

## Signed Unknotting Number and Knot Chirality Discrimination via Strand Passage

Chris SOTEROS,<sup>1,\*</sup> Kai ISHIHARA,<sup>2,\*\*</sup> Koya SHIMOKAWA,<sup>3,\*\*\*</sup>  
Michael SZAFRON<sup>4,†</sup> and Mariel VAZQUEZ<sup>5,††</sup>

<sup>1</sup>*Department of Mathematics and Statistics, University of Saskatchewan,  
Saskatoon, SK, Canada, S7N 5E6*

<sup>2</sup>*Department of Mathematics, Imperial College London, London SW7 2AZ, UK*

<sup>3</sup>*Department of Mathematics, Saitama University, Saitama 338-8570, Japan*

<sup>4</sup>*School of Public Health, University of Saskatchewan,  
Saskatoon, SK, Canada, S7N 5E5*

<sup>5</sup>*Department of Mathematics, San Francisco State University,  
San Francisco, CA 94132, USA*

(Received May 27, 2011)

Which chiral knots can be unknotted in a single step by a  $+$  to  $-$  ( $+-$ ) crossing change, and which by a  $-$  to  $+$  ( $-+$ ) crossing change? Numerical results suggest that if a knot with 6 or fewer crossings can be unknotted by a  $+-$  crossing change then it cannot be unknotted by a  $-+$  one, and vice versa. However, we exhibit one chiral 8-crossing knot and one chiral 9-crossing knot which can be unknotted by either crossing change. Furthermore, we address the question analytically using results of Taniyama and Traczyk. We apply Taniyama's classification of unknotting operations to chiral rational knots and fully classify all those which, in a single step, can be unknotted by either type of crossing change; the first of these is  $8_{13}$ . As a corollary, we obtain Stoimenow's result that all chiral twist knots can be unknotted by only one of the two crossing change types,  $+-$  or  $-+$ . Thus, as was observed numerically, all chiral knots with unknotting number one, and seven or fewer crossings, can be unknotted by only one of the two crossing change types. Traczyk's results allow us to address the question for some non-rational chiral unknotting number one knots with 9 or fewer crossings, however, for others the question remains open. We propose a numerical approach for investigating the latter type of knot. We also discuss the implications of our work in the context of DNA topology.

### §1. Introduction

DNA topology is the study of geometrical (supercoiling) and topological (knotting and linking) properties of closed DNA molecules.<sup>1)</sup> Important biological processes such as DNA replication and transcription alter the supercoiling of their DNA substrates. For example, replication of circular DNA interlinks the two newly replicated molecules. The resulting links are all  $(2, 2p)$ -torus links, which need to be unlinked to allow the cell to survive.<sup>2)</sup> Other processes, such as DNA packing and site-specific recombination, yield knotted DNA (e.g. see Refs. 3)–6)). It has been

---

\*) E-mail: soterios@math.usask.ca

\*\*) E-mail: k.ishihara@imperial.ac.uk

\*\*) E-mail: kshimoka@rimath.saitama-u.ac.jp

†) E-mail: michael.szafron@usask.ca

††) E-mail: mariel@math.sfsu.edu

shown experimentally that DNA knots interfere with vital cellular processes and may lead to cell death.<sup>7),8)</sup> The cellular issues resulting from DNA knot or link formation are resolved by type II topoisomerases.

Type II topoisomerases are essential enzymes found in every organism. They play crucial unknotting, unlinking and supercoiling simplification roles that help facilitate important cellular processes and ensure stable chromosome and plasmid inheritance. Certain type II topoisomerases are also able to knot, link and supercoil DNA. For example gyrase of *Escherichia coli* is the only type II topoisomerase known to introduce negative supercoils into its circular DNA substrate. Type II topoisomerases are reviewed in Refs. 9)–12).

Type II topoisomerases change the topology of DNA by passing one DNA segment through another (*strand-passage*). The strand-passage mechanism is reviewed in Refs. 13), 14). This strand passage activity permits linking or unlinking, knotting or unknotting, as well as relaxing or supercoiling of DNA molecules. Members of the type-2 class of topoisomerases include bacterial DNA gyrase, bacterial topoisomerase IV (topo IV) and eukaryotic topoisomerase II (topo II), all of which have similar structures (reviewed in Ref. 15)).

Here, we are interested in the potential chirality discrimination abilities (the ability to distinguish between mirror images) of type II topoisomerases. With regards to the mathematics of this, we assume that the reader is familiar with the standard knot theory definitions and results from Refs. 42), 43) and 44). However, when it comes to questions of chirality it is important to establish which convention is being used. For this, given a diagram  $D$  of a knot we define the *chirality* or *sign* of a crossing in  $D$  to be either positive (+) or negative (−) according to the right-hand rule sign convention of Fig. 1. Then, a  $+−$  *strand passage* (or  $+−$  *sign change*) is a strand passage based on a diagram  $D$  that converts a positive crossing in  $D$  to a negative one. By interchanging the +’s and −’s in this definition, a  $−+$  *strand passage* is analogously defined. In §2, we give a brief summary of some other knot theory definitions and results relevant to this paper. In particular, we review the definition for *chiral knot* and define a convention for assigning a “sign” (either − or +) to each chiral knot we consider.

Returning to type II topoisomerases, it has been reported that some exhibit chirality discrimination by acting more efficiently on molecules with a given topology (summarized in Ref. 12)). Experimentally it has been observed that some type II topoisomerases preferentially relax one type of supercoiling over the other.<sup>12),16),17)</sup> In the case of gyrase, the enzyme does not seem to have a binding preference, but it mainly introduces (−) supercoils into DNA by forcing the inversion of (+) cross-

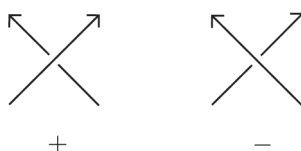


Fig. 1. Right-hand rule sign convention.

ings formed before strand-passage.<sup>18),19)</sup> Shaw and Wang reported in Ref. 20) that the knotting of nicked DNA rings (i.e. relaxed DNA circles) by an excess of type II topoisomerase from *Saccharomyces cerevisiae* (a type of yeast) produces more negative-noded than positive-noded trefoils. Several models have been proposed to explain the chirality preferences of different topoisomerases: reviews of those for the chiral action of bacterial gyrase are given in Refs. 18), 19), 21)–24); for bacterial topo IV, in Refs. 25)–28); and for other topoisomerases, in Refs. 16), 17).

Recent numerical results of Szafron and Soteros for a simplified lattice model of the type II topoisomerase strand-passage reaction provide evidence that selecting a synapse of specific chirality at the strand-passage site could account for knot chirality discrimination.<sup>29)–31)</sup> For example, from their simulations, whenever an unknotted polygon is converted into a trefoil via a  $+−$  strand-passage, then the trefoil is always negative. Similarly, when trefoils are produced from an unknot after a single  $−+$  strand-passage, only positive trefoils result. The same chirality discrimination is observed for other transitions from the unknot to a knot  $K$ , where  $K = 5_2, 6_1, 6_2$  (modulo mirror image). These results prompted us to address the following question: Does the sign of the crossing at a strand-passage site in an unknot determine the chirality-type of the post-strand-passage knot? For example, if a positive trefoil can be obtained from the unknot by a single  $−+$  strand-passage, can it also be obtained from the unknot by a  $+−$  strand-passage? More generally, we consider the following question: if a chiral knot  $K$  can be obtained from the unknot by a  $+−$  strand-passage, can it also be obtained from the unknot by a  $−+$  strand-passage?

