

Hard Unknots and Collapsing Tangles

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0 Introduction

Classical knot theory is about the classification, up to isotopy, of embedded closed curves in three-dimensional space. Two closed curves embedded in three-dimensional space are said to be *isotopic* if there is a continuous family of embeddings starting with one curve and ending with the other curve. This definition of isotopy captures our intuitive notion of moving a length of elastic rope about in space without tearing it. Given a closed loop of rope in space, it can sometimes be deformed in this way to a simple flat circle. In such a case we say that the loop is *unknotted*.

So it is not absurd if we sometimes ask, Is this knot unknotted? The question is not only non-contradictory, it is often hard. Look ahead to Figures 5 and 6. The shapes illustrated are unknots, but most people's intuition does not allow recognizing the unknotting, although it will present itself if one makes a rope model and shakes it. Recognizing unknots is a starting point for all of knot theory.

Corresponding to the physical models, one can make mathematical models of knots by formalizing the diagrams that one naturally draws for them, as in Figure 2. The study based on the diagrams is called *combinatorial knot theory*. The diagrams are well defined as mathematical structures, namely, planar graphs with four edges incident to each vertex and with extra structure: indication at each vertex of which strand crosses over and which under.

This paper is both an exposition of combinatorial knot theory, intended to be self-contained and readable by a beginner in the theory of knots and links, and a research paper. The new material is the presentation of an infinite collection of examples of unknot diagrams (and also knot and link diagrams) that are *hard*, in a precise sense shortly to be explained, and a beautiful characterization of a certain class of unknots in terms of continued fractions and their convergents (Theorems 6 and 7). We pinpoint the smallest hard unknot

diagrams (Theorem 8). We apply our results in a discussion of DNA recombination. Along the way, we rely heavily on John H. Conway's theory of *rational tangles*. Rational tangles allow algebraic operations, leading to connections with matrices and continued fractions.

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1 Culprits

Combinatorial knot theory got its start in the hands of Kurt Reidemeister [26], who discovered a set of moves on planar diagrams that capture the topology of knots and links embedded in three dimensional space. Reidemeister proved that if we have two knots or links in three-dimensional space, then they are isotopic if and only if corresponding diagrams for them can be obtained, one from the other, by a sequence of moves of the types shown in Figure 1.

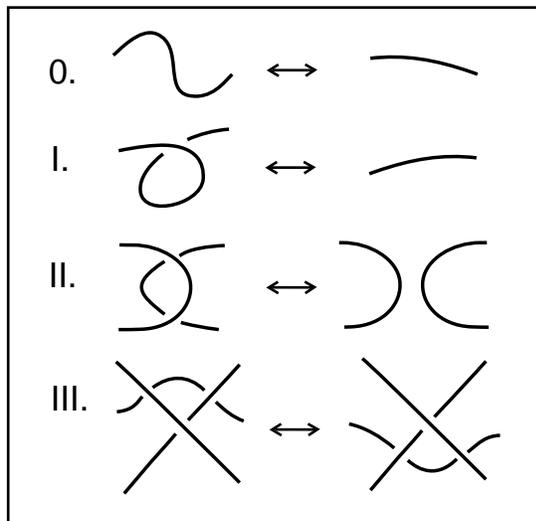


Figure 1 - The Reidemeister Moves

The moves are local and they are performed on the diagrams in such a way that the rest of the diagram is left fixed. This means that when one searches

for available Reidemeister moves on a diagram, one searches for one-sided, two-sided, and three-sided regions with the appropriate crossing patterns as shown in Figure 1. It is important to note that knot and link diagrams are taken to be on the surface of a two dimensional sphere that is standardly embedded in three-dimensional space. Thus the outer region of a planar diagram is handled just like any other region in that diagram, and can be the locus of any of the moves. In this section, we discuss the unknotting of knot diagrams using the Reidemeister moves.

Definition 1 We shall call a diagram of the unknot *hard* if it has the following three properties, where a move is *simplifying* if it reduces the crossing number of the diagram:

1. There are no simplifying type I or type II moves on the diagram.
2. There are no type III moves on the diagram.

Hard unknot diagrams must be made more complex before they will simplify to the unknot, if we use Reidemeister moves.

Here is an example of a hard unknot diagram (originally due to Ken Millett [22]), in Figure 2. We like to call this diagram the “Culprit”. The Culprit is a knot diagram that represents the unknot, but as a diagram, and using only the Reidemeister moves, it must be made more complicated before it can be simplified to an unknotted circle. We define the *complexity* of a knot or link diagram K to be the number of crossings, $C(K)$, in the diagram. The Culprit has 10 crossings, and in order to be undone, we definitely have to increase the number of crossings before decreasing them to zero. The reader can verify this for himself by checking each region in the diagram of the Culprit. A simplifying Reidemeister II-move can occur only on a two-sided region, but no two-sided region in the diagram admits such a move. Similarly, on the Culprit diagram there are no simplifying Reidemeister I-moves and there are no Reidemeister III-moves (note that a III-move does not change the complexity of the diagram).

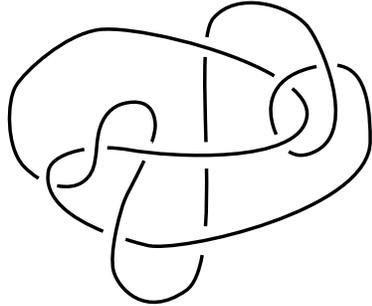


Figure 2 - The Culprit

View Figure 3 for an unknotting sequence for the Culprit. Notice that we undo it by swinging the arc that passes underneath most of the diagram outward, and that in this process the number of crossings in the intermediate diagrams increases. In the diagrams of Figure 3 the largest increase is to a diagram of 12 crossings. This is the best possible result for the initial diagram in the figure.

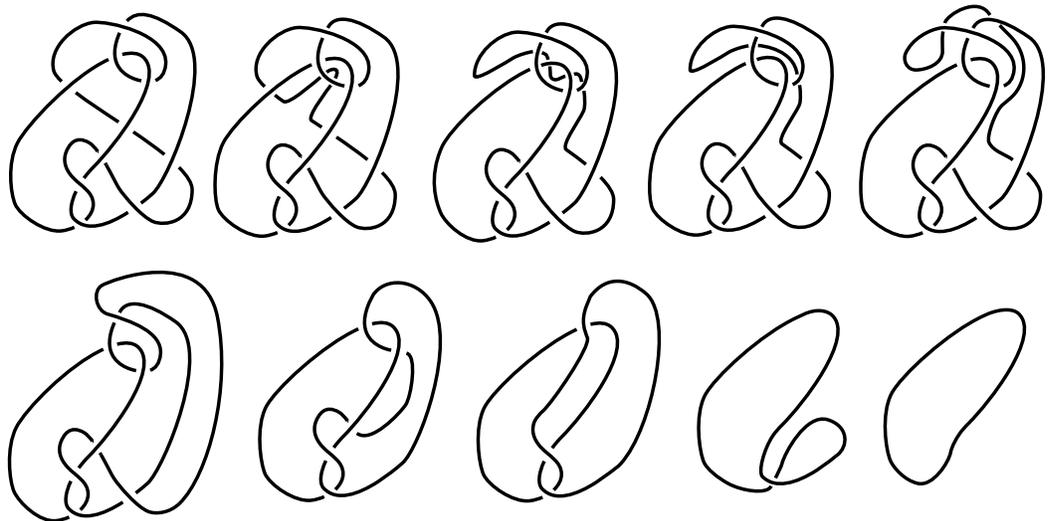


Figure 3 - The Culprit Undone

In contrast to the Culprit, view Figure 4 for an example of an easy unknot. This one simplifies after Reidemeister III-moves unlock further moves of type I and type II. The reader can probably just look at the diagram in Figure 4 and see at once that it is unknotted.

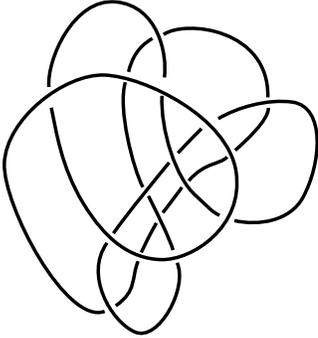


Figure 4 - An Easy Unknot

It is an unsolved problem just how much complexity can be forced by a hard unknot.

Definition 2 Recall that the *complexity* of a diagram K is the number of crossings, $C(K)$, of that diagram. Let K be a hard unknot diagram. Let K' be a diagram isotopic to K such that K' can be simplified to the unknot. For any unknotting sequence of Reidemeister moves for K there will be a diagram K'_{max} with a maximal number of crossings. Let $Top(K)$ denote the minimum of $C(K'_{max})$ over all unknotting sequences for K . Let

$$R(K) = Top(K)/C(K)$$

be called the *recalcitrance* of the hard unknot diagram K . Very little is known about $R(K)$.

In the case of our Culprit, $Top(K) = 12$, while $C(K) = 10$. Thus $R(K) = 1.2$. A knot that can be simplified with no extra complexity has recalcitrance equal to 1. We shall have more to say about the recalcitrance later.

In [12] Hass and Lagarias show that there exists a positive constant c_1 such that, for each $n > 1$, any unknotted diagram D with n crossings can be transformed to the trivial knot diagram using less than or equal to $2^{c_1 n}$ Reidemeister moves. As a corollary to this result, they conclude that any unknotted diagram D can be transformed by Reidemeister moves to the trivial knot diagram through a sequence of knot diagrams each of which has at most $2^{c_1 n}$ crossings. In our language, this result says that

$$R(D) \leq \frac{2^{c_1 C(D)}}{C(D)}.$$

The authors of [12] prove their result for $c_1 = 10^{11}$, but remark that this is surely too large a constant. Much more work needs to be done in this domain. We should also remark that the question of the knottedness of a knot is algorithmically decidable, due to the work of Haken and Hemion [13]. This algorithm is quite complex, but its methods are used in the work of Hass and Lagarias.

The next example is illustrated in Figure 5, a three-dimensional rendering of an unknot. This example is interesting psychologically, because it looks knotted to most observers. The three-dimensional picture is a frame from a deformation of this example in the energy minimization program KnotPlot [28]. It is illuminating to run the program on this example and watch the knot self-repel and undo itself. We leave the verification that this is an unknot as an exercise for the reader.

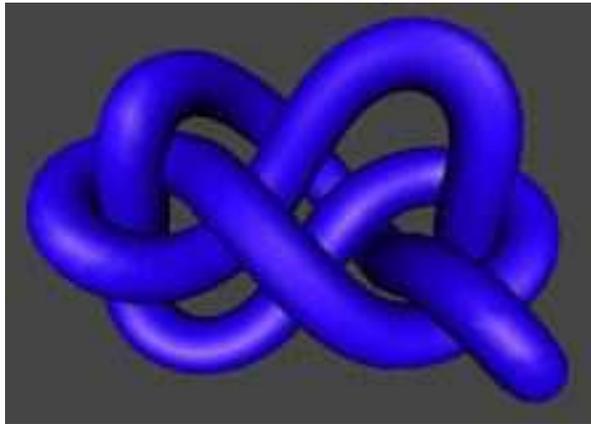


Figure 5 - Three-Dimensional Unknot

Finally, in Figure 6 we give an example of a hard unknot that is of a different type than the sort that we are considering in this paper. (It is not the closure of the sum of two rational tangles.) There are many knots and many hard unknots. We only scratch the surface of this subject.

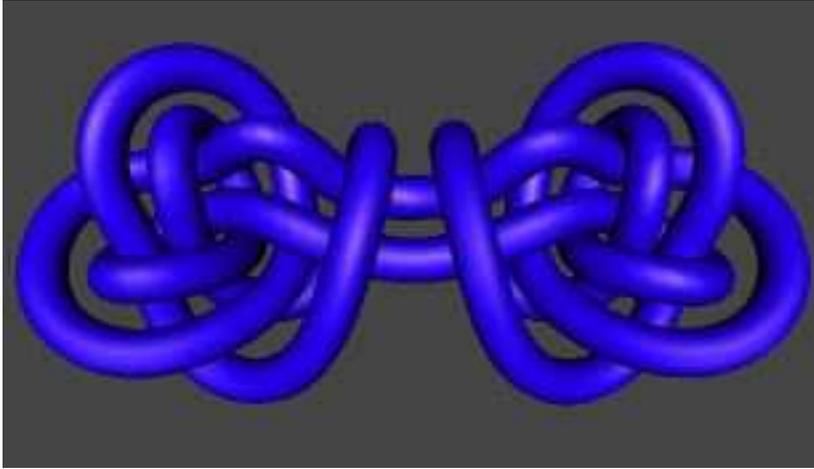


Figure 6 - Another Hard Unknot

For work on unknots related to braids see [23]. See also the work of Dynnikov [4] for a remarkable diagramming system for knots and links in which unknot diagrams can be detected by simplification only. Finally, another approach to detecting unknots is the use of invariants of knots and links. For example, it is conjectured that the Jones polynomial [15, 16] of a knot diagram is equal to one, only when that knot is unknotted.

2 Rational Tangles, Rational Knots and Continued Fractions

In this section we recall the subject of rational tangles and rational knots and their relationship with the theory of continued fractions. By the term “knots” we will refer to both knots and links, and whenever we really mean “knot” we shall emphasize it. Rational knots comprise the simplest class of knots. They are also known in the literature as Viergeflechte, four-plats or 2-bridge knots depending on their geometric representation. The theory of tangles was introduced in 1967 by Conway [3] in his work on enumerating and classifying knots and links.

A *2-tangle* is a proper embedding of two unoriented arcs and a finite number of circles in a 3-ball B^3 , so that the four endpoints lie in the boundary of B^3 . A *tangle diagram* is a regular projection of the tangle on a cross-sectional disc of B^3 . By “tangle” we will mean “tangle diagram”. A *rational tangle* is a special

case of a 2-tangle obtained by applying consecutive twists on neighbouring endpoints of two trivial arcs. Such a pair of arcs comprise the $[0]$ or $[\infty]$ tangles (see Figure 8), depending on their position in the plane. We shall say that such a tangle is in *twist form*. For an example see Figure 7. Conway defined the rational knots as “numerator” or “denominator” closures of the rational tangles. See Figure 7. Conway [3] also defined *the fraction* of a rational tangle to be a rational number or ∞ , obtained via a continued fraction that is associated with the tangle. We discuss this construction below.

