Supplementary information for "Characterising knotting properties of polymers in nanochannels"

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Note: Some Results in this document are duplicates of those in the main article – in these cases the numbering is the same. Citations and references to Figures in this document are self-contained.

Outlines of proofs of Results 4 and 5

Result 4. *For any given knot type K, K admits a proper non-local knot pattern in a tube $\mathbb{T}_{L,M}$ for L, M sufficiently large, and admits a proper local knot pattern in a tube $\mathbb{T}_{L',M'}$ for L', M' sufficiently large. Any tube $\mathbb{T}$ which accommodates a local knot pattern for K also accommodates a non-local knot pattern.*

We will prove here a more precise version of Result 4. First, we need a new definition. The *trunk* of a knot or link K is an invariant defined by $\mathrm{trunk}(K) = \min_E \max_{t\in\mathbb{R}} |h^{-1}(t) \cap E|$, where E is any embedding of K in $\mathbb{R}^3$ and $h : \mathbb{R}^3 \to \mathbb{R}$ is any given height function [1,3]. For another invariant, the bridge number $b(K)$ of K, $\mathrm{trunk}(K)$ satisfies $\mathrm{trunk}(K) \leq 2b(K)$.

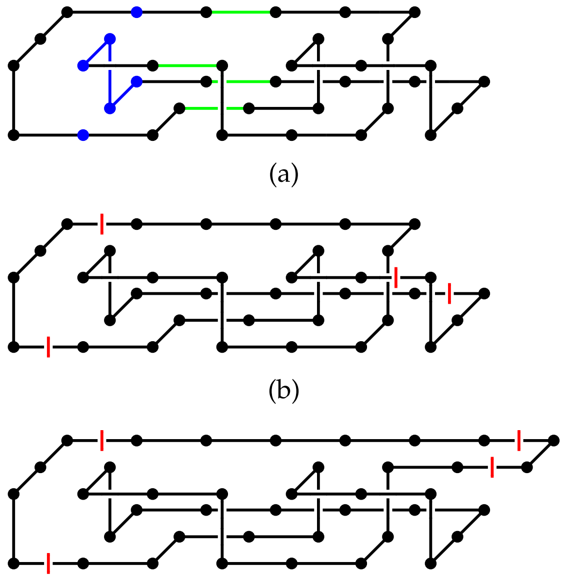
Result 4*. ***(A)*** *A knot K admits a proper non-local knot pattern in $\mathbb{T}_{L,M}$ if and only if* $\mathrm{trunk}(K) < (L+1)(M+1)$. ***(B)*** *A knot K admits a proper local knot pattern in $\mathbb{T}_{L,M}$ if* $\mathrm{trunk}(K) < (L+1)(M+1) - 2$.

Given a polygon $\pi \in \mathcal{P}_{\mathbb{T}}$, 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 $\{(x,y,z) : x = k\}$. See Figure 1(a) for an example.

Proof of Result 4.* **(A)** By [1, Theorem 1], we can construct a polygon of knot type K in $\mathbb{T}_{L,M}$ if and only if $\mathrm{trunk}(K) < (L+1)(M+1)$. Then we can obtain a proper knot pattern from such a polygon by opening its ends, i.e. by removing an edge or edges (as appropriate) in each of the left-most and right-most hinges. See Figure 2(a). We will show that there is a polygon which can be opened at each end to yield a proper non-local knot pattern.

First we consider the case where $\mathrm{trunk}(K) \geq 6$. Take a height function h and an embedding of K, π_K, in $\mathbb{T}$ such that $\mathrm{trunk}(K)$ is attained and such that π_K has the minimal number of critical points with respect to h. We can choose one maximal point p and one minimal point q to make a proper knot pattern so that each of the two arcs of $\pi_K - \{p,q\}$ has at least two critical points. See Figure 2(b). Let K_1 and K_2 be the components of the link obtained by taking the numerator closure of $\pi_K - \{p,q\}$. Then neither of K_1 nor K_2 is K by the minimality of the number of critical points of π_K. It follows that the pattern is non-local. We can construct a polygonal model of K satisfying the above conditions in a given tube.

