On toroidal knots, chirality, and molecules

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On Toroidal Knots, Chirality, and Molecules

by

Ramiro Garza

A Thesis Presented to the Graduate Faculty of the College of Science, Mathematics, and Technology in Partial Fulfillment of the Requirements for the Degree of

Master of Science

in the Field of Mathematics

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On Toroidal Knots, Chirality, and Molecules

A Thesis Presented to the
Faculty of the College of Science, Mathematics, and Technology
The University of Texas at Brownsville

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by
Ramiro Garza
April 2014
For Mom.

For Stacey.

For the directionless—may we be useful as we wander.
Acknowledgement

Mr. Mosh: Thank you for making math challenging and fun, again.

Dr. Zieschang: Thank you for the entrancing introduction to strange math with so few numbers in it, and for inviting me to the unforgettable Iowa R.E.U.

Dr. Vatchev and Dr. Glazyrin: Thank you for the feedback and for accepting the responsibility of being members in my thesis committee. I should have asked you more questions.

Dr. Mogilski: Thank you for the countless hours of counsel and patience; I could not have asked for better.
Abstract

The inspiration for this thesis came from two sources: the book *When topology meets chemistry: a topological look at molecular chirality*, by Erica Flapan [7], which discusses topologically interesting molecules; and the paper *All toroidal embeddings of polyhedral graphs in 3-space are chiral*, by T. Castle et al., which proves that toroidal embeddings of polyhedra are chiral.

Their proof is examined in detail. A possible application of this work, as discussed by the team, would be in molecules which have the structure of a toroidal polyhedral embedding. Various methods of seeking such an example are attempted and discussed.
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Chapter 1

Introduction

1.1 Knots and Chemistry

Chemistry and math are clearly parts of the same puzzle. In fact, knot theory came about due to a theory proposed by chemists [7] (here, a knot is defined as an embedding of the circle in 3-space which cannot be deformed into a plane—i.e., deformed in such a way that the entire object can be placed on a single plane). The theory was that an ether made up all matter, and it would become knotted; then, from different knots, came different elements. After this theory was disproven, chemists quickly lost interest in knots—but topologists picked up where they left off.

In chemistry, it is important to find similar compounds. Either pure fluorine (F₂) or hydrogen fluoride (HF) can be used to synthesize tetrafluoromethane [13] (CF₄); however, hydrogen fluoride is far safer and far cheaper to use than pure fluorine, despite performing comparably.

The reason HF and F₂ are similar is because they both contain the same element: fluorine (F); however, some compounds share similar traits simply because they share similar structure. Beta blockers are a class of drugs which inhibit beta receptors.
When beta receptors are affected by stress hormones, the heart can overreact and arrest [9]. Beta blockers dampen the effect of stress hormones so that a person can deter this situation, and they do this by being structured similarly enough to the stimulant to take its place in the beta receptors, which blocks the stimulant’s access.

![Figure 1.1: Adrenaline](image1)

![Figure 1.2: Propanolol](image2)

### 1.2 Chirality

A property of interest, which many chemical compounds have, is chirality. A compound which cannot be superimposed onto its mirror image is called chiral (e.g., Hands—it is impossible to place one’s hands, palms down, one atop the other, wrist-on-wrist, so that the fingers align with their analogues). Mirror image pairs are called enantiomers.

Sometimes, the effect of chirality is entertaining: The compound limonene smells of lemons, while its mirror image smells of oranges [7]. Other times, there is little to no noticeable effect: When drugs are produced in the lab, the yield is typically a
1:1 ratio between the enantiomers; one compound gives the desired effect, while the other does nothing or produces a mild side-effect [7]. However, sometimes, the effect is harrowing: In the 1960s, thalidomide was given to pregnant women to treat morning sickness; one compound eased the morning sickness, while the other enantiomer was responsible for horrible birth defects [7].

Knots may also be described as chiral, such as the simplest, non-trivial knot: the trefoil [6]. This raises the question: What properties, if any, might be shared between chemical compounds which both contain the same knot(s) within their structures?

Analysis can be quite difficult, especially because there is no known algorithm for determining if a knot is chiral. There is also the added difficulty in actually synthesizing a compound with a knot in it. The Hopf link, which is simply two interlocked circles, took fifty years to synthesize [7, 8].