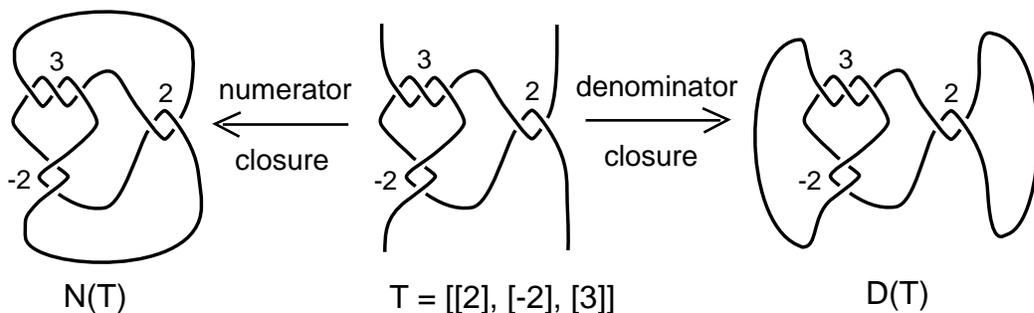


Figure 7 - A Rational Tangle and its Closures to Rational Knots

We are interested in tangles up to isotopy. Two tangles, T, S are *isotopic*, denoted by $T \sim S$, if and only if they have identical configurations of their four endpoints, and they differ by a finite sequence of the Reidemeister moves which take place in the interior of the projection disc. Of course, each twisting operation used in the definition of a rational tangle changes the isotopy class of the tangle to which it is applied. Rational tangles are classified by their fractions by means of the following theorem, different proofs of which are given in [24], [1, 2], [11] and [17].

Theorem 1 (Conway, 1975) *Two rational tangles are isotopic if and only if they have the same fraction.*

2.1 The Tangle Fraction

We shall now recall from [17] the main properties of rational tangles and of continued fractions, which illuminate the classification of rational tangles. The elementary rational tangles are displayed as either horizontal or vertical twists, and they are enumerated by integers or their inverses, see Figure 8.

The crossing types of 2-tangles (and of unoriented knots) follow the *checkerboard rule*: shade the regions of the tangle in two colors, starting from the left

outside region with grey, and so that adjacent regions have different colors. Crossings in the tangle are said to be of “positive type” if they are arranged with respect to the shading as exemplified in Figure 8 by the tangle $[+1]$, i.e. they have the region on the right shaded as one walks towards the crossing along the over-arc. Crossings of the reverse type are said to be of “negative type” and they are exemplified in Figure 8 by the tangle $[-1]$. The reader should note that our crossing type conventions are the opposite of those of Conway in [3]. Our conventions agree with those of Ernst and Sumners [5, 6], [31] which in turn follow the standard conventions of biologists.

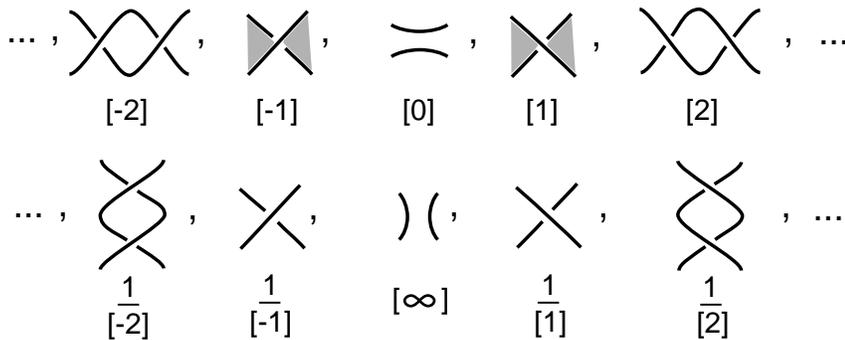


Figure 8 - The Elementary Rational Tangles and the Types of Crossings

In the class of 2-tangles we have the operations *addition* and *multiplication*, as illustrated in Figure 9, which are denoted by “+” and “*” respectively. These operations are well-defined up to isotopy. In order to read out a rational tangle we transcribe it as an algebraic expression using horizontal and vertical twists. For example, Figure 10 illustrates the rational tangle in twist form: $[1] + ([1] * [3] * \frac{1}{[-3]}) + [1]$, and also an isotopic form of the same tangle with expression $(([3] * \frac{1}{[-2]}) + [2])$. The decomposition of this last tangle is shown in Figure 11.

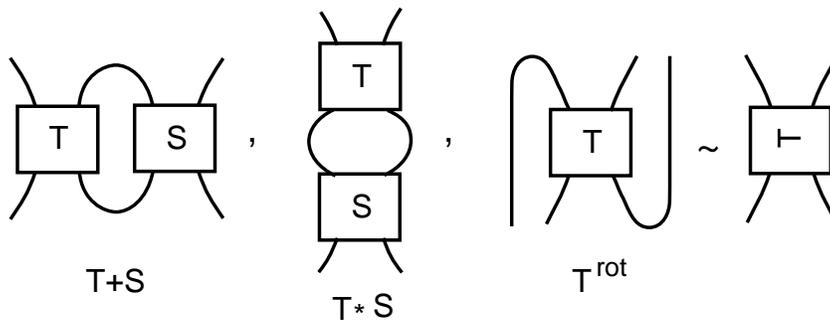


Figure 9 - Addition, Multiplication and Rotation of 2-Tangles

Note that addition and multiplication do not, in general, preserve the class of rational tangles. For example, the 2-tangle $\frac{1}{[3]} + \frac{1}{[3]}$ is not rational. The sum (product) of two rational tangles is rational if and only if one of the two consists in a number of horizontal (vertical) twists.

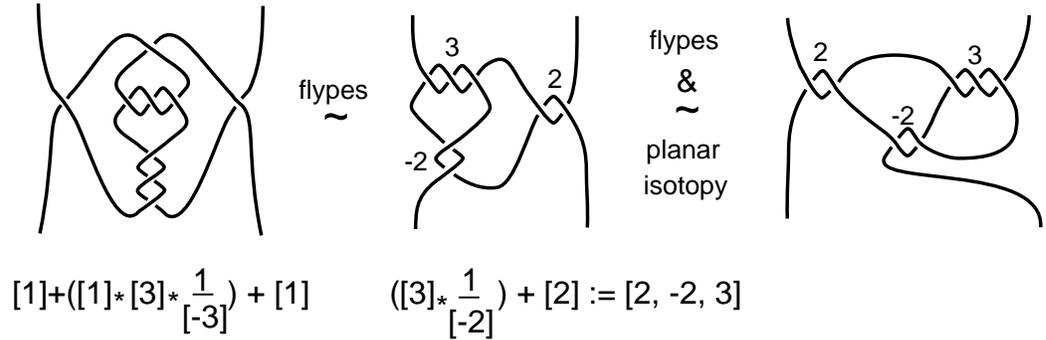


Figure 10 - A Rational Tangle in Twist Form Converted to Its Standard Form and to Its 3-Strand-Braid Representation

The *mirror image* of a tangle T , denoted $-T$, is T with all crossings switched. For example, $-[n] = [-n]$ and $-\frac{1}{[n]} = \frac{1}{[-n]}$. Then, the *subtraction* is defined as $T - S := T + (-S)$. The *rotation* of T , denoted T^{rot} , is obtained by rotating T on its plane counterclockwise by 90° . The *inverse* of T is defined to be $-T^{rot}$. Thus, inversion is accomplished by rotation and mirror image. Note that T^{rot} and the inverse of T are in general not isotopic to T and they are order 4 operations. But for rational tangles the inversion is an operation of order 2. (This follows from *the remarkable property of rational tangles that they are isotopic to their horizontal or vertical flip in space by 180°* . Note that a flip switches the endpoints of the tangle and, in general, a flipped tangle is not isotopic to the original one.) For this reason we shall denote the inverse of a rational tangle T by $1/T$, and hence the rotation of the tangle T will be denoted by $-1/T$. This explains the notation for the tangles $\frac{1}{[n]}$.

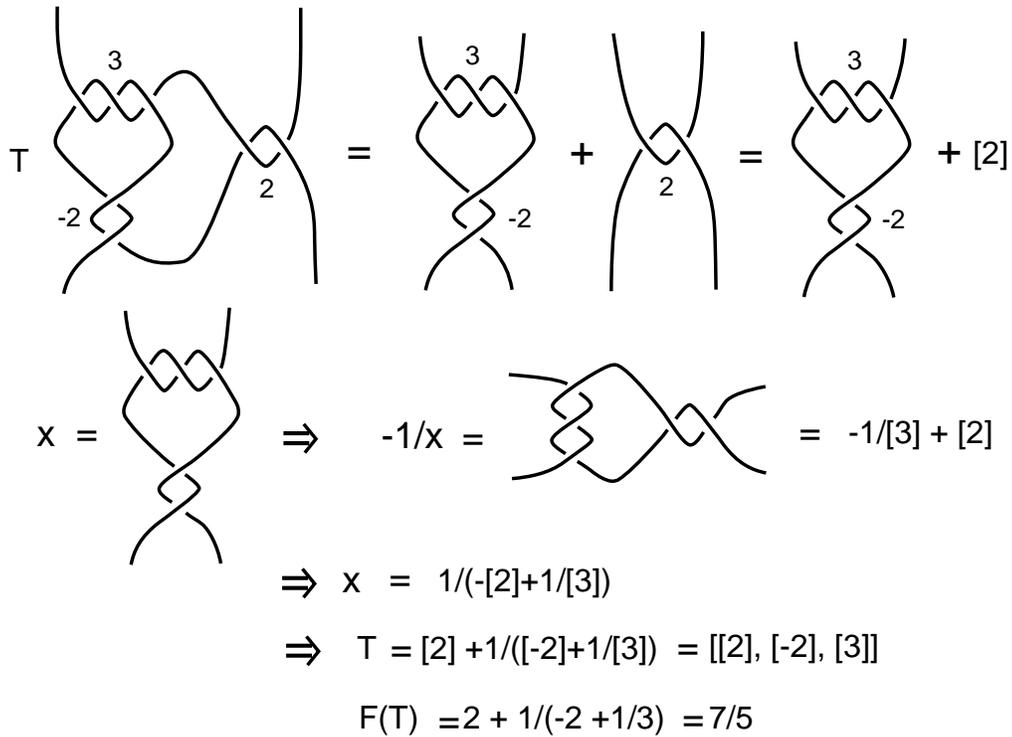


Figure 11 - Finding the Fraction

As we said earlier, there is a fraction associated to a rational tangle which characterizes its isotopy class (Theorem 1). In fact, the fraction is defined for any 2-tangle and always has the following three properties.

1. $F([\pm 1]) = \pm 1$.
2. $F(T + S) = F(T) + F(S)$.
3. $F(T^{rot}) = -1/F(T)$.

If $T = [\infty]$, we assign $F([\infty]) := \infty = \frac{1}{0}$, as a formal expression.

These rules suffice for computing the fraction inductively for rational tangles. So they will serve as the definition of the tangle fraction for rational tangles. In Figure 11 we illustrate the computation of a specific tangle fraction using

the above three rules. For this purpose we observe that a certain tangle's 90° rotate is immediately recognizable as a sum of tangles. Generalizing, the reader can easily deduce the formula below:

$$T * \frac{1}{[n]} = \frac{1}{[n] + \frac{1}{T}}$$

Indeed, rotate $T * \frac{1}{[n]}$ by 90° and note that it becomes $-[n] - \frac{1}{T}$. The original tangle is the negative reciprocal of this tangle. This formula implies that the two operations: addition of $[+1]$ or $[-1]$ and inversion between rational tangles suffice for generating the whole class of rational tangles. As for the fraction, we have the corresponding formula:

$$F(T * \frac{1}{[n]}) = \frac{1}{n + \frac{1}{F(T)}}.$$

For example, in Figure 11, the fraction associated with the tangle T is

$$F(T) = 2 + \frac{1}{-2 + \frac{1}{3}}.$$

Starting from a rational tangle in twist form, one can always bring the twists alternately to the right and to the bottom of the tangle using only isotopy moves on subtangles, called *flypes*. See Figure 12 for an abstract illustration of flypes. Note that in a flype the endpoints of the subtangle remain fixed; this is not true for a flip of the tangle in space. One can then associate to the rational tangle a vector of integers (a_1, a_2, \dots, a_n) , where the first entry denotes the place where the tangle starts untwisting and the last entry where it begins to twist. For example the tangle of Figure 7 corresponds to the vector $(2, -2, 3)$. We then say that the rational tangle is in *standard form* and we denote it by $T = [[a_1], [a_2], \dots, [a_n]]$. We also call this standard form the *continued fraction form* of the tangle, since it can literally be written in the form of a continued fraction involving the elementary integer tangles $[a_i]$.

From the above discussion it follows that for a rational tangle in standard form,

$$T = [[a_1], [a_2], \dots, [a_n]] = [a_1] + \frac{1}{[a_2] + \dots + \frac{1}{[a_{n-1}] + \frac{1}{[a_n]}}$$

for $a_1 \in \mathbb{Z}$, $a_2, \dots, a_n \in \mathbb{Z} - \{0\}$, its fraction is the numerical continued fraction

$$F(T) = [a_1, a_2, \dots, a_n] := a_1 + \frac{1}{a_2 + \dots + \frac{1}{a_{n-1} + \frac{1}{a_n}}}.$$

Since fractions and rational tangles correspond, we will, from now on, use the notation $[a_1, \dots, a_n]$ to denote both the continued fraction and a rational tangle in continued fraction form.



Figure 12 - The Flype Moves

The subject of continued fractions is of perennial interest to mathematicians. See for example [20], [25], [21], [33]. Here we only consider continued fractions of the above type, with all numerators equal to 1. As in the case of rational tangles, we allow the term a_1 to be zero. Clearly, the two simple algebraic operations *addition of +1 or -1* and *inversion* generate inductively the whole class of continued fractions, starting from zero.

If a rational tangle T changes by an isotopy, the associated continued fraction form may also change, while the fraction remains invariant. For example, $[2, -2, 3] = [1, 2, 2] = \frac{7}{5}$, see Figure 13. Indeed, the rational tangles $[2, -2, 3]$ and $[1, 2, 2]$ are isotopic as shown by the swing moves of Figure 13. A *swing move* is an isotopy move in which we swing an arc joining two consecutive crossings of opposite type across a subtangle box. See the first move in Figure 13. For the isotopy type of a rational tangle T with fraction $\frac{p}{q}$ we shall use the notation $[\frac{p}{q}]$.

The key to the exact correspondence of fractions and rational tangles lies in the construction of a canonical alternating form for the rational tangle. A tangle is said to be *alternating* if it is isotopic to a tangle where *the crossings alternate from under to over as we go along any component or arc of the weave*. Similarly, a knot is alternating if it possesses an alternating diagram. Using the swing moves and an induction argument, one shows that rational tangles (and rational knots) are alternating. We shall say that the rational tangle $S = [\beta_1, \beta_2, \dots, \beta_m]$ is in *canonical form* if S is alternating and m is odd. From the above, S alternating implies that the β_i 's are all of the same sign. It turns out that the canonical form for S is unique. In Figure 13 we bring our working rational tangle $T = [2, -2, 3]$ to its canonical form $S = [1, 2, 2]$.



