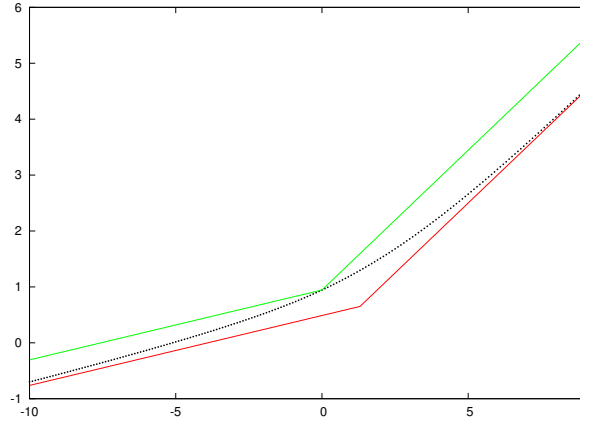
In this section we focus on the free energy $\mathcal{F}_{\mathbb{T}}(f)$. In particular, we determine its behaviour in the two large-force limits, $f \rightarrow \pm\infty$. There are a number of results from [27, Chapter 3] (see also [28, Chapter 3] and [17] for modified presentations) which will be important in this section. For this reason we explicitly state them here. We begin with some necessary assumptions.

Assumptions 1 (Assumptions 3.1 of [27]). Let $u_k(m)$ be the number of objects of size k and energy m . Assume that $u_k(m)$ satisfies the following properties:

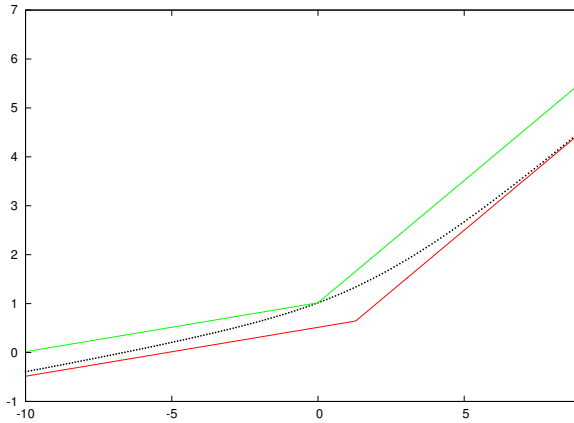
- (1) There exists a constant $K > 0$ such that $0 \leq u_k(m) \leq K^k$ for each value of k and m .
- (2) There exist finite integers A_k and B_k and a real constant C satisfying $0 \leq A_k \leq B_k \leq Ck$ such that $u_k(m) > 0$ for $A_k \leq m \leq B_k$ and $u_k(m) = 0$ otherwise.



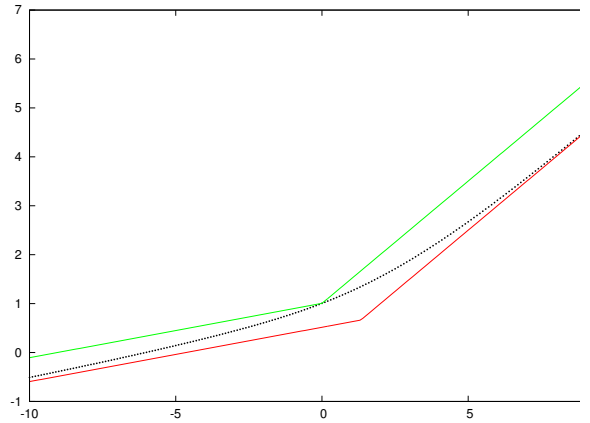
(a) Free energies in the 2×1 tube.



(b) Free energies in the 3×1 tube.



(c) Free energies in the 4×1 tube.



(d) Free energies in the 2×2 tube.

Figure 2: Numerical calculations of the free energies of polygons in three-dimensional tubes, plotted against the force f . The black points are calculations of $\mathcal{F}_{\mathbb{T}}(f)$ (numerically accurate to $\pm 10^{-5}$). The red and green curves are respectively lower and upper bounds for $\mathcal{F}_{\mathbb{T}}(f)$, as given by (5). Observe that in all cases, the black points appear to be asymptotic to the lower bounds for both $f \rightarrow \infty$ and $f \rightarrow -\infty$.

(3) $u_k(m)$ satisfies a supermultiplicative inequality of the type

$$u_{k_1}(m_1)u_{k_2}(m_2) \leq u_{k_1+k_2}(m_1 + m_2). \quad (6)$$

We now add a further assumption which is not required in [27], but will make calculations here somewhat simpler.

Assumptions 2. The limits

$$A = \lim_{k \rightarrow \infty} \frac{A_k}{k} \quad \text{and} \quad B = \lim_{k \rightarrow \infty} \frac{B_k}{k}$$

exist, with $A < B$.

Theorem 1 (Theorems 3.4 and 3.5 of [27]). *Let $u_k(m)$ be a sequence satisfying Assumptions 1 and 2. Then if $\epsilon \in (A, B)$, the density function $\mathcal{D}(\epsilon)$ is defined by the limit*

$$\log \mathcal{D}(\epsilon) = \lim_{k \rightarrow \infty} \frac{1}{k} \log u_k(\lfloor \epsilon k \rfloor).$$

The function $\log \mathcal{D}(\epsilon)$ is a concave function of ϵ on (A, B) , and is thus continuous and almost-everywhere differentiable. Moreover, there exists a number $\eta_k \in \{0, 1\}$ such that for each k ,

$$\frac{1}{k} \log u_k(\lfloor \epsilon k \rfloor + \eta_k) \leq \log \mathcal{D}(\epsilon).$$

We next define partition functions and relate them to the density function $\mathcal{D}(\epsilon)$. Let

$$U_k(z) = \sum_m u_k(m) e^{zm}.$$

Theorem 2 (Theorems 3.6, 3.17 and 3.19 of [27]). *The limit*

$$\mathcal{F}(z) = \lim_{k \rightarrow \infty} \frac{1}{k} \log U_k(z)$$

exists for all z . Moreover,

$$\mathcal{F}(z) = \sup_{A < \epsilon < B} \{\log \mathcal{D}(\epsilon) + \epsilon z\}$$

and

$$\log \mathcal{D}(\epsilon) = \inf_{-\infty < z < \infty} \{\mathcal{F}(z) - \epsilon z\}.$$

Our next preliminary result is a generalisation of [27, equation (3.4)].

Lemma 1. *Let T_k be a sequence satisfying $A_k \leq T_k \leq B_k$ and $T_k = Bk + o(k)$. Moreover, assume that $B_k < Bk$ for all k sufficiently large. Then*

$$\log \mathcal{D}(B^-) \equiv \lim_{\epsilon \rightarrow B^-} \log \mathcal{D}(\epsilon) \geq \limsup_{k \rightarrow \infty} \frac{1}{k} \log u_k(T_k).$$

Proof. Define $\epsilon_k = T_k/k$. Then because $T_k \leq B_k < Bk$, we have $\epsilon_k < B$ for all k sufficiently large and $\lim_{k \rightarrow \infty} \epsilon_k = B$.

Fix any k such that $\epsilon_k < B$. Let $N \in \mathbb{N}$, and put $r = Nk$. Since $\epsilon_k r$ is an integer, the supermultiplicativity assumption (6) can be used repeatedly to split up $u_r(\epsilon_k r)$ a total of $N - 1$ times, to obtain

$$u_r(\epsilon_k r) \geq u_k(\epsilon_k k)^N = u_k(T_k)^N.$$

Take logs, divide by $r = Nk$, and take $N \rightarrow \infty$ (keeping k fixed). The limit of the left-hand-side exists, and is the log of the density function, so

$$\log \mathcal{D}(\epsilon_k) \geq \frac{1}{k} \log u_k(T_k).$$

Taking the lim sup as $k \rightarrow \infty$ of both sides then gives

$$\begin{aligned} \limsup_{k \rightarrow \infty} \frac{1}{k} \log u_k(T_k) &\leq \limsup_{k \rightarrow \infty} \log \mathcal{D}(\epsilon_k) \\ &\leq \lim_{\epsilon \rightarrow B^-} \log \mathcal{D}(\epsilon) \\ &= \log \mathcal{D}(B^-), \end{aligned}$$

where the final limit exists due to the concavity of $\log \mathcal{D}(\epsilon)$. □

We also note the following consequences of the concavity of $\log \mathcal{D}(\epsilon)$ and Theorem 2 (see for example [20, Corollary 4] and [9, Chapter VI] for further background on convex functions and Legendre transforms):

$$\lim_{z \rightarrow \infty} (F(z) - Bz) = \lim_{\epsilon \rightarrow B^-} \log \mathcal{D}(\epsilon) \equiv \log \mathcal{D}(B^-) \tag{7}$$

$$\lim_{z \rightarrow -\infty} (F(z) - Az) = \lim_{\epsilon \rightarrow A^+} \log \mathcal{D}(\epsilon) \equiv \log \mathcal{D}(A^+). \tag{8}$$

3.1 $f \rightarrow \infty$

The main result of this section is the following theorem.

Theorem 3. *For any tube size $L \times M$, in the limit $f \rightarrow \infty$ the free energy $\mathcal{F}_{\mathbb{T}}(f)$ is asymptotic to $f/2$. That is,*

$$\lim_{f \rightarrow \infty} \left(\mathcal{F}_{\mathbb{T}}(f) - \frac{f}{2} \right) = 0. \tag{9}$$

Theorem 3 is in fact a corollary of a more general result. We restrict polygons to the half-space of \mathbb{Z}^3 defined by $x \geq 0$. Let \mathcal{P} be the subset of these polygons which contain at least one edge in the plane $x = 0$; the number of such polygons (counted up to y - and z -translations) is equal to p_n as previously defined in Section 2. The span of these polygons is defined in the same way as for those in \mathbb{T} ; let $p_n(s)$ be the number with length n and span s , and define the partition function

$$Z_n(f) = \sum_{s \geq 0} p_n(s) e^{fs}.$$

It is well-known [29] that the free energy

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

exists for all f and is a convex function.

Theorem 4. *In the limit $f \rightarrow \infty$, the free energy $\mathcal{F}(f)$ is asymptotic to $f/2$. That is,*

$$\lim_{f \rightarrow \infty} \left(\mathcal{F}(f) - \frac{f}{2} \right) = 0. \quad (10)$$

Before commencing the proof, we introduce some new definitions. Let \mathcal{P}^* be the set of polygons $\pi \in \mathcal{P}$ which satisfy the additional constraints:

- π has span $s \geq 2$,
- π contains the edge $(0, 0, 0) — (0, 1, 0)$ (called its left-most-edge) and no other edges in the plane $x = 0$,
- π contains the edge $(s, y, z) — (s, y + 1, z)$ for some y and z (called its right-most-edge), and contains no other edges in the plane $x = s$, and
- π contains no edges in the plane $x = s - 1$.