In this paper we first address this question by reviewing what is known about unknotting operations and about signed unknotting numbers. The *unknotting number* of a knot  $K$ , denoted by  $u(K)$ , is the minimal number of crossing changes (regardless of their sign) needed to unknot  $K$ . In this definition the minimum is taken over all knot diagrams of  $K$ . Using the right-hand rule sign convention of Fig. 1, we define the *positive unknotting number*,  $u_+(K)$ , to be the minimal number (over all knot diagrams of  $K$ ) of  $+−$  sign changes needed to unknot a knot  $K$  when no  $−+$  changes are allowed. Correspondingly, the *negative unknotting number*,  $u_-(K)$ , is taken to be the minimum number of  $−+$  sign changes needed to unknot  $K$  when no  $+−$  changes are allowed. If a knot cannot be unknotted with such crossing changes only, we define the corresponding signed unknotting number to be  $∞$ . In this context, the question above can be rephrased as follows.

**Main Question** Given a chiral unknotting number one knot  $K$ , is exactly one of  $u_+(K)$  and  $u_-(K)$  equal to 1?

In order to address this question, we use results about (unsigned) unknotting numbers,  $u(K)$ , and about knots with unknotting number one. Unknotting numbers have been of considerable interest to knot theorists (cf. Refs. 32), 33)). For the set of rational knots (see §2 for a definition), all unknotting number one knots have been characterized by Kanenobu-Murakami.<sup>34)</sup> Unknotting operations for such knots have been classified up to equivalence by Taniyama.<sup>35)</sup> Motegi<sup>36)</sup> showed that the unknotting number of a Montesinos knot defined with at least four non-integral rational tangles is strictly greater than 1, while there are Montesinos knots defined

with three rational tangles with unknotting number one. Recently, the papers by Gordon-Luecke<sup>32)</sup> and Ozsváth-Szabó<sup>33)</sup> complete the table of unknotting numbers of prime knots up to 10 crossings.

The concept of signed unknotting numbers was introduced and studied by Cochran and Lickorish.<sup>37)</sup> More recently, Traczyk<sup>38)</sup> tabulated information related to signed unknotting numbers (he denotes  $u_+(K)$  and  $u_-(K)$ , respectively by  $u_{++}(K)$  and  $u_{--}(K)$ ) for knots up to nine crossings. Also, Stoimenow<sup>39)</sup> has a recent result for rational knots. Darcy<sup>40)</sup> and Moon<sup>41)</sup> have looked at generalizations to signed distances between knots. Here we use the results of Taniyama and Traczyk to address the Main Question above. We show an affirmative answer for all knots up to seven crossings. However, we exhibit one eight crossing and one nine crossing knot for which  $u_+ = u_- = 1$ , thus indicating that this is not a universal property. We also address the question for all rational knots. To do this, we use Taniyama's classification of unknotting operations for rational knots to classify the signed unknotting operation for chiral rational unknotting number one knots. Using this classification we provide an answer to the Main Question for all chiral rational knots. In particular, for every chiral twist knot, the answer is yes (this was also established by Stoimenow using a different approach), and the first rational knot for which the answer is negative is an eight-crossing knot.

The paper is structured as follows. We first give a brief overview of some relevant knot theory definitions. Next, we review the numerical strand-passage results which motivated the Main Question. Then we prove that Taniyama's classification scheme for unknotting operations can be used to fully classify signed unknotting operations for chiral unknotting number one rational knots. We then combine this result with results from Traczyk to address the Main Question for all rational knots and for each of the non-rational knots (up to 9 crossings) investigated by Traczyk. We find two such knots for which the answer to the Main Question remains open, and for those, we address the Main Question using a numerical approach.

## §2. Knot theory definitions

In this section we give a cursory review of some relevant knot theory definitions and direct the interested reader to Refs. 42), 43) and 44) for fuller details.

A *knot* is defined as the image of an embedding of the 1-dimensional sphere into  $\mathbb{R}^3$  or  $S^3$ . A disjoint union of knots is called a *link*. Two knots are *equivalent* if they are ambient isotopic, i.e. one can be deformed continuously into the other without any intersections. A knot is said to be *chiral* if it is not ambient isotopic to its mirror image. Otherwise it is called *achiral*. A *knot diagram* is a regular (only transverse double-point intersections allowed) projection of the knot with over and under strand information indicated at each crossing. The sign of a crossing is obtained by assigning an arbitrary orientation to the knot and using the right-hand rule of Fig. 1). The least number of crossings over all knot diagrams for a given knot  $K$  is invariant for  $K$  and is called its *crossing number*. A *minimal diagram* for a knot  $K$  is one with the least possible number of crossings. A knot diagram is said to be *alternating* if, when walking along the knot, the strands alternate between

being over and under at the diagram crossings. A knot which has an alternating diagram is said to be an *alternating knot*. In order to define other classes of knots that are relevant here, we discuss some tangle theory results and definitions next.

A *2-string tangle*, or simply *tangle*, is a 3-dimensional ball with two properly embedded arcs. There are three classes of tangles: rational, locally knotted, and prime. *Rational tangles* are the simplest class of tangles (see Fig. 2 for examples). There is a one-to-one correspondence between the set of rational tangles and  $\mathbb{Q} \cup \{\infty\}$ , where  $\infty$  corresponds to the tangle shown on the left of Fig. 2.<sup>45)</sup> In particular, any rational tangle can be arranged in a canonical form, which can be untied by a finite number of horizontal and vertical half twists; the corresponding rational number is then obtained by inserting the numbers of horizontal and vertical half-twists sequentially into a continued fraction. A tangle is said to be *integral* if it consists of a horizontal row of  $k$ -half twists and is denoted by  $(k)$ , where  $k$  is an integer.

The *numerator operation* on a tangle  $T$  is obtained by connecting the top two endpoints of  $T$  by an arc and the two lower endpoints of  $T$  by another arc (see Fig. 3). The result,  $N(T)$ , is a knot or link. From two tangles  $T_1$  and  $T_2$ , a new tangle can be obtained by connecting the two right endpoints of  $T_1$  to the two left endpoints of  $T_2$  as is shown in Fig. 4. The resulting tangle is called the *sum* of  $T_1$  and  $T_2$ , and is denoted by  $T_1 + T_2$ . *Rational knots and links* are those obtained from rational tangles via the numerator operation. Furthermore, the numerator of the tangle sum of two rational tangles is also a rational knot.<sup>46)</sup> The set of rational knots coincides with that of *2-bridge knots*, and that of *4-plats*. One important subclass of rational knots are the *twist knots*, which each have a knot diagram as shown in Fig. 5.

In this paper, when referring to a chiral knot, we need to be able to distinguish between the knot and its mirror image. For the trefoil, we use the notation  $3_1^+$  to refer to the trefoil whose minimal diagram has three positive crossings and  $3_1^-$

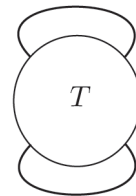
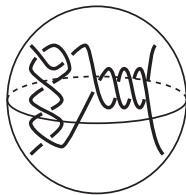
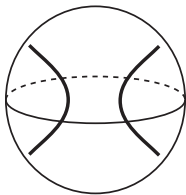


Fig. 2. Rational tangles: trivial tangle  $\infty$  on the left and tangle  $-30/7$  (which can be untied by  $-4$  horizontal,  $-3$  vertical and then  $-2$  horizontal half-twists) on the right.

Fig. 3. The numerator  $N(T)$ .

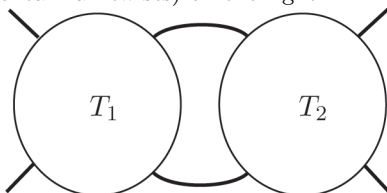


Fig. 4. The tangle sum  $T_1 + T_2$ .

