Journal of Knot Theory and Its Ramifications
Vol. 21, No. 7 (2012) 1250074 (9 pages)

DOI: 10.1142/S0218216512500745

UNRAVELLING TANGLED GRAPHS

CATHERINE FARKAS
Department of Mathematics,
University of Illinois at Chicago,
Chicago, IL 60607, USA

ERICA FLAPAN* and WYNN SULLIVAN
Department of Mathematics, Pomona College,
Claremont, CA 91711, USA
**ELF04747@pomona.edu*

Received 22 March 2011
Accepted 24 October 2011
Published 19 March 2012

ABSTRACT

Motivated by proposed entangled molecular structures known as *ravels*, we introduce a method for constructing such entanglements from 2-string tangles. We then show that for most (but not all) arborescent tangles this construction yields either a planar θ_4 graph or contains a knot.

Keywords: Spatial graphs; almost unknotted graphs; tangles; ravels; θ_n.

Mathematics Subject Classification 2010: 57M25, 57M15, 05C10

1. Introduction

The geometry of a molecule determines many of its properties, and for non-rigid molecules the topology can play a role as well. In order to better understand the effects of topology on molecular behavior, chemists have targeted topologically complex molecular structures for synthesis. Knotted and linked molecules, which were once such targets, have been successfully synthesized. However, chemists continue to develop new techniques to synthesize different types of knotted and linked molecules as well as other non-planar structures. Castle, Evans, and Hyde [2] define a *ravel* as a "local entanglement" of edges around a vertex which contains no knots or links (see for example Fig. 1), and propose such structures as targets of molecular synthesis. They assert that ravels may eventually be found within metal organic frameworks as well as within other extended molecular frameworks. Furthermore, since knotting and linking have been found in proteins and DNA-protein complexes, they suggest that it is reasonable to look for ravels in biochemical structures as well.

The informal definition of a ravel given above can be formalized in several ways. We give the following definition. Note that when we say a graph embedded in

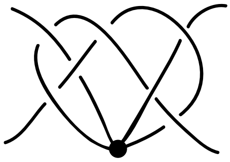

Fig. 1. An example of a ravel.

S^3 is "planar" we mean that the embedding of the graph is isotopic to a planar embedding.

Definition 1.1. Let B be a ball containing a graph G consisting of a vertex with n edges whose second vertices lie in ∂B. Let Γ denote the graph obtained by bringing these n vertices together within ∂B. If Γ is a θ_n graph which is non-planar but contains no knots then the pair (B, G) is said to be an n-***ravel*** and the embedded graph Γ is said to be ***raveled***.

Consider the relationship between a raveled graph and an almost unknotted graph defined below.

Definition 1.2. Let Γ denote an abstractly planar graph embedded in S^3. Suppose that Γ is non-planar, yet for any edge e, the embedded graph $\Gamma - e$ is planar. Then we say Γ is ***almost unknotted*** (equivalently, ***almost trivial***, ***minimally knotted***, or ***Brunnian***).

If a θ_n graph embedded in S^3 is almost unknotted, then it is also raveled. Conversely, any raveled θ_3 graph is almost unknotted. However, if $n > 3$, then the definition of a raveled θ_n graph is weaker than that of an almost unknotted θ_n graph. In fact, for any n, starting with a raveled θ_n we can obtain a raveled θ_{n+1} which is not almost unknotted by adding an edge which is isotopic to an existing edge.

Suzuki [7] gave the first example of an almost unknotted graph in 1970 by finding a non-planar embedding of a handcuff graph which contained no knots or links. Shortly afterward, Kinoshita [5] created an example of an almost unknotted θ_3 graph, which has since been known as *Kinoshita's θ-curve*. Later, Suzuki [8] generalized Kinoshita's θ-curve by defining a family of almost unknotted θ_n graphs for all $n \geq 3$. More recently Kawauchi [4] and Wu [9] have independently shown that every planar graph with no vertices of valence one has an almost unknotted embedding in S^3.

