Supercoiled DNA Tangles and Stick Number of Montesinos Links

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ABSTRACT. A circular DNA molecule uses twist and writhe to transmute into the supercoil state where specific topoisomerase enzymes are able to cut the DNA strand(s) to reduce the effect of supercoiling. The goal of this paper is to cut a rational link the represents *n* number of supercoiled integral tangles with a crossing number *c* which composes a total of *m* rational tangles. The combination of rational tangles configures a Montesinos knot where we obtain an upper bound stick number *s*. The upper bound for the stick number gives a rational number that represents how many sticks are required to turn a Montesinos knot into a stick Montesinos knot. We only focus on alternating Montesinos link can have an upper bound stick number *s* with $s \le c + 1$. However, this paper shows an improved upper bound of *s* for an alternating Montesinos knot when there is a 'large' *c*. Let *K* be an alternating Montesinos knot or link with the number of half-twist *e*, the crossing number *c*, the supercoiled integral tangles *n*, rational tangles *m*, and the stick number *s*. Shown as: $s \le \frac{2}{3}c + 2n + 3m + e + 1$.

1. Introduction

The inspiration for this project is examining how knot theory correlates to molecular biology. **DNA** (deoxyribonucleic acid) is located in the cell nucleus which makes up all (with some exceptions) living things including plants, animals, and bacteria. DNA is formed from two molecular strands twisted and knotted together that form a right-handed double helix. The **linking number** (*Lk*) is the number of times two sugar-phosphate chains of DNA wrap around each other. Another way to describe *Lk* is the number of turns or twists needed to unwind in a circular DNA molecule. To find the *Lk*, we count the number of **twist** (*Tw*) and the **writhe** (*Wr*). This is depicted as *Lk*=*Tw*+*Wr*. Insko and Trapp [1] took advantage of twist and writhe to assemble integral tangles with an efficient upper bound stick number *s* when each twist has more than seven crossings, roughly. They show it as $s \le \frac{2}{3}c + 2n + 3$. Note that Insko and Trapp utilized this approach to construct stick 2-bridge links formed from these integral tangles. However, by cutting two strands in a 2-bridge link diagram, we can configure a stick rational tangle that uses the same stick number as the 2-bridge link construction [1].

Now thanks to Lee, Oh, and No [3], they devised a way of putting a stick rational tangle inside a virtual box. After following a set of specific conditions, a virtual box can be added together with other virtual boxes. Meaning we can add any number of stick rational tangles together. Referring again to [3], as we combine virtual boxes together to an arbitrary θ , it is possible to form an alternating Montesinos knot. Note that not all Montesinos knots are alternating, however, this paper will only consider alternating Montesinos knots. Stick Montesinos knots provide an upper bound for the stick number. The upper bound for the stick number gives a rational number that represents how many sticks are required to turn a Montesinos knot or link into a stick Montesinos knot or link. Lee, Oh, and No [3] demonstrates an upper bound for the stick number *s* of an alternating Montesinos link given by $s \le c + 1$. However, this paper demonstrates an improved upper bound for *s* that uses fewer sticks when the crossing number is 'large' enough. The main topic of this paper is **Theorem 1**, which utilizes the twist and writhe to construct an improved *s* for alternating Montesinos knots.

Theorem 1. Let *K* be an alternating Montesinos knot or link with the number of half-twist e, the crossing number c, the supercoiled integral tangles n, rational tangles m and the stick number s. Then

$$s \leq \frac{2}{3}c + 2n + 3m + e + 1.$$

Section 2 describes supercoiled integral tangles, rational links, and Montesinos links. Readers should skip this section if they are already comfortable with the concepts or can refer back to section if they need any clarifications. Then Section 3 explains what stick rational tangles are as well as how to convert a rational link into a stick rational tangle. After, we transition over to placing a stick rational tangle inside of a virtual box and adding any number of virtual boxes together in section 4. Section 5 discusses stick Montesinos knots and how to find an improved upper bound stick number

s by applying the **Theorem 1**. We end this paper in section 6 where we further elaborate on DNA and leave some open questions for people to ponder.