While the first chemical knots analyzed were synthetic, knots have since been found to manifest naturally; DNA, for example, has been found to become enzymatically knotted and unknotted [3]. Small molecules, such as water or butane, don’t have much flexibility; their bonds do vary slightly in length and angle, but negligibly so. However, in long molecules, such as a 30-carbon chain or a DNA molecule, these tiny degrees of freedom can compound for a pliable composition.

1.3 When Chemistry Meets Topology

In her book, *When Chemistry Meets Topology*, Erica Flapan discusses on what she calls topologically complex molecules. These are molecules which, under the assumption of complete flexibility, cannot be deformed into a plane. Until the 1960s, there were no known compounds of this sort; for this reason, chemistry required geometry to study these non-topologically-distinct molecules. In 1961, the molecular Hopf link
was synthesized; 20 years later, the Simmons-Paquette molecule (Figure 1.3).

Both of these molecules, and many others since, are topologically complex—\textit{i.e.}, they can’t be deformed into a plane. However, if one of the rings of the Hopf link were cut, the one left intact could be taken out, then the first could be closed again. Now, the two rings are separate, which is a planar graph. In graph theory, a graph is called non-planar if there is \textit{no} possible combination of the same set of vertices and edges that can be deformed into a plane. The Hopf link graph was just shown to be not non-planar; however, the graph of the Simmons-Paquette molecule is.

In 1930 \cite{11}, Kuratowski published the characterization of planar graphs—now called Kuratowski’s Theorem. It is thus: A graph is non-planar if, and only if, it contains $K_5$ or $K_{3,3}$ as a subgraph.

If one refers back to Figure 1.3, it has points labeled 1-5 to show that it contains $K_5$.
as a subgraph. \( K_5 \) is the complete graph on five vertices (complete, here, means that there is an edge between any two vertices); \( K_{3,3} \) is the graph on two groups of three vertices such that there is an edge between every two vertices which are in different groups (see Figure 1.4).

![Figure 1.4: Three-runged Möbius ladder compound](image1)

In 1982, the first molecular Möbius ladder was synthesized by Walba et al. [16] (Figure 1.5). If all of the atoms which have two or fewer edges are removed, Figure 1.6 results, which is the three-runged Möbius ladder, \( M_3 \). It has labels 1, 2, 3 and a, b, c to demonstrate that it contains \( K_{3,3} \) as a subgraph.

![Figure 1.6: \( M_3 \), the three-runged Möbius ladder](image2)

Again, a broad definition of a chiral object is one which cannot be superimposed onto its mirror image; however, there are certain variations of this definition. Because molecules are rigid, the definition in chemistry allows only physically plausible manipulations in superimposition; e.g.: no rotations about double-bonds or meddling with bond angles. The topological definition differs from the former by assuming complete flexibility of objects. Therefore, if a molecular graph is analyzed and found to be topologically chiral, it must also be chemically chiral—and the Möbius ladder was proven to be topologically chiral [14].
Walba believed that the molecular Möbius ladder was topologically chiral, but he could not prove it. Jon Simon was inspired by this conjecture, and, in 1986, proved the statement, himself: If rungs go to rungs and sides go to sides, then the Möbius ladder is topologically chiral. The condition that rungs go to rungs and sides go to sides is important because they each represent different atoms and bonds. Flapan generalizes this statement by proving that any embedding of $M_3$ is chiral \[7\].

This brings us to what is called intrinsic chirality. A graph is just a set of vertices and edges; how one chooses to draw these edges in 3-space is called an embedding of the graph. A graph is intrinsically chiral if there is no achiral embedding of it. Flapan’s generalization, then, can be called a proof of $M_3$’s intrinsic chirality—but, are all Möbius ladders intrinsically chiral? As it turns out, if ladders of three or more rungs are considered, then all odd-runged ladders are intrinsically chiral, while the even-runged ones are not.

1.4 Toroidal Polyhedra

A polyhedral graph is simple, 3-connected, and planar. A simple graph is one which has edges only between two unique vertices, and has, at most, one edge between any two vertices. To be connected, a path of edges must be constructable from any one vertex to any other. To be $k$-connected, at least $k$ vertices (along with their edges) must be removed from a graph to make it no longer connected. To be planar, a graph must have at least one planar embedding.

In 2009 \[4\], Castle et al. conjectured that toroidal polyhedra are intrinsically chiral. Here, toroidal polyhedra are embeddings of polyhedral graphs which can be deformed into the surface of a torus, but not into plane (or, equivalently, a sphere).