There is a natural relationship between 4-ravels and 2-string tangles. In particular, by starting with a projection of a 2-string tangle B and replacing a crossing with a vertex we obtain a pair (B, G) where G consists of a vertex with 4 edges. For example, we replace a crossing of the tangle in Fig. 2 by a vertex and bring the endpoints together within ∂B to get a raveled θ_4 graph. Note, we color

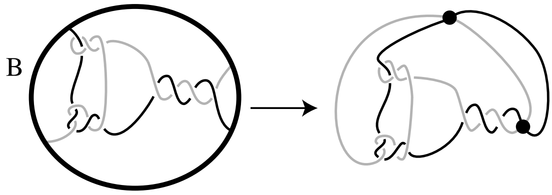

Fig. 2. We obtain a ravel from this tangle by replacing a crossing by a vertex as indicated.

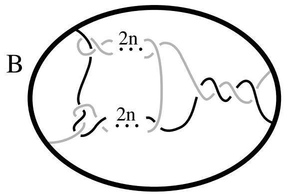

Fig. 3. An infinite family of ravels can be obtained from this infinite family of tangles.

the strings with different colors to make it easier to see. We can obtain infinitely many similar raveled θ_4 graphs by starting with any of the tangles in the family illustrated in Fig. 3.

The general question that we are interested in here is which families of 2-string tangles can produce a 4-ravel in this way. We show that (in spite of the above examples) in most cases a projection of an arborescent tangle does not yield a ravel in this way.

2. Background

A 2-string tangle (B, T) is said to be *rational* if it is homeomorphic to a trivial tangle by an orientation preserving map of pairs. Given a tangle (B, T), the *numerator closure* $N(T)$ is obtained by joining the North endpoints of (B, T) and joining the South endpoints of (B, T) both within ∂B. The *denominator closure* $D(T)$ is obtained by joining the East endpoints of (B, T) and joining the West endpoints of (B, T) both within ∂B.

Definition 2.1. A projection of a rational tangle A is said to be in ***alternating*** 3-***braid form*** if it looks like Fig. 4, where each box labeled A_i contains a_i horizontal twists with $a_i \neq 0$ for $i > 1$, and the signs of the rows of twists alternate.

It follows from Kauffman and Lambropoulou [3] that any projection of a rational tangle can be isotoped fixing its endpoints to a projection which is in alternating 3-braid form.

Definition 2.2. Let A be a projection of a 2-string tangle. We let A' denote the graph obtained by replacing a crossing of A by a vertex. We define the ***vertex***

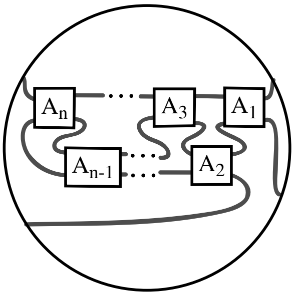

Fig. 4. A projection of a rational tangle in 3-braid form.

closure $V(A')$ as the graph obtained by joining all four endpoints to a vertex within the boundary of the tangle ball.

Observe that $V(A')$ is only a θ_4 graph if the crossing of A replaced by a vertex is between two different strings (see Fig. 5). If $V(A')$ is not a θ_4 graph, then by definition A' cannot be a ravel. In particular, if $V(A')$ contains a link then A' is not a ravel.

Definition 2.3. Let R and S be tangles. We define the sum $R + S$ and product $R \times S$ to be the tangles illustrated in Fig. 6.

Definition 2.4. A tangle of the form $S = S_1 + \cdots + S_n$ where each S_i is rational is said to be ***Montesinos***. The sum $S_1 + \cdots + S_n$ is said to be in ***reduced form*** if S cannot be written as a sum of fewer than n rational tangles.

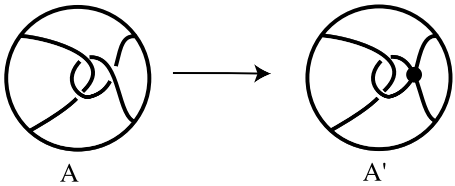

Fig. 5. In this example, $V(A')$ is not a θ_4 graph.