2. Background of Tangles, Rational Links, and Monesinos Links

2.1. Rational tangles, Rational Knots, Rational Links

Any reader who is unaccustomed to knot theory must first understand the concept of a knot and link. Imagine there is a person with a piece of string. If the person were to tie a knot with the two end strands and glued the two endpoints of the string together, this would form a knotted loop. A **knot** is a knotted loop of string with its cross-section being at a single point. A knot is considered a closed curve in three dimensions that does not intersect on itself anywhere. The areas where the knot (K) crosses over itself is known as the **crossings** of the projection. The crossing number c of K is the smallest number of crossings in a projection of any K. The picture below is considered a **projection** of K.



Examining the picture above, from left to right, c = 0 (unknot/trivial knot), 1 (trivial knot), 4 (figure-eight knot). A **link** is a collection of knotted loops that all intertwine with each other which does not cut through itself. A **linking number** *Lk* depicts the number of times that each curve winds around the other. A reader who is unfamiliar with knot theory should know that not all links are knots, but all knots are links since a knot can be described as a link with one component. However,

when knots or links are mentioned in certain parts of the reading, sometimes we are referring to both knots and links .

John H. Conway introduced a notation for knots that is related to knotting in DNA called *tangles*. A two string tangle can be thought up as two-strands contained in a three dimensional ball with the strands penetrating the sphere four times. A **tangle** in a knot (K) or link (L) is a region in the projection plane surrounded by a circle (or box) where the K or L crosses the circle precisely four times. One can think of the four points where the tangle crosses the circle as the compass directions Northwest (NW), Northeast (NE), Southeast (SE), and Southwest (SW). I want to point out the tangle diagrams in Figure 1 has the tangles inside of a box rather than a circle. The concept of a tangle still holds true inside of a box and the purpose of this box concept is to help the reader better visualize the notions of a *virtual box* in Section 4.



Click me - Figure 1. Examples of Rational Tangles

An example of a tangle is to imagine two strings (arcs) that are horizontally parallel to each other. This is known as the **empty tangle** or as the 0 tangle (shown in Figure 1a). The empty tangle consists of two horizontal strands where the four endpoints penetrate the adjacent vertices of a box. One strand connects the endpoints NW to NE and the second strand connects the endpoints SW to SE. Keep in mind that any *rational tangle* can be constructed out of an *empty tangle* through two moves known as the twist move and a rotation move. The first tangle move is known as a *twist*. A **twist** (starting from Figure 1a.) is when we disconnect the north easternmost vertex (NE) and south easternmost vertex (SE), move the NE strand *over* the SE strand, and reattach the vertices to obtain a new tangle that is illustrated in Figure 1b. The second tangle move is known as a **rotation**. A rotation is when the entire tangle is rotated 90° clockwise. An example of a rotation is take Figure 1a and rotate the tangle 90° clockwise. This creates the ∞ tangle (depicted in Figure 1c) that is two vertical strings. A tangle can also be represented as a rational number or an *integer tangle*. **Examples of an integer tangle.**



An integer tangle is two strands that wrap around each other and identifies the number of half-twists or crossings within the tangle. Connecting integral tangles together forms rational tangles which can be represented by Conway notation $[c_1, c_2, ..., c_n]$. All three tangles in Figure 1

are rational tangles. A **rational tangle** can be unwound by twisting and rotating the endpoints and be represented as a continued fraction $\frac{\beta}{\alpha}$ which depicts a rational number, hence the name. An important fact is that continued fractions has a canonical form of which all the integers used to form the continued fraction have to properties:

- 1. The integers can all have the same sign of either being all positive or all negative.
- The number of integers used to form the continued fraction is odd. Now closing the ends of a rational tangle can build a rational knot or a rational link. An example of a rational link is a 2-bridge link.



FIGURE 2. Diagram of supercoiled integral tangles in a rational link converted to rational tangle. Figure 2a illustrates an integral tangle. When the number of crossings *c* is positive, the over strand has a positive slope. When c is negative, the over strand has a negative slope. Figure 2b depicts a supercoiled integral tangle inside a 3 dimensional sphere. Figure 2c displays a 2-bridge link [1]. Figure 2d shows what strands to cut to find the rational tangle depicted in Figure 2e.