Fig. 5. A knot diagram for a twist knot.

denotes its mirror image. A similar approach can be used for many alternating knots. Specifically, for an alternating knot the projected writhe of a minimal diagram (obtained by summing over its crossings, with a  $+$  crossing contributing  $+1$  and a  $-$ , contributing  $-1$ ) is known to be invariant over all minimal diagrams (see for example Ref. 47)). Let  $sWr(D) \in \{-, 0, +\}$  denote the sign of the writhe of a minimal knot diagram  $D$ , with  $sWr(D) = 0$  if the writhe is 0. Thus, for each chiral alternating knot  $K$ , if the projected writhe in a minimal diagram  $D$  is non-zero, then  $sWr(K) \equiv sWr(D)$  can be used to distinguish between the knot and its mirror image. For example,  $3_1^+$  has a minimal diagram with three crossings all of which are positive and hence  $sWr(3_1^+) = +$ , while for  $3_1^-$ ,  $sWr(3_1^-) = -$ . All rational knots are alternating (see for example Ref. 42)) and all knots with seven or fewer crossings are rational. Furthermore, all the chiral alternating knots considered here satisfy  $sWr(K) \neq 0$ , and hence we can use  $sWr$  to distinguish an alternating knot from its mirror image. However, since this is not universally applicable, we use  $sWr(K) \equiv sWr(D)$  where  $D$  is the minimal diagram given in Rolfsen's knot table (hereafter referred to as Table R) to assign a sign to each chiral knot. Specifically, for each chiral pair of knots,  $K$  and its mirror image  $K^*$ , only one diagram is given in Table R, however, non-zero  $sWr(K)$  and  $sWr(K^*)$  are necessarily opposite in sign. Thus, here, the notation  $K^+$  will refer either to the knot  $K$  whose diagram appears in Table R with  $sWr(K) = +$  or to the knot  $K^*$  whose mirror image diagram appears in Table R with  $sWr(K) = -$ . The notation  $K^-$  is defined analogously. We will also use Table R as a reference point for naming knots and, unless stated otherwise, the unsuperscripted notation  $m_j$  will refer to the  $j$ th knot with crossing number  $m$  whose minimal diagram is labelled  $m_j$  in Table R, while  $m_j^*$  will refer to its mirror image. Note that Portillo et al.<sup>48)</sup> propose using the sign of the *overall mean writhe*, calculated over sets of random polygons with a given chiral knot-type, to distinguish between a chiral knot and its mirror image. Specifically given a set of random polygons with knot-type  $K$ : they define the *writhe* of a polygon to be the average of its projected writhe taken over all possible projections; the *mean writhe* of  $K$  for some specific length  $n$  is then the writhe averaged over all  $n$ -edge polygonal realizations of  $K$ ; and the *overall mean writhe* of  $K$  is the mean writhe averaged over all such realizations of  $K$  and over all lengths. In Ref. 48), they have estimated overall mean writhes (using two distinct sets of random polygons (simple cubic lattice self-avoiding and off-lattice equilateral random polygons)) for all knots up to 8-crossings and have recently extended this to 9-crossing knots. For the knots studied in this paper, we found that calculating  $sWr(K)$  from the minimal diagram for the knot as given in Rolfsen<sup>44)</sup> yields the same sign as that obtained for the knot by the approach of Portillo et al.<sup>48)</sup>

### §3. A lattice model for crossing-sign dependent strand passage

In Refs. 29), 49), Szafron and Soteris developed a simple cubic lattice self-avoiding polygon model to model local strand passage. In the model, it is assumed that two strands of the polygon have already been brought close (i.e. pinched) to-

gether to facilitate strand-passage. The pinched portion of the polygon is modelled by a fixed structure anchored at the origin, denoted by  $\Theta$  (Fig. 6(a)). Any self-avoiding polygon (SAP) containing  $\Theta$  is called a  $\Theta$ -SAP. Strand-passage at  $\Theta$  replaces it with the structure  $\Theta_s$ , shown on the right in Fig. 6(a). Note that this process only yields a lattice polygon if the sites marked with open circles around  $\Theta$  are unoccupied by the original polygon. In the case where these sites are unoccupied,  $\Theta$  is referred to as  $\Theta_0$ , and any polygon containing it, as a  $\Theta_0$ -SAP. The left diagram of Fig. 6(b)

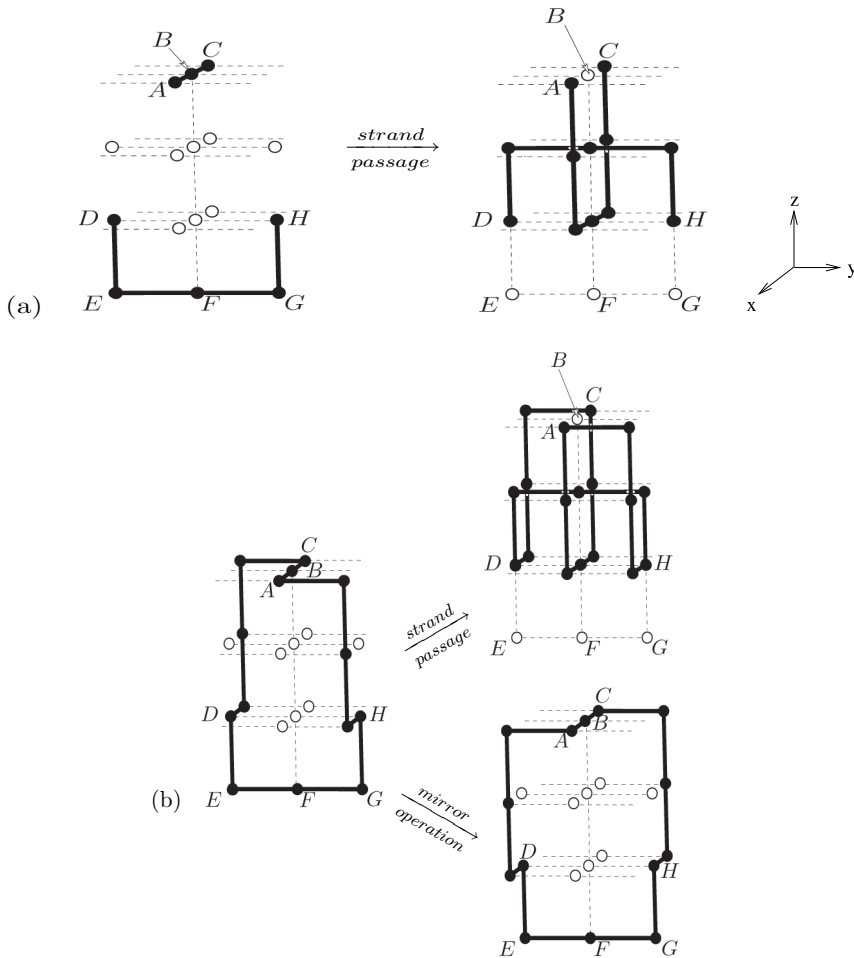


Fig. 6. (a) The left diagram shows the strand-passage structure  $\Theta$  anchored at the origin (i.e.  $B = (0, 0, 0)$ ).  $\Theta$ 's vertices and edges are indicated by solid circles and bonds, respectively. Dashed lines and open circles represent, respectively, lattice edges and vertices which may or may not be occupied in a  $\Theta$ -SAP. In the case where the open circles are not occupied, the strand-passage structure is called  $\Theta_0$ . The after-strand-passage structure  $\Theta_s$  is shown on the right. (b) An unknotted 14-edge  $\Theta_0$ -SAP  $\omega$  (on left) and the corresponding 18-edge after-strand-passage polygon  $\omega_s$  (top right). The diagram on the bottom right is the  $\Theta_0^+$ -SAP  $\tilde{\omega}$  obtained from the  $\Theta_0^-$ -SAP  $\omega$  via the mirror operation  $\sim$ .

shows a 14-edge  $\Theta_0$ -SAP  $\omega$ . The upper right diagram of the same figure shows the after-strand-passage lattice polygon  $\omega_s$  obtained from  $\omega$  by replacing  $\Theta_0$  with  $\Theta_s$ .