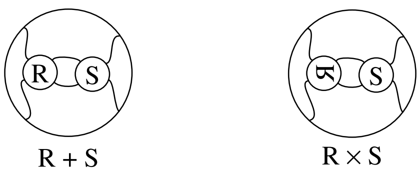

Fig. 6. The sum and product of tangles R and S.

Observe that if $S_1 + \cdots + S_n$ is a Montesinos tangle in reduced form and $n > 1$, then none of the S_i is a horizontal tangle.

Definition 2.5. An ***arborescent tangle*** is a tangle obtained by addition and multiplication of rational tangles. The algebraic expression for an arborescent tangle S is said to be in ***reduced form*** if it contains a minimum number of rational tangles and a minimum number of parentheses.

Note an arborescent tangle is also referred to as an ***algebraic tangle*** by some authors.

3. Results

Proposition 3.1. *Let A be a projection of a rational tangle in alternating* 3*-braid form, and let A' be obtained by replacing a crossing of A by a vertex v such that $V(A')$ is a θ_4 graph. Then $V(A')$ is either planar or contains a non-trivial knot, and hence A' cannot be a ravel.*

Proof. We label the boxes of A as in Fig. 4. Let A_i be the box which contains the vertex v. Let w be the vertex of $V(A')$ in the boundary of the tangle ball. By isotoping the edges of $V(A')$ around w we can consecutively remove the crossings in all of the A_j with $j < i$. Thus without loss of generality, we can assume that either $i = 1$ or both $i = 2$ and $a_1 = 0$. Furthermore, by isotoping the edges around v, we can remove all of the crossings in A_i so that A' looks like one of the illustrations in Fig. 7.

Let R be the tangle obtained from Fig. 7 by replacing a neighborhood of v with a 0-tangle as illustrated in Fig. 8. Then the two possibilities for R are illustrated in Fig. 9. Observe that if $i = 1$, then the denominator closure $D(R)$ is homeomorphic to a subgraph of $V(A')$, and if $i = 2$ and $a_1 = 0$, then the numerator closure $N(R)$ is homeomorphic to a subgraph of $V(A')$.

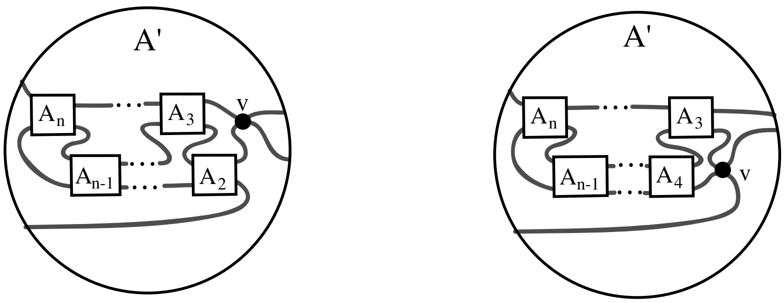

Fig. 7. If $i = 1$ then A' is illustrated on the left, and if $i = 2$ and $a_1 = 0$ then A' is illustrated on the right.

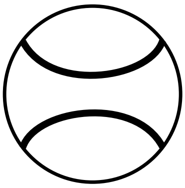

Fig. 8. We replace a neighborhood of v with this 0-tangle.

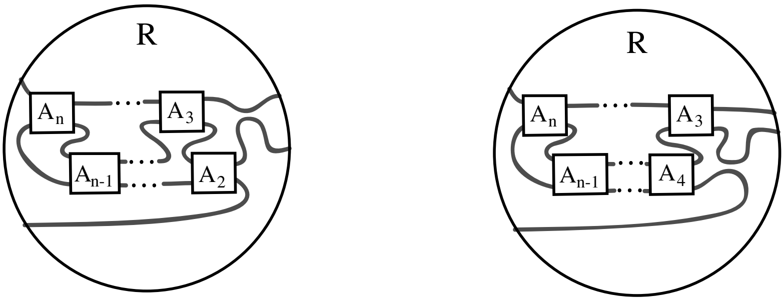

Fig. 9. If $i = 1$ then R is illustrated on the left, and if $i = 2$ and $a_1 = 0$ then R is illustrated on the right.