In the toroidal tetrahedron in Figure 1.7, the path $ABDCA$ forms a trefoil knot.
What Castle and his team have encountered through their extensive study is that there does not seem to be a single toroidal entanglement on the torus which doesn’t contain a knot or a link. An entanglement is an anomaly in a non-planar embedding of a graph which, if removed, would result in a planar embedding. Knots and links are common entanglements, but another kinds is that of ravels [5].

The teams believes that an entanglement which is not a knot or a link is not possible, here, but that fact remains to be proved. However, Castle’s team proved that toroidal polyhedra are chiral, provided that they contain either a knot or a link. The proof is segmented into three cases: trefoils, general torus knots and links, then the Hopf link (which is excluded from the second segment). What follows is an overview of the proof which will be detailed in the thesis.

If an achiral graph embedding contains a chiral knot as a subgraph, it must also contain the knot’s mirror image as a subgraph. Thus, for the first two cases, a minimal graph embedding is made using a chiral knot and its mirror image, which makes the embedding achiral. These embeddings are each proved to be non-planar, which implies that they cannot be embeddings of a polyhedral graph. This is done using Euler’s formula, $V - E + F = 2$, and universal covers. The universal cover is a 2-dimensional representation of a torus.

One can visualize the creation of a universal cover by cutting the torus, from the center, outward—like a cake. The severed donut shape can then be straightened into
tetrahedral isotope is indeed chiral.

knots and one (ACBDA) graph; if this contains only chirally knotted or linked cycles, the topological invariant that consists of all cycles in the knotted tetrahedron embedding is chiral, we use Kau's spherical tetrahedron in \( S^2 \), Fig. 1. An infinite number of toroidal tetrahedral graphs are possible. The simplest example contains a single trefoil knot as a subgraph, as shown in Fig. 1.

The trefoil winds around the two fundamental cycles of the torus, the Euclidean plane, \( \mathbb{E}^2 \). Toroidal isotopes can be 'unrolled' into the universal cover of the spherical tetrahedron in \( S^2 \). The universal cover of toroidal isotopes \( \mathbb{E}^2 \) is illustrated by a simple animation contained in the ESI.

The first objective of this thesis will be to delve into the details of Castle’s team’s proof, for much is omitted. A more thorough understanding will be sought and

1.5 Objective

The first objective of this thesis will be to delve into the details of Castle’s team’s proof, for much is omitted. A more thorough understanding will be sought and
discussed.

What Castle and his colleagues do not include, but speak of, is a molecular example. The objective of this thesis research will be to find one, beginning with their suggestion of carcerands—molecules which trap a guest molecule and will not release it, even at high temperatures. Carcerands can often be represented by polyhedral graphs, so templating one on a torus or ring would result in a chiral compound (if their conjecture is correct).

Initially, the computer applications KnotPlot and Avogadro were to be utilized in molecular analysis. KnotPlot allows manipulation of graphs and can even be asked to simplify a structure, which would make determining which if a knot is a subembedding of the structure almost effortless. However, the molecules in consideration contain far above the limit of vertices that KnotPlot can handle.

The application, Avogadro, has no problem displaying entire molecules, but it cannot manipulate them; thus, this software was also abandoned.
Chapter 2

Concepts

A few topological and graph theoretical concepts are addressed.

2.1 Definitions

Topology: Let $X$ be a set and let $\tau$ be a set of subsets of $X$. If the following hold:

1. $X$ and $\emptyset$ are in $\tau$
2. Any finite or infinite union of sets in $\tau$ is an element in $\tau$
3. Any finite intersection of sets in $\tau$ is an element in $\tau$

then $\tau$ is called a topology on $X$.

Topological Space: A set, $X$, with a topology, $\tau$, is called a topological space. It is sometimes denoted $(X, \tau)$, but $\tau$ is often omitted when no confusion will arise.

Graph: Let $V = \{v_1, v_2, \ldots \}$ be a finite or infinite set. Let $V_2 := \{\{v, w\} : \{v, w\} \subseteq V\}$.
If $E \subseteq V_2$, then the pair of sets, $(V, E)$, is called a graph. $G$ or $G(V, E)$ denotes the graph described by $(V, E)$; the elements of $V$ are called the graph’s vertices; the elements of $E$, its edges.
Let $G$ be a graph. A subgraph, $H$, of $G$, results when vertices and or edges are removed from $G$. Adjacent vertices may also be condensed into a single vertex. It is said that $H$ is a subgraph of $G$, or that $G$ contains $H$ as a subgraph.