Using  $\Theta_0$ -SAPs, in Refs. 29), 49), Szafron and Soteros investigate, both theoretically and numerically, the distribution of knots obtained after performing a single strand passage. For their numerical work, Markov Chain Monte Carlo was used to generate samples of  $\Theta$ -SAPs. In particular, in Ref. 49) an algorithm, called the  $\Theta$ -BFACF algorithm, was developed to generate  $\Theta$ -SAPs with varying lengths but fixed knot-type. In the case that the initial polygon is an unknotted  $\Theta$ -SAP, in Ref. 49) the  $\Theta$ -BFACF algorithm was proved to have exactly two ergodicity classes depending on the sign of the crossing at  $\Theta$  in a projection onto the  $xy$ -plane. If the crossing sign at  $\Theta$  in a given polygon is positive, the polygon is called a  $\Theta^+$ -SAP and otherwise, a  $\Theta^-$ -SAP. Thus, from the ergodicity proof in Ref. 49), if one starts with an unknotted  $\Theta^+$ -SAP, the  $\Theta$ -BFACF algorithm can, in the long run, generate any other unknotted  $\Theta^+$ -SAP. Likewise the  $\Theta$ -BFACF algorithm only generates  $\Theta^-$ -SAPs when starting with a  $\Theta^-$ -SAP. Furthermore, the transition probabilities can be chosen so that each equal-length  $\Theta^+$ -SAP (or  $\Theta^-$ -SAP) is equally likely to occur in the equilibrium distribution. Thus the  $\Theta$ -BFACF algorithm provides a way to investigate knot distributions after a unidirectional crossing-sign change in an unknotted polygon.

Figure 6(b) shows a 14-edge  $\Theta_0^-$ -SAP  $\omega$  on the left and a 14-edge  $\Theta_0^+$ -SAP  $\tilde{\omega}$  on the bottom right.  $\tilde{\omega}$  can be obtained from  $\omega$  by the simple “mirror” operation which takes  $(x, y, z) \in \mathbb{Z}^3$  to  $(-x, y, z)$ . It is also proved in Ref. 49) that this mirror operation provides a one-to-one mapping between unknotted  $\Theta^-$ - and  $\Theta^+$ -SAPs which preserves their after-strand-passage knot-types, except with opposite chirality. Thus the after-strand-passage knot distribution for unknotted  $\Theta^+$ -SAPs can be obtained from that for unknotted  $\Theta^-$ -SAPs, and vice versa.

A composite (a.k.a. multiple) Markov Chain (CMC) version of the  $\Theta$ -BFACF algorithm has been used to generate 2,491,776,147 unknotted  $\Theta_0^-$ -SAPs whose lengths vary from 14 to 5000.<sup>29),30)</sup> Strand passage was performed once on each of these sample polygons and the after-strand-passage knot-type was assessed using both the Alexander and the HOMFLY polynomials. For unknotting number one knots up to  $10_{42}$ , no two knots (ignoring chirality) have the same Alexander polynomial<sup>50)</sup> and the HOMFLY polynomial can be used to distinguish between a knot and its mirror image. We expect the occurrence of high crossing number knots to be rare and make the assumption that the only knots possible are those up to  $10_{42}$ . Based on this, the chiral knot distribution that resulted consisted of knots of only one chirality type, e.g. only  $3_1^+$  (31,161,421),  $5_2^+$  (36,596),  $6_1^+$  (417) and  $6_2^+$  (436) were observed. This was one of the main motivations for investigating the Main Question.

The CMC  $\Theta$ -BFACF algorithm has also been used to generate trefoil  $\Theta_0^-$ -SAPs.<sup>31)</sup> The  $\Theta$ -BFACF algorithm is known to preserve the initial polygon’s knot-type (including chirality) as well as its crossing-sign at  $\Theta$ . We generated 1,501,867,897  $\Theta_0^+$ -SAPs with knot type  $3_1^-$ . Among these, we never observed an after strand-passage knot with trivial Alexander polynomial and hence we never observed an after strand-passage unknot. This gives numerical support to the conjecture that a  $+ -$  crossing change on a  $3_1^-$  knot cannot yield the unknot. This is consistent with



the fact that no after-strand-passage  $3_1^-$  knots were observed in the unknot  $\Theta_0^-$ -SAP simulation. These results provided further motivation for investigating the Main Question.

### §4. Main Question results

In this section, we first review known results and theorems related to unknotting operations and signed unknotting number, and then we apply them to address the Main Question.

From the literature, knot theorists primarily study signed unknotting numbers and signed distances between knots to resolve questions about unsigned unknotting numbers and distances. In fact, in the knot theory literature very few knot tables exist which provide signed unknotting number or signed distance information.<sup>38),41)</sup> Traczyk appears to be the first to present a table of knots along with signed unknotting information.<sup>38)</sup> More recently, Stoimenow<sup>39)</sup> proved a theorem for rational unknotting number one knots which can be used to obtain information about their signed unknotting numbers. Prior to this, Taniyama<sup>35)</sup> completely classified, up to equivalence, the unknotting operation of rational knots with unknotting number one. We show first that for such knots that are chiral, the  $+-$  unknotting operation is not equivalent to the  $-+$  unknotting operation. Thus Taniyama’s results can be used to completely answer the Main Question for rational knots. We then use Traczyk’s results to address the question for the non-rational unknotting number one, chiral knots in his table.

#### 4.1. Taniyama’s results and their consequences

First we review the equivalence class definitions for crossing change and unknotting operation given by Taniyama.<sup>35)</sup> Let  $K$  be a knot in  $S^3$ . Suppose a 3-ball  $B^3$  in  $S^3$  meets  $K$  in a rational tangle  $T$  as on the left of Fig. 7. If we replace  $(B^3, T)$  by the rational tangle  $(B^3, T')$  (as shown in Fig. 7), we have another knot  $K'$ . This operation on  $K$  at  $(B^3, T)$  is considered a crossing change on  $K$ . Let  $(B_1^3, T_1)$  and  $(B_2^3, T_2)$  be the initial rational tangles for any two crossing changes on  $K$ . Two such crossing changes are considered equivalent if there is a homeomorphism  $h : S^3 \rightarrow S^3$  such that  $h(K) = K$ ,  $h(B_1^3) = B_2^3$  and  $h(T_1) = T_2$ . Since an unknotting operation is a crossing change, we can also define equivalence for unknotting operations in the same way.

Taniyama classified the unknotting operation for unknotting number one rational knots up to this equivalence. Note that from the definition of knot equivalence in

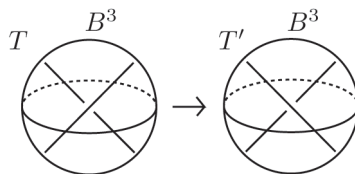


Fig. 7. Crossing change.

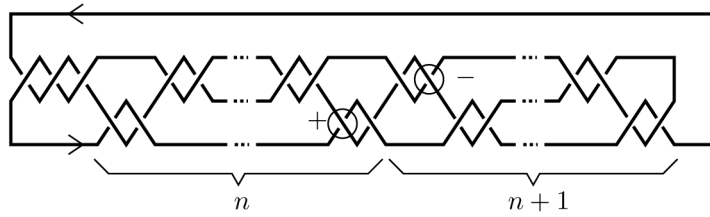


Fig. 8.  $C(3, 2, 2, \dots, 2, -2, -2, \dots, -2)$  with odd  $n$  has two inequivalent unknotting operations with opposite sign, cf. Fig. 5 in Taniyama’s paper.<sup>35)</sup>

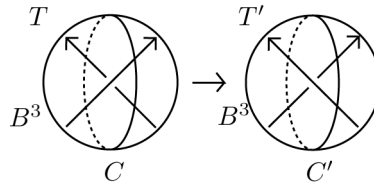


Fig. 9. Crossing change circle.

his paper, a knot and its mirror image are equivalent, but, by our definition of knot equivalence they are distinct. Taniyama showed for a rational knot that the number of equivalence classes of unknotting operations is either 0, 1, or 2. Moreover he showed an unknotting operation for a twist knot is unique up to equivalence, and that a rational knot has two inequivalent unknotting operations if and only if the knot can be expressed using 4-plat notation (see Ref. 42) for the notation definition) as

$$C(3, 2, 2, \dots, 2, -2, -2, \dots, -2), \tag{4.1}$$

or its mirror image, where the number of 2’s is  $n$  and that of  $-2$ ’s is  $n + 1$ , for some positive integer  $n$ . For the case that  $n$  is odd, the knot with 4-plat notation  $C(3, 2, 2, \dots, 2, -2, -2, \dots, -2)$  is depicted in Fig. 8.

