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Knots, Rational Tangles and DNA Topology

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Abstract The topology of DNA information management via the action of topoisomerase enzymes during recombination and replication is modelled using rational tangles, a complete knot invariant analysing knot subsegments. This project examined the algebraic structure of rational tangles, with special attention to proofs of Conway's Theorem, which posits a bijection between rational tangles and rational numbers via continued fractions. One result of this investigation is that the precision and uniqueness of rational tangle arithmetic is generated by its correspondence with the modular group $\mathrm{PSL}(2,\mathbb{Z})$. The DNA application's validity is also ensured by a deeper topological result about Dehn surgery which relates quantitative DNA models to rational tangles.

Contents

1 Introduction

Knot theory relates to 3-manifolds and three-dimensional movements, and hence many applications in our three-dimensional world. Rational tangles are a knot segment, defined as two strands inside a 'box' with ends fixed to the boundary, and knotted inside this 'box' by means of horizontal and vertical twists only. My research project uses the rational tangles' quantitative descriptions of DNA topology as a starting point to examine how rational tangle symmetries lead to an arithmetic which provides the only currently known complete knot invariant. Being based on twists makes rational tangles well suited to describe the 'knottedness' of DNA. Being a long macromolecule packed into a small space, and in constant motion, topoisomerase enzymes need to knot and unknot DNA segments for information management. This occurs by cutting and healing, which can be modelled as rational tangle surgery, i.e., replacing one rational tangle by another, and is numerically described by a system of linear equations based on knot invariants which are derived from rational tangle arithmetic. The model is based on Conway's Theorem (1970) that two rational tangles are isotopic if and only if they have the same fraction. Conway's Theorem implies a bijection between rational tangles and the extended rational numbers, without proof other than a demonstration that if you calculate a tangle's fraction in a certain way, you can use this fraction to 'unknot' every tangle described by the same fraction by the same sequence of moves (the 'Conway dance'). Conway's intermediate between fraction and rational tangle are the continued fractions, and a specific notation which quantifies rational tangles as an ordered series of horizontal and vertical twists.

In this form, rational tangles have their own symmetry-based arithmetic. While efficient, this arithmetic is also unusual - it does not immediately form a group, and it is easy to accidentally leave the class of rational tangles. To understand this arithmetic was the main focus of my research, with the intention of exploring (and perhaps in the future strengthening) connections between different areas of mathematics, and diverse applications, as rational tangles are also used in quantum topology, gauge theory, statistical mechanics and fluid mechanics.

Several proofs of Conway's Theorem were examined, and one (Kauffmann and Lambropoulou, 2004) studied in depth. It turns out that the wide applicability of rational tangle models is based on the correspondence of the rational tangle arithmetic with the projective modular group $\mathrm{PSL}(2, \mathbb{Z})$. Understanding this relationship was the main achievement of my project. Links to topological Dehn surgery and lens spaces were noted, and may hopefully be investigated in further research. Without results about Dehn surgery, rational tangles could not be used to model DNA topoisomerase action. Topoisomerases and, by implication, rational tangles are an area of high current research interest, being relevant for the improvement of cancer treatments and many other processes where transmitting or corrupting genetic information is of relevance.

Methods of this project were literature review, research, and working on knot and tangle problems with my supervisor.

Statement of Authorship This project was developed and researched with the help of my supervisor Dr. Jelena Schmalz. Core results are from Kauffmann and Lambropoulou's 'On the Classification of Rational Tangles' (2004), Kauffmann's *Knots and Physics* (2001) and a literature review. Main sources are listed in the **Reference** section.

2 Knot Invariants and DNA Topology

Some definitions to begin:

2.1 Definition:

A *knot* is a circle embedded in $\mathbb{R}^3$ or equivalently the sphere S^3.

2.1.1 Definition:

A *knot diagram* is the planar projection of a 3-dimensional knot with ends tied together and the strand assumed to be infinitely elastic.

The main issue in knot theory is to find out whether two apparently different knots are in fact the same knot, i.e., isotopic. Establishing knot isotopy is surprisingly difficult.

2.2 Definition:

Two knots are isotopic if and only if one knot can be transformed into the other using finitely many *Reidemeister moves*, which are set out in Figure 1:

Knots can become more complex during Reidemeister moves. We can only show sameness, not difference using Reidemeister moves, since we cannot exclude that a further sequence of moves may establish isotopy. Hence Reidemeister moves are only an important first tool for calculating knot invariants.