Let $p_n^*(s)$ be the number of polygons in \mathcal{P}^* with length n and span s . Then $p_n^*(s)$ satisfies Assumptions 1, with length corresponding to size and span corresponding to energy. To see this, note the following.

- (1) $K = 6$ satisfies condition (1).
- (2) The numbers A_n and B_n are

$$A_n = \begin{cases} 2 & n = 6 \\ 3 & n = 8 \\ 4 & n \geq 10 \end{cases} \quad B_n = \frac{n-2}{2}.$$

The n -edge polygon $\tilde{\pi}_n \in \mathcal{P}^*$ consisting of the edges $(0, 0, 0) — (0, 1, 0)$, $(\frac{n-2}{2}, 0, 0) — (\frac{n-2}{2}, 1, 0)$ and $(i, 1, 0) — (i + 1, 1, 0)$, $(i, 0, 0) — (i + 1, 0, 0)$, $i = 0, \dots, \frac{n-2}{2} - 1$ has span B_n . Note that $A_n = B_n$ for $n \leq 8$. For $n \geq 10$, an n -edge polygon in \mathcal{P}^* with span $s \in [A_n, B_n)$ can be obtained from $\tilde{\pi}_{2s+2}$ by concatenating an appropriately rotated and translated version of $\tilde{\pi}_{n-2s-2}$ at the edge $(1, 1, 0) — (2, 1, 0)$ of $\tilde{\pi}_{2s+2}$. Thus $p_n^*(s) > 0$.

- (3) Any two polygons $\pi_1, \pi_2 \in \mathcal{P}^*$ can be concatenated (by translating π_2 so that its left-most-edge coincides with the right-most-edge of π_1 and then deleting the two coincident edges) in a way that preserves total length and total span, giving

$$p_{n_1}^*(s_1) p_{n_2}^*(s_2) \leq p_{n_1+n_2}^*(s_1 + s_2).$$

Now define $P_n^*(f) = \sum_s p_n^*(s)e^{fs}$. By Theorem 2, the free energy

$$\mathcal{F}^*(f) = \lim_{n \rightarrow \infty} \frac{1}{n} \log P_n^*(f)$$

exists. Since $p_n^*(s) \leq p_n(s)$, we have $\mathcal{F}^*(f) \leq \mathcal{F}(f)$. Moreover, there exist constants n_0 and s_0 such that any polygon $\pi \in \mathcal{P}$ of length n and span s can be converted into a unique polygon $\pi' \in \mathcal{P}^*$ with length $n + n_0$ and span $s + s_0$. So

$$p_n(s) \leq p_{n+n_0}^*(s + s_0).$$

Multiply this by $e^{f(s+s_0)}$, sum over s , take logs, divide by n and take $n \rightarrow \infty$ to obtain $\mathcal{F}(f) \leq \mathcal{F}^*(f)$, so that we in fact have

$$\mathcal{F}^*(f) = \mathcal{F}(f). \quad (11)$$

Proof of Theorem 4. By Theorems 1 and 2, the Legendre transform of \mathcal{F}^* ,

$$\log \mathcal{S}^*(\epsilon) = \inf_{-\infty < f < \infty} \{\mathcal{F}^*(f) - \epsilon f\} = \lim_{n \rightarrow \infty} \frac{1}{n} \log p_n^*(\lfloor \epsilon n \rfloor), \quad (12)$$

exists and is finite and concave for $\epsilon \in (0, 1/2)$, where $\mathcal{S}^*(\epsilon)$ can be viewed as the growth rate of polygons with ‘‘span density’’ ϵ , that is, those polygons whose span is asymptotically ϵ times their length.

Then by Theorem 2,

$$\mathcal{F}^*(f) = \sup_{0 < \epsilon < 1/2} \{\log \mathcal{S}^*(\epsilon) + f\epsilon\}. \quad (13)$$

Then as f gets large, it follows from (7) that the behaviour of $\mathcal{F}^*(f)$ is obtained by taking $\epsilon \rightarrow (1/2)^-$. We thus need to examine the behaviour of $\log \mathcal{S}^*(\epsilon)$ in this limit.

First note that by applying Lemma 1 with the sequence $T_n = (n - 2)/2$, we have

$$\lim_{\epsilon \rightarrow 1/2^-} \log \mathcal{S}^*(\epsilon) \geq \limsup_{n \rightarrow \infty} \frac{1}{n} \log p_n^*\left(\frac{n-2}{2}\right) = 0. \quad (14)$$

Now polygons in \mathcal{P}^* can be unambiguously rooted and oriented (let $(0, 0, 0)$ be the root, with the first step in the positive y direction), so we can view such a polygon as a walk which is self-avoiding except for the start and end vertex. Given $\pi \in \mathcal{P}_n^*$, let $\omega(\pi)$ be the resulting walk composed of the sequence of vertices $v_0 = (0, 0, 0), v_1, \dots, v_n, v_{n+1} = v_0$. We define an *increasing step* of π to be any step (v_i, v_{i+1}) of $\omega(\pi)$ in the positive x direction which increases the span of the walk (i.e. the maximum x -coordinate of the vertices in the subwalk from v_0 to v_{i+1} is one greater than that for the subwalk from v_0 to v_i). So a polygon with span s has exactly s increasing steps. Likewise, define the *decreasing steps* of π to be the increasing steps of $\omega(\pi)'$, where $\omega(\pi)'$ is the walk obtained by reversing the orientation of $\omega(\pi)$ (but maintaining the same root). A polygon of span s will thus also have s decreasing steps.

To obtain an upper bound on $\log \mathcal{S}^*(\epsilon)$ as $\epsilon \rightarrow 1/2^-$, we define

$$k_n^*(t) = \sum_{s \geq t} p_n^*(s),$$

that is, the number of polygons of length n and span at least t .

Given any fixed $r \leq n$, we can write $n = pr + q$ with $0 \leq q < r$, so any polygon $\pi \in \mathcal{P}_n^*$ can be divided into p or $p + 1$ subwalks, the first p of which have length r . If the polygon’s span is at least t then it has at least t increasing and at least t decreasing steps, and thus at most $n - 2t$ steps which are neither increasing

nor decreasing. So at most $n - 2t$ of its p length- r subwalks contain non-increasing or non-decreasing steps, and the rest (for $p > n - 2t$) must be composed entirely of increasing or decreasing steps. A subwalk that contains only increasing or decreasing steps must only have steps in the x direction (positive or negative), and hence (due to self-avoidance) the subwalk must be either entirely increasing or entirely decreasing. Hence there are only two types of such subwalks of length r ; one consists of r positive x -steps and the other r negative x -steps. Letting $u = n - 2t$, we thus have

$$k_n^*(t) \leq \sum_{i=0}^u \binom{p}{i} c_r^i 2^{p-i} c_q, \quad (15)$$

where c_n is the number of SAWs of length n .

Given any $\delta > 0$, take r sufficiently large ($\geq N_\delta$) so that $2 \leq e^{\delta r}$ and $c_r \leq e^{(\delta+\kappa)r}$ (this is possible due to (4)). Then

$$\begin{aligned} k_n^*(t) &\leq \sum_{i=0}^u \binom{p}{i} \left(e^{(\delta+\kappa)r} \right)^i \left(e^{\delta r} \right)^{p-i} c_q \\ &= e^{\delta r p} c_q \sum_{i=0}^u \binom{p}{i} e^{\kappa r i}. \end{aligned} \quad (16)$$

Let $t = \lfloor \epsilon n \rfloor$ so that $u = n - 2\lfloor \epsilon n \rfloor$. Noting that $p \sim n/r$, let ϵ be sufficiently close to $1/2$ so that $u < p/2$ (for $p \geq 4$, $\epsilon > (1/2) - 1/(3r)$ is sufficient). Then the largest summand of (16) is the last one, so

$$k_n^*(\lfloor \epsilon n \rfloor) \leq e^{\delta r p} c_q (u+1) \binom{p}{u} e^{\kappa r u}.$$

Take logs, divide by n and apply Stirling's formula:

$$\begin{aligned} \frac{1}{n} \log k_n^*(\lfloor \epsilon n \rfloor) &\leq \frac{1}{n} \log(u+1) + \frac{\delta r p}{n} + \frac{1}{n} \log c_q + \frac{\kappa r u}{n} \\ &\quad - \frac{p}{n} \log \left(\frac{p-u}{p} \right) + \frac{u}{n} \log \left(\frac{p-u}{u} \right) + O \left(\frac{\log n}{n} \right). \end{aligned}$$

Then for $r > N_\delta$ and $\epsilon > (1/2) - 1/(3r)$ fixed, take $p \rightarrow \infty$ and hence $n \rightarrow \infty$ (note that $u \sim (1 - 2\epsilon)n$):

$$\begin{aligned} \log \mathcal{S}^*(\epsilon) &\leq \limsup_{n \rightarrow \infty} \frac{1}{n} \log k_n^*(\lfloor \epsilon n \rfloor) \\ &\leq \delta + \kappa r(1 - 2\epsilon) - \frac{1}{r} \log(1 - r + 2r\epsilon) + (1 - 2\epsilon) \log \left(\frac{1 - r + 2r\epsilon}{r - 2r\epsilon} \right). \end{aligned}$$

Taking $\epsilon \rightarrow 1/2^-$ gives

$$\limsup_{\epsilon \rightarrow 1/2^-} \log \mathcal{S}^*(\epsilon) \leq \delta.$$

Let δ be arbitrarily small, and combine with (14), to obtain

$$\lim_{\epsilon \rightarrow 1/2^-} \log \mathcal{S}^*(\epsilon) = 0. \quad (17)$$

Finally by taking $f \rightarrow \infty$ in (13), and using (7) and (11), we obtain the result. \square

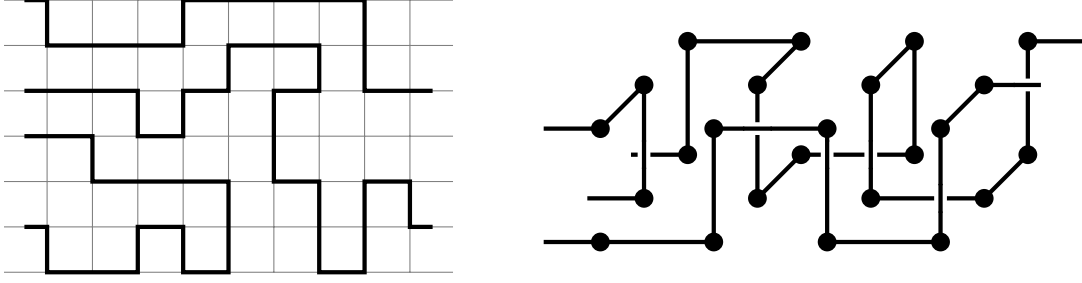


Figure 3: Left: A 9-block of the 6×0 tube. This 9-block has length 50. Right: A full 4-block of the 2×1 tube. This 4-block has length 24.