Suppose $\mathrm{trunk}(K) = 4$. First we consider the case where K is prime, i.e., K is a 2-bridge knot. Take a Conway's normal form with the minimal crossing number. Then there are at least two strings of the 4-braid corresponding to the Conway's normal form that contain crossings. Then we can make a proper knot pattern so that both K_1 and K_2, the components of the numerator closure, contain one each of such strings. Then the crossing numbers of K_1 and K_2 are strictly



(a)

(b)

(c)

Figure 1: (a) A 36-edge polygon π that fits inside $\mathbb{T}_{L,M}$ with $L \geq 2$ and $M \geq 1$; the tube extends without bound to the right and the span $s(\pi) = 6$. Blue vertices and edges denote the hinge H_1 of π, and green edges denote the section S_3 of π. (b) The locations of the two pairs of vertical red lines indicate the locations of the two 2-sections in this polygon; in this example, the polygon can be decomposed into a start unknot pattern, a proper trefoil knot pattern, and an end unknot pattern. The proper knot pattern is classified as non-local in this case. (c) A local proper knot pattern in the same tube with span 7.

less than that of K. Hence neither of K_1 nor K_2 is K. We can construct a polygonal model of K satisfying the above conditions in a given tube and it gives a non-local pattern. Suppose K is a composite knot. Let L_1 and L_2 be knots such that $K = L_1 \# L_2$ and L_1 is a prime knot. Then by the above argument, we can create a non-local pattern for L_1. By a connected sum operation, we can then construct a polygon of K that gives a non-local proper knot pattern.

(B) Suppose trunk$(K) < (L+1)(M+1) - 2$. Then by using a method of [1, Theorem 1], we can construct a polygon inside a region in $\mathbb{T}_{L,M}$ as in Figure 2(c) (left). Then by pulling out a part as in Figure 2(c) (right) we have a local proper knot pattern. □

Result 5. *Given a prime knot $K \neq 0_1$ that can occur in a 2×1 tube, there exists at least one proper local knot pattern and at least one proper non-local knot pattern. Furthermore, at least for $K \in \{3_1, 4_1, 5_1, 5_2\}$, the span of a smallest proper local knot pattern of K in $\mathbb{T}_{2,1}$ is greater than that of a smallest proper non-local knot pattern of K in $\mathbb{T}_{2,1}$.*

Proof. Any prime knot that can occur in a 2×1 tube is 2-bridge [1]. It is well known that any 2-bridge knot is represented by Conway's normal form $C(a_1, \cdots, a_n)$, which is a closure of a 4-braid using only two generators σ_1 and σ_2 [2]. Since there is no σ_3 and the fourth string in