Figure 13 - Reducing to Alternating Form Using the Swing Moves

On the other hand, by Euclid’s algorithm and keeping all remainders of the same sign, one can show that every continued fraction $[a_1, a_2, \dots, a_n]$ can be transformed to a unique canonical form $[\beta_1, \beta_2, \dots, \beta_m]$, where all β_i ’s are positive or all negative integers and m is odd. For example, $[2, -2] = [1, 1, 1] = \frac{3}{2}$. There is also an algorithm that can be applied directly to the initial continued fraction to obtain its canonical form, which works in parallel with the algorithm for the canonical form of rational tangles. Indeed, we have:

Proposition 1 *The following identity is true for continued fractions and it is also a topological equivalence of the corresponding tangles:*

$$[\dots, a, -b, c, d, e, \dots] = [\dots, (a - 1), 1, (b - 1), -c, -d, -e, \dots].$$

This identity gives a specific inductive procedure for reducing a continued fraction to all positive or all negative terms. In the case of transforming to all negative terms, we can first flip all signs and work with the mirror image. Note also that

$$[\dots, a, b, 0, c, d, e, \dots] = [\dots, a, b + c, d, e, \dots]$$

will be used in these reductions.

Proof. The identity in the Proposition follows immediately from the formula:

$$a + 1/(-b) = (a - 1) + 1/(1 + 1/(b - 1)).$$

If a and b are positive, this formula allows the reduction of negative terms in a continued fraction. □

For the study of rational knots it is easier to use another way of representing an abstract rational tangle in standard form, illustrated in Figure 10. This is the *3-strand-braid representation*. As illustrated in Figure 10, the 3-strand-braid representation is obtained from the standard representation by planar rotations of the vertical sets of crossings, thus creating a lower row of horizontal crossings. By the checkerboard shading convention, the signs of the crossings in the lower row do not change under these rotations.

Note that the set of twists of a rational tangle may be always assumed *odd*. Indeed, let n be even and let the left-most twist $[a_1]$ be on the upper part of the 3-strand braid representation. Up to the ambiguity (upper or lower row) of the right-most crossing, the vector associated to a rational tangle is *unique*, i.e. $(a_1, a_2, \dots, a_n) = (a_1, a_2, \dots, a_n - 1, 1)$, if $a_n > 0$, and $(a_1, a_2, \dots, a_n) = (a_1, a_2, \dots, a_n + 1, -1)$, if $a_n < 0$.

Remark 1 We have omitted here the proof of the invariance of the fraction. The interested reader can consult [3], [11], [17] for various proofs of this fact. One definition of the fraction of a general 2-tangle is:

$$F(T) = i \langle N(T) \rangle / \langle D(T) \rangle,$$

where $i^2 = -1$ and $\langle L \rangle = \langle L \rangle (A)$ denotes the bracket polynomial [16] of a link L with $A = i^{1/2}$. Here $N(T)$ and $D(T)$ are the numerator and denominator closures of the tangle T , as illustrated in Figure 7.

2.2 Rational Knots and Continued Fractions

By joining with simple arcs the two upper and the two lower endpoints of a 2-tangle T , we obtain a knot called the *Numerator* of T , denoted $N(T)$. Joining with simple arcs each pair of the corresponding top and bottom endpoints of T we obtain the *Denominator* of T , denoted by $D(T)$, see Figure 7. Note that $N(T) = D(T^{rot})$ and $D(T) = N(T^{rot})$. As we shall see in the next section, the numerator closure of the sum of two rational tangles is still a rational knot. But the denominator closure of the sum of two rational tangles is not necessarily a rational knot. For example, consider the denominator of the sum $\frac{1}{[3]} + \frac{1}{[3]}$.

A rational knot is defined to be the numerator of a rational tangle. Given two different rational tangle types $[\frac{p}{q}]$ and $[\frac{p'}{q'}]$, when do they close to isotopic rational knots? More than one rational tangle can yield isotopic rational knots. The corresponding equivalence relation between the rational tangles is reflected by an arithmetic equivalence of their corresponding fractions. Rational knots and links are one of the few cases in knot theory where we have a complete classification story. Indeed, we have the following theorem:

Theorem 2 (Schubert, 1956) *Suppose that rational tangles with fractions $\frac{p}{q}$ and $\frac{p'}{q'}$ are given. Here p and q are relatively prime, similarly for p' and q' . If $K(\frac{p}{q})$ and $K(\frac{p'}{q'})$ denote the corresponding rational knots obtained by taking numerator closures of these tangles, then $K(\frac{p}{q})$ and $K(\frac{p'}{q'})$ are isotopic if and only if*

1. $p = p'$ and
2. either $q \equiv q' \pmod{p}$ or $qq' \equiv 1 \pmod{p}$.

Different proofs of Theorem 2 are given in [29], [1], [18].

Schubert classified rational knots by finding canonical forms via representing them as 2-bridge knots. In [18] we gave a new combinatorial proof of Theorem 2, by posing the question: given a rational knot diagram, at which places may one cut it so that it opens to a rational tangle? We then pinpoint two distinct categories of cuts that represent the two cases of the arithmetic equivalence of Schubert's theorem. The first case corresponds to the *special cut*, as illustrated in Figure 14. The two tangles $T = [-3]$ and $S = [1] + \frac{1}{[2]}$ are non-isotopic by the Conway Theorem (Theorem 1), since $F(T) = -3 = 3/(-1)$, while $F(S) = 1 + 1/2 = 3/2$. But they have isotopic numerators: $N(T) \sim N(S)$, the left-handed trefoil. Now $-1 \equiv 2 \pmod{3}$, confirming Theorem 2. See [18] for a complete analysis of the special cut.

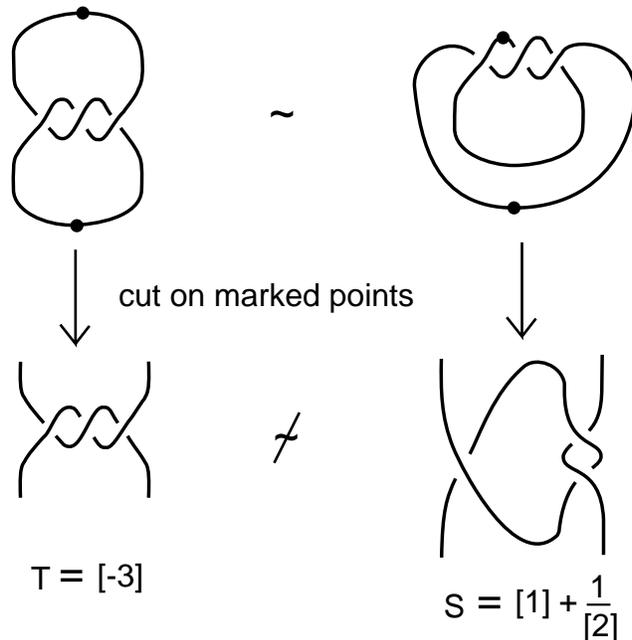


Figure 14 - An Example of the Special Cut

The second case of Schubert's equivalence corresponds to the *palindrome cut*, an example of which is illustrated in Figure 15. Here we see that the tangles

$$T = [2, 3, 4] = [2] + \frac{1}{[3] + \frac{1}{[4]}}$$

and

$$S = [4, 3, 2] = [4] + \frac{1}{[3] + \frac{1}{[2]}}$$

both have the same numerator closure. Their corresponding fractions are

$$F(T) = 2 + \frac{1}{3 + \frac{1}{4}} = \frac{30}{13} \quad \text{and} \quad F(S) = 4 + \frac{1}{3 + \frac{1}{2}} = \frac{30}{7}.$$

Note that $7 \cdot 13 \equiv 1 \pmod{30}$, again confirming Theorem 2.

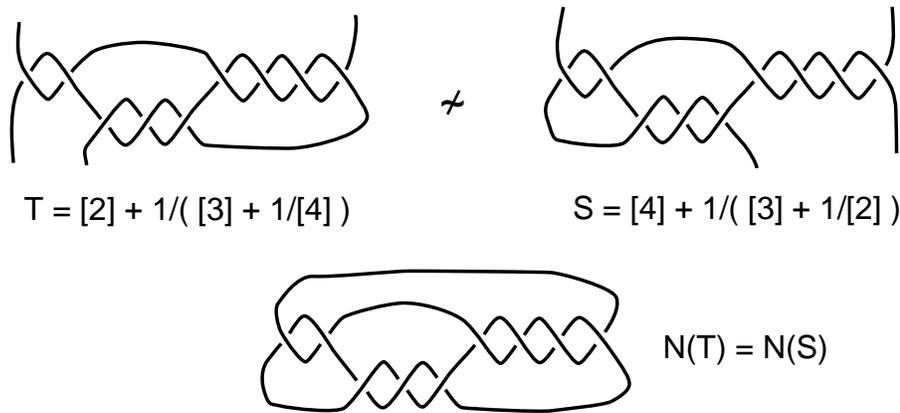


Figure 15 - An Instance of the Palindrome Equivalence

In the general case if $T = [a_1, a_2, \dots, a_n]$, we shall call the tangle $S = [a_n, a_{n-1}, \dots, a_1]$ *the palindrome of T*. Clearly these tangles have the same numerator. In order to check the arithmetic in the general case of the palindrome cut we need to generalize this pattern to arbitrary continued fractions and their palindromes (obtained by reversing the order of the terms).

Theorem 3 below is a known result about continued fractions. See [17], [30] or [19]. We shall give here our proof of this statement. For this we will first present a way of evaluating continued fractions via 2×2 matrices (compare with [9], [21]). This method of evaluation is crucially important for the rest of the paper. We define matrices $M(a)$ by the formula

$$M(a) = \begin{pmatrix} a & 1 \\ 1 & 0 \end{pmatrix}.$$

These matrices $M(a)$ are said to be the *generating matrices* for continued fractions, as we have:

Theorem 3 (The Palindorome Theorem) *Let $\{a_1, a_2, \dots, a_n\}$ be a collection of n integers, and let*

$$\frac{P}{Q} = [a_1, a_2, \dots, a_n]$$

and

$$\frac{P'}{Q'} = [a_n, a_{n-1}, \dots, a_1].$$

Then $P = P'$ and $QQ' \equiv (-1)^{n+1} \pmod{P}$.

Moreover, for any sequence of integers $\{a_1, a_2, \dots, a_n\}$ the value of the corresponding continued fraction

$$\frac{P}{Q} = [a_1, a_2, \dots, a_n]$$

is given through the following matrix product

$$M = M(a_1)M(a_2) \dots M(a_n)$$

via the identity

$$M = \begin{pmatrix} P & Q' \\ Q & U \end{pmatrix}$$

where this matrix also gives the evaluation of the palindrome continued fraction

$$[a_n, a_{n-1}, \dots, a_1] = \frac{P}{Q'}.$$

Proof. Let

$$\frac{R}{S} = [a_2, a_3, \dots, a_n].$$

Then

$$\frac{P}{Q} = [a_1, a_2, \dots, a_n] = a_1 + \frac{1}{\frac{R}{S}} = a_1 + \frac{S}{R} = \frac{Ra_1 + S}{R}.$$

By induction we may assume that

$$M(a_2)M(a_3) \dots M(a_n) = \begin{pmatrix} R & S' \\ S & V \end{pmatrix}.$$

Hence

$$M(a_1)M(a_2) \dots M(a_n) = \begin{pmatrix} a_1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} R & S' \\ S & V \end{pmatrix} = \begin{pmatrix} a_1R + S & a_1S' + V \\ R & S' \end{pmatrix}.$$

This proves by induction that

$$M = M(a_1)M(a_2)\dots M(a_n) = \begin{pmatrix} P & Q' \\ Q & U \end{pmatrix}.$$

To see the result about the palindrome continued fraction (and the terms P and Q' in the matrix), let M^T denote the transpose of M . Then

$$M^T = M(a_n)M(a_{n-1})\dots M(a_1),$$

from which the statement about the palindrome follows by a repeat of the above calculation. Note also that $Det(M) = (-1)^n$ since M is a product of n matrices of determinant equal to -1 , and $Det(M) = PU - QQ'$. Hence

$$PU - QQ' = (-1)^n.$$

This last equation implies the congruence stated at the beginning of the Theorem, and completes the proof of the Theorem. \square

3 The Return of the Culprit

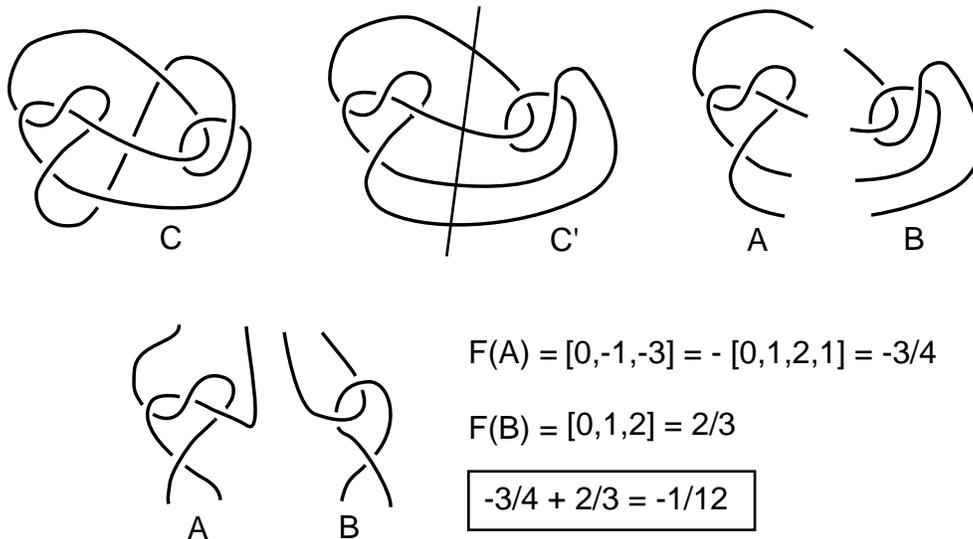


Figure 16 - The Culprit Analysis

In order to see the Culprit in a way that allows us to understand why it is unknotted, we shall use the language and technique of the theory of tangles as explained in the previous section.