The corresponding result for polygons in \mathbb{T} then follows in a straightforward manner as described next.

Proof of Theorem 3. Since $\mathcal{P}_{\mathbb{T},n}$ contains at least one polygon of span $(n-2)/2$ for every even n (specifically $\tilde{\pi}_n$), we have $\mathcal{F}_{\mathbb{T}}(f) \geq f/2$.

Every polygon in \mathbb{T} also occurs in the half-space, but certain polygons which are only counted once in $Z_n(f)$ may be counted multiple times in $Z_{\mathbb{T},n}(f)$, because translations of a polygon in the y and/or z directions (but still staying in \mathbb{T}) are all counted separately. However, the number of possible translations is bounded above by a constant c depending only on L and M , so

$$Z_{\mathbb{T},n}(f) \leq cZ_n(f).$$

Taking logs, dividing by n and sending $n \rightarrow \infty$, we have

$$\mathcal{F}_{\mathbb{T}}(f) \leq \mathcal{F}(f),$$

and the result follows. □

3.2 $f \rightarrow -\infty$

In this section we consider the case of compressed polygons. Some preliminary definitions and results are required before the main theorem can be stated.

Given a polygon $\pi \in \mathbb{T}$, a *hinge* H_k of π is the set of edges and vertices lying in the intersection of π and the y - z plane defined by $\{(x, y, z) : x = k\}$. A *section* S_k is the set of edges in π , in the x direction, connecting H_{k-1} and H_k . A *half-section* of S_k is the set of half-edges in S_k with either $k-1 \leq x \leq k-\frac{1}{2}$ or $k-\frac{1}{2} \leq x \leq k$.

A *1-block* of \mathbb{T} is any non-empty hinge which can occur in a polygon π in \mathbb{T} , together with the half-edges of π in the two adjacent half-sections. The *length* of a 1-block is the sum of the lengths of all its polygon edges and half-edges. It is thus natural to view a 1-block as the part of a polygon between two half-integer x -coordinates $k \pm \frac{1}{2}$ for some $k \in \mathbb{Z}$.

An *s-block* is then any connected sequence of s 1-blocks, the entirety of which can occur in a polygon in \mathbb{T} . (It is also possible, if the first and last half-sections of the s -block are empty, for the s -block itself to be a polygon.) The length of an s -block is the sum of the lengths of its constituent 1-blocks. Let $b_{\mathbb{T},s}$ be the number of s -blocks in \mathbb{T} , counted up to translation in the x -direction. See Figure 3 for an example of a 9-block in a 6×0 tube.

Lemma 2. *The limit*

$$\beta_{\mathbb{T}} = \lim_{s \rightarrow \infty} \frac{1}{s} \log b_{\mathbb{T},s} \quad (18)$$

exists and is finite.

Proof. Any $(s + t)$ -block can be cut into an s -block and a t -block; we thus have

$$b_{\mathbb{T},s+t} \leq b_{\mathbb{T},s} b_{\mathbb{T},t}.$$

So $\{\log b_{\mathbb{T},s}\}$ is a subadditive sequence, and the limit (18) exists. We clearly have $b_{\mathbb{T},s} \geq 1$ for all $s \geq 1$, so that $\beta_{\mathbb{T}}$ is finite. \square

A 1-block is *full* if its length is equal to $W = (L + 1)(M + 1)$. Equivalently, a 1-block is full if every vertex in a plane $\{(x, y, z) : x = k\}$ is in its hinge. An s -block is full if every one of its constituent 1-blocks is full. See Figure 3 for an example. Let $b_{\mathbb{T},s}^{\text{F}}$ be the number of full s -blocks in \mathbb{T} .

Lemma 3. *The limit*

$$\beta_{\mathbb{T}}^{\text{F}} = \lim_{s \rightarrow \infty} \frac{1}{s} \log b_{\mathbb{T},s}^{\text{F}} \quad (19)$$

exists and is finite.

Proof. The reasoning is the same as in Lemma 2. A full $(s + t)$ -block can be cut into a full s -block and a full t -block, so

$$b_{\mathbb{T},s+t}^{\text{F}} \leq b_{\mathbb{T},s}^{\text{F}} b_{\mathbb{T},t}^{\text{F}}.$$

The sequence $\{\log b_{\mathbb{T},s}^{\text{F}}\}$ is thus subadditive, and the limit (19) exists. Likewise (consider for example s -blocks obtained from Hamiltonian polygons) $b_{\mathbb{T},s}^{\text{F}} \geq 1$ for all $s \geq 1$. \square

We are now able to state the main theorem of this section.

Theorem 5. *For any tube size $L \times M$, in the limit $f \rightarrow -\infty$ the free energy $\mathcal{F}_{\mathbb{T}}(f)$ is asymptotic to $(\beta_{\mathbb{T}}^{\text{F}} + f)/W$, where $W = (L + 1)(M + 1)$. That is,*

$$\lim_{f \rightarrow -\infty} \left(\mathcal{F}_{\mathbb{T}}(f) - \frac{f}{W} \right) = \frac{\beta_{\mathbb{T}}^{\text{F}}}{W}. \quad (20)$$

The proof of Theorem 5 will require, at least at first, a different approach to that of Theorem 3. We begin with some more definitions.

Let $\mathcal{P}_{\mathbb{T}}^*$ be the set of those polygons $\pi \in \mathcal{P}_{\mathbb{T}}$ which satisfy the additional constraints:

- π has span $s \geq 2$,
- π contains the edge $(0, 0, 0) — (0, 1, 0)$ and no other edges in the plane $x = 0$,
- π contains the edge $(s, 0, 0) — (s, 1, 0)$ and no other edges in the plane $x = s$, and
- π contains no edges in the plane $x = s - 1$.

Let $p_{\mathbb{T},n}^*(s)$ be the number of polygons in $\mathcal{P}_{\mathbb{T}}^*$ with length n and span s . We define a partition function analogous to $Z_{\mathbb{T},n}(f)$:

$$Z_{\mathbb{T},n}^*(f) = \sum_s p_{\mathbb{T},n}^*(s) e^{fs}.$$

Lemma 4. *The free energy*

$$\mathcal{F}_{\mathbb{T}}^*(f) = \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_{\mathbb{T},n}^*(f)$$

exists and is equal to $\mathcal{F}_{\mathbb{T}}(f)$.

Proof. If $(L, M) = (1, 0)$ then $Z_{\mathbb{T},n}^*(f) = e^{f(n-2)/2}$, and the result is trivial. Otherwise, at least one of the statements $L \geq 2$ or $M \geq 1$ is true.

We show that the sequence $p_{\mathbb{T},n}^*(s)$ satisfies Assumptions 1 with size $k = n$ and energy $m = s$, so that Theorem 2 can be applied.

1. Using $K = 6$ suffices to satisfy condition (1).
2. The numbers A_n and B_n (respectively the minimum and maximum possible spans for a $\mathcal{P}_{\mathbb{T}}^*$ polygon of length n) are

$$A_n = \begin{cases} 2 & n = 6 \\ 3 & n = 8 \\ \max \{4, \lceil \frac{n-6}{W} \rceil + 2\} & n \geq 10 \end{cases} \quad B_n = \frac{n-2}{2}.$$

Using specific hinges such as those defined in Section 4 for the proof of Theorem 6, it is possible to prove that $p_{\mathbb{T},n}^*(s) > 0$ for each integer $s \in [A_n, B_n]$.

3. The set $\mathcal{P}_{\mathbb{T}}^*$ has been defined so that any two polygons π_1, π_2 in $\mathcal{P}_{\mathbb{T}}^*$ can be concatenated in a way that preserves both total length and total span. Let π_1 have span s_1 , and define e_1 to be the single edge of π_1 with maximal x -coordinate and e_2 to be the single edge of π_2 with minimal x -coordinate. Then
 - i. Translate π_2 so that e_1 and e_2 coincide, and delete those two edges.
 - ii. If $L \geq 2$ then replace the edge $(s_1 - 1, 1, 0) — (s_1, 1, 0)$ with the three edges

$$(s_1 - 1, 1, 0) — (s_1 - 1, 2, 0) — (s_1, 2, 0) — (s_1, 1, 0).$$

Otherwise if $(L, M) = (1, 1)$ then replace the edge $(s_1 - 1, 1, 0) — (s_1, 1, 0)$ with the three edges

$$(s_1 - 1, 1, 0) — (s_1 - 1, 1, 1) — (s_1, 1, 1) — (s_1, 1, 0).$$

See Figure 4 for an illustration. So any two polygons π_1, π_2 in $\mathcal{P}_{\mathbb{T}}^*$ of lengths n_1 and n_2 and spans s_1 and s_2 , can be concatenated to give another polygon in $\mathcal{P}_{\mathbb{T}}^*$ of length $n_1 + n_2$ and span $s_1 + s_2$. Thus

$$p_{\mathbb{T},n_1}^*(s_1)p_{\mathbb{T},n_2}^*(s_2) \leq p_{\mathbb{T},n_1+n_2}^*(s_1 + s_2), \quad (21)$$

and condition (3) is satisfied.