Next we consider unknotting operations of chiral knots. From now on we assume that knots are oriented. Let  $D$  be a properly embedded disk in  $B^3$  such that  $D$  meets  $K$  in the opposite direction. We call  $D$  a *crossing disc*. The boundary  $\partial D = C$  is called a *crossing circle* (see Fig. 9). Since a positive to negative crossing change is given by a right handed twist along  $D$  and a negative to positive crossing change is given by a left handed twist, a positive to negative crossing change can be realized by a  $+1$ -Dehn surgery on  $C$  and a negative to positive by  $-1$ -Dehn surgery.<sup>51)</sup> Note that the crossing circle is determined up to isotopy in  $\partial B^3 - T$ . Let  $C'$  denote the surgery core of the Dehn surgery. Let  $C_1$  and  $C_2$  be the crossing change circles of two equivalent crossing changes and let  $\gamma_1$  and  $\gamma_2$  be their respective surgery slopes. Then we can assume that the homeomorphism  $h$  will send  $C_1$  to  $C_2$  and  $\gamma_1$  to  $\gamma_2$ .

**Proposition 1.** *Suppose a knot  $K$  is chiral. Then a positive to negative crossing change of  $K$  is not equivalent to a negative to positive crossing change of  $K$ .*

*Proof.* Let  $C_+$  and  $\gamma_+$  be the crossing change circle and the surgery slope for a positive to negative crossing change and  $C_-$  and  $\gamma_-$  be those for a negative to

positive crossing change. Suppose the two crossing changes are equivalent. Let  $h : S^3 \rightarrow S^3$  be a homeomorphism which gives the equivalence. Then we can assume that  $h$  sends  $C_+$  to  $C_-$  and  $\gamma_+$  to  $\gamma_-$ . Since the slopes  $\gamma_+$  and  $\gamma_-$  have opposite signs,  $h$  reverses the orientation of the meridian-longitude coordinate. Hence  $h$  reverses the orientation of  $S^3$ . Since  $h(K) = K$ ,  $K$  is achiral.<sup>52)</sup> This completes the proof.  $\square$

As a consequence of Proposition 1, if a chiral knot can be unknotted by switching crossings of either signs, it has at least two equivalence classes of unknotting operations. Taniyama showed there is only one equivalence class of unknotting operations for twist knots. As twist knots other than the figure-8-knot are chiral, this establishes, by a different argument, Stoimenow’s result:

**Result 1** (Proposition 3.21<sup>39)</sup>). *The only twist knot which unknots by switching crossings of either signs (not necessarily in the same diagram) is the figure-8-knot.*

Taniyama also showed for rational knots that the number of equivalence classes is at most two and a rational knot with two equivalence classes has the form given in (4.1) or its mirror image. If we put an orientation on such a knot, we can see that the crossings of the two unknotting operations have the same sign if  $n$  is even and opposite sign if  $n$  is odd (see Fig. 8 for the case that  $n$  is odd, and Figs. 10 and 11 for the cases that  $n = 1$  and 3, respectively). Moreover by, for example, Proposition 4 in Ref. 53),  $C(3, 2, 2, \dots, 2, -2, -2, \dots, -2)$  is chiral for each  $n$ . Hence we have the following result.

**Result 2.** *A chiral unknotting number one rational knot can be unknotted by switching crossings of either signs (not necessarily in the same diagram) if and only if it can be expressed as:  $C(3, 2, 2, \dots, 2, -2, -2, \dots, -2)$ , or its mirror image, where the number of 2’s is  $n$  and that of  $-2$ ’s is  $n + 1$ , for some positive odd integer  $n$ .*

*Remark:* In Refs. 54) and 39), it is shown that for any alternating diagram of an unknotting number one rational knot, there is a crossing corresponding to an unknotting operation. If we apply a similar move to those shown in Figs. 10 and 11 to Fig. 8 (or Fig. 5 in Ref. 35)), we obtain an alternating diagram with two crossings which correspond to inequivalent unknotting operations. By the affirmative answer to the Tait flying conjecture by Menasco and Thistlethwaite,<sup>47)</sup> any reduced (i.e. without nugatory crossings) alternating diagram of the knot can be obtained by a

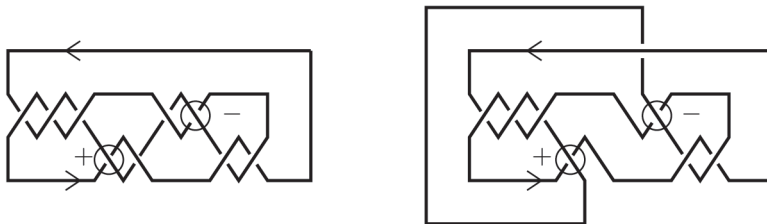


Fig. 10.  $C(3, 2, -2, -2)$  is  $8_{13}$ . By a move in a paper by Nakanishi,<sup>54)</sup> two inequivalent unknotting operations can be seen in alternating diagrams. The diagram in Fig. 12 can be obtained by a flype and isotopy on  $S^2$ .

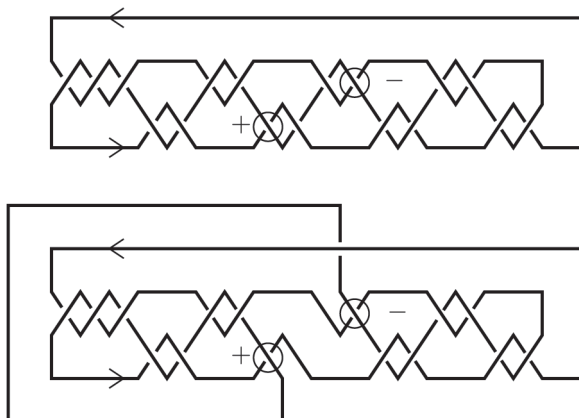


Fig. 11.  $C(3, 2, 2, 2, -2, -2, -2, -2)$  has crossing number 16. The bottom diagram is a reduced alternating diagram with 16 crossings. Hence this knot has crossing number 16 (cf. Murasugi,<sup>55)</sup> Thistlethwaite,<sup>56)</sup> and Kauffman<sup>57)</sup>).

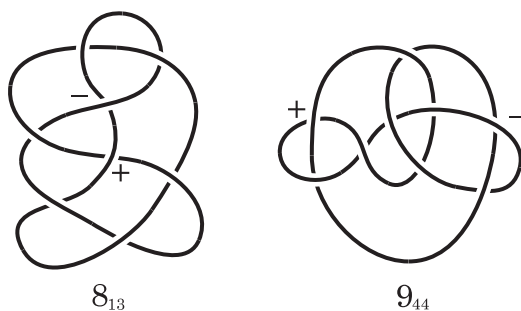


Fig. 12.  $8_{13}$  (left) and  $9_{44}$  (right) with both types of crossing changes marked.

sequence of flypes from this diagram. Since crossings which correspond to unknotting operations do not disappear after a flype, for any alternating diagram of the knot we can always find two crossings which correspond to inequivalent unknotting operations. Recall that all rational knots are alternating. Hence, for any of the chiral unknotting number one rational knots which can be unknotted by switching crossings of either sign, there do exist diagrams in which either crossing change can be applied to unknot the knot.