View Figure 16. In Figure 16 we have a drawing C of the Culprit and next to it we have a drawing C' of the result of part of Figure 3, where the undercrossing arc in C has been moved (making the complexity rise) until it has been drawn outside the rest of the diagram. Concentrate on C' . Notice that we can cut C' into two pieces, as shown in Figure 16. These two pieces, A and B , are rational tangles, and this cutting process shows that C' is the numerator closure of the tangle sum of A and B . This is written $C' = N(A + B)$. Each rational tangle T has a rational fraction $F(T)$ that tells all about it. In this case,

$$F(A) = \frac{1}{-1 + \frac{1}{-3}} = -3/4$$

and

$$F(B) = \frac{1}{1 + \frac{1}{2}} = 2/3.$$

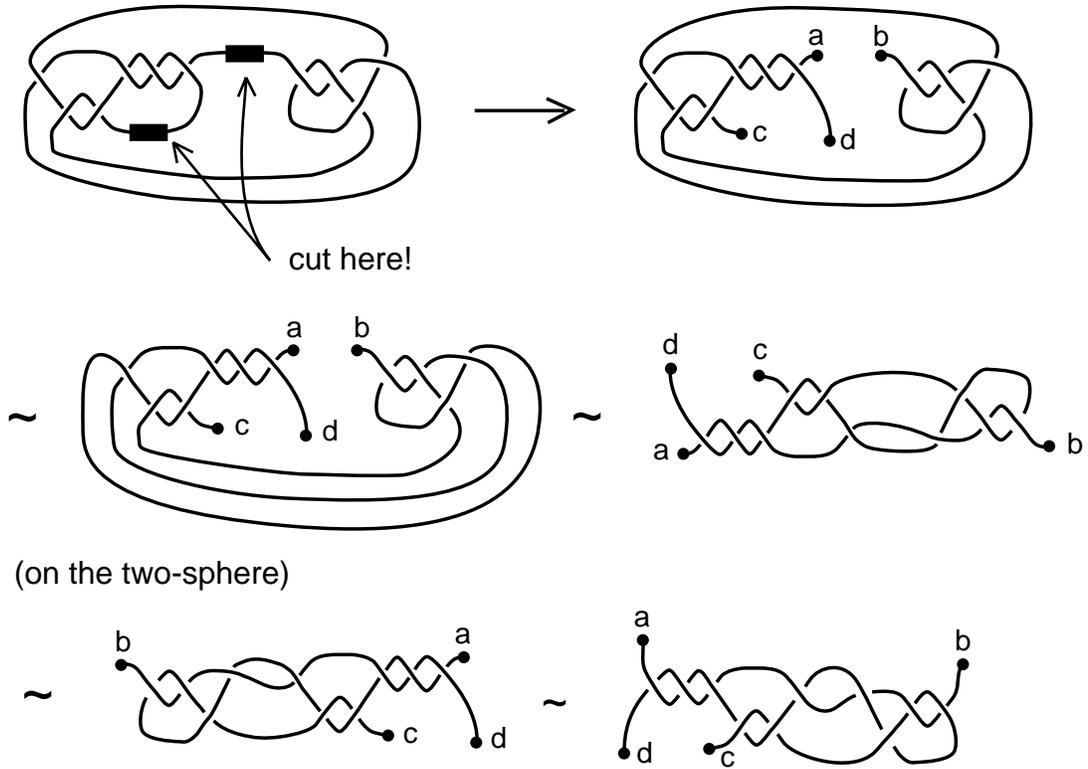
We know that the numerator of $A + B$ is unknotted and we would like to understand why it is unknotted. We notice that the sum of the fractions of A and B is

$$F(A) + F(B) = -3/4 + 2/3 = -1/12.$$

Thus the numerator of the sum of the fractions of A and B is -1 . Does this -1 imply the unknottedness of the numerator of $A + B$? Well, the answer is that it does, and that will be the subject of much of the rest of the paper. See Theorem 6.

4 Collapsing to Unknots

In this section we first prove that the numerator of the sum of two rational tangles is a rational knot or link. We identify the knot or link, and use the result to characterize in Theorem 6 those unknots that arise as numerators of the sum of two rational tangles.



$$N([1,2,3] + [1,1,2]) = N([3,2,1+1,1,2])$$

Figure 17 - The Numerator of a Sum of Rational Tangles is a Rational Link

Theorem 4 (Addition of Rational Tangles) Let $\frac{P}{Q} = [a_1, a_2, \dots, a_n]$ and $\frac{R}{S} = [b_1, b_2, \dots, b_m]$. Let $A = [\frac{P}{Q}]$ and $B = [\frac{R}{S}]$ be the corresponding rational tangles. Then the knot or link $N(A + B)$ is rational. In fact

$$N(A + B) = N([a_n, a_{n-1}, \dots, a_2, a_1 + b_1, b_2, \dots, b_m]).$$

Proof. View Figure 17. In this figure we illustrate a special case of the Theorem. The general case is clear from this illustration. \square

Definition 3 Given continued fractions $\frac{P}{Q} = [a_1, \dots, a_n]$ and $\frac{R}{S} = [b_1, \dots, b_m]$, let

$$[a_1, \dots, a_n] \# [b_1, \dots, b_m] := [a_n, \dots, a_2, a_1 + b_1, b_2, \dots, b_m].$$

If

$$\frac{F}{G} = [a_n, \dots, a_2, a_1 + b_1, b_2, \dots, b_m],$$

we shall write

$$\frac{P}{Q} \# \frac{R}{S} = \frac{F}{G}.$$

By Theorem 4, $N([\frac{P}{Q} \# \frac{R}{S}]) = N([\frac{P}{Q}] + [\frac{R}{S}])$.

Remark 2 The reader should note that $N([\frac{P}{Q}] + [\frac{R}{S}])$ is *not*, in general, isotopic to $N([\frac{P}{Q} + \frac{R}{S}]) = N([\frac{PS+QR}{QS}])$. This is the whole point of the previous Theorem. When we add two rational tangles we do not in general get a rational tangle, but the closure of this sum is a rational knot. This rational knot is the closure of a rational tangle distinct from $[\frac{P}{Q} + \frac{R}{S}]$. A good example is $P/Q = [3, 2, 1] = 10/3$ and $R/S = [2, 2, 1] = 7/3$. Then $P/Q + R/S = 51/9$, while $(P/Q) \# (R/S) = [1, 2, 3 + 2, 2, 1] = 51/35$. We have $N([10/3] + [7/3]) = N([51/35])$, which is not isotopic to $N([51/9])$ by the Schubert Theorem. Nevertheless, the numerator of $(P/Q) \# (R/S)$ is equal to $PS + QR$. This is the import of the next Theorem.

Theorem 5 *If P/Q has matrix*

$$M = M(\vec{a}) = M(a_1) \dots M(a_n)$$

and R/S has matrix

$$N = M(\vec{b}) = M(b_1) \dots M(b_m),$$

then $[a_1, \dots, a_n] \# [b_1, \dots, b_m]$ has matrix

$$M \# N := M^T N^E,$$

where N^E denotes the matrix obtained by interchanging the rows of N . This gives an explicit formula for $[a_1, \dots, a_n] \# [b_1, \dots, b_m]$. This formula can be used to determine not only when $N([\frac{P}{Q}] + [\frac{R}{S}])$ is unknotted but also to find its knot type as a rational knot via Schubert's Theorem. In particular, we find that

$$N([\frac{P}{Q}] + [\frac{R}{S}]) = N([\frac{PS + QR}{QS + UR}]) = N([\frac{Num(P/Q + R/S)}{Num(Q'/U + R/S)}])$$

where $|PU - QQ'| = 1$.

Proof. We know from Theorem 3 that

$$M(\vec{a}) = M(a_1) \dots M(a_n) = \begin{pmatrix} P & Q' \\ Q & U \end{pmatrix},$$

and that

$$M(\vec{b}) = M(b_1) \dots M(b_m) = \begin{pmatrix} R & S' \\ S & V \end{pmatrix}.$$

Let

$$F/G = [a_n, \dots, a_2, a_1 + b_1, b_2, \dots, b_m] = \frac{P}{Q} \# \frac{R}{S}.$$

Then we have, by Theorem 4, that

$$N\left(\left[\frac{P}{Q}\right] + \left[\frac{R}{S}\right]\right) = N\left(\left[\frac{F}{G}\right]\right),$$

and

$$M(\vec{c}) = M(a_n) \dots M(a_2)M(a_1 + b_1)M(b_2) \dots M(b_m) = \begin{pmatrix} F & G' \\ G & W \end{pmatrix}.$$

Now note the identity

$$\begin{pmatrix} a_1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} b_1 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} a_1 + b_1 & 1 \\ 1 & 0 \end{pmatrix}.$$

Thus

$$M(\vec{c}) = M(\vec{a})^T \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} M(\vec{b}) = M(\vec{a})^T M(\vec{b})^E$$

where M^E denotes the matrix obtained from M by interchanging its two rows. In particular, this formula implies that

$$\begin{pmatrix} F & G' \\ G & W \end{pmatrix} = \begin{pmatrix} P & Q \\ Q' & U \end{pmatrix} \begin{pmatrix} S & V \\ R & S' \end{pmatrix} = \begin{pmatrix} PS + QR & PV + QS' \\ Q'S + UR & Q'V + US' \end{pmatrix}.$$

Thus

$$N\left(\left[\frac{P}{Q}\right] + \left[\frac{R}{S}\right]\right) = N\left(\left[\frac{PS+QR}{Q'S+UR}\right]\right) = N\left(\left[\frac{Num(P/Q + R/S)}{Num(Q'/U + R/S)}\right]\right)$$

where $|PU - QQ'| = 1$. This completes the proof of the Theorem. \square

Theorem 6 (Unknot Theorem) *Let $\frac{P}{Q} = [a_1, \dots, a_n]$ and $\frac{R}{S} = [b_1, \dots, b_m]$ be as in Theorem 5. Then $N\left(\left[\frac{P}{Q}\right] + \left[\frac{R}{S}\right]\right)$ is unknotted if and only if $PS + QR = \pm 1$, that is, PS and QR are consecutive integers.*

Proof. It follows from Theorem 5 and the Schubert Theorem that $N([\frac{P}{Q}])$ is unknotted if and only if $PS + QR = \pm 1$. \square

Remark 3 Suppose, as in Theorem 6, that $|PS + QR| = 1$ so that $N([\frac{P}{Q}] + [\frac{R}{S}])$ is an unknot. Then it follows from Theorem 6 that $N([\frac{Q}{P}] + [\frac{S}{R}])$ is also an unknot. Thus, the pair of fractions $(\frac{P}{Q}, \frac{R}{S})$ yields an unknot if and only if the pair of inverse fractions $(\frac{Q}{P}, \frac{S}{R})$ yields an unknot. In fact, the reader will enjoy proving the following identity for any rational tangles A and B :

$$N(\frac{1}{A} + \frac{1}{B}) = -N(A + B)$$

where the minus sign denotes taking the mirror image of the diagram $N(A+B)$, and equality is isotopy. Thus, for any pair of fractions $(\frac{P}{Q}, \frac{R}{S})$ (not necessarily forming an unknot)

$$N([\frac{P}{Q}] + [\frac{R}{S}]) = -N([\frac{Q}{P}] + [\frac{S}{R}]).$$

We end this section with a way to produce infinitely many unknots. Consider a rational number, its corresponding continued fraction, and its matrix representation:

$$P/Q = [a_1, \dots, a_n]$$

with

$$M = M(\vec{a}) = M(a_1) \dots M(a_n) = \begin{pmatrix} P & Q' \\ Q & U \end{pmatrix}.$$

Note that since the determinant of this matrix is $(-1)^n$, we have the formula $PQ - QQ' = (-1)^n$ from which it follows that

$$P/Q - Q'/U = (-1)^n / QU.$$

Hence, by Theorem 6, the rational knot

$$N([P/Q] - [Q'/U])$$

is unknotted and, as we shall see later, is a good candidate to produce a hard unknot.

5 Continued Fractions, Convergents and Lots of Unknots

In this section we'll show that we can do even better than the example above for producing infinitely many unknots. Remarkably, the fraction Q'/U (at the end of the last section) has an interpretation as the truncation of our continued fraction $[a_1, \dots, a_n]$.

Lemma 1 *Let $P/Q = [a_1, \dots, a_n]$ with corresponding matrix $M = M(\vec{a}) = M(a_1) \dots M(a_n) = \begin{pmatrix} P & Q' \\ Q & U \end{pmatrix}$. Then $Q'/U = [a_1, \dots, a_{n-1}]$. Conversely, if $R/S = [a_1, \dots, a_{n-1}]$ is a reduced fraction, then $|R| = |Q'|$ and $|S| = |U|$. So, we can choose signs for R and S so that*

$$\begin{pmatrix} P & R \\ Q & S \end{pmatrix} = \begin{pmatrix} P & Q' \\ Q & U \end{pmatrix}.$$

Proof. To see this formula, let

$$N = M(a_1) \dots M(a_{n-1}) = \begin{pmatrix} R & S' \\ S & V \end{pmatrix},$$

so that

$$R/S = [a_1, \dots, a_{n-1}].$$

Then

$$\begin{aligned} \begin{pmatrix} P & Q' \\ Q & U \end{pmatrix} &= M(a_1) \dots M(a_{n-1})M(a_n) = NM(a_n) \\ &= \begin{pmatrix} R & S' \\ S & V \end{pmatrix} \begin{pmatrix} a_n & 1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} Ra_n + S' & R \\ Sa_n + V & S \end{pmatrix}. \end{aligned}$$

This shows that $Q'/U = R/S = [a_1, \dots, a_{n-1}]$, as claimed. For the converse, note that the pairs $(P, Q), (Q', U), (R, S)$ are pairs of relatively prime integers. Note also that $Q'/U = R/S$. Thus $|R| = |Q'|$ and $|S| = |U|$. \square

Definition 4 One says that $[a_1, \dots, a_{n-1}]$ is a *convergent* of $[a_1, \dots, a_{n-1}, a_n]$. We shall say that two fractions P/Q and R/S are *convergents* if the continued fraction of one of them is a convergent of the other.

We have, so far, proved the following result.

Proposition 2 *Let $P/Q = [a_1, \dots, a_{n-1}, a_n]$ and let $Q'/U = [a_1, \dots, a_{n-1}]$, a convergent of P/Q . Then*

$$N([P/Q] - [Q'/U]) = N([a_1, \dots, a_{n-1}, a_n] - [a_1, \dots, a_{n-1}])$$

is an unknot.

Remark 4 Another, more direct way to see this result is illustrated in Figure 18. In this figure we show $N([2, 3, 4] - [2, 3])$ with the second tangle written as a 180° turn of the standard form for $[2, 3]$ (this is isotopic to the standard form since we are working with rational tangles). In this form, we see clearly that the braidings of the two tangles cancel in the back of the 2-sphere to form an unknot.

The reader should note that

$$\begin{aligned} N([a_1, \dots, a_n] - [a_1, \dots, a_{n-1}]) &= N([a_1, \dots, a_n] \sharp [-a_1, \dots, -a_{n-1}]) \\ &= N([a_n, \dots, a_2, a_1 - a_1, \dots, -a_{n-1}]) = N([a_n, \dots, a_2, 0, -a_2, \dots, -a_{n-1}]) \\ &= N([a_n, \dots, a_2 - a_2, \dots, -a_{n-1}]) = \dots \\ &= N([a_n, a_{n-1} - a_{n-1}]) = N([a_n, 0]) = U \end{aligned}$$

where U is the unknotted circle. Thus we see directly that a continued fraction and the negative of its convergent will yield an unknot when we take the numerator of the sum of the corresponding tangles.