Since $\mathcal{P}_{\mathbb{T}}^* \subseteq \mathcal{P}_{\mathbb{T}}$, we have $\mathcal{F}_{\mathbb{T}}^*(f) \leq \mathcal{F}_{\mathbb{T}}(f)$. To obtain the reverse inequality, we use the fact that any $\mathcal{P}_{\mathbb{T}}$ polygon can be converted into a unique $\mathcal{P}_{\mathbb{T}}^*$ polygon by adding a fixed number n_0 of edges, which increase the span by at most a constant number s_0 (see for example [2, 26]). (Both n_0 and s_0 depend on the dimensions of the tube \mathbb{T} .) Thus

$$p_{\mathbb{T},n}(s) \leq \sum_{s'=s}^{s+s_0} p_{\mathbb{T},n+n_0}^*(s').$$

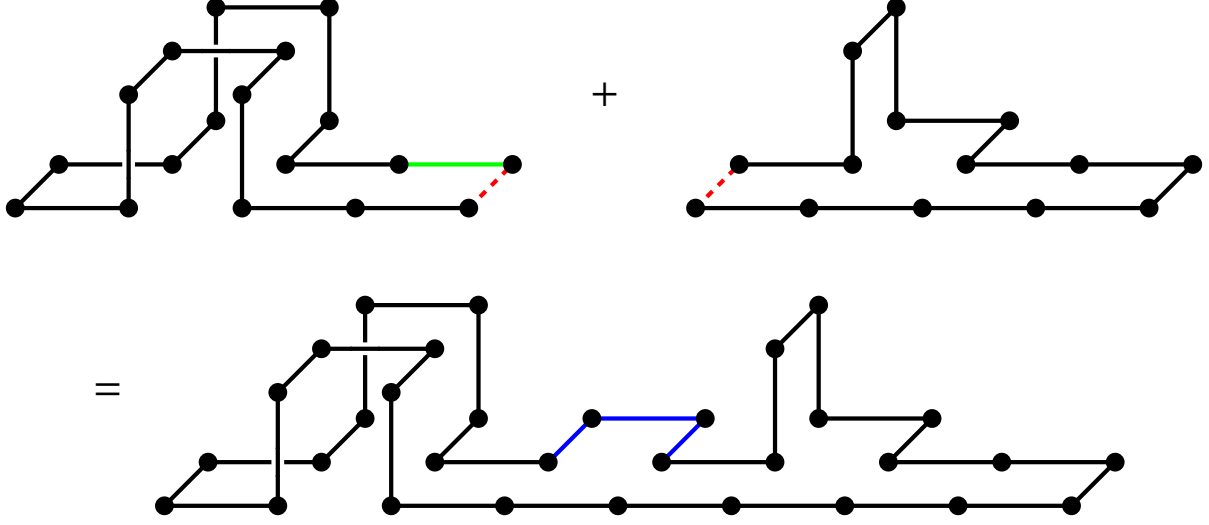


Figure 4: The concatenation operation of $\mathcal{P}_{\mathbb{T}}^*$ polygons described in the proof of Lemma 4, in the 2×1 tube. The second polygon is translated so that the red edges coincide. These edges are then removed, and the green edge is replaced by the three blue edges. Note that the total length, 32, and the total span, 8, are preserved.

Multiplying by e^{fs} and summing over s ,

$$\begin{aligned}
Z_n(f) &= \sum_s p_{\mathbb{T},n}(s) e^{fs} \leq \sum_s e^{fs} \sum_{s'=s}^{s+s_0} p_{\mathbb{T},n+n_0}^*(s') \\
&= \sum_s \sum_{s'=s}^{s+s_0} p_{\mathbb{T},n+n_0}^*(s') e^{fs'} e^{f(s-s')} \\
&= \left(1 + e^{-f} + \dots + e^{-fs_0}\right) \sum_s p_{\mathbb{T},n+n_0}^*(s) e^{fs} \\
&\leq (s_0 + 1) \max\{1, e^{-fs_0}\} Z_{\mathbb{T},n+n_0}^*(f).
\end{aligned}$$

Taking logs, dividing by n and letting $n \rightarrow \infty$ provides the required result. \square

Polygons in $\mathcal{P}_{\mathbb{T}}^*$ then have a density function, similar to $\mathcal{S}^*(\epsilon)$ as defined in (12):

$$\log \mathcal{S}_{\mathbb{T}}^*(\epsilon) = \inf_{-\infty < f < \infty} \{\mathcal{F}_{\mathbb{T}}^*(f) - \epsilon f\} = \lim_{n \rightarrow \infty} \frac{1}{n} \log p_{\mathbb{T},n}^*(\lfloor \epsilon n \rfloor)$$

for $\epsilon \in (1/W, 1/2)$, with

$$\mathcal{F}_{\mathbb{T}}^*(f) = \sup_{1/W < \epsilon < 1/2} \{\log \mathcal{S}_{\mathbb{T}}^*(\epsilon) + \epsilon f\}. \quad (22)$$

The approach to proving Theorem 5 will involve the ‘dual’ object to $\mathcal{F}_{\mathbb{T}}^*(f)$. Let $q_{\mathbb{T},s}^*(n) = p_{\mathbb{T},n}^*(s)$. (We introduce this quantity to make it clear that we are now interpreting the span of a polygon as its ‘size’ and the length of a polygon as its ‘energy’.) Define

$$Q_{\mathbb{T},s}^*(z) = \sum_n q_{\mathbb{T},s}^*(n) e^{zn}.$$

Lemma 5. *The free energy*

$$\mathcal{G}_{\mathbb{T}}^*(z) = \lim_{s \rightarrow \infty} \frac{1}{s} \log Q_{\mathbb{T},s}^*(z)$$

exists for all z . It is a convex function of z , and is thus continuous and almost-everywhere differentiable.

Proof. If $(L, M) = (1, 0)$ then the result is again trivial, so we can assume that at least one of the statements $L \geq 2$ or $M \geq 1$ is true.

We show that the sequence $q_{\mathbb{T},s}^*(n)$ satisfies Assumptions 1, with one minor caveat.

- (1) Since $q_{\mathbb{T},s}^*(n) \leq b_{\mathbb{T},s+1} \leq (b_{\mathbb{T},1})^{s+1}$, using $K = (b_{\mathbb{T},1})^2$ suffices to satisfy condition (1).
- (2) The numbers A_s and B_s (respectively the minimum and maximum possible lengths of a $\mathcal{P}_{\mathbb{T}}^*$ polygon of span s) are

$$A_s = 2(s+1) \quad B_s = \begin{cases} A_s & \text{if } s = 2, 3 \\ W(s-2) + 6 & \text{if } W \text{ or } s \geq 4 \text{ even} \\ W(s-2) + 5 & \text{if } W \text{ and } s > 4 \text{ odd.} \end{cases}$$

However, note that $q_{\mathbb{T},s}^*(n) > 0$ only if n is even. Condition (2) can then be met by letting the energy of a polygon be its *half-length*, rather than its length. Adjusting everything to account for this essentially amounts to taking $n \mapsto n/2$ in the definitions of $q_{\mathbb{T},s}^*(n)$ and $Q_{\mathbb{T},s}^*(z)$, and likewise dividing the values of A_s and B_s by 2. This is straightforward, so we will in general continue to use length instead of half-length.

- (3) The inequality (21) can be rewritten as

$$q_{\mathbb{T},s_1}^*(n_1)q_{\mathbb{T},s_2}^*(n_2) \leq q_{\mathbb{T},s_1+s_2}^*(n_1+n_2),$$

so condition (3) is satisfied.

By Theorem 2, the free energy $\mathcal{G}_{\mathbb{T}}^*(z)$ exists. A standard application of the Cauchy-Schwarz inequality (see for example [14, Section 2.3]) demonstrates the convexity of $\mathcal{G}_{\mathbb{T}}^*(z)$. \square

Remark. A similar argument to that of the proof of Lemma 4 can be used to show that $\mathcal{G}_{\mathbb{T}}^*(1) = \beta_{\mathbb{T}}$; that is, $\mathcal{P}_{\mathbb{T}}^*$ polygons and s -blocks in \mathbb{T} (counted by span) have the same growth rate. Moreover, if s -blocks in \mathbb{T} are equipped with a fugacity z measuring their length, it is also possible to show that they have a well-defined free energy, and that that free energy is equal to $\mathcal{G}_{\mathbb{T}}^*(z)$. The same arguments *do not* allow one to establish the same relationship between full s -blocks and Hamiltonian polygons (polygons of span s which occupy every vertex in their $s+1$ hinges) – see Section 4 and Figure 7 for details.

We will now determine the asymptotic behaviour of $\mathcal{G}_{\mathbb{T}}^*(z)$ as $z \rightarrow \infty$, and will see later that this is related, in a very simple way, to the behaviour of $\mathcal{F}_{\mathbb{T}}(f)$ as $f \rightarrow -\infty$. We once again make use of a density function. By Theorem 2 there is a ‘length density’ function, analogous to $\mathcal{S}^*(\epsilon)$ as defined in (12):

$$\log \mathcal{L}_{\mathbb{T}}^*(\alpha) = \inf_{-\infty < z < \infty} \{ \mathcal{G}_{\mathbb{T}}^*(z) - \alpha z \} = \lim_{s \rightarrow \infty} \log q_{\mathbb{T},s}^*(\lfloor \alpha s \rfloor). \quad (23)$$

The function $\log \mathcal{L}_{\mathbb{T}}^*(\alpha)$ is finite and concave for $\alpha \in (2, W)$. The inverse Legendre transform is then

$$\mathcal{G}_{\mathbb{T}}^*(z) = \sup_{2 < \alpha < W} \{ \log \mathcal{L}_{\mathbb{T}}^*(\alpha) + \alpha z \}. \quad (24)$$

We will determine the behaviour of $\log \mathcal{L}_{\mathbb{T}}^*(\alpha)$ as $\alpha \rightarrow W^-$, which, together with (7), informs the behaviour of $\mathcal{G}_{\mathbb{T}}^*(z)$ for $z \rightarrow \infty$. For readability we split the result into an upper and lower bound.

Lemma 6. For any tube size $L \times M$, the density function $\mathcal{L}_{\mathbb{T}}^*(\alpha)$ satisfies

$$\log \mathcal{L}_{\mathbb{T}}^*(W^-) \equiv \lim_{\alpha \rightarrow W^-} \log \mathcal{L}_{\mathbb{T}}^*(\alpha) \leq \beta_{\mathbb{T}}^F. \quad (25)$$

Proof. The following argument is inspired by a proof of [24] regarding adsorbing self-avoiding walks.

Define

$$j_{\mathbb{T},s}^*(m) = \sum_{n \geq m} p_{\mathbb{T},s}^*(n),$$

that is, the number of $\mathcal{P}_{\mathbb{T}}^*$ polygons of span s and length at least m .

