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 $T_{L,M}$ for $L, M$ sufficiently large, and admits a proper local knot pattern in a tube $T_{L',M'}$ for $L', M'$ sufficiently large. Any tube $T$ 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 $\text{trunk}(K) = \min_E \max_{t \in \mathbb{R}} |h^{-1}(t) \cap E|$, 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 $K$, trunk($K$) satisfies trunk($K$) $\leq 2b(K)$.

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

Given a polygon $\pi \in \mathcal{P}_T$, a hinge $H_k$ of $\pi$ is the set of edges and vertices lying in the intersection of $\pi$ 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 $T_{L,M}$ if and only if 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 trunk($K$) $\geq 6$. Take a height function $h$ and an embedding of $K, \pi_K$, in $T$ such that trunk($K$) is attained and such that $\pi_K$ 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 $\pi_K$. 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 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
Figure 1: (a) A 36-edge polygon $\pi$ that fits inside $T_{L,M}$ 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 $\pi$, and green edges denote the section $S_3$ of $\pi$. (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 $T_{L,M}$ 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 $2 \times 1$ 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 $T_{2,1}$ is greater than that of a smallest proper non-local knot pattern of $K$ in $T_{2,1}$.

**Proof.** Any prime knot that can occur in a $2 \times 1$ tube is 2-bridge [1]. It is well known that any 2-bridge knot is represented by Conway’s normal form $C(a_1, \ldots, a_n)$, which is a closure of a 4-braid using only two generators $\sigma_1$ and $\sigma_2$ [2]. Since there is no $\sigma_3$ and the fourth string in
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 $2 \times 1$ tube with the smallest span we can obtain a proper knot pattern with the smallest span in the $2 \times 1$ 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

Figure 3: (a) Two polygons of $3_1$ in $2 \times 1$ 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 $2 \times 1$ tube with the smallest span 8; this consists of 50 edges. (c) Two polygons of $5_1$ in $2 \times 1$ tube with the smallest span 10; these consist of 60 edges. (d) A polygon of $5_2$ in $2 \times 1$ tube with the smallest span 10; this consists of 62 edges.