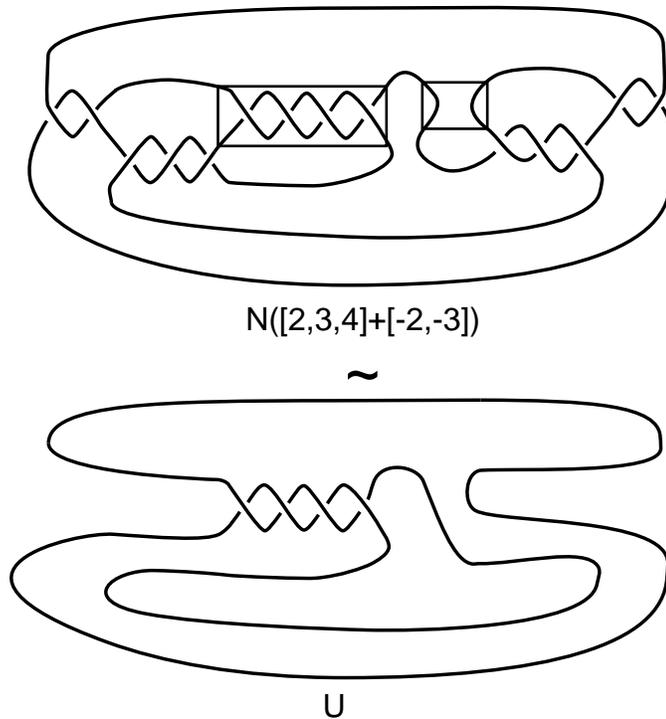


Figure 18 - Braid Cancellation to an Unknot

We see from the above that the two consecutive integers PU and QQ' produce two continued fractions $P/Q = [a_1, \dots, a_n]$ and $Q'/U = [a_1, \dots, a_{n-1}]$ so that the second fraction is a convergent of the first. *The property of one fraction being a convergent of the other is in fact, always a property of fraction pairs produced from consecutive integers.* For example, consider the integers 90 and 91. We have $90 = 10 \times 9$ and $91 = 13 \times 7$. Thus

$$13 \times 7 - 10 \times 9 = 1.$$

Hence

$$13/9 - 10/7 = 1/63,$$

so that $N([13/9] + [-10/7])$ is an unknot by Theorem 6. We see that

$$13/9 = [1, 2, 4] = [1, 2, 3, 1]$$

and

$$10/7 = [1, 2, 3]$$

so that $13/9$ and $10/7$ are convergents. We will now prove this statement about convergents. For the next Lemma see also [7].

Lemma 2 *Let P and Q be relatively prime integers and let s and r be a pair of integers such that $Ps - Qr = \pm 1$. Let $R = r + tP$ and $S = s + tQ$ where t is any integer. Then $\{R, S\}$ comprises the set of all solutions to the equation $PS - QR = \pm 1$. Similarly, all solutions of the equation $PS - QR = \mp 1$ are given in the form $R = -r + tP$ and $S = -s + tQ$.*

Proof. Without loss of generality we can assume that $Ps - Qr = 1$. We leave it to the reader to formulate the case where $Ps - Qr = -1$. Certainly R and S as given in the statement of the Lemma satisfy the equation $PS - QR = 1$. Suppose that R and S is some solution to this equation. Then it follows by taking the difference with the equation $Ps - Qr = 1$ that $P(S - s) = Q(r - R)$. Since P and Q are relatively prime, it follows at once from this equation and the uniqueness of prime factorization of integers that $R = r + tP$ and $S = s + tQ$ for some integer t . The last part of the Lemma follows by the same form of reasoning. This completes the proof. \square

Lemma 3 *Let P and Q be relatively prime integers and let $P/Q = [a_1, \dots, a_n]$ be a continued fraction expansion for P/Q . Let also $r/s = [a_1, \dots, a_{n-1}]$ be a convergent for $[a_1, \dots, a_n]$. Let $R = r + tP$ and $S = s + tQ$ where t is any integer. Then $R/S = [a_1, \dots, a_n, t]$, and thus P/Q is a convergent of R/S .*

Proof. By Lemma 1, we have

$$M(\vec{a}) = M(a_1) \dots M(a_n) = \begin{pmatrix} P & r \\ Q & s \end{pmatrix}.$$

Moreover, we have:

$$M(\vec{a})M(t) = \begin{pmatrix} P & r \\ Q & s \end{pmatrix} \begin{pmatrix} t & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} Pt + r & P \\ Qt + s & Q \end{pmatrix}.$$

By Lemma 2 for $\{R = r + tP, S = s + tQ\}$ we have $PS - QR = (-1)^{n+1}$. So $R/S = [a_1, \dots, a_n, t]$, and P/Q is a convergent of R/S . Thus all such solutions correspond to continued fractions of which P/Q is a convergent. This completes the proof. \square

Finally, we can sum up by pointing out that we have proved the following result.

Theorem 7 (Unknotting Convergents) *Let P/Q and R/S be reduced fractions. Then*

$$N([P/Q] - [R/S])$$

is an unknot if and only if P/Q and R/S are convergents.

Remark 5 In this sense Theorems 6 and 7 show us that the simplest method of collapse to the unknot is the only way that the collapse can occur when we take the numerator of the sum of two rational tangles. The reader will enjoy verifying that this class of unknots can be obtained from a closed loop of rope by consecutive twisting of adjacent strands of the rope, followed by a separation of the rope into the numerator sum of two rational tangles. Such processes occur naturally in situations involving DNA topology as described later in this paper.

Infinite Continued Fractions. Note that if we start with an infinite continued fraction

$$[a_1, a_2, a_3, \dots]$$

and define the *truncations*

$$P_n/Q_n = [a_1, \dots, a_n],$$

then we have

$$P_n/Q_n - P_{n-1}/Q_{n-1} = (-1)^n / Q_n Q_{n-1}.$$

This equation is usually used to analyze the convergence of the truncations of the continued fraction to a real number. Here we see a *single infinite continued fraction*, whether or not convergent, *producing an infinite family of unknot diagrams*:

$$K_n = N([P_n/Q_n] - [P_{n-1}/Q_{n-1}]).$$

Surely, the simplest instance of this phenomenon occurs with the infinite continued fraction for the Golden Ratio:

$$\frac{1 + \sqrt{5}}{2} = [1, 1, 1, \dots].$$

Here the convergents are $f_n/f_{n-1} = [1, 1, 1, \dots, 1]$ (with n 1's) and f_n is the n -th Fibonacci number where $f_0 = 1, f_1 = 1$ and $f_{n+1} = f_n + f_{n-1}$ for $n \geq 1$. The matrices are

$$M(1)^n = \begin{pmatrix} f_n & f_{n-1} \\ f_{n-1} & f_{n-2} \end{pmatrix}.$$

Thus we have

$$f_n/f_{n-1} - f_{n-1}/f_{n-2} = (-1)^n/f_{n-1}f_{n-2}.$$

In this instance, this formula shows that the sequence of truncations is convergent (to the Golden Ratio).

In Figure 19 we illustrate a hard unknot based on the eighth and seventh truncations of the Golden Ratio continued fraction. This example is produced by using the standard closure of $N([f_8/f_7] - [f_7/f_6]) = N([34/21] - [21/13])$. By this same pattern, we can extract from the infinite continued fraction for the golden ratio an infinite family of hard unknots. Note the unavailability of Reidemeister moves on the first diagram. In Figure 19 the first diagram illustrates the numerator of the sum of the two tangles $[f_8/f_7] = [1, 1, 1, 1, 1, 1, 1, 1]$ and $-[f_7/f_6] = [-1, -1, -1, -1, -1, -1, -1]$ with each tangle in 3-strand braid form with the integer 1-twist on the left. In this form the diagram is a hard unknot, and this generalizes to infinitely many examples of the same type. The second example has one tangle turned by 180° so that the integer 1-twists face one another, giving an easy unknot. The third example has one tangle turned by 180° so that both integer 1-twists face into the outer region. This diagram is an easy unknot on the 2-sphere, since there is a Reidemeister II-move in the outer region. If we were to restrict moves to the plane, then this Reidemeister move would not be available. The third diagram is a hard unknot in the plane.

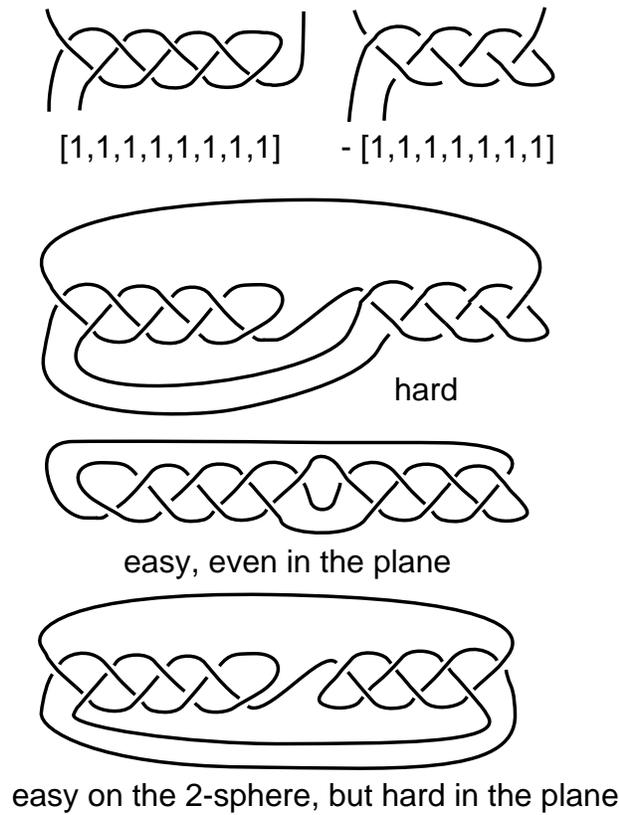


Figure 19 - $N([f_8/f_7] - [f_7/f_6]) = N([34/21] - [21/13])$

6 Constructing Hard Unknots

In this section we indicate how to construct hard unknots by using positive alternating tangles A and B such that $N(A - B)$ is unknotted. By our main results we know how to construct infinitely many such pairs of tangles by taking a continued fraction and its convergent, with the corresponding tangles in reduced (alternating) form.

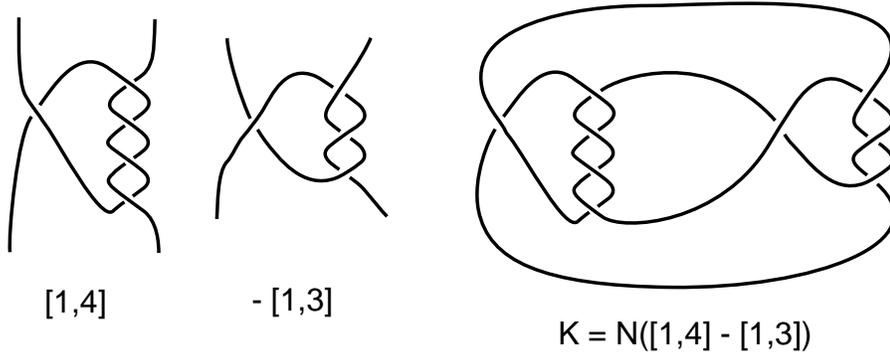


Figure 20 - $K = N([1, 4] - [1, 3])$

Let's begin with the case of $5/4 = [1, 4] = [1, 3, 1]$ and $4/3 = [1, 3]$. In Figure 20 we show the standard representations of $[1, 4]$ and $-[1, 3]$ as tangles, and $K = N([1, 4] - [1, 3])$. The reader will note that this diagram is a hard unknot with 9 crossings, one less than our original Culprit of Figure 16. In Figure 24 we give a diagram H that is isotopic to the mirror image of K . In Theorem 8 we show that H is one of a small collection of minimal hard unknot diagrams having the form $N(A - B)$ for reduced positive rational tangle diagrams A and B . In most cases, if one takes the standard representations of the tangles A and B , and forms the diagram for $N(A - B)$, the resulting unknot diagram will be hard. There are some exceptions however, and the next example illustrates this phenomenon.

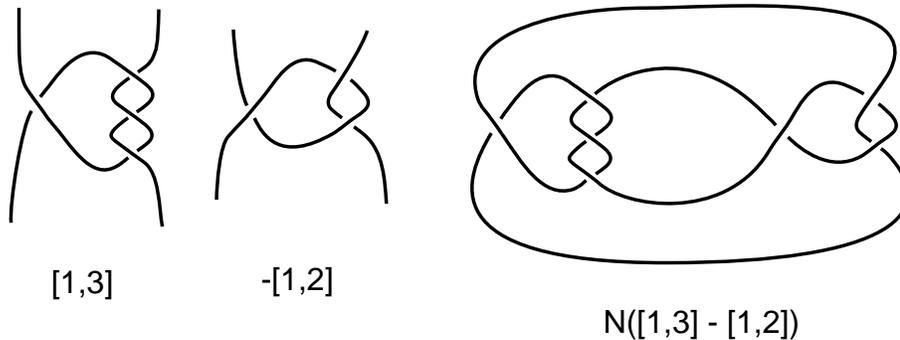


Figure 21 - $N([1, 3] - [1, 2])$

In Figure 21 we show the standard representations of $[1, 3]$ and $[1, 2]$ as tangles, and the diagram of $N([1, 3] - [1, 2])$. This diagram, while unknotted, is not a

hard unknot diagram due to the three-sided outer region. This outer region allows a type III Reidemeister move on the surface of the 2-sphere.

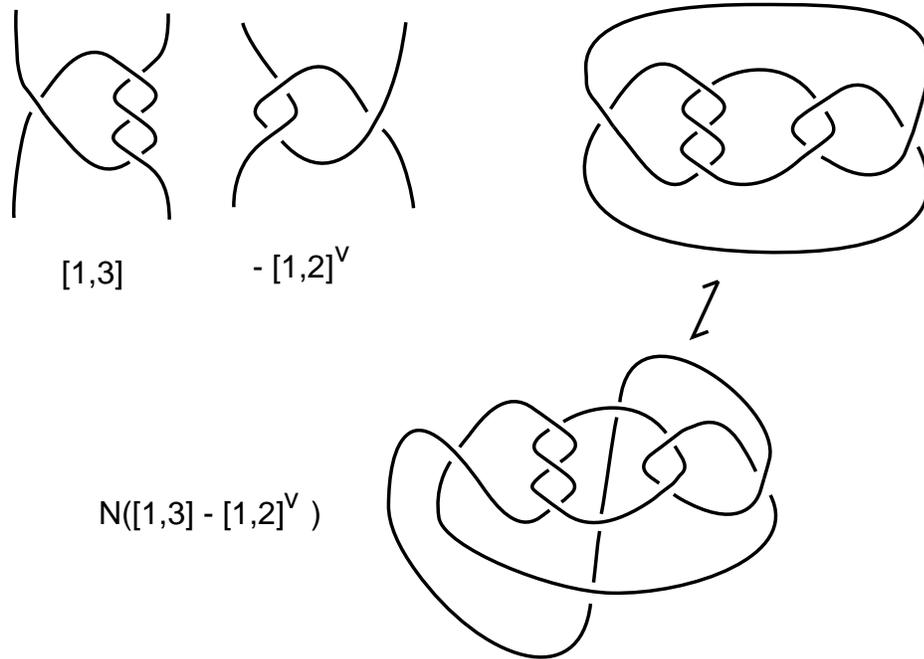


Figure 22 $-N([1, 3] - [1, 2]^v)$

The Tucking Construct. In Figure 22 we have replaced $[1, 2]$ by $[1, 2]^v$, the 180° turn of the tangle $[1, 2]$ about the vertical direction in the page. Now we see that the literal diagram of $N([1, 3] - [1, 2]^v)$ is of course still unknotted and is also not a hard unknot diagram. However this diagram can be converted to an unknot diagram by tucking an arc as shown in the Figure. The resulting hard unknot is the same diagram of 10 crossings that we had in Figure 16 as our initial Culprit. Note that a direct tuck on Figure 21 does not work (there would be a type III move made available). Note also that the other possibilities of flipping both tangles in Figure 21 or flipping the first tangle do not lead to hard unknots. We call this strategem the *tucking construct*. The tucking prevents the appearance of a type II move in the outermost region of the diagram.