In summary, Result 1 tells us that the Main Question is answered affirmatively for all chiral twist knots; this is consistent with the results from the  $\Theta$ -SAP simulation since the knots  $3_1$ ,  $5_2$  and  $6_1$  are all chiral twist knots. Result 2 tells us that there is exactly one rational knot with 15 or fewer crossings for which the Main Question is not answered affirmatively. Specifically this is  $8_{13}$  (see Fig. 12), which is  $C(3, 2, -2, -2)$  (see Fig. 10). The next such knot is a 16 crossing knot  $C(3, 2, 2, 2, -2, -2, -2, -2)$  (see Fig. 11). This explains the  $\Theta$ -SAP simulation results regarding  $6_2$ , which is rational but not twist.

4.2. *Traczyk’s results and their consequences*

In this section, we review the results of Traczyk<sup>38)</sup> to address the Main Question of this paper. We thus focus on the knots up to 9 crossings as tabulated in section 5 in Ref. 38) (hereafter we refer to this tabulation as Table T). Of these, the only chiral unknotting number one knots are

$$3_1, 5_2, 6_1, 6_2, 7_2, 7_6, 7_7, 8_1, 8_7, 8_{11}, 8_{13}, 8_{14}, 8_{20}, 8_{21}, \\ 9_2, 9_{12}, 9_{14}, 9_{19}, 9_{21}, 9_{22}, 9_{24}, 9_{26}, 9_{27}, 9_{28}, 9_{30}, 9_{33}, 9_{34}, 9_{39}, 9_{42}, 9_{44}, 9_{45}. \quad (4.2)$$

(In Table T, the unknotting numbers of  $8_{10}$  and  $8_{16}$  are listed as uncertain, however, their unknotting numbers have since been resolved as two.<sup>33),58),59)</sup> In this section we present a table (see Table I) for these knots which is similar to Table T except that we have used Results 1 and 2 of this paper to update the information. Since signed unknotting number information is chirality-class dependent, knowing to which chirality class each of the knots in the table belongs is important. As discussed in §2, we use the sign of the projected writhe, denoted  $sWr(K)$ , of the knot diagrams in Table R to distinguish between a chiral knot  $K$  and its mirror image  $K^*$ . We understand from Traczyk that the naming convention in Table T is related to that given in Jones [60], Table 15.9], which is not the same as that in Table R.<sup>44)</sup> Here, in column one of Table I, we specify the name of the knot according to Table R, where a \* superscript indicates that it is the mirror image of the knot in Table R; the value of  $sWr$  (as calculated using KnotPlot<sup>61)</sup>) for the specified knot is given in the fourth column of our table.

Following Ref. 38), we define the function  $f_K(n)$  (for a knot  $K$ ) to be the minimum number of  $-+$  changes necessary to unknot  $K$  if at most  $n$   $+ -$  changes are allowed. Thus for a chiral unknotting number one knot  $K$ , the answer is yes to the Main Question if either

$$f_K(0) = f_K(1) = 1,$$

since this means that  $u_- = 1$  and  $u_+ > 1$ ; or

$$f_K(0) > 1 \text{ and } f_K(1) = 0,$$

since this means that  $u_+ = 1$  and  $u_- > 1$ . Meanwhile the answer to the Main Question is no if

$$f_K(0) = 1 \text{ and } f_K(1) = 0,$$

since this means that  $u_+ = u_- = 1$ . To determine  $f_K(n)$ , Traczyk uses at least two results. First, if the signature,  $\sigma_K$ , (as defined by Murasugi<sup>62)</sup>) of the knot is positive then a  $+ -$  change cannot decrease the signature and hence, since  $\sigma_{0_1} = 0$ ,  $K$  cannot be unknotted by any number of only  $+ -$  changes. Second, he establishes a criterion [38), Theorem 3.1] for the positive signed unknotting number of a knot  $K$  based on  $u(K)$  and the evaluation of the Jones polynomial,  $V_K$ , at  $\omega = e^{2\pi i/6}$  (see also Lemma 2.1 of Ref. 63)). For an unknotting number one knot  $K$ , the criterion yields that: if  $K$  is unknotted by a  $+ -$  change, then  $V_K(\omega) \in \{\pm 1, i\sqrt{3}\}$  while if it is unknotted by a  $- +$  change, then  $V_K(\omega) \in \{\pm 1, -i\sqrt{3}\}$ . Except for the cases of  $8_{13}$ ,  $9_{33}$  and  $9_{44}$  discussed below, we have used the definition of  $V_K$  as in Ref. 63)

Table I. Signed unknotting information for the chiral unknotting number one knots of Table T [38], section 5]. Items marked with a † are corrections to Table T; details of the corrections are given in the text. The column titled “Main Question” gives the answer to our Main Question.  $sWr$  denotes the sign of the projected writhe from the Table R diagram of the knot  $K$ , or its opposite sign for  $K^*$ .  $V_K(\omega) = \pm(i\sqrt{3})^v$  is reported as  $\pm v$  in column 6.

$K$	$f_K(0)$	$f_K(1)$	$\sigma_K$	$sWr$	$\pm v$	$u_-$	$u_+$	Main Question	Knot Class
3 <sub>1</sub>	1	1	2	−	−1	1	> 1	YES	twist
5 <sub>2</sub>	1	1	2	−	−0	1	> 1	YES	twist
6 <sub>1</sub>	2	0	0	−	−0	> 1	1	YES	twist
6 <sub>2</sub>	1	1	2	−	+0	1	> 1	YES	rational
7 <sub>2</sub>	1	1	2	−	+0	1	> 1	YES	twist
7 <sub>6</sub>	1	1	2	−	−0	1	> 1	YES	rational
7 <sub>7</sub> <sup>*</sup>	2	0	0	−	+1	> 1	1	YES	rational
8 <sub>1</sub>	∈ {2, 3}	0	0	−	+0	> 1	1	YES	twist
8 <sub>7</sub> <sup>*</sup>	1	1	2	−	+0	1	> 1	YES	rational
8 <sub>11</sub>	1	1	2	−	−1	1	> 1	YES	rational
8 <sub>13</sub>	1	0 <sup>†</sup>	0 <sup>†</sup>	+	−0	1	1	NO	rational
8 <sub>14</sub>	1	1	2	−	−0	1	> 1	YES	rational
8 <sub>20</sub>	1	1	0	−	−1	1	> 1	YES	not rational
8 <sub>21</sub>	1	1	2	−	−1	1	> 1	YES	not rational
9 <sub>2</sub>	1	1	2	−	−1	1	> 1	YES	twist
9 <sub>12</sub>	1	1	2	−	+0	1	> 1	YES	rational
9 <sub>14</sub>	∈ {2, 3}	0	0	+	+0	> 1	1	YES	rational
9 <sub>19</sub>	1	1 <sup>†</sup>	0	−	−0	1	> 1	YES	rational
9 <sub>21</sub> <sup>*</sup>	1	1	2	−	−0	1	> 1	YES	rational
9 <sub>22</sub> <sup>*</sup>	1	1	2	−	−0	1	> 1	YES	not rational
9 <sub>24</sub>	1	1	0	−	−1	1	> 1	YES	not rational
9 <sub>26</sub> <sup>*</sup>	1	1	2	−	+0	1	> 1	YES	rational
9 <sub>27</sub>	2 <sup>†</sup>	0	0	−	+0	> 1	1	YES	rational
9 <sub>28</sub>	1	1	2	−	−1	1	> 1	YES	not rational
9 <sub>30</sub>	∈ {1, 2}	0	0	−	−0	> 1?	1	?	not rational
9 <sub>33</sub> <sup>*</sup>	∈ {1, 2}	0 <sup>†</sup>	0	+	+0	> 1?	1	?	not rational
9 <sub>34</sub>	2	0	0	−	+1	> 1	1	YES	not rational
9 <sub>39</sub> <sup>*</sup>	1	1	2	−	−0	1	> 1	YES	not rational
9 <sub>42</sub> <sup>*</sup>	1	1	2	−	−0	1	> 1	YES	not rational
9 <sub>44</sub>	1	0	0	−	−0	1	1	NO	not rational
9 <sub>45</sub>	1	1	2	−	+0	1	> 1	YES	not rational

along with the values of  $f_K$  in Table T to establish the correspondence between the knots in Table T and those of Table R and we indicate this in column one of Table I. Consistent with Table T, the value of  $V_K(\omega) = \pm(i\sqrt{3})^v$  for a knot is presented (in column 6) in the form  $\pm v$ . Table I also shows updated values for  $f_K(0)$  and  $f_K(1)$  for the chiral unknotting number one knots, where we have used updated unknotting number information and Results 1 and 2 of this paper. The last column indicates which knots are rational and amongst those which are twist knots.