Figure 2.1: From left to right, let the graphs be called $G$, $H$, and $J$. $H$ is a subgraph of $G$ by edge and vertex removal, while $J$ is a subgraph of $G$ because the vertices 2, 5, and 1 are condensed into a single vertex, labeled $1'$.

Informally, while a graph is thought of as a visual object, this depiction is only a representation of the graph; a graph is only defined by its vertices and edges.

**Path:** Let $G(V,E)$ be a graph. A $k$-tuple, $(v_1, v_2, \ldots, v_k)$ is called a path if, for $i \in \{1, 2, \ldots, k - 1\}$, \(\{v_i, v_{i+1}\} \in E\). It is typically denoted $v_1v_2\ldots v_k$.

**Cycle:** A path of the form $v_1v_2\ldots v_k$ such that $v_1 = v_k$ is called a cycle.

**Graph Realization:** Let $\rho : V \rightarrow \mathbb{R}^3$ be a map such that \(\{\rho(v_1), \rho(v_2), \ldots\}\) is a set of distinct points in $\mathbb{R}^3$ such that any plane in $\mathbb{R}^3$ contains, at most, three of these points. Let $[\rho(v_i), \rho(v_j)]$ denote the straight line segment from $\rho(v_i)$ to $\rho(v_j)$. Let $G(V,E)$ be a graph. The topological space

$$R(G) = \bigcup \{[\rho(v_i), \rho(v_j)] : \{v_i, v_j\} \in E\}$$

is called a realization of $G$.

**Simple:** A graph is simple if there is no edge connecting a vertex to itself. It is noted that, in the literature, a graph is often defined to allow more than one edge between the same two vertices. With this definition, it must be explicitly stated that a simple graph allows, at most, one edge between any two vertices.
**k-connected:** A graph is called connected if there is a path between any two vertices. A graph is called \(k\)-connected if no less than \(k\) vertices, along with the corresponding edges, must be removed to make the graph no longer connected.

**Planar:** Let \(G\) be a graph and let \(R(G)\) be its realization in \(\mathbb{R}^3\). \(G\) is planar if there is an embedding of \(R(G)\) in \(\mathbb{R}^2\). Graphs which are not planar are called non-planar. One may notice that a graph is planar if, and only if, its realization can be embedded in \(S^2 = \{(x, y, z) : x^2 + y^2 + z^2 = 1\}\).

**Polyhedral:** A graph is called polyhedral if it is simple, 3-connected, and planar. Any such graph can be embedded in 3-space as a convex polygon.

**Homotopy:** If \(f\) and \(f'\) are continuous maps from the space \(X\) to the space \(Y\), then it is said that \(f\) is homotopic to \(f'\) if there is a continuous map, \(F : X \times [0, 1] \to Y\), such that
\[
F(x, 0) = f(x) \quad \text{and} \quad F(x, 1) = f'(x)
\]
for each \(x \in X\). \(F\) is called a homotopy between \(f\) and \(f'\).

**Null-Homotopic:** If \(f\) is homotopic to a constant function, then \(f\) is called null-homotopic. Null-homotopic cycles will be focused upon; informally, these are the cycles which can be deformed to a single point (the constant function). In the universal cover (to be defined), a null-homotopic cycle is a typical cycle; i.e., the cycle begins and ends with the same, exact vertex, in the plane. Non-null-homotopic cycles, like a ring around the minor axis, cannot be condensed into a single point without leaving the toroidal surface; in the universal cover, these cycles begin and end with distinct copies of the same vertex (see Figure 2.2).

**Homeomorphism:** Let \(X\) and \(Y\) be topological spaces. Let \(f : X \to Y\) be a bijection, and let \(f^{-1} : Y \to X\) denote its inverse function. If \(f\) and \(f^{-1}\) are both continuous, then \(f\) is called a homeomorphism from \(X\) to \(Y\); \(X\) is said to be homeo-
Figure 2.2: The cycle $ADCBA$ is null-homotopic, while the cycle $ACBDA$ isn’t [4].

morphic to $Y$, and vice versa.

**Embedding:** Let $f : X \rightarrow Y$ be an injective, continuous map between the topological spaces, $X$ and $Y$. Let $Z$ be the image set, $f(X)$, considered as a subspace of $Y$. Then, $f' : X \rightarrow Z : x \mapsto f(x)$ is a continuous bijection. If $f'$ is a homeomorphism between $X$ and $Z$, then the map $f$ is called an embedding of $X$ in $Y$.