The Culprit Revisited. Let's consider the example in Figure 16 again. Here we have $P/Q = -3/4$ and $R/S = 2/3$. We have $P/Q + R/S = -3/4 + 2/3 = -1/12$. Thus $N([-3/4] + [2/3])$ is an unknot by Theorem 6. This is exactly the unknot C' illustrated in Figure 16. Note that C is the tucking construct applied to C' .

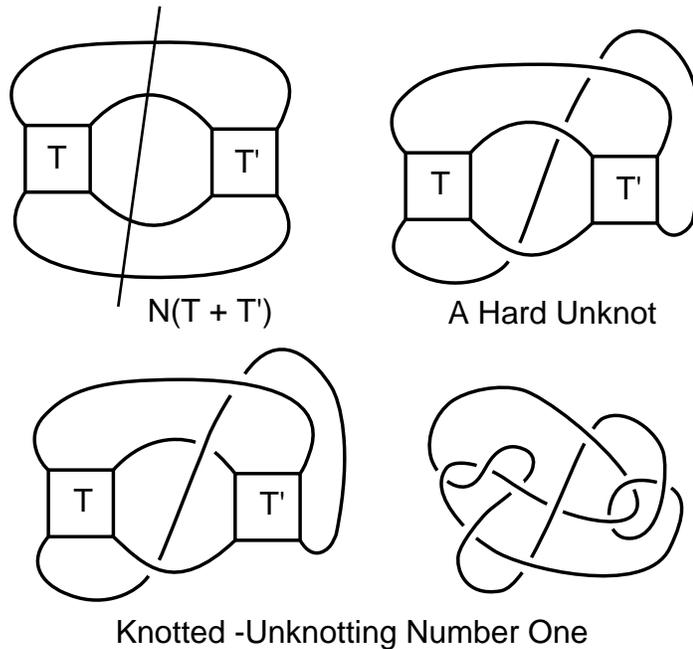


Figure 23 - The Tucking Construct

We can make infinitely many examples of this type. View Figure 23. The pattern is as follows. Suppose that $T = [P/Q]$ and $T' = [R/S]$ are rational tangles such that $PS + QR = \pm 1$. Then we know that $N(T + (T')^v)$ is an unknot. Furthermore we can assume that each of the tangles T and T' are in alternating form. The two tangle fractions have opposite sign and hence the alternation of the weaves in each tangle will be of opposite type. We create a new diagram for $N(T + (T')^v)$ by putting an arc from the bottom of the closure entirely underneath the diagram as shown in Figure 23. This is the general form of the tucking construct.

Remark 6 View the bottom of Figure 23 and note that we have indicated that the hard unknot becomes an alternating and hence knotted diagram (this can be proved by applying the results in [16]) by switching one crossing in the tucking construction. Thus the tucking construction is also an infinite source of knots of unknotting number one.

Hard Unknots Recipe. In a tangle $[a_1, \dots, a_n]$, call a_1 the *integer part* of the tangle. Here we use tangles $T = [a_1, \dots, a_n]$ and $T' = [-a_1, \dots, -a_{n-1}]$ with all a_i positive. Except for very few cases with small number of total crossings, the following hold:

1. If the integer parts both face in the same direction, then $N(T + T')$ is a hard unknot diagram.
2. If the integer parts both face the outside region, thus making a type II move available on the 2-sphere, then the tucking construct will create a hard unknot.
3. If the integer parts both face the inside region, then we do not get a hard unknot and we cannot remedy this fact using tucking.

The reader should compare these remarks to the contents of Figure 19.

7 The Smallest Hard Unknots

Figure 24 illustrates two hard unknot diagrams H and J with 9 crossings ($K = -H$ appears earlier in Figure 20).

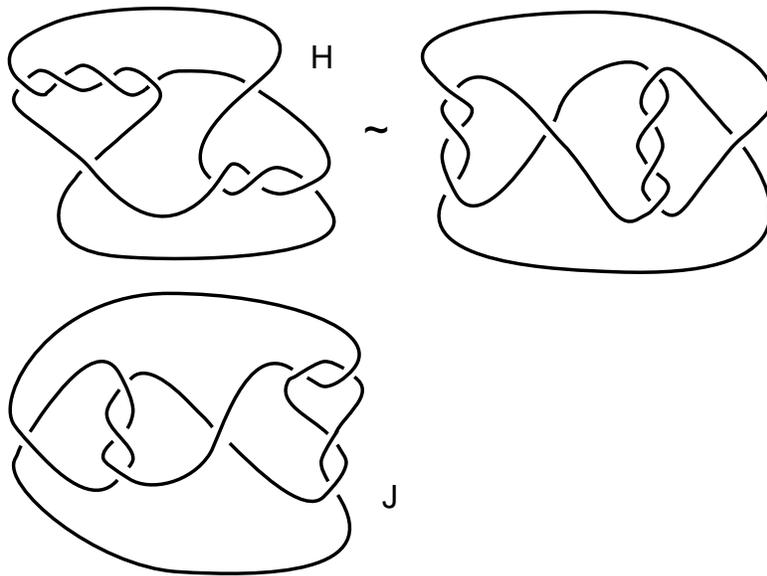


Figure 24 - H and J are Hard Unknots of 9 Crossings

Two equivalent versions of the diagram H appear in Figure 24. The right-hand version of H in this figure is of the form:

$$H = N([1, 3] - [1, 4]) = N([4/3] - [5/4]).$$

Note that $[1, 3]$ and $[1, 4] = [1, 3, 1]$ are convergents. Thus H and K are mirror images of each other. The diagram J in Figure 24 is of the form:

$$J = N([1, 3] - [1, 2, 2]) = N([4/3] - [7/5]).$$

Note that $[1, 3] = [1, 2, 1]$ and $[1, 2, 2] = [1, 2, 1, 1]$ are convergents. Note also that the crossings in J corresponding to 1 in $[1, 3]$ and -1 in $[-1, -2, -2]$ can be switched and we will obtain another diagram J' , arising as sum of two alternating rational tangles, that is also a hard unknot. This diagram can be obtained from the diagram J without switching crossings, by performing flypes (Figure 12) on the subtangles $[1, 3]$ and $[-1, -2, -2]$ of J , and then doing an isotopy of this new diagram on the 2-sphere. (We leave the verification of this statement to the reader.) Thus the diagram J' can be obtained from J by flyping. A similar remark applies to the diagram H , giving a corresponding diagram H' , but in this case H' is easily seen to be equivalent to H by a planar isotopy that does not involve any Reidemeister moves. Thus, up to these sorts of modifications, we have produced essentially two hard unknot diagrams with 9 crossings.

We have the following result.

Theorem 8 *The diagrams H and J shown in Figure 24 are, up to flyping subtangle diagrams and taking mirror images, the smallest hard unknot diagrams in the form $N(A - B)$ where A and B are rational tangles in reduced positive alternating form.*

Proof. It is easy to see that we can assume that $A = [P/Q]$ where P and Q are positive, relatively prime and P is greater than Q . We leave the proof that one can choose P greater than Q to the reader.

We then know from Theorem 7 that $B = [-R/S]$ where one of P/Q and R/S is a convergent of the other. We can now enumerate small continued fractions. We know the total of all terms in A and B must be less than or equal to 9 since H and J each have nine crossings.

In order to make a 9-crossing unknot example of the form $N(A - B)$ where A and B are rational tangles in reduced positive alternating form, we must partition the number 9 into two parts corresponding to the number of crossings in each tangle. It is not hard to see that we need to use the partition $9 = 4 + 5$ in order to make a hard unknot of this form. Furthermore, 4 must correspond to the continued fraction $[1, 3]$, as $[2, 2]$ will not produce a hard unknot when combined with another tangle. Thus, for producing 9 crossing examples we must take $A = [1, 3]$. Then, in order that A and B be convergents,

and B have 5 crossings, the only possibilities for B are $B = [1, 4]$ and $B = [1, 2, 2]$. These choices produce the diagrams H, H', J, J' . It is easy to see that no diagrams with less than 9 crossings will suffice to produce hard unknots, due to the appearance of Reidemeister moves related to the smaller partitions. This completes the proof. \square

Conjecture 1 *Up to mirror images and flyping tangles in the diagrams, the hard unknot diagrams H and J of 9 crossings, shown in Figure 24, have the least number of crossings among all hard unknot diagrams.*

This conjecture has been verified for us by Slavik Jablan, using his program “Linknot” [14].

8 The Goeritz Unknot

The earliest appearance of a hard unknot is a 1934 paper of Goeritz [10]. In this paper Goeritz gives the hard unknot G shown in Figure 25. As the reader can see (for example by flyping vertically the tangle $[-3]$ twice), this example is a variant on $N([4] + [-3])$ which is certainly unknotted. The Goeritz example has 11 crossings, due to the extra 2-twists that make it a hard unknot. It is part of an infinite family based on the pattern $N([n] + [-n + 1])$.

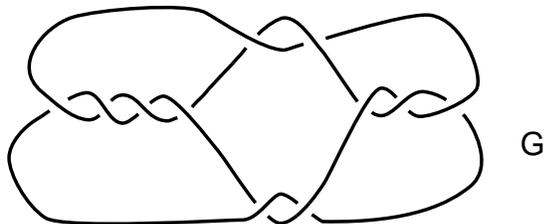


Figure 25 - The Goeritz Hard Unknot

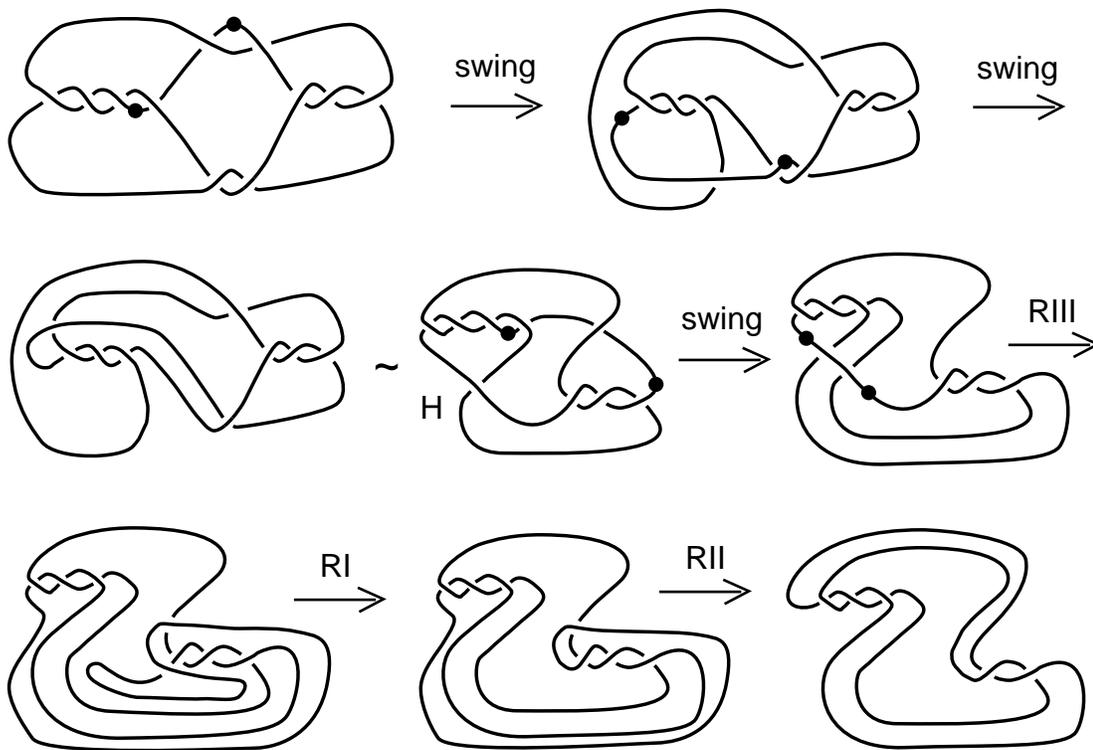
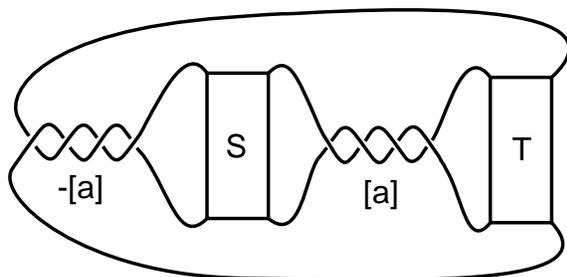


Figure 26 - Unknotting the Goeritz Unknot

In Figure 26 we illustrate the steps in another unknotting process for G . A move labeled *swing* consists in swinging the corresponding marked arc in the diagram. A swing move when realized by Reidemeister moves will complicate the diagram before taking it to the indicated simplification. After two swing moves G has been transformed into the diagram H of the previous section that is again a hard unknot diagram, but with 9 crossings rather than 11!

9 Recalcitrance Revisited



$$K[a] = N(-[a] + S + [a] + T) = N(S + T)$$

Figure 27 - Twisting Up the Recalcitrance

Suppose that $K[a]$ denotes the knot diagram shown in Figure 27, so that

$$K[a] = N(-[a] + S + [a] + T).$$

We shall assume that $K[0] = N(S + T)$ is unknotted. We also assume that the diagram $K[a]$ is hard, a generalization of the form of the hard diagram H in Figure 24. Let's also assume that it takes N Reidemeister moves to transform $[-1] + S + [1]$ to S . This transformation is easily accomplished in three dimensions by one full rotation, but may require many Reidemeister moves in the plane (keeping the ends of the tangle fixed). It is certainly possible to produce alternating rational tangles S and T with this property that no less than N Reidemeister moves can accomplish an isotopy from $[-1] + S + [1] + T$ to $S + T$. Let $C = C(S) + C(T)$ denote the total number of crossings in the tangles S and T . Then the recalcitrance (Definition 2) of $K[0]$ is $R(0) = k/C$ for some k and the recalcitrance of $K[a]$ is generically given by the formula

$$R(a) = \frac{aN + k}{2a + C}$$

since each extra turn of S will add N Reidemeister moves to the untying, and the number of crossings of $K[a]$ is equal to $2a + C$. We conclude from this that *for large a the recalcitrance $R(a)$ is as close as we like to $N/2$* . This shows that *the recalcitrance of an unknotted diagram can be arbitrarily large*. There is no upper limit for the ratio of the number of moves needed to undo the knot in relation to the number of crossings in the original knot diagram.