It follows from Schubert's classification of 2-bridge knots and links [6] that for any rational tangle R, $D(R)$ is a trivial knot or link if and only if R is a horizontal tangle and $N(R)$ is a trivial knot or link if and only if R is a vertical tangle. However, if either $i = 1$ and R is horizontal or $i = 2$, $a_1 = 0$, and R is vertical, then $V(A')$ is planar. Since $V(A')$ is a θ_4 graph $V(A')$ cannot contain a link of more than one component. Thus $V(A')$ is either planar or contains a non-trivial knot. □

Proposition 3.2. *Let $S_1, \ldots, S_n$ be rational tangles and let $S = S_1 + \cdots + S_n$ be a Montesinos tangle in reduced form with $n > 1$. Let S' be obtained from a projection of S by replacing a crossing by a vertex v such that $V(S')$ is a θ_4 graph. Then $V(S')$ contains a non-trivial knot, and hence S' cannot be a ravel.*

Proof. Let S_i be the tangle in the sum $S_1 + \cdots + S_n$ that contains v. Since $n > 1$, $S_1 \neq S_n$. Hence, without loss of generality, we can assume that v is not contained in S_n. Since S is in reduced form, S_n is a rational tangle which is not horizontal. Thus it follows from Schubert [6] that $D(S_n)$ is a non-trivial knot or link. Let e_1 and e_2 denote the edges of $V(S')$ which are disjoint from all S_j with $j < i$.

Then, we see from Fig. 10 that the simple closed curve $e_1 \cup e_2$ contains $D(S_n)$ as a connected summand (possibly with a trivial knot). Since $V(S')$ is a θ_4 graph, it cannot contain a link with more than one component. Thus $V(S')$ contains a non-trivial knot as required. □

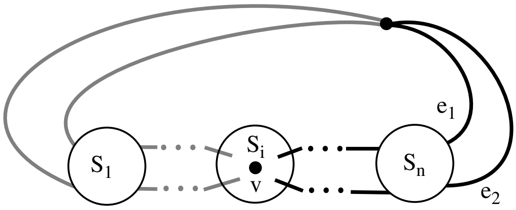

Fig. 10. The black simple closed curve $e_1 \cup e_2$ contains the knot $D(S_n)$ as a connected summand.

By contrast with rational tangles and Montesinos tangles, replacing a crossing in an arborescent tangle may create a ravel (see for example Fig. 2). Observe that the arborescent tangles in Fig. 3 have the form $(Q+P)\times R$ where R, P, and Q are rational tangles. To avoid arborescent tangles of this type, we make the following definition.

Definition 3.3. Let S be an arborescent tangle written in reduced form such that it contains one of the expressions: $(R + (Q \times P))$, $((Q \times P) + R)$, $(R \times (Q + P))$, or $((Q + P) \times R)$, where R and at least one of P or Q is rational. Then we say S contains a ***bad triangle***.

Theorem 3.4. *Let S be a non-rational arborescent tangle written in reduced form with no bad triangles, and let S' be obtained from a projection of S by replacing a crossing by a vertex v such that $V(S')$ is a θ_4 graph. Then $V(S')$ contains a non-trivial knot, and hence S' cannot be a ravel.*

Proof. Since S is written in reduced form the number r of rational tangles in the algebraic expression for S is minimal. Also, since S is not rational, $r > 1$. We prove the theorem by strong induction on r. If $r = 2$, then S is a Montesinos tangle in reduced form and hence the theorem follows from Proposition 3.2. Thus we assume that $r > 2$.

Suppose the theorem is true for any arborescent tangle satisfying the hypotheses which can be expressed algebraically with fewer than r rational tangles. Now without loss of generality, we can assume that $S = S_1 + \cdots + S_n$ where $2 \leq n \leq r$ and each S_i is a (possibly rational) arborescent tangle in reduced form containing no bad triangles. Furthermore, without loss of generality, the vertex v replaces a crossing in $T = S_1 + \cdots + S_{n-1}$.