**Ambient Isotopic:** Let $X$ and $Y$ be topological spaces, and let $g$ and $h$ be embeddings of $X$ in $Y$. If, for a continuous map,

$$F : Y \times [0, 1] \rightarrow Y,$$

the following hold:

1. $F(y, 0) = y$
2. $F| \ Y \times \{t\}$ is a homeomorphism from $Y \times \{t\}$ onto $Y$ for all $t \in [0, 1]$
3. $F(g(x), 1) = h(x)$

then $F$ is called an ambient isotopy taking $g$ to $h$; $g$ is said to be ambient isotopic to $h$, and vice versa.

**Mirror Image:** Let $G$ be an embedding in $\mathbb{R}^3$. Let $s : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ be a symmetry about the plane, $L := \{(x, y, z) \in \mathbb{R}^3 : x = 0\}$. I.e., $s$ is the map of $\mathbb{R}^3$ onto itself, defined by $(x, y, z) \mapsto (-x, y, z)$. The image of $G$, $s(G)$, is called the mirror image of $G$ in $\mathbb{R}^3$. 

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Informally, a mirror image is what one would expect: a reflection of an object through a plane, like one’s face in a mirror.

**Chirality:** Let $G$ be an embedding in $\mathbb{R}^3$ and let $G' = s(G)$ be its mirror image with the mirror reflection $s$. If there is an ambient isotopy, $h: \mathbb{R}^3 \times [0,1] \to \mathbb{R}^3$, such that

$$h(x,0) = x \text{ for } x \in X \quad \text{and} \quad h(g,1) = s(g) \text{ for } g \in G,$$

then $G$ is called achiral. If no such ambient isotopy exists, then $G$ is called chiral.

**Knot:** Let $S^1 = \{(x,y,0) : x^2 + y^2 = 1\}$. An embedding, $\alpha: S^1 \to \mathbb{R}^3$, of $S^1$ into $\mathbb{R}^3$ is called a knot. Two knots are considered equivalent if they are ambient isotopic to each other. The unknot embedding is $\sigma: S^1 \to \mathbb{R}^3 : x \mapsto x$. If a knot is ambient isotopic to $\sigma$, then it is called the unknot (also, the trivial knot).

**Link:** Let $\alpha_i$, $i = 1,2,\ldots,k$, be knots such that $\alpha_i(S^1) \cap \alpha_j(S^1) = \emptyset$ for $i \neq j$. Then $\alpha: S^1 \times \{1,2,\ldots,k\} \to \mathbb{R}^3$, defined by $\alpha(x,i) = \alpha_i(x)$ is called a link. Two links are considered equivalent if they are ambient isotopic to each other. If $\alpha$ is ambient isotopic to $\upsilon$, where $\upsilon$ is the embedding $\upsilon: S^1 \times \{1,2,\ldots,k\} \to \mathbb{R}^3$, defined by $\upsilon(x,i) = (x,i-1)$ then it is called the unlink.

**Universal Cover:** Let $\sim$ be a relation on $\mathbb{R}^2$, such that $(x_1,y_1) \sim (x_2,y_2)$ if, and only if, $x_1 - x_2 \in \mathbb{Z}$ and $y_1 - y_2 \in \mathbb{Z}$. The quotient space, $\mathbb{R}^2/\sim$, of this relation is homeomorphic to the torus; it’s quotient map, $q: \mathbb{R}^2 \to \mathbb{R}^2/\sim$, is called the universal cover of the torus.

Informally, the torus’ minor axis is the copy of $S^1$ within the torus, while the major axis is the outer, straight line which goes through the hole of the torus, perpendicular to the plane containing the minor axis. To visualize the universal cover, a torus is cut perpendicularly to the minor axis; after which, it can be be straightened into a tube. This tube can be cut laterally, then unrolled like wrapping paper, into a flat square.
Because the opposite sides of the square are equivalent, the square can be tiled in $\mathbb{R}^2$ thus: one side of the square is labeled north, the sides adjacent to north are west and east, and the final side is labeled south. In the tiling, north sides only touch south sides; east sides only touch west sides; and each side touches only one other square.