2.2. 2-Bridge Knot

The bridge number b(k) of a knot K is the minimal number of unknotted arcs on either side of the

projection plane that is bisecting *K*. The b(k) of *K* is the least bridge number of all of the projections of the knot K. An example of a 2-bridge link is shown in Figure 3.



FIGURE 3. 2-Bridge Knot

Figure 3 has a projection plane cutting through a knot towards the middle. The bridge-number of the knot is 2 since there are 2 arcs below the bisecting plane and 2 arcs above the bisecting plane. Counting the number of each individual unknotted arc above and below the plane can determine the bridge number of a knot. Knots that have a bridge number 2 are a classified as **two-bridge knots**. All 2-bridge links have the following properties:

- 1. Any Rational link has a bridge number of 2.
- 2. Every two bridge link is a Rational link.

Knowing this, if a knot does not have a bridge number of two, then it will not be a rational knot. For clarification, a knot K or link L is said to be a *two-bridge knot* or *link* when it is constructed out of a rational tangle. The set of 2-Bridge links is a subset of the set of Montesinos links.

2.3. Montesinos Link

A Montesinos link produces a diagram composed of *m* rational tangle diagrams $R_1, R_2, ..., R_m$, and *e* half-twists.



FIGURE 4. Montesinos knot

Viewing Figure 4, we can see on the far left we have three half-twist or e = 3. On the far right, the boxes $(R_1, R_2, ..., R_m)$ are *m* rational tangles where there is a total of *m*. Refer to Lee, Oh, and No [3] for more information about Montesinos knots as we shall be applying their definitions of a Montesinos knot.

If a Montesinos knot diagram is alternating, then it is has a reduced Montesinos diagram. This means

- If $e \ge 0$, then $R_1, ..., R_m$ are positively alternating.
- If *e* = 0, then *R*₁,...,*R_m* are positively alternating and *R_{t+1},...,R_n* are negatively alternating for some *t*, where 1 ≤ *t* < *m*.

3. Converting Supercoiled Integral Tangles to Stick Rational Tangles

Insko and Trapp took advantage of twist and writhe to construct 2-bridge knots out of supercoiled integral tangles. A **supercoiled integral tangle** uses both twisting (Tw) and writhing (Wr) to count the number of crossings or **link number** (Lk) of a tangle.



The image on the far left is a rational link or **integral tangle**. The image to the right adds writhe to the integral tangle making a supercoiled integral tangle. To solve the linking number (Lk) for a supercoiled tangle is Lk = Tw + Wr.



The image above on the left side illustrates an tangle with writhe. When the tangle loses writhe or Wr = 0, the number of twist increases, however, *Lk* has not changed. Examine section 6 for further

details.

We can replace the arcs in a knot or link with straight line segments or *sticks* to create a **stick knot**. Every knot or link has a **stick number** *s* which represents the lowest number of sticks needed to form the link. Insko and Trapp [1] shown that a two bridge rational link has a stick number *s* by knowing the number of crossings *c* and the number of supercoiled integral tangles *n* using $s \le \frac{2}{3}c + 2n + 3$. It is written as follows.

Theorem 1. Let *L* be a rational link given by the integers $c_1, c_2, ..., c_n$, and suppose *P* of the integers satisfy $c_i \equiv 0 \pmod{3}$, *Q* satisfy $c_i \equiv 1 \pmod{3}$, and *R* satisfy $c_i \equiv 2 \pmod{3}$. Then the stick number s(L) of *L* satisfies

$$s(L) \leq \frac{2}{3}c(L) + 2n + 3 - \frac{2}{3}Q - \frac{1}{3}R.$$

By building off of his notation, we can turn an integral tangle into a stick rational tangle diagram using the same number of sticks as [1]. They show how to construction of supercoilded integral tangle and how to glue the tangles together to build polygonal 2-bridge links. Their result was an improved upper bound for the stick number of 2-bridge links with crossing number roughly six times the number of tangles or more.