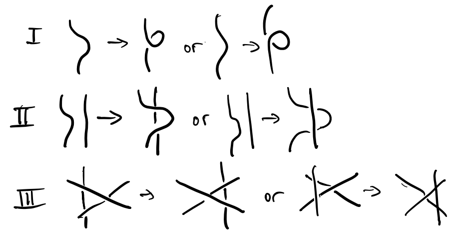

Figure 1: Reidemeister moves RI, RII, RIII

2.3 Definition:

A *knot invariant* distinguishes between knots, usually by assigning a unique quantity to a given knot.

There exists a number of different knot invariants, which are usually tailored around their particular application. There is no single complete knot invariant which can reliably distinguish all knots in all circumstances.

2.3.1 Example:

Writhe Number. A simple example of a knot invariant is the writhe number. Oriented crossings are assigned signs, as shown in Figure 2. The signs are summed over all crossings of the knot diagram c(K) to calculate the writhe :

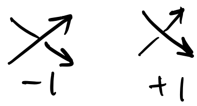

Figure 2: Sign of oriented crossings

$$w(K) = \sum_{p \in c(K)} \text{sign}(p)$$

Built up from these are knot polynomials such as the bracket (Kauffmann) polynomial and the Jones Polynomial. These knot polynomials generate all possible states of a knot while keeping a numerical track record of the required transformations. These quantities are then averaged or integrated over all states (Kauffmann, 2001, pp.25). For example, the bracket polynomial for knot K defines A as opening a crossing of K so it becomes two horizontal strands, and B as opening a crossing to obtain two vertical strands, in each case joining up the strands in the location where they had previously crossed (i.e., connecting previously unconnected strands to create two new, uncrossed strands running beside each other either horizontally or vertically). This produces two new knots, one after the application of A, and one after B. This process is repeated, creating a family of descendants of K. The diagrams are labelled so as to keep track of how many A and B splices were undertaken. With this information, one can reconstruct the ancestor knot K from any of its descendants (labelled as σ). The descendants are called the *states* of K in analogy to the energetic states of a physical system. The labels are commutative. To average, consider a single state of K, denoted σ , and define $\|\sigma\|$ as the number of loops minus one in this state σ. Then form a polynomial for the variable d^n , with exponent $n = \|\sigma\|$, and A, B the coefficients assigned to the correct order of d^n for the state they are labelling:

$$\langle K \rangle = \langle K \rangle (A, B, d) = \sum_{\sigma} \langle K \mid \sigma \rangle \cdot d^{\|\sigma\|} \tag{1}$$

The bracket polynomial is therefore only invariant under the second and third Reidemeister moves, and clearly affected by the number of crossings. This is dealt with by the *normalised bracket polynomial*,

$$L_K = \left(-A^3\right)^{-w(K)} \langle K \rangle \tag{2}$$

In the regular bracket polynomial, a single crossing (Reidemeister I) is denoted as either $-A^3$ or by $-A^{-3}$, which once exponentiated with the negative writhe will normalise the polynomial with respect to the number of loops (as each loop adds +1 to the writhe in the positive case. In the negative case, the multiple negatives of loop, writhe, and $-A^{-3}$ lead to the same normalisation.)

The bracket yields the same quantitative invariant as the Jones polynomial, which is calculated slightly differently, but follows an equivalent principle. There exist other, differently calculated polynomials, such as HOMFLYPT. The choice of polynomial depends on its purpose. No polynomial is a complete invariant, meaning that, while precise and successfully used in physical applications, knot polynomials cannot distinguish **every** knot from another.

2.4 DNA as an information storage, distribution and management system

DNA is a complex macromolecule consisting of a backbone of sugar-phosphate molecules which hold in place four bases (Adenine, Cytosine, Guanine, Thymine), which by their order encode vast amounts of information. The actual molecule is more diverse and complex, however, most forms of DNA can be modelled in this highly simplified way (Tubiana, Alexander et.al. , 2024, p.38). We picture the bases like rungs on a ladder, which is flexible, and multiply twisted around itself. Being over 2 meters long (in humans) and coiled into a cell nucleus by means of complex molecular-energetic interactions , this coiled structure is again spiralled around itself and thus multiply twisted, a state biologists describe as supercoiled. DNA information access and distribution occurs in two ways, replication and recombination (see Figure 3). Again, in a highly simplified model, for replication the DNA molecule is opened like a zipper, and a copy of the contents is taken. This typically happens during cell division. For recombination, a small segment of DNA is exchanged for another in a specific location. This typically happens during sexual reproduction.