The column titled “Main Question” in Table I includes the answer to the Main Question for the given knot. Result 2 of this paper is used to obtain the answer for all the rational knots, and the  $f_K$  values are used to answer the question for the

non-rational knots. Thus there is at least one non-rational knot for which the answer to the Main Question is negative, namely  $9_{44}$ . Figure 12 exhibits a knot diagram (equivalent to the minimal diagram in Rolfsen’s book) for this knot with the two relevant crossings marked.

For the knots  $9_{30}$  and  $9_{33}^*$  the answer to the Main Question remains uncertain. These knots have been investigated via the CMC  $\Theta$ -BFACF algorithm. For each of these two knot-types, after testing over 25 million essentially independent  $\Theta_0^-$ -SAPs of varying lengths, no unknots were obtained after a  $-+$  strand passage. In addition, we investigated these knots using another strand passage model. Specifically, the Hua et al.<sup>64)</sup> strand passage model has recently been extended to include a topological filter with a chirality bias.<sup>65)</sup> Using numerical results from this model for 20000 essentially independent lattice polygons of length 100, neither  $9_{30}$  nor  $9_{33}^*$  was unknotted by a  $-+$  strand passage. All this leads us to conjecture that the answer to the Main Question is yes for these two knots.

Values in Table I marked by a dagger have been modified from Table T. These modifications are as follows. Table T had an uncertainty regarding  $f_{9_{27}}(0)$ , namely  $1 \leq f_{9_{27}}(0) \leq 2$ . Since  $9_{27}$  is rational, this can be resolved, using Result 2, to  $f_{9_{27}}(0) = 2$ . In particular, for  $f_{9_{27}}(0)$  to be 1, it would mean that  $u_-(9_{27}) = 1$  and  $u_+(9_{27}) = 1$ , contradicting Result 2. Similarly for  $9_{19}$ , the uncertainty in Table T for  $f_{9_{19}}(1)$  is resolved.

There is also an uncertainty in Table T regarding  $9_{33}$ , namely  $1 \leq f_{9_{33}}(0) \leq 2$ . Table T also indicates  $f_K(1) = 1$  for this knot. Based on the uncertainty in  $f_K(0)$ , we believe the knot in Table T corresponds to  $9_{33}^*$ . This knot can be unknotted in a single  $+ -$  crossing change as seen directly from its minimal diagram, and hence  $f_K(1) = 0$ ; we have reported this in Table I. However, the uncertainty in  $f_K(0)$  remains.

Finally  $8_{13}$  (regardless of its chirality-class) has signature 0 and  $f_K(1) = 0$  (by Result 2) hence the entries for these two quantities are incorrect in Table T and have been corrected here.

Thus all the knots other than  $8_{13}, 9_{30}, 9_{33}$  and  $9_{44}$  have been proved to satisfy the property that exactly one of  $u_+$  and  $u_-$  is 1. These knots are

$$\begin{aligned}
 &3_1, 5_2, 6_1, 6_2, 7_2, 7_6, 7_7, 8_1, 8_7, 8_{11}, 8_{14}, 8_{20}, 8_{21}, \\
 &9_2, 9_{12}, 9_{14}, 9_{19}, 9_{21}, 9_{22}, 9_{24}, 9_{26}, 9_{27}, 9_{28}, 9_{34}, 9_{39}, 9_{42}, 9_{45}. \tag{4.3}
 \end{aligned}$$

### §5. Discussion

Because of the supercoiled nature of DNA in the cell, twist knots are expected to be the most likely non-trivial knots produced after a single strand passage on an unknotted substrate. Result 1 of this paper tells us that a twist knot  $K$  can either be unknotted in one step by a  $+ -$  crossing change or by a  $- +$  crossing change but not by both. In particular, if  $K$  can only be unknotted by a  $+ -$  crossing change, then its mirror image  $K^*$  can only be unknotted by a  $- +$  crossing change. Thus this gives another way to distinguish between a twist knot and its mirror image. Furthermore, if a hypothetical topoisomerase is selective for a positive crossing (say)

at a strand passage site, then after a single strand passage, selectivity for twist knots of only one chirality class (those unknotted by a  $-+$  crossing change) is guaranteed. This is because only these twist knots could result from a  $+ -$  strand passage on the unknot, and no  $+ -$  strand passage on such a twist knot could unknot it (however knots which have the twist knot in their prime decomposition could result). Result 2, gives a similar conclusion for all rational knots with seven or fewer crossings. Furthermore, there is only one 8 crossing knot for which there could be knots of both chirality classes after a single strand passage. Although topoisomerases appear only to have a preferential (as opposed to selective) chirality bias, our results imply that this will influence the chirality of the post-strand-passage knots.

With respect to strand passage models, the  $\Theta$ -SAP and the recent He et al. model<sup>65</sup>) both incorporate a chirality bias and are hence useful for studying knot chirality discrimination via strand passage. They can and have been used to model the chirality preferences of enzyme action on DNA and to investigate knot theoretic questions such as the Main Question of this paper. Furthermore, the knot theory results of this paper can be used to better understand the models. For example, with respect to the  $\Theta$ -BFACF algorithm, the affirmative answer to the question for each knot  $K$  in (4.3) makes it clear that the after-strand-passage knot distribution for  $\Theta_0^+$ -SAPs can be very different from that for  $\Theta_0^-$ -SAPs (for positive trefoils, for example, the latter contains unknots, while the former does not). However the mirror operation defined previously still gives a one-to-one mapping between a knot-type  $K$   $\Theta_0^+$ -SAP and a knot-type  $K^*$   $\Theta_0^-$ -SAP which preserves the after-strand-passage knot-type but with opposite chirality, and hence the after-strand-passage knot distribution for  $\Theta_0$ -SAPs can be investigated using  $\Theta_0$ -SAPs of either type ( $\Theta_0^+$  or  $\Theta_0^-$ ).

### Acknowledgements

CS acknowledges financial support from NSERC and a WestGrid resource allocation from Compute Canada. KI is supported by a postdoctoral fellowship from EP-SRC Grant EP/H031367/1 to D. Buck. KS is supported by KAKENHI (22540066). MV is supported by NSF grants DMS0920887 and DMS1057284, and by NIH grant 2S06GM052588-12. The authors acknowledge Kevin He for providing numerical results from Ref. 65).