Now based off their research, we can turn links into stick rational tangles using the same number of sticks. The reasoning is as follows. Any 2-bridge knot or link has a reduced alternating diagram form and it is easy to change a rational tangle diagram so that the number of tangles *n* can always be odd. Moreover, the projection can be assumed reduced and alternating, so it has minimal crossing number. [1. PG 6] We will now explain how to convert a rational link into a stick rational tangle.



FIGURE 5. Converting Rational Link to Stick Rational Tangle

First, start off with a 2-bridge link as depicted in Figure 5a. If we have already have a rational tangle we can skip to Figure 5b, else refer to Figure 2 on how to turn a 2-bridge link into a rational tangle. By examining Figure 5b, we start replacing all the arcs with straight lines or *sticks* which leads to Figure 5c. After we replace all the arcs with sticks, we obtain a stick rational tangle as shown in Figure 5d. We shall now describe a stick rational tangle.



FIGURE 6. Stick Rational Tangle

Once we acquire a stick rational tangle, we are going to label the end points as a, b, c and d. Examine Figure 6a on how to properly label each end point. Figure 6b depicts how to properly insert positive and negative (reflection of the positive) integral tangles. For more detail, see [1]. We shall now give an example to explain how to count the stick number of a stick rational tangle.

Example.

Assume Figure 6a, has 49 crossings *c* and 7 integral tangles *n*. Use $s \le \frac{2}{3}c + 2n + 3$ [1] to find the upper bound for the stick number. Thus,

$$s \le \frac{2}{3}(49) + 2(7) + 3$$
$$s \le 32\frac{2}{3} + 14 + 3$$
$$s \le 49\frac{2}{3}$$

This means the upper bound for the stick number stick number is $s \le 49\frac{2}{3}$ or rather $s \le 49$.

4. Stick Rational Tangle Confined Inside a Virtual Box

4.1 Virtual Boxes together with Stick Tangles

We have shown in the previous section that a 2-bridge link can be converted into a stick rational tangle using the same amount of sticks as a 2-bridge link. In this section, we show that a stick rational tangle can fit inside a *virtual box*. To accomplish this, we use the Lee, No, and Oh [3] method in which they were able to contain a stick rational tangle inside a *virtual box*. In a specific manner, we label the four end points of the stick rational tangle as a, b, c, and d. Next, appropriately denote the end sticks where the four end points are attached as L_a, L_b, L_c , and L_d . Now think of a *virtual box* as a three dimensional box that surrounds a rational tangle. Applying the same technique Lee, No, and Oh utilized in their paper [3], we are able to contain a stick rational tangle R inside a *virtual box* B_R .



Click me - Figure 7. Rational Tangle Confined Inside a Virtual Box

Examining Figure 7, we are able to confine R inside of B_R following the three given conditions:

- 1. L_a passes through the back side (face) of B_R , and L_b passes through the left side (face) of B_R ,
- 2. The point *c* lies on the common edge between the back side (face) and the left side (face) of B_R , and
- 3. L_d passes through the back side (face) of B_R near the position of c.

Note, in Figure 7, the dotted lines represent sticks outside of B_R and the filled line segments are inside of B_R . In addition of those three conditions, the three end points a, b, and d do not lie inside of B_R , but c lies on the corner edge. Also, L_a, L_b, L_c , and L_d can extend to any necessary length, but L_a, L_b , and L_d lies out side of B_R and L_c cannot leave the area of B_R . From here on, consider a stick rational tangle comprised of supercoiled integral tangles as a stick rational tangle inside a virtual box.

4.2 Combining Virtual Boxes

A stick rational tangle R_1 inside a virtual box B_{R1} can be added together with R_2 inside B_{R2}

without having to add any sticks. Following Lee, Oh, and No method [3] for combining B_R together, we can combine supercoiled integral tangles without having to add any sticks. Observe Figure 8 for an illustration.



Click me - Figure 8. Technique for combining virtual boxes containing Rational Tangle

Once again, we have the four end points of the stick rational tangle as a, b, c, and d and the end sticks as L_a, L_b, L_c , and L_d . First place down B_{R1} . Next, position B_{R2} away from B_{R1} (where the do not touch) on the right backside side or where L_{a1} is sticking out of B_{R1} . If we angled the virtual boxes and stick rational tangles correctly, L_{a1} and L_{b2} will merge into one stick. Also, the points d_2 and c_1 will merge into one stick but make sure L_{d2} does not cross through the virtual box B_{R1} . We can then manipulate B_{R2} to extend downwards to any necessary length shown in Figure 8. Following these steps, any number of virtual boxes can be added together.