Given any fixed $r \leq s + 1$, we write $s + 1 = pr + t$ with $0 \leq t < r$, and think of a polygon of span s as a connected sequence of p r -blocks and (possibly) one t -block. If a polygon has span s and length n then it has $W(s + 1) - n$ unoccupied vertices within its $s + 1$ hinges. Letting $u = W(s + 1) - m$, the maximum number of unoccupied vertices in a polygon with at least length m , and then by considering all possible choices for the number i of r -blocks with unoccupied vertices, we have

$$j_{\mathbb{T},s}^*(m) \leq \sum_{i=0}^u \binom{p}{i} (b_{\mathbb{T},r})^i (b_{\mathbb{T},r}^F)^{p-i} b_{\mathbb{T},t}.$$

For any fixed $\delta > 0$ take r sufficiently large ($> N_\delta$) so that $b_{\mathbb{T},r} \leq e^{(\beta_{\mathbb{T}} + \delta)r}$ and $b_{\mathbb{T},r}^F \leq e^{(\beta_{\mathbb{T}}^F + \delta)r}$. Then

$$\begin{aligned} j_{\mathbb{T},s}^*(m) &\leq b_{\mathbb{T},t} \sum_{i=0}^u \binom{p}{i} e^{ir(\beta_{\mathbb{T}} + \delta)} e^{(p-i)r(\beta_{\mathbb{T}}^F + \delta)} \\ &= b_{\mathbb{T},t} e^{rp(\beta_{\mathbb{T}}^F + \delta)} \sum_{i=0}^u \binom{p}{i} e^{ir(\beta_{\mathbb{T}} - \beta_{\mathbb{T}}^F)}. \end{aligned} \quad (26)$$

Now let $m = \lfloor \alpha s \rfloor$, so that $u = W(s + 1) - \lfloor \alpha s \rfloor$. Noting that $p \sim s/r$, take α sufficiently close to W so that $u < p/2$ ($\alpha > W - 1/(2r + 4)$ is sufficient). Then the largest summand of (26) is the last one, so

$$j_{\mathbb{T},s}^*(\lfloor \alpha s \rfloor) \leq b_{\mathbb{T},t} e^{rp(\beta_{\mathbb{T}}^F + \delta)} (u + 1) \binom{p}{u} e^{ru(\beta_{\mathbb{T}} - \beta_{\mathbb{T}}^F)}.$$

Take logs, divide by s and apply Stirling's formula:

$$\begin{aligned} \frac{1}{s} \log j_{\mathbb{T},s}^*(\lfloor \alpha s \rfloor) &\leq \frac{1}{s} \log b_{\mathbb{T},t} + \frac{rp(\beta_{\mathbb{T}}^F + \delta)}{s} + \frac{ru(\beta_{\mathbb{T}} - \beta_{\mathbb{T}}^F)}{s} + \frac{1}{s} \log(u + 1) \\ &\quad - \frac{p}{s} \log \left(\frac{p - u}{p} \right) + \frac{u}{s} \log \left(\frac{p - u}{u} \right) + O \left(\frac{\log s}{s} \right). \end{aligned}$$

With $r > N_\delta$ and $\alpha > W - 1/(2r + 4)$ fixed, take a lim sup as $p \rightarrow \infty$ (and hence $s \rightarrow \infty$) to find

$$\begin{aligned} \log \mathcal{L}_{\mathbb{T}}^*(\alpha) &\leq \limsup_{s \rightarrow \infty} \frac{1}{s} \log j_{\mathbb{T},s}^*(\lfloor \alpha s \rfloor) \\ &\leq \beta_{\mathbb{T}}^F + \delta + r(W - \alpha)(\beta_{\mathbb{T}} - \beta_{\mathbb{T}}^F) - \frac{1}{r} \log(1 - r(W - \alpha)) + (W - \alpha) \log \left(\frac{1}{r(W - \alpha)} - 1 \right). \end{aligned}$$

In the limit $\alpha \rightarrow W^-$,

$$\log \mathcal{L}_{\mathbb{T}}^*(W^-) \leq \beta_{\mathbb{T}}^F + \delta.$$

Since δ can be arbitrarily small, the proof is complete. \square

The proof of the other bound makes use of Lemma 1.

Lemma 7.

$$\log \mathcal{L}_{\mathbb{T}}^*(W^-) \equiv \lim_{\alpha \rightarrow W^-} \log \mathcal{L}_{\mathbb{T}}^*(\alpha) \geq \beta_{\mathbb{T}}^F.$$

Proof. By definition, any s -block or full s -block can be ‘completed’, by adding edges at one or both of its ends, to create a self-avoiding polygon of span $\geq s + 1$. In particular, there are constants s_0 and n_0 (dependant on the dimensions of the tube \mathbb{T}) such that any full s -block can be completed into a unique $\mathcal{P}_{\mathbb{T}}^*$ polygon of span $s + s_0$ and length between Ws and $Ws + n_0$. So

$$b_{\mathbb{T},s}^F \leq \sum_{n=Ws}^{Ws+n_0} q_{\mathbb{T},s+s_0}^*(n).$$

Now let $n_{s+s_0}^{\max}$ be the value of n between Ws and $Ws + n_0$ which maximises $q_{\mathbb{T},s+s_0}^*(n)$ (if there are multiple such values, take the smallest one). We then have

$$b_{\mathbb{T},s}^F \leq (n_0 + 1) q_{\mathbb{T},s+s_0}^*(n_{s+s_0}^{\max}).$$

Observe that n_s^{\max} is a sequence which satisfies the conditions of Lemma 1: it is by definition a value between the minimum and maximum lengths for $\mathcal{P}_{\mathbb{T}}^*$ polygons of span s , and $n_s^{\max} = Ws + o(s)$. So

$$\begin{aligned} \log \mathcal{L}_{\mathbb{T}}^*(W^-) &\geq \limsup_{s \rightarrow \infty} \frac{1}{s} \log q_{\mathbb{T},s}^*(n_s^{\max}) \\ &\geq \limsup_{s \rightarrow \infty} \frac{1}{s} \log \left(\frac{b_{\mathbb{T},s-s_0}^F}{n_0 + 1} \right) \\ &= \lim_{s \rightarrow \infty} \frac{1}{s} \log b_{\mathbb{T},s}^F \\ &= \beta_{\mathbb{T}}^F. \end{aligned} \quad \square$$

Now Lemmas 6 and 7, together with (24) and (7), imply the following.

Corollary 1. *In the limit as $z \rightarrow \infty$, the free energy $\mathcal{G}_{\mathbb{T}}^*(z)$ is asymptotic to $Wz + \beta_{\mathbb{T}}^F$. That is,*

$$\lim_{z \rightarrow \infty} (\mathcal{G}_{\mathbb{T}}^*(z) - Wz) = \beta_{\mathbb{T}}^F.$$

We are now able to complete the proof of the main theorem of this section.

Proof of Theorem 5. For given rational $\alpha \in (2, W)$, we have

$$\log \mathcal{L}_{\mathbb{T}}^*(\alpha) = \lim_{s \rightarrow \infty} \frac{1}{s} \log q_{\mathbb{T},s}^*(\lfloor \alpha s \rfloor).$$

If we take this limit through values of s such that s/α is an integer, then this can be written as

$$\begin{aligned} \log \mathcal{L}_{\mathbb{T}}^*(\alpha) &= \lim_{s \rightarrow \infty} \frac{1}{s/\alpha} \log q_{\mathbb{T},s/\alpha}^*(s) \\ &= \lim_{s \rightarrow \infty} \frac{\alpha}{s} \log p_{\mathbb{T},s}^*(s/\alpha) \\ &= \alpha \log \mathcal{S}_{\mathbb{T}}^*(1/\alpha). \end{aligned}$$

Continuity allows us to extend this result to all $\alpha \in (2, W)$, and it can alternatively be written as

$$\epsilon \log \mathcal{L}_{\mathbb{T}}^*(1/\epsilon) = \log \mathcal{S}_{\mathbb{T}}^*(\epsilon) \quad (27)$$

for $\epsilon \in (1/W, 1/2)$.

Now consider (22) in the case that $f \rightarrow -\infty$. By (8), the behaviour of $\mathcal{F}_{\mathbb{T}}^*(f)$ in this limit will be determined by the behaviour of $\log \mathcal{S}_{\mathbb{T}}^*(\epsilon)$ as $\epsilon \rightarrow (1/W)^+$. By (27) and Lemmas 6 and 7,

$$\begin{aligned} \log \mathcal{S}_{\mathbb{T}}^*((1/W)^+) &\equiv \lim_{\epsilon \rightarrow (1/W)^+} \log \mathcal{S}_{\mathbb{T}}^*(\epsilon) = \frac{1}{W} \log \mathcal{L}_{\mathbb{T}}^*(W-) \\ &= \frac{\beta_{\mathbb{T}}^F}{W}, \end{aligned}$$

so that by (8), $\mathcal{F}_{\mathbb{T}}^*(f)$ is asymptotic to $f/W + \beta_{\mathbb{T}}^F/W$ as $f \rightarrow -\infty$. Since $\mathcal{F}_{\mathbb{T}}(f) = \mathcal{F}_{\mathbb{T}}^*(f)$, the theorem is complete. \square

4 Hamiltonian polygons

Theorem 5 establishes that, in the limit of a large compressive force, the free energy of polygons in an $L \times M$ tube is related to the growth rate $\beta_{\mathbb{T}}^F$ of full s -blocks in the tube. At first, this may seem peculiar: one might expect that the $f \rightarrow -\infty$ asymptote should be related to the growth rate of some easily described class of *polygons*, not *blocks*. In fact we do expect this to be the case. The precise statement of our conjecture, corroborated by numerical analysis for small tube sizes, is presented later in this section (Conjecture 1).

Recall that, if the first and last half-sections of an s -block are empty, the s -block itself forms a polygon of span $s - 1$. Conversely, any polygon π of span s corresponds to a unique $(s + 1)$ -block. If that $(s + 1)$ -block is full, we will say that π is *Hamiltonian*. Note that, since π occupies every vertex in its $s + 1$ hinges, it must have length $n = (s + 1)W = (s + 1)(L + 1)(M + 1)$. Then because n must be even, we conclude that Hamiltonian polygons of span s can exist only if W is even or s is odd.

Let $p_{\mathbb{T},n}^H$ be the number of Hamiltonian polygons of length n in the tube \mathbb{T} , defined up to translation in the x -direction. Note that $p_{\mathbb{T},n}^H = 0$ if n is not a multiple of W ; moreover, if W is odd then n must be a multiple of $2W$.

The following result establishes that Hamiltonian polygons have a growth rate, and is proved here using arguments adapted from [10, Chapter 4].

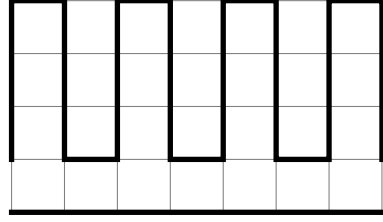
Theorem 6 ([10, Chapter 4]). *The limit*

$$\kappa_{\mathbb{T}}^H = \lim_{n \rightarrow \infty} \frac{1}{n} \log p_{\mathbb{T},n}^H \quad (28)$$

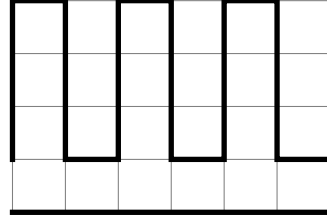
exists, where the limit is taken through values of n which are multiples of W (resp. $2W$) when W is even (resp. odd). The limit is finite.

The proof of Theorem 6 will follow from a concatenation argument. Before we begin, it will be convenient to introduce two special hinges, constructed via a process called *zig-zagging*. This process, operating in an $L \times M$ rectangle of the y - z plane (i.e. a hinge of \mathbb{T} , with $0 \leq y \leq L$ and $0 \leq z \leq M$), generates a self-avoiding walk via the following algorithm.