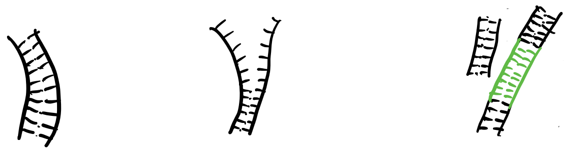

Figure 3: DNA, replication, recombination

2.5 Topoisomerase enzymes use rational tangles.

For both replication and recombination, the highly compressed information encoded in the supercoiled macromolecules needs to be accessed. This required untwisting or unknotting of DNA is achieved by topoisomerase enzymes in an (untopological) unwinding – the DNA strand is cut, relevant strands are threaded through, and the cut healed again. Alternatively, overly tight supercoiling is 'relaxed' by a similar process.

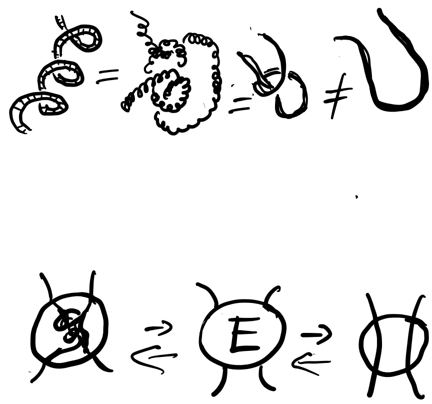

Figure 4: Supercoiled DNA (the problem), and tangle surgery (the solution)

Topoisomerase action is modeled as the enzyme re-arranging DNA by *tangle surgery*, which means that an entire tangle is removed, and another tangle inserted in its place to create the required strand arrangement (Figure 4). This has been experimentally established by placing a DNA strand onto a gel on top of a positive charge. As the DNA molecule is negatively charged, it will move toward the positive charge, and will travel faster the more coiled, i.e., smaller it is. Afterwards, the DNA molecule can be examined under an electron microscope to determine shape and changes in shape. It is possible to thus quantify the recombination process as a series of linear equations. Thanks to experimental observations and topological results on Dehn surgery, it can be assumed that the whole-number relationships observed in the linear system of transformation equations imply that the tangles are (mostly) rational (Ernst and Sumner, 1990, p.490). Dehn surgery is a topological technique whereby a knot along with its tubular neighborhood is removed from a 3-manifold, and a solid torus is glued in by a homeomorphism of its boundary to the torus boundary of the removed neighbourhood. This homeomorphism is specified by a slope (p, q) which represents a simple closed curve on the boundary torus. The values of p, q relate to the knot invariants.

3 Rational Tangle Arithmetic and $\mathrm{PSL}(2, \mathbb{Z})$

John Conway (1970) introduced rational tangles as an alternative tool for analysing knots and defining knot invariants. Tangles are part of a knot, treated as two (or more) separate links inside a 'box' which holds the strands' ends in place. As with knots, we work with the planar projection diagram, which takes note of over- and under crossings (Figure 5).

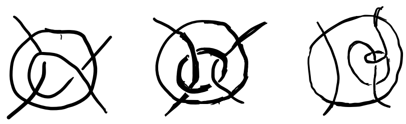

Figure 5: Rational, prime, and locally knotted tangles

3.1 Definition:

Rational Tangles are defined as two arcs embedded in a 3-ball with the arcs' ends fixed on the boundary, and conventionally labelled with compass directions. The trivial (unlinked) tangles are labelled as **0** or ∞ (see Figure 6).