10 Collapsing to Knots and Links

In this section we point out that our results about unknotted closures of sums of rational tangles can be generalized to collapses to arbitrary knots and links. This leads to the concept of a *hard knot diagram*. We shall say that a knot or link diagram D is *hard* if it admits no type III moves and has no simplifying type I or type II moves. Any sequence of Reidemeister moves that takes this diagram to a smaller diagram for that knot or link must first increase the number of crossings of D . The concepts of this paper, such as recalcitrance, can be generalized to this domain. We can ask, given any diagram D for the least number of Reidemeister moves that will transform D to some minimal diagram for the knot type of D . Many questions can be asked at this juncture. In this section we formulate some collapse results and give examples. We encourage the reader to explore further!

It is worth putting these results in perspective. In this paper we are exploring the combinatorial space of all knot and link diagrams by using the Reidemeister moves. Hard unknots and hard knots are local minima in this combinatorial space. The problem with a local minimum is that it may not be a global minimum. Hard knots can often be made smaller (we want a minimal diagram for the knot), but again must be made larger before becoming smaller. Each time we find a local minimum we may have to face the complex possibilities involved in climbing up out of it before things can be simplified. These features are fundamental to the study of knots and links via diagrams.

Notation. Let R be *any* 2-tangle. We shall write

$$S = [a_1, \dots, a_n, R]$$

to denote the tangle

$$[a_1] + \frac{1}{[a_2] + \frac{1}{\dots + \frac{1}{[a_n] + \frac{1}{R}}}}$$

Note that we will occasionally replace $[a]$ by a in the notation for continued fraction forms of tangles. Note that if R is an arbitrary tangle, then $(R^{rot})^{rot} = R^\pi$ where R^π denotes the result of turning R by 180° around an axis perpendicular to the page. In the case of rational tangles R , we know that $R^\pi = R$, but in the general case the tangle and its 180° rotate may be distinct topologically. This means that $1/(1/R) = R^\pi$ in the general case. Similar remarks apply to R^v , the result of rotating R about the vertical axis and R^h , the result of rotating R about the horizontal axis. Many of the isotopies that we use for rational tangles may replace R by rotations of R by 180° about horizontal or vertical axes or both. Note that $R^\pi = R^{hv}$.

Definition 5 Letting $P/Q = [a_1, a_2, \dots, a_n]$ and $V/W = [b_1, b_2, \dots, b_m]$, it is convenient to make the following definitions for any tangles T and S :

1. $[P/Q]\sharp T = [a_n, a_{n-1}, \dots, a_1 + T]$.
2. $[a_1, a_2, \dots, a_n, T]\sharp[b_1, b_2, \dots, b_n, S] = [T, a_n, a_{n-1}, \dots, a_1 + b_1, b_2, \dots, b_m, S]$

Note that this generalizes our previous definitions of the \sharp operation. In fact, we have a generalization of the Theorem 4, that the numerator closure of the sum of two rational tangles is a rational knot, to the following statement:

Theorem 9 *For any tangles T and S (not necessarily rational) the following equation expresses the numerator of the sum of the tangles indicated below. In this statement we have used the symbol $\hat{=}$ to mean that T and S on the right may differ from their counterparts on the left-hand side of the equation by 180° rotations (as discussed above). In the case of S and T rational or invariant under such rotations, the sign $\hat{=}$ may be replaced by $=$.*

$$N([a_1, a_2, \dots, a_n, T] + [b_1, b_2, \dots, b_n, S]) \hat{=} N([T, a_n, a_{n-1}, \dots, a_1 + b_1, b_2, \dots, b_m, S]).$$

In particular,

$$N([a_1, a_2, \dots, a_n, T] + [-a_1, -a_2, \dots, -a_n, S]) \hat{=} N(T + S).$$

In the special case where $T = [\infty]$ and $S = [0]$ this last equation becomes

$$N([a_1, a_2, \dots, a_n] + [-a_1, -a_2, \dots, -a_{n-1}]) = U$$

where U is unknotted, recovering Proposition 2. Similarly we have

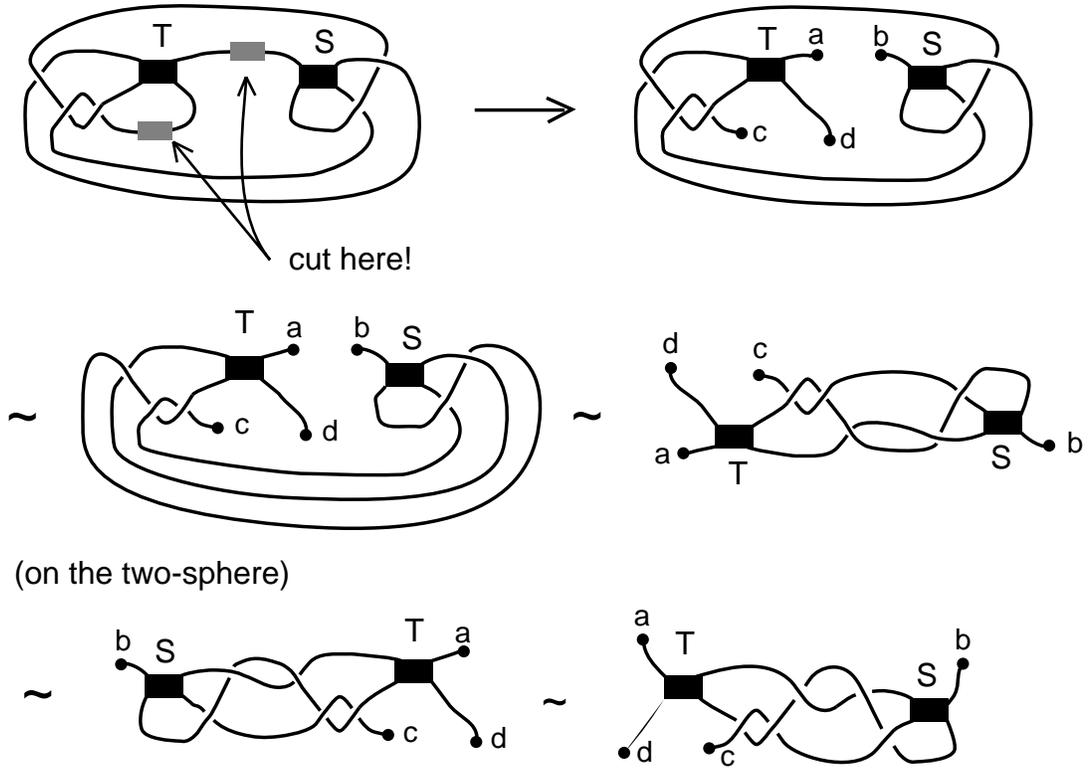
$$N([a_1, \dots, a_n + T] + [-a_1, \dots, -a_n]) \hat{=} N(T)$$

and

$$N([a_1, \dots, a_n, T] + [-a_1, \dots, -a_n]) \hat{=} D(T).$$

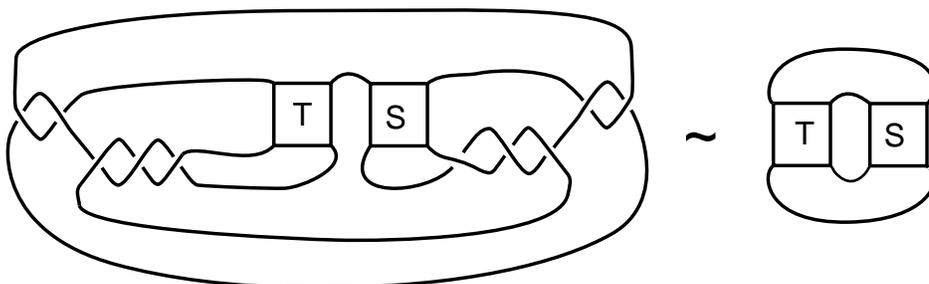
Note that since T and S are arbitrary tangles, we can also regard this Theorem as a statement about black boxes called T and S that are connected as in Figure 28 to form rationally extended tangles and closures. This is the same as considering tangles that contain 4-valent rigid graphical vertices. Such graphs can be modelled as embeddings in three-dimensional space by attaching strings to rigid bodies (such as geometrical balls) in place of the vertices.

Proof. The proof follows from the isotopies indicated in Figure 28 and the identities $[a_1, \dots, a_n, 0] = [a_1, \dots, a_{n-1}]$ and $[a_1, \dots, a_n, \infty] = [a_1, \dots, a_n]$. \square



$$N([1, 2, T] + [1, 1, S]) = N([T, 2, 1+1, 1, S])$$

Figure 28 - The Black Boxes



$$N([2, 3, T] + [-2, -3, S^V]^V) \sim N(T + S)$$

Figure 29 - Black Boxes and Braid Cancellation

Remark 7 For T and S any 2-tangles, the cancellation to $N(T + S)$ in Theorem 9 can be stated more precisely as follows:

$$N([a_1, a_2, \dots, a_n, T] + [-a_1, -a_2, \dots, -a_n, S^v]^v) = N(T + S).$$

See Figure 29 for a direct illustration of this result. Note that this formula tells us that we have rational collapses to any knot or link, since we can always cut such a knot or link into one tangle or a sum of two tangles and embed these in cancelling rational patterns. Just as we have constructed hard unknot diagrams, we can construct hard *knot* diagrams.

The next Theorem is a direct consequence of Theorem 9. We leave its proof to the reader.

Theorem 10 (i) *Letting*

$$M = M(\vec{a}) = M(a_1)M(a_2) \dots M(a_n) = \begin{pmatrix} P & Q' \\ Q & U \end{pmatrix},$$

and given F/G , a fraction in reduced form, then there exists a unique reduced fraction R/S such that

$$N([F/G]) = N([P/Q] + [R/S]),$$

and

$$\frac{F}{G} = \frac{\text{Num}(P/Q + R/S)}{\text{Num}(Q'/U + R/S)}$$

where $\text{Num}(a/b + c/d) = ad + bc$. Note that Q'/U is a convergent of P/Q , so we see that a combination of a fraction and its convergent appears in the decomposition of an arbitrary rational knot, fully generalizing our results about the unknot.

(ii) For any 2-tangle T ,

$$N([P/Q] + [-P/Q']\sharp T) = N(T).$$

This is another generic form of the collapse result, and this one specializes directly to our unknot theorem when we take $T = [1/N]$ so that $N(T)$ is an unknot. In that case the fractions P/Q and $(P/Q')\sharp(1/N)$ are convergents.

(iii) If T and S are arbitrary 2-tangles and $[P/Q]$ denotes a specific rational tangle with a given continued fraction expansion, as above, then

$$N([P/Q]\sharp T + [-P/Q']\sharp S) = N(T + S).$$

Example 1. View Figure 30. This figure illustrates the identity

$$N\left(\frac{1}{[m] + \frac{1}{[n]+T}} - \frac{1}{[m]}\right) = D(T)$$

where $D(T)$ denotes the denominator of T , and T is any tangle. The example is due to DeWitt Sumners and is fashioned to illustrate that an equation

$$N(A + B) = K$$

for fixed K and variable A and B may have infinitely many solutions, as we have proved above. Let's analyse the class of examples in Figure 30 in our formalism. Note that for any tangle T ,

$$N([T, 0]) = N(T + 1/[0]) = N(T + [\infty]) = D(T).$$

Then we have

$$\begin{aligned} N\left(\frac{1}{[m] + \frac{1}{[n]+T}} - \frac{1}{[m]}\right) &= N([0, m, [n] + T] + [0, -m]) = N([[n] + T, m, 0 + 0, -m]) \\ &= N([n + T, m, 0, -m]) = N([[n] + T, 0]) = D([n] + T) = D(T), \end{aligned}$$

making this class a special case of the first part of the Proposition.

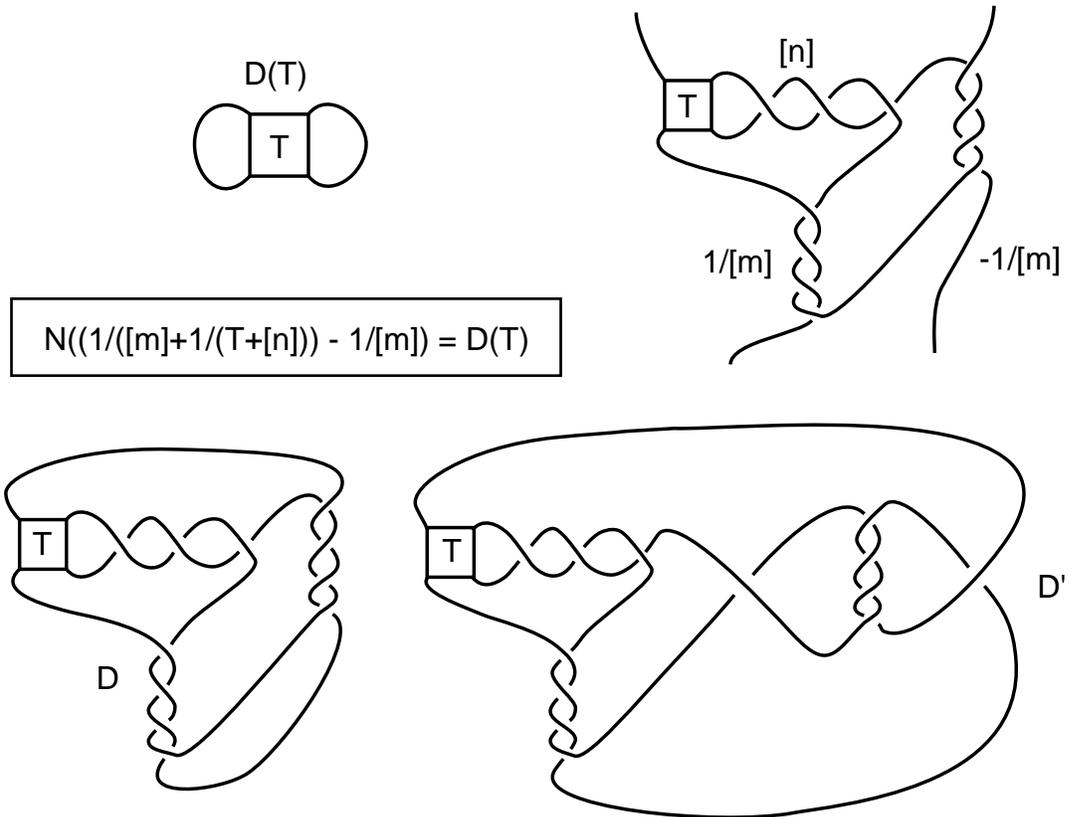


Figure 30 - Sumners' Example

Example 2. View Figure 31. Here we have a knot $K = N(T + S)$ and have constructed three diagrams associated with K . The first diagram is $N([2, 3, T] + [-2, -3, S])$, which by the results of this section is isotopic to K , and it is a hard diagram. The next diagram is made by applying a 180° turn and replacement to one of the subtangles of the previous diagram. It is hard in the plane but not on the 2-sphere. In the third diagram we remedy this situation by using the tucking construct, obtaining another hard diagram related to K .