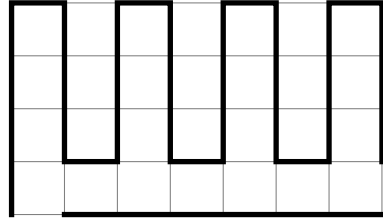
1. Begin at initial vertex (x, y_0, z_0) .



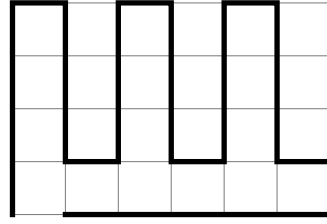
(a) The hinge $H_{\mathbb{T}}^A(x)$ in a 7×4 tube.



(b) The hinge $H_{\mathbb{T}}^A(x)$ in a 6×4 tube.



(c) The hinge $H_{\mathbb{T}}^B(x)$ in a 7×4 tube.



(d) The hinge $H_{\mathbb{T}}^B(x)$ in a 6×4 tube.

Figure 5: Hinges $H_{\mathbb{T}}^A(x)$ and $H_{\mathbb{T}}^B(x)$ in the y - z plane, when L is odd or even. The bottom left corner in each is the vertex $(x, y, z) = (x, 0, 0)$.

2. If possible (without violating self-avoidance), take steps in the positive z -direction, without passing $z = M$. Go to step 3.
3. If possible (without violating self-avoidance), take steps in the negative z -direction, without passing $z = 0$. Go to step 4.
4. If possible (without violating self-avoidance or passing $y = L$), take a step in the positive y -direction, and return to step 2. If not, terminate the process.

The two special hinges are then defined as follows.

- $H_{\mathbb{T}}^A(x)$ consists of the edges $(x, 0, 0) — (x, 1, 0) — \dots — (x, L, 0)$, together with a zig-zagging starting at $(x, 0, 1)$.
- $H_{\mathbb{T}}^B(x)$ consists of the edges $(x, 1, 0) — (x, 2, 0) — \dots — (x, L, 0)$, together with a zig-zagging starting at $(x, 0, 0)$.

See Figure 5 for examples. Note that if $M = 0$ then $H_{\mathbb{T}}^A(x)$ is just a line of edges from $(x, 0, 0)$ to $(x, L, 0)$, while $H_{\mathbb{T}}^B(x)$ is the vertex $(x, 0, 0)$ together with edges from $(x, 1, 0)$ to $(x, L, 0)$.

Proof of Theorem 6. We will show that $p_{\mathbb{T},n}^H$ is a supermultiplicative sequence, by demonstrating that any two Hamiltonian polygons in \mathbb{T} can be concatenated to give a third.

Let π be a Hamiltonian polygon in \mathbb{T} of length n and span s . Since π is Hamiltonian, the vertex $(0, 0, 0)$ must be occupied, and thus at least one of the edges $(0, 0, 0) — (0, 1, 0)$ and $(0, 0, 0) — (0, 0, 1)$ must also be occupied. (Clearly if $M = 0$ then it must be the former.) We say that π is of *type* S_1 if $(0, 0, 0) — (0, 1, 0)$ is occupied, otherwise it is of *type* S_0 . Similarly, at least one of the edges $(s, 0, 0) — (s, 1, 0)$ and $(s, 0, 0) — (s, 0, 1)$ must be occupied by π ; if the former is occupied then π is of *type* F_1 , otherwise it is of *type* F_0 . (The S and F stand for *start* and *finish*.)

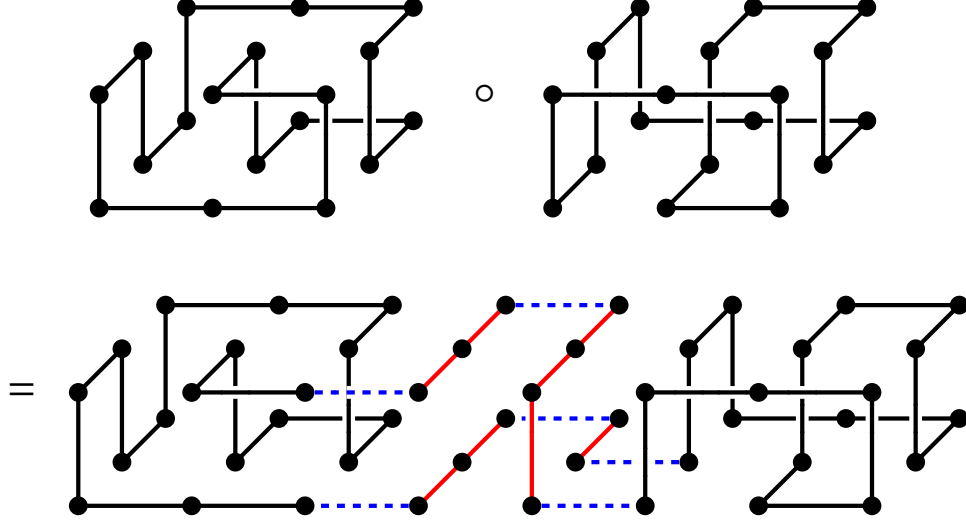


Figure 6: The concatenation operation of two Hamiltonian polygons in the 2×1 tube, as described in the proof of Theorem 6. This is case (c), where the first polygon is of type F_0 and the second is of type S_1 . The red edges are the two special hinges $H_{\mathbb{T}}^A(3)$ and $H_{\mathbb{T}}^B(4)$, and the blue edges connect these special hinges to the two polygons and to each other.

Now let π_1 and π_2 be two Hamiltonian polygons in \mathbb{T} , of lengths n_1 and n_2 and spans s_1 and s_2 respectively. We will define a new polygon $\pi_1 \circ \pi_2$ generated by concatenation. There are four cases to consider, depending on whether π_1 is of type F_0 or F_1 , and whether π_2 is of type S_0 or S_1 . In all cases, we begin by translating π_2 a distance of $s_1 + 3$ in the positive x -direction.

- (a) (π_1, π_2) of types (F_1, S_1) : Insert hinges $H_{\mathbb{T}}^B(s_1 + 1)$ and $H_{\mathbb{T}}^B(s_1 + 2)$. Delete edges $(s_1, 0, 0) - (s_1, 1, 0)$ in π_1 and $(s_1 + 3, 0, 0) - (s_1 + 3, 1, 0)$ in (the translation of) π_2 . Insert the two edges required to join π_1 to $H_{\mathbb{T}}^B(s_1 + 1)$, the two edges required to join $H_{\mathbb{T}}^B(s_1 + 2)$ to π_2 , and the two edges required to join $H_{\mathbb{T}}^B(s_1 + 1)$ to $H_{\mathbb{T}}^B(s_1 + 2)$.
- (b) (π_1, π_2) of types (F_1, S_0) : Insert hinges $H_{\mathbb{T}}^B(s_1 + 1)$ and $H_{\mathbb{T}}^A(s_1 + 2)$. Delete edges $(s_1, 0, 0) - (s_1, 1, 0)$ in π_1 and $(s_1 + 3, 0, 0) - (s_1 + 3, 0, 1)$ in π_2 . Insert the three pairs of edges required to join π_1 to $H_{\mathbb{T}}^B(s_1 + 1)$, $H_{\mathbb{T}}^A(s_1 + 2)$ to π_2 , and $H_{\mathbb{T}}^B(s_1 + 1)$ to $H_{\mathbb{T}}^A(s_1 + 2)$.
- (c) (π_1, π_2) of types (F_0, S_1) : Insert hinges $H_{\mathbb{T}}^A(s_1 + 1)$ and $H_{\mathbb{T}}^B(s_1 + 2)$. Delete edges $(s_1, 0, 0) - (s_1, 0, 1)$ in π_1 and $(s_1 + 3, 0, 0) - (s_1 + 3, 1, 0)$ in π_2 . Insert the three pairs of edges required to join π_1 to $H_{\mathbb{T}}^A(s_1 + 1)$, $H_{\mathbb{T}}^B(s_1 + 2)$ to π_2 , and $H_{\mathbb{T}}^A(s_1 + 1)$ to $H_{\mathbb{T}}^B(s_1 + 2)$.
- (d) (π_1, π_2) of types (F_0, S_0) : Insert hinges $H_{\mathbb{T}}^A(s_1 + 1)$ and $H_{\mathbb{T}}^A(s_1 + 2)$. Delete edges $(s_1, 0, 0) - (s_1, 0, 1)$ in π_1 and $(s_1 + 3, 0, 0) - (s_1 + 3, 0, 1)$ in π_2 . Insert the three pairs of edges required to join π_1 to $H_{\mathbb{T}}^A(s_1 + 1)$, $H_{\mathbb{T}}^A(s_1 + 2)$ to π_2 , and $H_{\mathbb{T}}^A(s_1 + 1)$ to $H_{\mathbb{T}}^A(s_1 + 2)$.

See Figure 6 for an example. In each of these four cases, we have constructed a unique Hamiltonian polygon of length $n_1 + n_2 + 2W$ and span $s_1 + s_2 + 3$. We thus have

$$p_{\mathbb{T}, n_1}^H p_{\mathbb{T}, n_2}^H \leq p_{\mathbb{T}, n_1 + n_2 + 2W}^H. \quad (29)$$

Subtracting $2W$ from each of n_1 and n_2 gives

$$p_{\mathbb{T}, n_1 - 2W}^H p_{\mathbb{T}, n_2 - 2W}^H \leq p_{\mathbb{T}, n_1 + n_2 - 2W}^H,$$

so that $\left\{ \log p_{\mathbb{T}, n - 2W}^H \right\}$ is a subadditive sequence. It follows that the limit (28) exists. Moreover, it is straightforward to connect up sequences of $H_{\mathbb{T}}^A(x)$ hinges (or alternatively, sequences of $H_{\mathbb{T}}^B(x)$ hinges) in order to show that, for any n a multiple of W (resp. $2W$) when W is even (resp. W is odd), there exists a Hamiltonian polygon of length n . So for those values of n ,

$$1 \leq p_{\mathbb{T}, n}^H \leq p_{\mathbb{T}, n} \implies 0 \leq \kappa_{\mathbb{T}}^H \leq \mathcal{F}_{\mathbb{T}}(0) < \infty. \quad \square$$

As with general polygons in \mathbb{T} , one can associate a force f with the span of Hamiltonian polygons, to obtain a partition function $Z_{\mathbb{T}, n}^H(f)$. Moreover, since all Hamiltonian polygons of length n have the same span $s = n/W - 1$, we have

$$Z_{\mathbb{T}, n}^H(f) = p_{\mathbb{T}, n}^H e^{f(n/W - 1)}.$$

The corresponding free energy then has a simple form:

$$\mathcal{F}_{\mathbb{T}}^H(f) = \lim_{n \rightarrow \infty} \frac{1}{n} \log Z_{\mathbb{T}, n}^H(f) = \kappa_{\mathbb{T}}^H + \frac{f}{W},$$

where the limit is taken through values of n which are multiples of W or $2W$ as appropriate.