What makes a tangle rational is their construction, described here as the *rational tangle arithmetic*, which allows us to : (i) build up a knot from the two trivial tangles by means of a finite number of vertical and horizontal twists of the arc ends, with the number of twists recorded as invariants. Here, n twists if horizontal are marked as n , as $\frac{1}{n}$ if vertical, with the sign determined by the sign of the crossing induced by the twist, (ii) combine existing rational tangles either on the right hand side, labelled as $+$, or from underneath, labelled $*$, (iii) rotate by 90 degrees counterclockwise, denoted by R^r, (iv) take the mirror image, by which the signs of all crossings are reversed, (over to under, under to over), written by $-R$ (v) take the inverse, which combines rotation with reversed crossings, denoted as $R^i = -R^r$

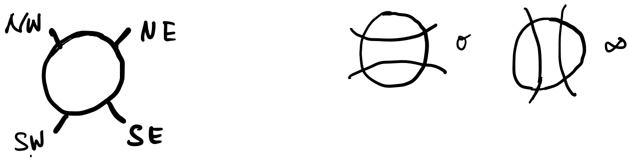

Figure 6: Tangle labelling conventions

This arithmetic can be used to construct, or analyse a rational tangle, as shown in Figure 7.

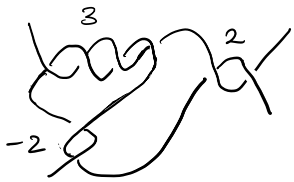

Figure 7: Example rational tangle: $([3] * \frac{1}{[-2]}) + [2]$

This leads to a *standard notation* for rational tangles:

$$R = ((([a_n] * \frac{1}{[a_{n-1}]}) + [a_{n-2}]) * \cdots * \frac{1}{[a_2]}) + [a_1] \tag{3}$$

for all

$$a_2, a_3, \ldots, a_{n-1} \in \mathbb{Z} \setminus \{0\} \tag{4}$$

(In this notation, a_1 can be zero, which becomes important in the next section, where tangles are brought into correspondence with canonical form continued fractions, which must have an odd number of elements. Note also that one could start with a vertical tangle, but this does not matter, as one could turn the 'page' the vertical tangle diagram is projected on sideways before starting, hence all rational tangles can be written as if they always start with a horizontal tangle. Note also that in this notation, division by infinity, i.e., the vertical tangle $\frac{1}{\infty}$, is defined as the tangle labelled [0], which makes intuitive sense if you recall that the vertical trivial tangle is a 90 degree rotation of the horizontal trivial tangle.)

3.2 Conway's Theorem: Rational Tangles invariant is a fraction

3.2.1 Definition:

A *continued fraction* $[a_1, a_2, ..., a_n]$ is in canonical form if it is termwise positive or negative and n is odd, however a_1 can be zero. Every fraction can be put into this canonical continued form. Being a parallel system of quotients and remainders, the uniqueness of canonical form continued fractions is guaranteed by the uniqueness of Euclid's algorithm.

If a rational tangle is written in the above standard notation, the values for all terms a_i can be written **in reverse order** as a canonical continued fraction. The value of this continued fraction as regular fraction is also the unique invariant for the tangle:

3.2.2 Theorem

(Conway, 1970) Two rational tangles are isotopic if and only if they have the same fraction.

$$R = a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \cfrac{1}{a_4 + \cdots + \cfrac{1}{a_n}}}} = \frac{p}{q} \tag{5}$$

This implies a bijection between rational tangles and the extended rational numbers. How is this possible? Sameness between tangles is described by isotopy, which implies that one object can be transformed into another in a series of homeomorphic deformations. Sameness between rational numbers is equivalence, which preserves more structures. For instance, a circle is isotopic, but not equal to an ellipse. At some point of Conway's method, isotopy is transformed into equality and vice versa. Another surprise is that all rational tangles described by the rational $\frac{p}{q}$ which is the short form of the relevant continued fraction are isotopic, making $\frac{p}{q}$ the fraction invariant. Again, something - and not just anything, but the invariant - jumps like a spark between mathematically different structures.

Since Conway's (unproven) theorem, various methods of proof have been put forward, mostly using heavy mathematical machinery based on algebraic topology (Burde and Zieschang, 1985, pp.214) or group theory (Aicardi, 2011). The proof by Kauffmann and Lambropoulou (2004) which I decided to study in depth is combinatorial, working entirely on the level of tangle and fraction operations and notations, exploiting the many symmetries of rational tangles in order to gradually push the notations of tangles and fractions into a shared space where the two concepts can rigorously be shown to connect. The main operation in Kauffmann and Lambropoulou (2004) is the *flype* , a move from 19th century knot theory. Think of the tangle as a flat piece of translucent material which is marked by a letter (e.g. R) which has no rotation or mirror symmetry. We can however see this letter from the other side, through the material, which is indicated in Figure as a *dotted* letter. For a flype, we attach strands at all four ends, cross one strand over the other on one side, and then pull the strings tight. This will most likely straighten out the twist, flip the flat surface over, and cause a twist to appear on the other side, as shown in Figure 8.