Label the arcs of T as in Fig. 11. Since $V(S')$ is a θ_4 graph, arc b cannot be connected to arc e within S_n. Thus, without loss of generality, we can assume that within S_n arc b is connected to arc c and arc e is connected to arc f. Hence the four edges of $V(S')$ are a, d, $b \cup c$, and $e \cup f$. Since $V(S')$ is a θ_4 graph, $V(T')$ must also be a θ_4 graph, and by a slight abuse of notation the edges of $V(T')$ are the arcs a, b, d, and e.

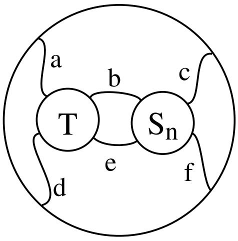

Fig. 11. Label the arcs of S as indicated.

First suppose that the tangle $T = S_1 + \cdots + S_{n-1}$ is not rational. Now T is written in reduced form with no bad triangles. Since T is expressed with fewer than r rational tangles, by our inductive hypothesis, $V(T')$ contains a non-trivial knot K. Without loss of generality, K is contained in one of the pairs of edges $a \cup d$, $b \cup e$, or $a \cup b$ of $V(T')$. Since a and d are also edges of $V(S')$, if K is in $a \cup d$ then K is a non-trivial knot in $V(S')$. If K is in the pair of edges $b \cup e$ of $V(T')$, then K is a connected summand (possibly with a trivial knot) of a knot in the pair of edges $(b \cup c) \cup (e \cup f)$ of $V(S')$. If K is in the pair of edges $a \cup b$ of $V(T')$, then K is a connected summand (possibly with a trivial knot) of a knot in the edges $a \cup (b \cup c)$ of $V(S')$. Thus if T is not rational, we are done.

Now suppose that T is a rational tangle. Since $S = T + S_n$ and $r > 2$, S_n cannot also be rational. Furthermore, since S is written in reduced form, $S_n = R_1 \times \cdots \times R_q$, where $q \geq 2$ and each R_i is an arborescent tangle. Since T is rational and S contains no bad triangles, if $q = 2$ then neither R_1 nor R_2 is rational. Now, it follows from Bonahon and Siebenmann [1] that for any arborescent tangle $R_1 \times \cdots \times R_q$ with either $q > 2$ or both $q = 2$ and neither R_1 nor R_2 rational, $D(R_1 \times \cdots \times R_q)$ contains a non-trivial knot or link. However, $D(S_n) = D(R_1 \times \cdots \times R_q)$ cannot be a link with more than one component since $V(S')$ is a θ_4 graph. Thus $V(S')$ contains a non-trivial knot in the pair of edges $(b \cup c)$ and $(e \cup f)$, and hence again we are done. □

Acknowledgments

The second author was partially supported by NSF Grant DMS-0905087.

References

[1] F. Bonahon and L. Siebenmann, New Geometric Splittings of Classical Knots, and the Classification and Symmetries of Arborescent Knots, available at http://www-bcf.usc.edu/fbonahon/Research/Preprints/BonSieb.pdf.

[2] T. Castle, M. Evans and S. T. Hyde, Ravels: knot-free but not free. Novel entanglements of graphs in 3-space, *New J. Chem.* **32** (2008) 1489–1492.

[3] L. H. Kauffman and S. Lambropoulou, On classification of rational tangles, *Adv. Appl. Math.* **33** (2004) 199–237.

[4] A. Kawauchi, Almost identical imitations of (3,1)-dimensional manifold pairs, *Osaka J. Math.* **26** (1989) 743–758.
[5] S. Kinoshita, On Elementary Ideals of Polyhedra in the 3-sphere, *Pacific J. Math.* **42** (1972) 89–98.
[6] H. Schubert, Die eindeutige Zerlegbarkeit eines Knotens in Primknoten, *S. B. Heidelberger Akad. Wiss. Math. Natur. Kl.* (1949) 57–104.
[7] S. Suzuki, On Linear Graphs in 3-sphere, *Osaka J. Math.* **7** (1970) 375–396.
[8] S. Suzuki, Almost Unknotted θ_n-curves in the 3-Sphere, *Kobe J. Math.* **1** (1984) 19–22.
[9] Y. Q. Wu, Minimally knotted embeddings of planar graphs, *Math. Z.* **214** (1993) 653–658.