Having established the existence of a growth rate $\kappa_{\mathbb{T}}^H$ and free energy $\mathcal{F}_{\mathbb{T}}^H(f)$, we are now able to state the conjectured relationship between compressed and Hamiltonian polygons.

Conjecture 1. *Hamiltonian polygons and full s -blocks in the $L \times W$ tube \mathbb{T} , counted by length instead of span, have the same growth rate. That is,*

$$\kappa_{\mathbb{T}}^H = \frac{\beta_{\mathbb{T}}^F}{W}$$

where $W = (L + 1)(M + 1)$. Consequently, in the limit $f \rightarrow -\infty$, the free energy $\mathcal{F}_{\mathbb{T}}(f)$ of polygons in the tube is asymptotic to $\mathcal{F}_{\mathbb{T}}^H(f) = \kappa_{\mathbb{T}}^H + f/W$. That is,

$$\lim_{f \rightarrow -\infty} \left(\mathcal{F}_{\mathbb{T}}(f) - \mathcal{F}_{\mathbb{T}}^H(f) \right) = 0.$$

Note that, since every Hamiltonian polygon of span s is a full $(s + 1)$ -block, it follows immediately that $\kappa_{\mathbb{T}}^H \leq \beta_{\mathbb{T}}^F/W$. It is the reverse inequality which is more challenging. As remarked in Section 3.2, it is possible to prove that polygons and s -blocks in \mathbb{T} have the same growth rate, by showing that every s -block can be “completed”, by adding edges at its start and end, to a polygon. This is not true for full s -blocks and Hamiltonian polygons, however; there exist full s -blocks which can never form a part of a Hamiltonian polygon. See Figure 7 for an example.

We next explore the validity of this conjecture for small tube sizes using transfer matrix calculations.

4.1 Transfer-matrices and Hamiltonian polygons

We focus first on defining 1-patterns in terms of 1-blocks, and then use 1-patterns to define a transfer matrix. To do this, first consider any $\omega \in \mathcal{P}_{\mathbb{T}}$ and let s be its span. The polygon ω uniquely defines a sequence of $s + 1$ connected 1-blocks: $E_0(\omega), E_1(\omega), \dots, E_s(\omega)$. Given a $j \in \{1, \dots, s\}$, ω can be thought of as a connected sequence of three embeddings $E_j^1, E_j(\omega)$ and E_j^3 where E_j^1 (resp. E_j^3) consists of the edges

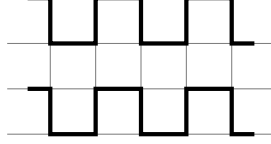


Figure 7: A full 5-block in the 3×0 tube which can never form of a part of a Hamiltonian polygon.

and half-edges of ω before (resp. after) the plane $x = j - \frac{1}{2}$ ($x = j + \frac{1}{2}$). Since ω is a polygon, the vertices of $E_j(\omega)$ in the plane $x = j - \frac{1}{2}$ are connected pairwise by sequences of edges in E_j^1 . To define a 1-pattern, it is unnecessary to keep the full details of these edge sequences; rather, it will be enough to store the connectivity information in terms of which of the left-most vertices of $E_j(\omega)$ are connected together in E_j^1 . For this, we first label the vertices of the left-most plane of $E_j(\omega)$ lexicographically as $v_1^j, \dots, v_{r_j}^j$. Next we obtain a pair-partition \mathcal{S}_j of the vertex labels $\{1, \dots, r_j\}$ from $V^j = \{v_1^j, \dots, v_{r_j}^j\}$, using the connectivity information from E_j^1 . We then define the *left connectivity information* for $E_j(\omega)$ by this pair partition $\mathcal{E}_j = \mathcal{S}_j$. For $E_0(\omega)$, because its left-connectivity information is completely determined by the 1-block we define its left-connectivity information to be $\mathcal{E}_0 = \phi$, the empty set. Now ω 's j th *proper 1-pattern* is defined to be the ordered pair $\omega_j = (\mathcal{E}_j, E_j(\omega))$, $j = 1, \dots, s-1$; its *right-most 1-pattern*, the ordered pair $\omega_s = (\mathcal{E}_s, E_s(\omega))$; and its *left-most 1-pattern*, $\omega_0 = (\mathcal{E}_0, E_0(\omega))$. Hence ω generates a unique sequence of 1-patterns $(\omega_0, \omega_1, \dots, \omega_{s-1}, \omega_s)$ and, for convenience, we write $\omega = (\omega_0, \omega_1, \dots, \omega_{s-1}, \omega_s)$. From this we can define \mathcal{A}_1 , \mathcal{A}_2 , and \mathcal{A}_3 , respectively, as the set of all distinct (up-to x -translation) left-most, proper, and right-most 1-patterns that result from some $\omega \in \mathcal{P}_{\mathbb{T}}$ with span $s \geq 1$. We also define \mathcal{A}_0 to be the set of all $\omega \in \mathcal{P}_{\mathbb{T}}$ with span $s = 0$.

Given two 1-patterns $\pi_1 = (S_{1,1}, E_1)$, and $\pi_2 = (S_{2,1}, E_2)$, we consider whether E_1 followed by E_2 is a possible 2-block of a polygon. Note that $S_{1,1}$ and E_1 induce a pair partitioning for the vertices in the right-most plane of E_1 , call this pair partition $S_{1,2}$. We thus say that π_2 can follow π_1 (or equivalently, π_1 can precede π_2) if $S_{1,2} = S_{2,1}$ and the right-most plane of E_1 is the same as the left-most plane of E_2 . (Note that we are allowing π_1 to be a left-most pattern or π_2 to be a right-most pattern.) We say a sequence of 1-patterns, $\pi_1, \pi_2, \dots, \pi_r$, is *properly connected* if π_{i+1} can follow π_i for each $i = 1, \dots, r-1$. We refer to the entire sequence π_1, \dots, π_r as an *r-pattern*. Let $t_{\mathbb{T}, r}$ be the number of r -patterns in the tube \mathbb{T} , and let $t_{\mathbb{T}, r}^F$ be the number of r -patterns whose underlying r -blocks are full. We refer to the latter as *full r-patterns*. Any r -pattern which consists of a sequence of proper 1-patterns is called a *proper r-pattern*. By definition, for each $\omega \in \mathcal{P}_{\mathbb{T}}$ (or $\mathcal{P}_{\mathbb{T}}^H$, the subset of Hamiltonian polygons) its sequence $\omega_0, \omega_1, \dots, \omega_{s-1}, \omega_s$ of 1-patterns gives an $(s+1)$ -pattern (a full $(s+1)$ -pattern), and for any $r \geq 2$, each r -pattern (or full r -pattern) starting with a left-most 1-pattern (full left-most 1-pattern) and ending with a right-most 1-pattern (full right-most 1-pattern) yields an element of $\mathcal{P}_{\mathbb{T}}$ ($\mathcal{P}_{\mathbb{T}}^H$).

Lemma 8. *Both r -patterns and full r -patterns have exponential growth rates, and these are equal to $\beta_{\mathbb{T}}$ and $\beta_{\mathbb{T}}^F$ respectively.*

Proof. Patterns are distinguished from blocks by the inclusion of left connectivity information. Each r -pattern corresponds to a unique r -block, but an r -block ω may correspond to multiple r -patterns, as there may be multiple valid sets of left connectivity information which can be matched to ω . However, observe that the number of valid sets of left connectivity information is bounded above by a function of the tube size; namely, the number of pair partitions of W (if W is even) or $W-1$ (if W is odd) vertices. This number is $(W-1)!!$ if W is even and $(W-2)!!$ if W is odd. Hence

$$b_{r, \mathbb{T}} \leq t_{r, \mathbb{T}} \leq (W-1)!! b_{r, \mathbb{T}}.$$

Take logs, divide by r and take $r \rightarrow \infty$, to find

$$\lim_{r \rightarrow \infty} \frac{1}{r} \log t_{\mathbb{T}, r} = \beta_{\mathbb{T}}.$$

Exactly the same arguments apply to full r -patterns, and we have

$$\lim_{r \rightarrow \infty} \frac{1}{r} \log t_{\mathbb{T}, r}^{\mathbb{F}} = \beta_{\mathbb{T}}^{\mathbb{F}}. \quad \square$$

With this definition of patterns, we can follow the approaches used in [10] to obtain transfer matrices. We will focus on full patterns, and hence define four sets $\mathcal{A}_0^{\mathbb{F}}, \mathcal{A}_1^{\mathbb{F}}, \mathcal{A}_2^{\mathbb{F}},$ and $\mathcal{A}_3^{\mathbb{F}}$ corresponding, respectively, to those elements of $\mathcal{A}_0, \mathcal{A}_1, \mathcal{A}_2,$ and \mathcal{A}_3 which are full. We assign a labelling to the elements of $\cup_{k=0}^3 \mathcal{A}_k^{\mathbb{F}}$ and denote them as $\pi_1, \pi_2, \dots, \pi_{r_{\mathbb{T}}}$. Then we obtain the $r_{\mathbb{T}} \times r_{\mathbb{T}}$ transfer matrix $T^{\mathbb{F}}(x)$ for full 1-patterns as follows:

$$[T^{\mathbb{F}}(x)]_{i,j} = \begin{cases} x^{n_{\pi_i} + n_{\pi_j}} = x^W & \text{if } \pi_j \text{ can follow } \pi_i \\ 0 & \text{otherwise,} \end{cases}$$

where n_{π} is the length of the 1-block from which the 1-pattern π was derived, which is W for full 1-blocks.