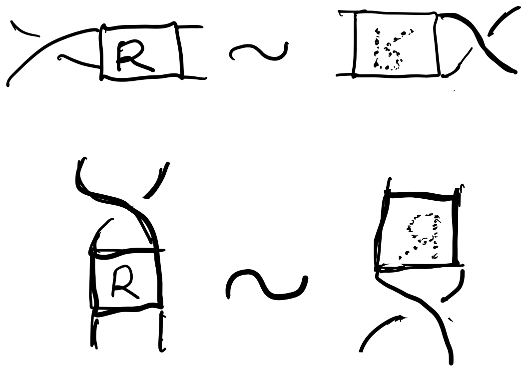

Figure 8: Horizontal and vertical flype

The letter marking which stands for the tangle inside the 'box' is now seen as if through the material. It is still the same tangle and evidently has not been changed by being flipped over. As the counterexample in Figure 9 shows, if a tangle is not rational, this flype symmetry will not occur.

Kauffmann and Lambropoulou (2004) use this aspect of the flype to show by induction that a rational tangle is isotopic to itself when reflected in both the horizontal and vertical axis, i.e., turned counterclockwise by 180 degrees. This is true for the base cases [0], [∞], [$\pm$1], i.e., the horizontal and sideways trivial (uncrossed) tangle and the single crossing of either sign. Then assuming a tangle R_n which is isotopic to its rotated self, the induction step to R_{n+1} is attained by adding a single crossing on the side , R_n +[$\pm$1]. As we know from the

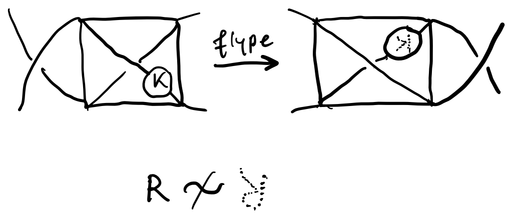

Figure 9: Counterexample: flype on a locally knotted, non-rational tangle

discussion of flypes that the tangle is not changed by being 'seen from inside the paper', and knowing that $[\pm 1]$ is isotopic to its rotated self, the same will be true for their combination. (A similar, slightly more elaborate procedure is employed for vertical flypes). Hence, as shown in Figure 10, a rational tangle is isotopic to itself when rotated by 90 degrees. Having established this symmetry, we gain a limited form of commutativity, as the

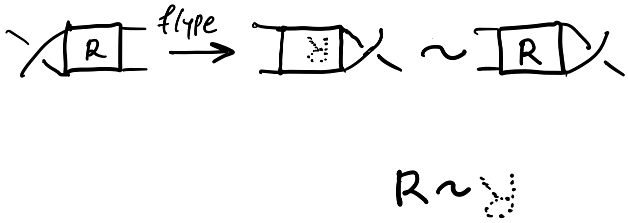

Figure 10: Induction by flype establishes isotopy between tangle and its upside down vertical reflection

flype symmetry implies that $(R + [\pm 1]) \sim ([\pm 1] + R)$. The same can be established for $*$, i.e., adding a vertical tangle from underneath. Using these results, Kauffmann and Lambropoulou (2004) show that every rational tangle can be transformed into the standard form

$$R = ((([a_n] * \frac{1}{[a_{n-1}]}) + [a_{n-2}]) * \cdots * \frac{1}{[a_2]}) + [a_1] \tag{6}$$

and once in standard form, can be written as a canonical form rational tangle, which leads to the unique invariant $\frac{p}{q}$, the value of the continued fraction. Uniqueness is slowly introduced as tangle notation becomes restricted to standard notation, until it becomes firmly established in the canonical continued fraction. Hence, despite the rational tangles' strange and limited arithmetic and their being only defined up to isotopy, rational tangles are shown to be bijective with $\mathbb{Q} \cup \{\infty\}$.