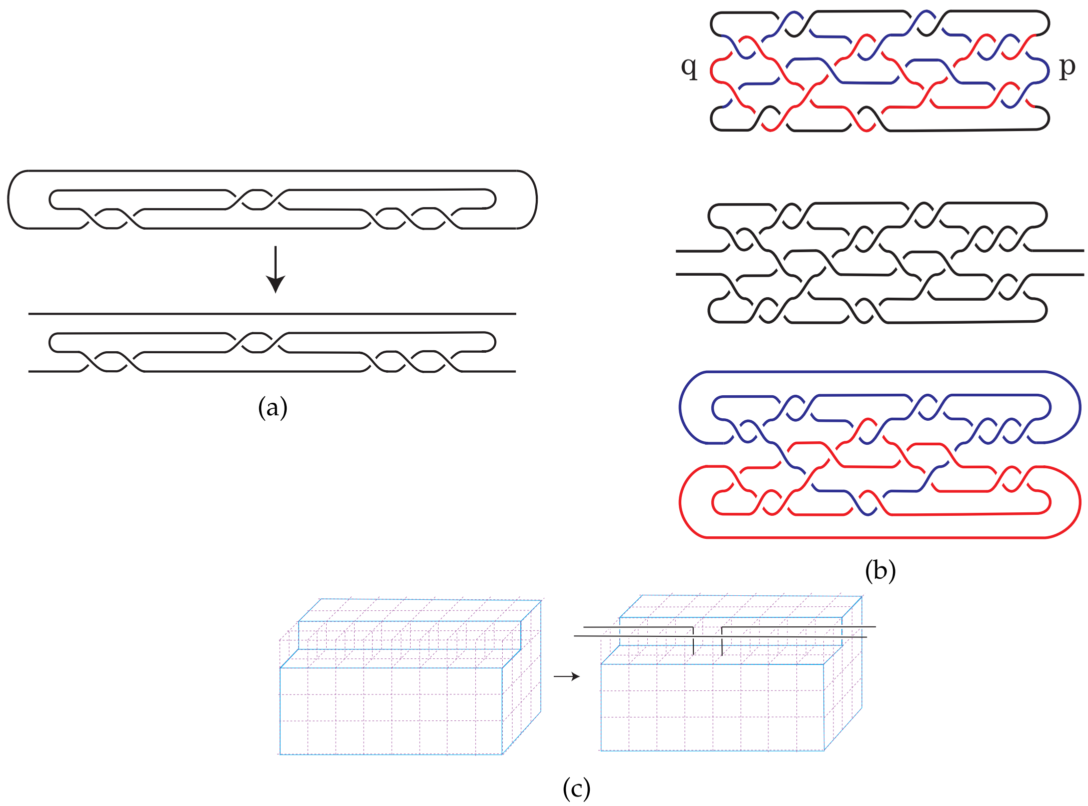


Figure 2: (a) A local 7_5 pattern obtained by opening ends of Conway's normal form. (b) When $\mathrm{trunk}(K) \geq 6$ we can choose p and q so that each arc of $\pi_K - \{p, q\}$ contains at least two critical points. (c) By pulling out a part, we can construct a local knot pattern.

the Conway's normal form is straight, we have a local knot pattern by opening both ends as in Figure 2(a).

By [1, Lemma 3(1)], from a knotted polygon in a 2×1 tube with the smallest span we can obtain a proper knot pattern with the smallest span in the 2×1 tube for that knot type by opening both ends of the polygon. For $K \in \{3_1, 4_1, 5_1, 5_2\}$, by applying the argument of [1, Theorem 4], we can completely characterise the configurations of K with smallest span, see Figures 3(a), (b), (c), (d) for examples. We can then conclude that the resulting proper knot patterns are all non-local. On the other hand, in these cases a local proper knot pattern can be constructed by increasing the span by one by the same method as in Figure 1(c). □

References

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[2] K Murasugi, *Knot Theory and its Applications*, Birkhäuser, 1996.

[3] M Ozawa, *Waist and trunk of knots*, Geometriae Dedicata **149** (2010), 85–94.

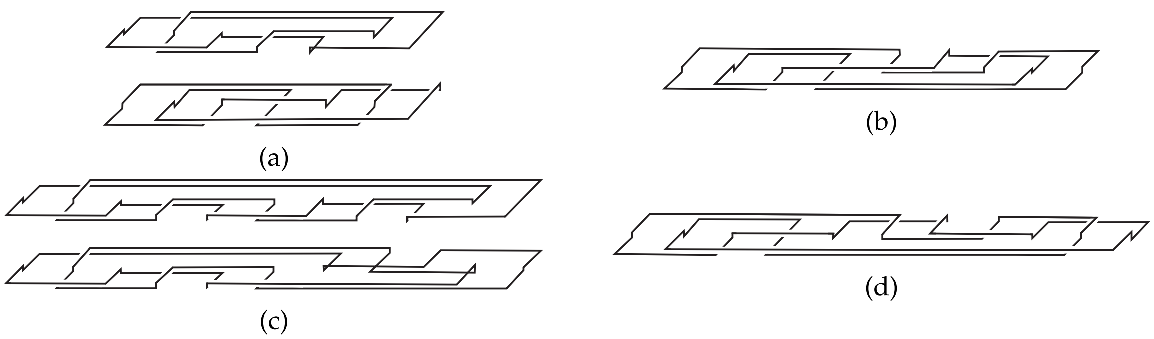

Figure 3: (a) Two polygons of 3_1 in 2×1 tube with the smallest span 6; the first consists of 36 edges and the second consists of 38 edges. (b) A polygon of 4_1 in 2×1 tube with the smallest span 8; this consists of 50 edges. (c) Two polygons of 5_1 in 2×1 tube with the smallest span 10; these consist of 60 edges. (d) A polygon of 5_2 in 2×1 tube with the smallest span 10; this consists of 62 edges.