Note that stick rational tangles $R_1, R_2, ..., R_m$ are formed up of *n* integral tangles. Also, $R_1, R_2, ..., R_m$ are able to merge together through linear transformation. Furthermore, the angle between two stick rational tangles (say R_1 and R_2) is an arbitrary angle θ . For more information, examine [3]. In the next section, we cover how we can combine $R_1, ..., R_m$ to form a stick Montesinos link.

5. Stick Montesinos Knot

Lee, No, and Oh [3] shown that *virtual boxes* containing stick rational tangles can be combined together to form a stick Montesinos knot. Let *K* be an alternating Montesinos knot with R_m stick rational tangles and *e* half-twist. Since *K* is an alternating Montesinos knot, then presume $R_1, ..., R_m$ are all positively alternating and $e \ge 0$.



FIGURE 9. Stick Montesinos Knot

Lee, No, and Oh [3] shown that an upper bound for the stick number of an alternating stick Montesinos knot is $s(K) \le c(K) + 1$. They constructed a crossing tangle *c* using c + 1 sticks with at least six crossings. However, we can construct an stick Montesinos link with an improved stick number for a 'large' number of crossings.

Theorem 1. Let *K* be an alternating Montesinos knot or link with the number of half-twist e, the crossing number c, the supercoiled integral tangles n, rational tangles m and the stick number s. Then

$$s \le \frac{2}{3}c + 2n + 3m + e + 1.$$

We will provide some examples to illustrate the theorem.

Example 1. Examine Figure 5 which we label as R_1 and assume there is 144 crossings c, 12 integral tangles n, and confined inside 1 rational tangle. Let there exist $R_1, R_2, R_3, R_4, R_5, R_6, R_7$ that are all duplicates of each other and we want to form an alternating Montesinos link with e = 0. We will show Insko method [1] first and show another example with Theorem 1.

Ex 1a. Applying [1] method ($s \le \frac{2}{3}(c) + 2(n) + 3$ to each rational tangle:

$$s \le \frac{2}{3}(144) + 2(12) + 3$$

 $s \le 96 + 24 + 3$
 $s \le 123$

Since all the boxes are duplicates of each other, we have to add 123 to itself eleven more times or multiple 123 by 12. This give the stick number $s \le 1476$ however, we must add an extra stick due to the construction of the alternating Montesinos link [3]. Thus, the upper bound stick number is $s \le 1477$

Ex 1b. Applying Theorem 1, c = 1728, n = 144, m = 12:

$$s \le \frac{2}{3}(1728) + 2(144) + 3(12) + 1$$
$$s \le 1152 + 288 + 36 + 1$$
$$s \le 1477$$

This shows using either [1] or Theorem 1 obtains the same stick number. Also, notice that employing Lee, Oh, and No method of $s \le c+1$ [3] provides a larger stick number that is $s \le 1729$.

Important! This formula does not work for all cases. As a possible future research topic, create a formula that finds the upper bound of a stick number for alternating and non alternating Montesinos links that is useful for 'large' crossing numbers. This is important as DNA involves has a 'large' number of crossings so creating a diagram of DNA with the least amount of sticks would be most efficient.

6. DNA



Reverting back to section 2, tangles are knots used to relate to DNA. In this section, we will describe what DNA is, DNA's relationship with supercoiling, and leave off on some open ended questions. All living things have DNA (deoxyribonucleic acid) located inside of their cells. However, DNA is too small to see with the naked eye thus scientist use special equipment such as X-rays, an atomic force microscope, and electron microscope to view DNA. The basic structure of duplex DNA or double-stranded DNA is formed from two molecular strands (sugar-phosphate strands) that twist and knot together and composed of 4 bases; (A) adenine, (G) guanine, (C) cytosine, and (T) thymine. DNA needs to untwist itself into two separate sugar-phosphate strands inside a cell for the process of DNA transcription and DNA replication.