This bijection is founded in the correspondence of rational tangle arithmetic with the modular group $\mathrm{PSL}(2, \mathbb{Z})$, which is defined by the two generators

$S : x \to -\frac{1}{x}$, in tangles the 90 degree anti-clockwise rotation R^r $T : x \to x + 1$, in tangles the adding of a twist $R + [1]$

This can also be described as matrices multiplied with the tangle invariant written as vector:

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{bmatrix} p \\ q \end{bmatrix} = (\frac{p+q}{q})$$

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{bmatrix} p \\ q \end{bmatrix} = (\frac{-q}{p})$$

and once considered as matrix multiplication, restrictions and gaps of rational tangle arithmetic immediately make more intuitive sense. Considering either fractions or rational tangles, we find the identity transformations, and hence define the group presentation

$$\mathrm{PSL}(2, \mathbb{Z}) = \langle S, T \mid S^2 = (ST)^3 = id \rangle$$

As Kauffmann and Lambropulou (2004) show, one can inductively generate $-[1]$, and thus all of the rational numbers using only the above two operators:

$$R - [1] = -\frac{1}{[1] + \left(-\frac{1}{(-\frac{1}{x}+[1])}\right)}$$

which as shown in Figure 11, can also be solved as a tangle equation, thus confirming the bijection of tangle arithmetic and canonical form continued fractions as group operations of $\mathrm{PSL}(2, \mathbb{Z})$.

3.3 Further Implications: Dehn surgery and DNA, lens spaces.

3.3.1 Definition:

A *torus* is a surface of revolution homeomorphic to $S^1 \times S^1$.

Two solid tori can be glued together to form S^3 by mapping the meridian curve of one torus to a longitude curve on the other torus.

3.3.2 Definition:

A *torus kno*t is a knot that lies on the surface of a solid torus surface without self-intersection. It is algebraically described as a (p, q) torus knot. As Figure 12 shows, p denotes the number of times the knot winds around the torus meridian, while q denotes the number of times it winds around the torus longitude.