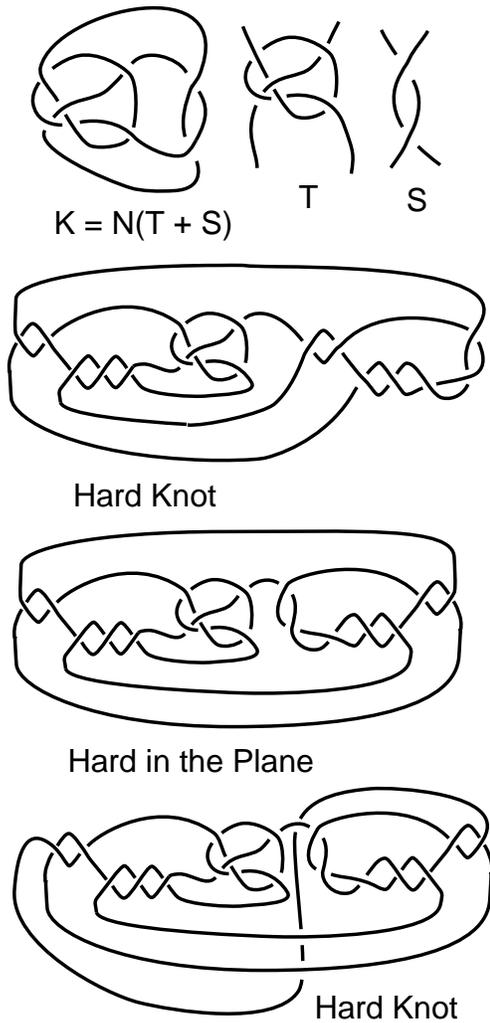


Figure 31 - A Hard Knot

11 Stability in Processive DNA Recombination

In this section we use the techniques of this paper to study properties of the topology of processive DNA recombination. We follow the tangle model of DNA recombination [5, 6, 31] developed by C. Ernst and D.W. Sumners. In this model the DNA is divided into two regions corresponding to two tangles O and I and a recombination site that is associated with I . This division

of the DNA is a model of how the enzyme that performs the recombination traps a part of the DNA, thereby effectively dividing it into the tangles O and I . The recombination site is represented by another tangle R . The entire arrangement is then a knot or link $K[R] = N(O + I + R)$. We then consider a single recombination in the form of starting with $R = [0]$, the zero tangle, and replacing R with a new tangle; for our purposes this will be the tangle $[1]$ or the tangle $[-1]$. Processive recombination consists in consecutively replacing again and again by $[1]$ or by $[-1]$ at the same site. Thus, in processive recombination we obtain the knots and links

$$K[n] = N(O + I + [n]).$$

The knot or link $K[0] = N(O + I)$ is called the *DNA substrate*, and the tangle $O + I$ is called the *substrate tangle*. It is of interest to obtain a uniform formula for knots and links $K[n]$ that result from the processive recombination.

In some cases the substrate tangle is quite simple and is represented as a single tangle $S = O + I$. For example, we illustrate processive recombination in Figure 32 with $R = [+1]$, $S = [-1/3] = [0, -3]$ and $I = [0]$ with $n = 0, 1, 2, 3, 4$. Note that by Proposition 1,

$$\begin{aligned} K[n] &= N(S + [n]) = N([0, -3] + [n]) = N([-3, 0 + n]) = N([-3, n]) \\ &= N(-[3, -n]) = N(-[2, 1, n - 1]). \end{aligned}$$

This formula gives the abstract form of all the knots and links that arise from this recombination process. This formula goes infinitely many steps further than Figure 32. Looking at Figure 32 we see that the sequence is: *Unknot, Hopf Link, Figure Eight Knot, Whitehead Link, Funny Twisty Diagram, and so on*. A single neat formula for the whole sequence is welcome.

We say that the formula

$$K[n] = N(-[2, 1, n - 1])$$

for $n > 1$ is *stabilized* in the sense that all the terms in the continued fraction have the same sign and the n is in *one single place* in the fraction. In general, a *stabilized fraction* will have the form

$$\pm[a_1, a_2, \dots, a_{k-1}, a_k + n, a_{k+1}, \dots, a_n]$$

where all the terms a_i are positive for $i \neq k$ and a_k is non-negative. It is not quite obvious that the output of a recombination process will be stabilized in this sense. We shall prove below that this is always the case. For another

example view Figure 33, where we show a process that stabilizes after the second term, with the transition from first to second term having its own idiosyncrasy.

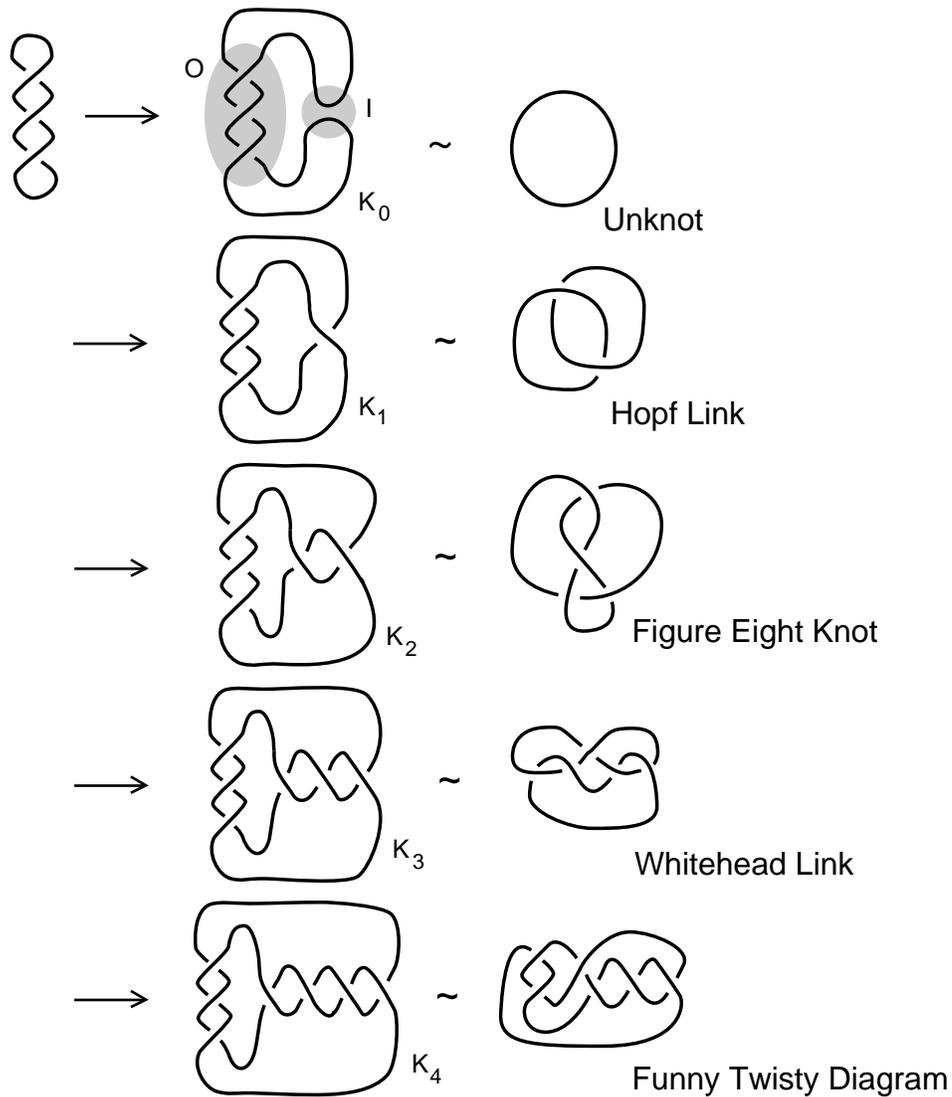


Figure 32 - Processive Recombination with $S = [-1/3]$

Let's see what the form of the processive recombination is for an arbitrary sequence of recombinations. We start with

$$O = [a_1, a_2, \dots, a_r]$$

$$I = [b_1, b_2, \dots, b_s].$$

Then

$$\begin{aligned} K[n] &= N(O + (I + [n])) = N([a_1, a_2, \dots, a_r] + [n + b_1, b_2, \dots, b_s]) \\ &= N([a_r, a_{r-1}, \dots, a_2, a_1 + n + b_1, b_2, \dots, b_s]). \end{aligned}$$

Proposition 3 *The formula*

$$K[n] = N([a_r, a_{r-1}, \dots, a_2, a_1 + n + b_1, b_2, \dots, b_{s-1}, b_s])$$

can be simplified to yield a stable formula (in the sense of the discussion above) for the processive recombination when n is sufficiently large.

Proof. Apply Proposition 1. □

Here is an example. Suppose we take $O = [1, 1, 1, 1]$ and $I = [-1, -1, -1]$ so that the DNA substrate is an (Fibonacci) unknot. Then by the above calculation:

$$K[n] = N([1, 1, 1, 1 + n + (-1), -1, -1]) = N([1, 1, 1, n, -1, -1]).$$

Suppose that n is positive. Applying Proposition 1, we get:

$$K[n] = N([1, 1, 1, n, -1, -1]) = N([1, 1, 1, n-1, 1, 0, 1]) = N([1, 1, 1, n-1, 2]),$$

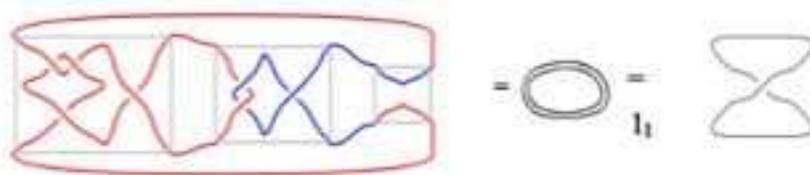
and this is a stabilized form for the processive recombination.

More generally, suppose that $O = [a_1, \dots, a_n]$ where all of the a_i are positive. Let $I = [-a_1, \dots, -a_{n-1}]$. Then $K[0] = N(O + I)$ is an unknotted substrate by our result about convergents (Proposition 2 and Theorem 7). Consider $K[n]$ for positive n . We have

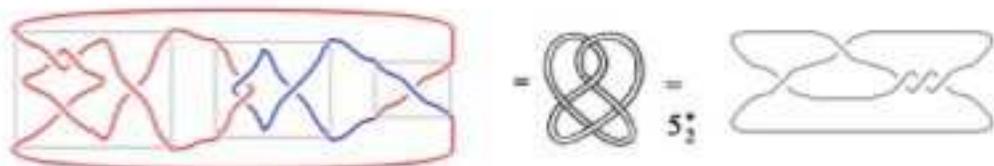
$$\begin{aligned} K[n] &= N([a_n, a_{n-1}, \dots, a_2, a_1 + n - a_1, -a_2, \dots, -a_{n-1}]) \\ &= N([a_n, a_{n-1}, \dots, a_2, n, -a_2, \dots, -a_{n-1}]) \\ &= N([a_n, a_{n-1}, \dots, a_2, (n-1), 1, (a_2-1), a_3, \dots, a_{n-1}]). \end{aligned}$$

If $a_2 - 1$ is not zero, the process terminates immediately. Otherwise there is one more step. In this way the knots and links resulting from the recombination process all have a uniform stabilized form. Further successive recombination just adds more twist in one entry in the continued fraction diagram whose closure is $K[n]$.

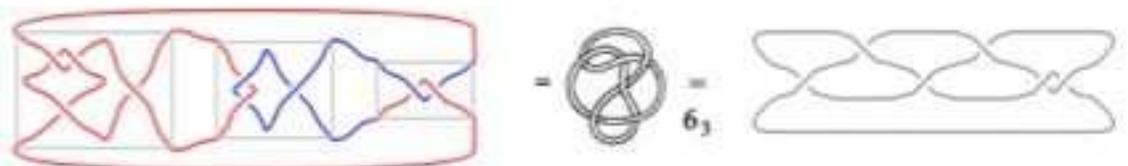
The reader may be interested in watching a visual demonstration of these properties of DNA recombination. For this we recommend the program *GINterface* (TangleSolver) [32] of Mariel Vasquez. Her program can be downloaded from the internet as a Java applet, and it performs and displays DNA recombination. Figure 33 illustrates the form of display for this program. The reader should be warned that the program uses the reverse order from our convention when listing the terms in a continued fraction. Thus we say $[1, 1, 2]$ while the program uses $(2, 1, 1)$ for the same structure.



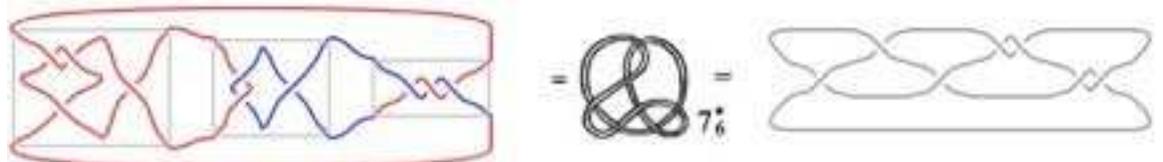
$N((2,1,1) + (-2,-1) + (0)) = (1)$ unknot



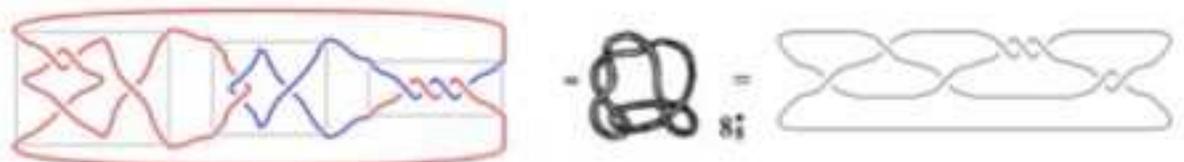
$N((2,1,1) + (-2,-1) + (1)) = (1,1,3) + 5$ twist knot



$N((2,1,1) + (-2,-1) + (2)) = (1,1,1,1,2)$ knot



$N((2,1,1) + (-2,-1) + (3)) = (1,1,1,2,2)$ knot



$N((2,1,1) + (-2,-1) + (4)) = (1,1,1,3,2)$ knot

Figure 33 - Processive Recombination with $S = O + I$ and
 $O = [1, 1, 1, 1]$, $I = [-1, -1, -1]$.

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