The generating function for full patterns can be expressed in terms of this transfer matrix as follows:

$$\begin{aligned} G^{\mathbb{F}}(x) &= \sum_{s \geq 1} t_{\mathbb{T}, s}^{\mathbb{F}} x^{sW} = t_{\mathbb{T}, 1}^{\mathbb{F}} x^W + x^W \sum_{i,j} \left[\sum_{t \geq 0} T^{\mathbb{F}}(x) \left(T^{\mathbb{F}}(x) \right)^t \right]_{i,j} \\ &= t_{\mathbb{T}, 1}^{\mathbb{F}} x^W + x^W \sum_{i,j} [T^{\mathbb{F}}(x)(I - T^{\mathbb{F}}(x))^{-1}]_{i,j}, \end{aligned}$$

where $t_{\mathbb{T}, 1}^{\mathbb{F}} = r_{\mathbb{T}}$. The radius of convergence of $G^{\mathbb{F}}(x)$ is given by $e^{-\beta_{\mathbb{T}}^{\mathbb{F}}/W}$ and can also be determined by the smallest value of $x > 0$ which satisfies $\det(I - T^{\mathbb{F}}(x)) = \det(I - x^W T^{\mathbb{F}}(1)) = 0$ or equivalently $\det(x^{-W} I - T^{\mathbb{F}}(1)) = 0$, that is, it is given by the largest eigenvalue of $T^{\mathbb{F}}(1)$. The generating function for Hamiltonian polygons can also be expressed in terms of this transfer matrix as follows:

$$\begin{aligned} G^{\mathbb{H}}(x) &= \sum_{s \geq 0} p_{\mathbb{T}, s}^{\mathbb{H}} x^{(s+1)W} = |\mathcal{A}_0^{\mathbb{F}}| x^W + p_{\mathbb{T}, 1}^{\mathbb{H}} x^{2W} + x^W \sum_{i,j} \left[\sum_{t \geq 0} A^{\mathbb{H}}(x) \left(T^{\mathbb{F}}(x) \right)^t B^{\mathbb{H}}(x) \right]_{i,j} \\ &= |\mathcal{A}_0^{\mathbb{F}}| x^W + p_{\mathbb{T}, 1}^{\mathbb{H}} x^{2W} + x^W \sum_{i,j} [A^{\mathbb{H}}(x)(I - T^{\mathbb{F}}(x))^{-1} B^{\mathbb{H}}(x)]_{i,j}, \end{aligned}$$

where the matrices $A^{\mathbb{H}}(x)$ (resp. $B^{\mathbb{H}}(x)$) are obtained by first labelling the elements of $\mathcal{A}_1^{\mathbb{F}}$ (resp. $\mathcal{A}_3^{\mathbb{F}}$) as $\pi_{1,1}, \pi_{1,2}, \dots, \pi_{1,r_{1,\mathbb{T}}}$ (resp. $\pi_{3,1}, \pi_{3,2}, \dots, \pi_{3,r_{3,\mathbb{T}}}$) and then, for each $j = 1, \dots, r_{\mathbb{T}}$: the i, j entry of $A^{\mathbb{H}}(x)$ is x^W if π_j can follow $\pi_{1,i}$ (0 otherwise), $i = 1, \dots, r_{1,\mathbb{T}}$; and the j, i entry of $B^{\mathbb{H}}(x)$ is x^W if $\pi_{3,i}$ can follow π_j (0 otherwise), $i = 1, \dots, r_{3,\mathbb{T}}$. We explain next that determining whether or not the conjecture holds is equivalent to determining whether or not the largest eigenvalue of $T^{\mathbb{F}}(1)$ gives the radius of convergence for $G^{\mathbb{H}}(x)$.

For two 1-patterns π_i and π_j in $\mathcal{A}^{\mathbb{F}} = \cup_{k=0}^3 \mathcal{A}_k^{\mathbb{F}}$, we say π_j is reachable from π_i if for some r there is a full r -pattern that starts with π_i and ends with π_j . $T^{\mathbb{F}}(x)$ is the weighted adjacency matrix for a directed graph $D^{\mathbb{F}}$ on the set of elements of $\mathcal{A}^{\mathbb{F}}$, and if π_j is reachable from π_i then there is a directed path from π_i to π_j in $D^{\mathbb{F}}$. We say π_i and π_j *communicate* if π_j is reachable from π_i and π_i is reachable from π_j . Communication is an equivalence relation which partitions $\mathcal{A}^{\mathbb{F}}$ into communication classes that correspond to the strongly

connected components of the digraph D^F . The elements of \mathcal{A}^F can then be relabelled in such a way that $T^F(x)$ is a block upper triangular matrix where the block matrices along the diagonal are the weighted adjacency matrices for the strongly connected components of D^F (this gives the Frobenius normal form of $T^F(x)$). Hence the characteristic polynomial of $T^F(x)$ is the product of the characteristic polynomials of the weighted adjacency matrices for the strongly connected components of D^F . (See for example [15, p29-7 and p27-6] or [7, Chapter 3].)

We define the Hamiltonian 1-patterns to be those elements of \mathcal{A}_2^F which can be part of a Hamiltonian polygon; call this subset \mathcal{A}_2^H . Note that by definition every element of \mathcal{A}_2^H is reachable from some element of \mathcal{A}_1^F . Further, if we consider any two elements π_i and π_j in \mathcal{A}_2^H , then there exists a Hamiltonian polygon ω_1 which contains π_i and another Hamiltonian polygon ω_2 which contains π_j . The concatenation construction defined earlier in this section can be used to concatenate polygon ω_1 to ω_2 (or vice versa) to create a new Hamiltonian polygon with π_j reachable from π_i (π_i reachable from π_j) through elements of \mathcal{A}_2^H . Thus the subdigraph of D^F generated by the elements of \mathcal{A}_2^H forms a strongly connected digraph D^H in which every 1-pattern is reachable from every other. We claim further that this subdigraph is a strongly connected component of D^F (i.e. it is a maximal strongly connected digraph). Suppose to the contrary that there exists a larger strongly connected subdigraph of D^F , call it D , which contains D^H as a proper subdigraph. Let π_i be in the vertex set of D but not in \mathcal{A}_2^H , then π_i does not occur in a Hamiltonian polygon, however, π_i communicates with every vertex of D^H . A contradiction results by taking a Hamiltonian polygon ω which contains $\pi_j \in \mathcal{A}_2^H$ and inserting at π_j a sequence of properly connected 1-patterns from π_j to π_i and then from π_i to π_j to create a Hamiltonian polygon that contains π_i . Thus D^H is a strongly connected component of D^F . We call its weighted adjacency matrix the Hamiltonian 1-pattern transfer matrix $T^H(x)$ and it is obtained by restricting $T^F(x)$ (all other rows and columns removed) to the elements of \mathcal{A}_2^H . Thus we also have:

$$\begin{aligned} G^H(x) &= \sum_{s \geq 0} p_{\mathbb{T},s}^H x^{(s+1)W} = |\mathcal{A}_0^F| x^W + p_{\mathbb{T},1}^H x^{2W} + x^W \sum_{i,j} \left[\sum_{t \geq 0} A^{H*}(x) \left(T^H(x) \right)^t B^{H*}(x) \right]_{i,j} \\ &= |\mathcal{A}_0^F| x^W + p_{\mathbb{T},1}^H x^{2W} + x^W \sum_{i,j} [A^{H*}(x)(I - T^H(x))^{-1} B^{H*}(x)]_{i,j}, \end{aligned}$$

where $A^{H*}(x)$ and $B^{H*}(x)$ are obtained from $A^H(x)$ and $B^H(x)$, respectively, by restricting to \mathcal{A}_2^H , and $T^H(x)$ will be one of the block matrices along the diagonal in the Frobenius normal form of $T^F(x)$. Thus $\det(I - T^F(x)) = \det(I - T^H(x)) \prod_{k \geq 1} \det(I - T_k(x))$ where $T_k(x), k \geq 1$ are the weighted adjacency matrices for the other strongly connected components of D^F . The component which corresponds to the smallest root will yield the radius of convergence of $G^F(x)$. The conjecture is that this root comes from $\det(I - T^H(x)) = \det(I - x^W T^H(1)) = 0$ and this corresponds to $T^H(1)$ having the largest eigenvalue amongst $T^H(1), T_k(1), k \geq 1$. For small tube sizes we have verified this conjecture by determining the strongly connected components and their corresponding adjacency matrices and determining which component(s) determine the radius of convergence. Table 1 shows the results. In addition to the numerical verifications provided in Table 1, in two dimensions (that is, when $M = 0$) this conjecture has been verified exactly for $L \leq 5$.

5 Summary and Discussion

We have studied a model of self-avoiding polygons restricted to a $L \times M$ rectangular tube \mathbb{T} of the cubic lattice \mathbb{Z}^3 , subject to a force f which acts in a direction parallel to the axis of the tube. Without loss of generality, we assume $L \geq M \geq 0$ and $L > 0$. When $f > 0$ the force effectively stretches the polygons,

\mathbb{T} size $L \times M$	$\kappa_{\mathbb{T}}^H$	next largest growth rate	\mathbb{T} size $L \times M$	$\kappa_{\mathbb{T}}^H$	next largest growth rate
3×0	0.232905	0	1×1	0.329239	0.173287
4×0	0.239939	0	2×1	0.440750	0.360063
5×0	0.288670	0.196889	3×1	0.488108	0.443274
6×0	0.288344	0.120645	4×1	0.515163	0.485601
7×0	0.314534	0.263113	2×2	0.516565	0.406593
8×0	0.313302	0.222208			
9×0	0.329583	0.296447			
10×0	0.328358	0.269453			
11×0	0.339448	0.316341			

Table 1: Evidence that $\kappa_{\mathbb{T}}^H = \beta_{\mathbb{T}}^F/W$ for small tube sizes.

while when $f < 0$ the force is compressive. For all values of f one can define a free energy $\mathcal{F}_{\mathbb{T}}(f)$. We have shown that in both limits $f \rightarrow \pm\infty$ the free energy $\mathcal{F}_{\mathbb{T}}(f)$ is asymptotic to a linear function of f , and we have proved the exact forms of both of these linear functions. In the $f \rightarrow -\infty$ case the asymptote can be written in terms of the growth rate of a class of objects we call full s -blocks; we conjecture that this value is in fact the same as the growth rate of a subclass of polygons, namely Hamiltonian polygons, which occupy all vertices within a $L \times M \times N$ rectangular prism. Using transfer matrix calculations related to full s -blocks, we establish that the conjecture is true for tube sizes including $M = 0$ and $1 \leq L \leq 11$, $M = 1$ and $1 \leq L \leq 4$, and $(L, M) = (2, 2)$.

Note that, if the conjecture holds, then essentially the order of the two limits $n \rightarrow \infty$ (polygon length grows to infinity) and $f \rightarrow -\infty$ (the force becomes infinitely compressive) can be interchanged. When the conjecture is true, there is at least one consequence of this with respect to the probability of knotting. Specifically, the properties of Hamiltonian polygons presented here in Section 4, have been used previously in [10, Theorem 4.3] to establish that: for any given proper r -pattern P obtained from a Hamiltonian polygon in \mathbb{T} , all but exponentially few sufficiently large Hamiltonian polygons in \mathbb{T} will contain P . Then for $L \geq 2$, $M \geq 1$, letting P be an appropriate full tight trefoil pattern c.f. [10, Figure 4.12], this establishes that all but exponentially few sufficiently large Hamiltonian polygons in \mathbb{T} are knotted. Combining this with the Atapour et al [3] results about knotting for finite forces f , we have that if the $f \rightarrow -\infty$ limit is dominated exponentially by Hamiltonian polygons, then for any force $f \in [-\infty, \infty)$, all but exponentially few sufficiently large polygons in \mathbb{T} will be knotted.

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