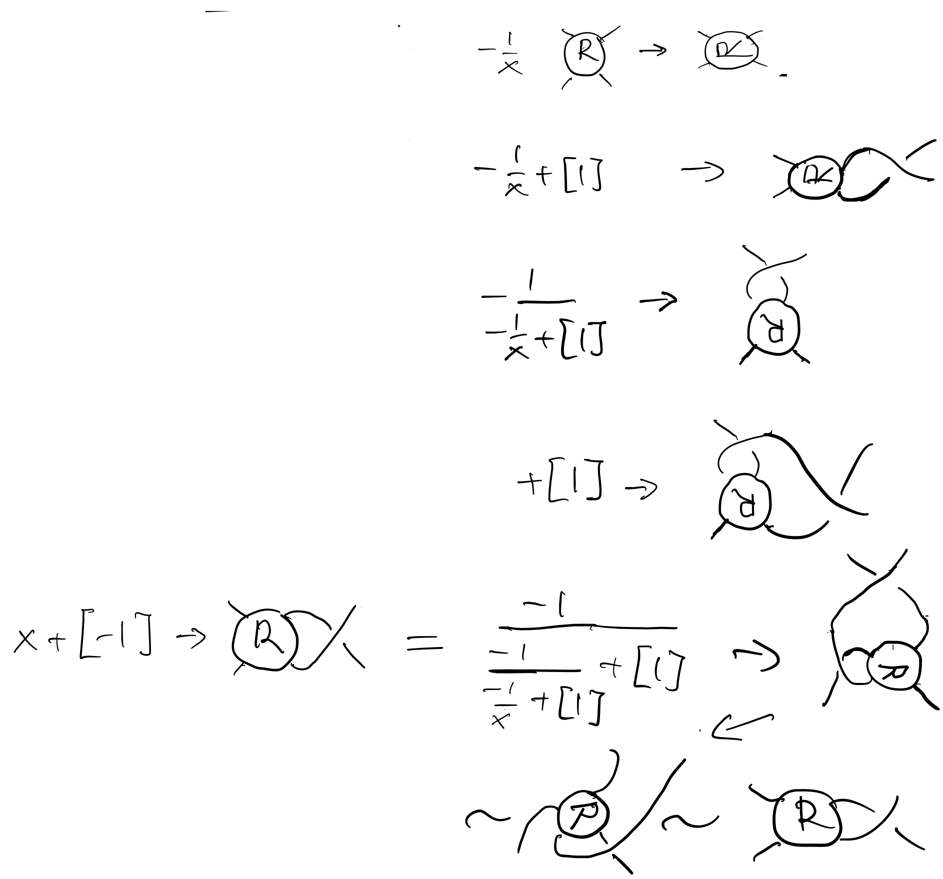

Figure 11: Group representation as tangle arithmetic

Topological *Dehn surgery* removes a tubular neighbourhood of a given knot and then glues in a solid torus such that the meridian curve of the solid torus maps to a (p, q)-curve on the torus boundary of the knot exterior (Adams, 1994, p.257). (To do this with a rational tangle, one turns the tangle into a 4-plat using denominator closure i.e., joining the tangle's two top strands and its two bottom strands). In the context of DNA topology, the values of the Dehn surgery slope (p, q) are often derived from the rational tangle invariant $\frac{p}{q}$. As indicated before, the results of Dehn surgery guarantee mathematically that (most of) the tangles involved in DNA processes are rational. This is a consequence of the whole number relations in the system of linear equations which is used to describe DNA recombination events (Ernst & Sumners, 1990, p.493).

The result of Dehn surgery is a compact 3-manifold without boundary called *lens space* $L(p, q)$, which is the quotient space of $\mathbb{Z}/p$ acting by cyclic group action on S^3 (here considered as the unit sphere in $\mathbb{C}^2$):

$$(z_1, z_2) \mapsto (e^{\frac{2\pi i}{p}} z_1, e^{\frac{2\pi i q}{p}} z_2)$$

The coprime integers p, q in the above equation are the integer values of p and q of the rational tangle invariant $\frac{p}{q}$. Thus, the rational tangle can also take us from analysing the arrangement of strands in a knot to an important (and compact) tool of low-dimensional topology and quantum field theory (Adams, 2004, p. 254).

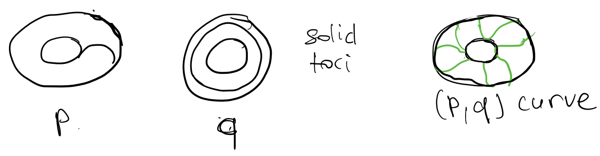

Figure 12: Torus meridian, longitude, (p,q) curve

4 Discussion and Conclusion

Mathematical knot theory is useful for many and diverse applications. Deep mathematical structures hide beneath the apparent simplicity of strings twisted around one another. Knot theory results apply especially to areas relating to 3-space, 3-spheres and complex half-spheres, particularly to movement and rotation in these spaces. Hence there are applications in many areas of physics, and as I have described here, biology, regarding the topology of DNA. For DNA information management, the supercoiled (i.e., multiply twisted around itself) molecule needs to be untwisted or unknotted. This is achieved by topoisomerase enzymes cutting the DNA strand and threading another strand through, followed by the enzyme healing the strand again. The enzyme achieves this by using the molecular equivalent of rational tangle surgery, that is, by removing one rational tangle and inserting another in its place. Rational tangles are defined as a knot segment consisting of two arcs inside a 3-ball, with the four ends fixed on the boundary. Rational tangles are created from the trivial tangle by twisting either on the right or from underneath, and possess an arithmetic which permits addition of other rational tangles from the right or below, rotation by 90 degrees counterclockwise, taking of the mirror image by changing the sign of all crossings, and inversion, which corresponds to a combination of taking the mirror image and rotation. Following Conway's (1970) Theorem which states that two rational tangles are isotopic if and only if they have the same fraction, rational tangles under their specific arithmetic can be shown to be bijective to the extended rational numbers. This seemed surprising, considering the tangle arithmetic is not commutative and basic addition can result in non-rational tangles. Kauffmann and Lambropoulou's (2004) combinatorial proof of Conway's theorem was examined at depth to investigate the underlying (and puzzling) algebraic structure of rational tangles. It was found that the bijection between the extended rational numbers and rational tangles is based on their shared algebraic structure of operations as modular group, $PSL(2, \mathbb{Z})$. This group is relevant to many areas of mathematics and diverse applications, such as Moebius transformations and Pauli matrices. The structure of Kauffmann's and Lambropoulou's proof showed me how different mathematical entities can be brought into connection by rigorous alignment of shared symmetries, and careful creation and manipulation of notation.

Further research could collect and examine more examples of structures shaped by $\mathrm{PSL}(2, \mathbb{Z})$ and study their relationship. As one can move between knots and signed graphs by checkerboard shading a knot and placing a vertex into each shaded region, further research might also investigate whether rational tangles might be useful for some graph theoretical applications.

5 Acknowledgment

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