### References

- 1) A. Bates and A. Maxwell, *DNA Topology* (Oxford University Press, New York, 2005).
- 2) J. B. Schwartzman and A. Stasiak, *EMBO Reports* **5** (2004), 256
- 3) J. Arsuaga, M. Vazquez, S. Trigueros, D. Sumners and J. Roca, *Proc. Natl. Acad. Sci. USA* **99** (2002), 5373.
- 4) L. F. Liu, J. L. Davis and R. Calendar, *Nucleic Acids Res.* **9** (1981), 3979.
- 5) S. A. Wasserman and N. R. Cozzarelli, *J. Biol. Chem.* **266** (1991), 20567.
- 6) D. W. Sumners, C. Ernst, S. J. Spengler and N. R. Cozzarelli, *Q. Rev. Biophys.* **28** (1995), 253.
- 7) J. Portugal and A. Rodriguez-Campos, *Nucleic Acids Res.* **24** (1996), 4890.
- 8) R. W. Deibler, J. K. Mann, D. W. L. Sumners and L. Zechiedrich, *BMC Mol. Biol.* **8** (2007), 44.
- 9) J. C. Wang, *Nat. Rev. Mol. Cell Biol.* **3** (2002), 430.
- 10) P. Forterre, S. Gribaldo, D. Gabelle and M. C. Serre, *Biochimie* **89** (2007), 427.



- 11) J. Roca, *Nucleic Acids Res.* **37** (2009), 721.
- 12) J. M. Fogg, D. J. Catanese, G. L. Randall, M. C. Swick and L. Zechiedrick, *IMA Vol. in Math. and its App.* **150** (2009), 73.
- 13) J. C. Wang, *Q. Rev. Biophys.* **31** (1998), 107.
- 14) A. Maxwell, L. Costenaro, S. Mittelheiser and A. D. Bates, *Biochem. Soc. Trans.* **33** (2005), 1460.
- 15) J. J. Champoux, *Annu. Rev. Biochem.* **70** (2001), 369.
- 16) K. C. Neuman, G. Charvin, D. Bensimon and V. Croquette, *Proc. Natl. Acad. Sci. USA* **106** (2009), 6986.
- 17) S. Trigueros, J. Salceda, I. Bermudez, X. Fernandez and J. Roca, *J. Mol. Biol.* **335** (2004), 723.
- 18) S. C. Kampranis, A. D. Bates and A. Maxwell, *Proc. Natl. Acad. Sci. USA* **96** (1999), 8414.
- 19) J. Gore, Z. Bryant, M. D. Stone, M. Nöllmann, N. R. Cozzarelli and C. Bustamante, *Nature* **439** (2006), 100.
- 20) S. Y. Shaw and J. C. Wang, *Proc. Natl. Acad. Sci. USA* **94** (1997), 1692.
- 21) M. Nöllmann, N. J. Crisona and P. B. Arimondo, *Biochimie* **89** (2007), 490.
- 22) A. D. Bates, M. H. O’Dea and M. Gellert, *Biochemistry* **35** (1996), 1408.
- 23) A. Vologodskii, *Biophys. J.* **87** (2004), 3066.
- 24) N. M. Baker, S. Weigand, S. Maar-Mathias and A. Mondragón, *Nucleic Acids Res.* **39** (2011), 755.
- 25) K. V. Klenin, J. Langowski and A. V. Vologodskii, *J. Mol. Biol.* **320** (2002), 359.
- 26) M. D. Stone, Z. Bryant, N. J. Crisona, S. B. Smith, A. Vologodskii, C. Bustamante and N. R. Cozzarelli, *Proc. Natl. Acad. Sci. USA* **100** (2003), 8654.
- 27) G. Charvin, T. R. Strick, D. Bensimon and V. Croquette, *Biophys. J.* **89** (2005), 384.
- 28) N. J. Crisona, T. R. Strick, D. Bensimon, V. Croquette and N. R. Cozzarelli, *Genes Dev.* **14** (2000), 2881.
- 29) M. L. Szafron, “Knotting Statistics After a Local Strand Passage in Unknotted Self-Avoiding Polygons in  $\mathbb{Z}^3$ ”, PhD Thesis, University of Saskatchewan (2009).
- 30) M. L. Szafron and C. E. Soteros, *J. of Phys. A* **44** (2011), 245003.
- 31) M. L. Szafron and C. E. Soteros, *J. of Phys. A* **44** (2011), 322001.
- 32) C. Gordon and J. Luecke, *Algebr. Geom. Topol.* **6** (2006), 2051.
- 33) P. Ozsváth and Z. Szabó, *Topology* **44** (2005), 705.
- 34) T. Kanenobu and H. Murakami, *Proc. Amer. Math. Soc.* **98** (1986), 499.
- 35) K. Taniyama, *Math. Ann.* **291** (1991), 579.
- 36) K. Motegi, *Rev. Mat. Univ. Complut. Madrid* **9** (1996), 151.
- 37) T. D. Cochran and W. B. L. Lickorish, *Trans. Amer. Math. Soc.* **297** (1986), 125.
- 38) P. Traczyk, *Contemp. Math.* **233** (1999), 215.
- 39) A. Stoimenow, *Math. Scand.* **94** (2004), 227.
- 40) I. Darcy, “Biological Metrics on DNA Knots and Catenanes”, PhD Thesis, Florida State University (1997).
- 41) H. Moon, “Calculating Knot distances and solving tangle equations involving Montesinos Links”, PhD Thesis, University of Iowa (2010).
- 42) K. Murasugi, *Knot theory and its applications* (Birkhäuser Boston, Inc., Boston, 2008).
- 43) C. C. Adams, *The knot book* (American Mathematical Society, Providence, 2004).
- 44) D. Rolfsen, *Knots and Links* (Publish or Perish, Houston, 1990).
- 45) J. H. Conway, “Computational Problems in Abstract Algebra”, *Proc. Conf., Oxford, 1967* (1970), p. 329.
- 46) G. Burde and H. Zieschang, *Knots* (Walter de Gruyter & Co., Berlin, 2003).
- 47) W. Menasco and M. B. Thistlethwaite, *Ann. Math.* **138** (1993), 113.
- 48) J. Portillo, Y. Diao, R. Scharein, J. Arsuaga and M. Vazquez, *J. of Phys. A* **44** (2011), 275004.
- 49) M. L. Szafron, “Monte Carlo Simulations of Strand Passage in Unknotted Self-Avoiding Polygons”, MSc Thesis, University of Saskatchewan (2000).
- 50) I. Darcy and D. W. Summers, *Math. Proc. Camb. Phil. Soc.* **128** (2000), 497.
- 51) M. Scharlemann, *Chaos, Solitons, and Fractals* **9** (1998), 693.
- 52) J. Hoste, M. Thistlethwaite and J. Weeks, *Math. Intelligencer* **20** (1998), 33.
- 53) C. Ernst and D.W. Summers, *Math. Proc. Camb. Phil. Soc.* **102** (1987), 303.

- 54) Y. Nakanishi, *Proceeding of the 5-th Korea-Japan School of Knots and Links* (1997), p. 213.
- 55) K. Murasugi, *Topology* **26** (1987), 187.
- 56) M. B. Thistlethwaite, *Topology* **26** (1987), 297.
- 57) L. Kauffman, *Topology* **26** (1987), 395.
- 58) A. Stoimenow, *Math. Res. Lett.* **11** (2004), 755.
- 59) H. Murakami and A. Yasuhara, *Proc. Amer. Soc.* **128** (2000), 3693.
- 60) V. F. R. Jones, *Ann. Math.* **126** (1987), 335.
- 61) R. Scharein, KnotPlot. <http://www.knotplot.com>  
Program for drawing, visualizing, manipulating, and energy minimizing knots.
- 62) K. Murasugi, *Trans. Amer. Math. Soc* **117** (1965), 387.
- 63) T. Kanenobu, *J. Knot Theory Ramifications* **19** (2010), 1535.
- 64) X. Hua, D. Nguyen, B. Raghavan, J. Arsuaga and M. Vazquez, *Topology and its Applications* **154** (2007), 1381.
- 65) K. He, R. Scharein, A. Chen and M. Vazquez, preprint.