Figure 10. DNA transcription and DNA replication

Supercoiling is important in biology because it allows long DNA strands to fit inside of a cell nucleus and helps unwind DNA allowing for synthesis of RNA strands or new DNA strands. In transcription (Figure 10a), DNA copies into the messenger-RNA which tells the cell how to make protein. In replication (Figure 10b), DNA copies itself into another DNA strand before a single cell divides into two cells. Even though figure 10 shows a brief moment in a cells life, both processes of which the unwound regions of DNA occurs fast. However, when a DNA is tightly supercoiled or cannot untangle itself, how does the DNA manage untangle in order to replicate? The answer is Topoisomerases.

Enzymes that regulate DNA supercoiling are known as topoisomerases.



Figure 11. Type I and Type II Topoisomerases

There are two types of topoisomerases known as Type I and Type II. Type I topoisomerases enzymes catalyze changes in DNA topology for single-stranded breaks in DNA. As shown in Figure 11 on the left side, Type I helps untangle a supercoiled integral tangle. Type II topoisomerases enzymes catalyze changes in DNA topology for double-stranded breaks in DNA. Shown on the right side of Figure 11, Type II turns an integral tangle or a relaxed DNA into a supercoiled integral tangle. Finally, we discuss the linking number of supercoiled integral tangle.



FIGURE 12. Integral Supercoiled DNA

The **linking number** (*Lk*) is the number of times two sugar-phosphate chains of DNA wrap around, or are 'linked', with one another. Another way to describe *Lk* is the number of turns or twists in a circular molecule. To find the linking number *Lk* of a double helix, we count the number of **twist** and the number of **writhe**. This is depicted as Lk = Tw + Wr.

Note that Tw and Wr can be integers and real numbers such as Tw = +0.5 and Wr = +2.5 Lk measures the total deficit or excess of double-helical turns in a molecule. Thus, when 'Lk = +5', we mean a DNA molecule is 'overwound by five turns' exactly. An interesting fact is DNA in living

cells is normally underwounded or more precisely Lk is negative. Therefore, when $Lk = \pm 1$ or any number that is not 0, shall have that many *more* double-helical turns.

6.2. Final Thoughts

On a final note, I want to leave some questions open for discussion. Please understand I am a mathematician, **not** a molecular biologist. My experience in the field of biology is epsilon (ε) small. However, doing this research has peaked my curiosity involving knot theory and DNA. I understand from a biologist point of view my ideology might seem controversial, but scientific discoveries are not made through rational thinking. Now we shall dive into topics left open for research.

- Since we are able to find an upper bound for the stick number of stick Montesinos knots, can we correlate this to DNA? Rather is it possible to reconstruct a strand of DNA but as a Montesinos knot/link? If not, can the set of a Montesinos links be a subset to another kind of knot (similarly to how 2-bridge links are subsets of Montesinos Links) that can translate into DNA?
- 2. Is it possible to find an even smaller stick number for rational tangles that have a large number of crossings?
- 3. If we can construct a long right-handed double helix as a Montesinos knot/link, would the stick number of the double helix tell us anything about the DNA? Is there an average range for the stick numbers to classify the DNA into a specific category (e.g. healthy, damaged,untangling DNA about to replicate)?
- 4. Could we create a DNA model using sticks? If we can, is there a difference between the number of sticks from a healthy strand of DNA from damaged strand of DNA? If we could determine the number of sticks, what is the stick number of cancer cells?
- 5. Another topic involves cancer cells. If we are able to locate cancer cells within the human body, can we create a supercoiled DNA strand that prevents the DNA from replicating?

(Thus stopping the cancer cell from spreading.) Obviously, we would have to disrupt the topoisomerases in cancer cells so they cannot untangle the DNA strand. Or maybe the question is there any knot a topoisomerases can't/ won't untangle?

7. Acknowledgement

I would like to give a big thanks to Dr. Rolland Trapp for his wonderful guidance and profound knowledge in knot theory as well as Dr. Corey Dunn for his thoughtful advising in this program. None of this would of ever happened without them. I also want to thank California State University, San Bernardino and the NSF research grant DMS-2050894 for funding the program.

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