![Figure 2.3: A graph, embedded on a torus (right) with its universal cover](image)

**Homotopy Type $\{p, q\}$:** Let the numbers $p$ and $q$ be co-prime. A cycle is of homotopy type $\{p, q\}$ (or called a $\{p, q\}$ knot) if it revolves about the major axis $|p|$ many times, and about the minor axis $|q|$ many times; $k\{p, q\}$ denotes a link with $k$ many components, each of homotopy type $\{p, q\}$.

In the universal cover, a $\{p, q\}$ cycle’s beginning and ending points are connected by the vector $(p, q)$. The difference between $\{p, q\}$ and $\{-p, q\}$ is the direction of rotation about the major axis; similarly, $\{p, q\}$, $\{p, -q\}$, and the minor axis. It is common practice to have the bottom-to-top direction be the positive rotation direction for the minor axis, and left-to-right for the major axis. Thus, if $p$ and $q$ are both positive, or both negative, the knot, $\{p, q\}$, will have a positive slope in the universal cover; if *only* $p$ or *only* $q$ is negative, then a negative slope will result.

**Curve:** Let $X$ be a topological space, and let $\gamma : [0, 1] \to X$ be a continuous map; then $\gamma$ is called a curve. If $\gamma$ is injective, then it is called simple; if $\gamma(0) = \gamma(1)$, then $\gamma$ is called closed. A simple, closed curve is often called a Jordan curve. A topological space, $X$, is called path-connected if, for any two points, $x, y \in X$, there is a curve,
\(\gamma\), such that \(\gamma(0) = x\) and \(\gamma(1) = y\).

**Surface**: A Hausdorff, topological space, \(S\), such that each \(s \in S\) has a neighborhood homeomorphic to an open set in \(\mathbb{R}^2\) is called a surface.

**Genus**: (plural: genera) Let \(S\) be a surface. The maximal number, \(k\), for which there are \(k\) pairwise-disjoint Jordan curves, \(\gamma_1, \gamma_2, \ldots, \gamma_k\), in \(S\) such that the complement, \(S \setminus \bigcup_{i=1}^{k} \gamma_i([0, 1])\), is path-connected is called the genus of \(S\).

Let \(\alpha : R(G) \to \mathbb{R}^3\) be an embedding. Let \(k := \min\{\text{genus}(S) : \alpha(R(G)) \subseteq S \subseteq \mathbb{R}^3\}\). This \(k\) will be called the genus of \(\alpha\).

**Toroidal Embedding**: An embedding of a graph in the torus (which means it has a genus of 1) will be referred to as a toroidal embedding (or a toroidal graph).

\(a\{b, c\} \otimes d\{e, f\}\): This notation will indicate a toroidal graph composed of the knots (composed of the links) \(a\{b, c\}\) and \(d\{e, f\}\); the intersections between the different knots (different links) will generate the vertices.

### 2.2 Facts

The following facts will be used heavily in the proof:

**Theorem 1 (Kaufmann’s Topological Invariant)** If an achiral graph realization contains a cycle which, if embedded alone, is ambient isotopic to a chiral knot, then this graph also contains another cycle which, if embedded alone, is ambient isotopic to the first knot’s mirror image.

**Theorem 2 (Kuratowski’s Theorem)** A graph is non-planar if, and only if, it contains either \(K_5\) or \(K_{3,3}\) (or both) as a subgraph. \(K_5\) is the complete graph on five vertices, which means that there is an edge between any two vertices. \(K_{3,3}\), similarly, is a graph on six vertices, separated into two groups of three vertices each, such that there is an edge between every pair of vertices which are in different groups.
Figure 2.4: $K_5$ and $K_{3,3}$ [7].
Chapter 3

Proof

For clarity on vocabulary: graph will mean the abstract object defined above; a graph realization is a representation of a graph in 3-space (it is an embedding); and a toroidal embedding is an embedding of a graph realization into the toroidal surface.

Theorem 3 Let $G$ be a simple, 3-connected, planar graph—i.e., a polyhedral graph. Let $\gamma$ be an embedding of $G$ into the toroidal surface, such that there is no ambient isotopy which takes $\gamma$ into the spherical surface—then $\gamma$ is chiral. It is assumed that, for $\gamma$ to be embedded into the torus such that it is not ambient isotopic to a spherical embedding, it must contain a knot or a link as a subembedding.

In order to cover every scenario in Theorem 3 all possibilities are broken down into three categories, which will each be considered separately. These categories are: gemini trefoils, $k\{p,q\}$ pairs, and, finally, the Hopf link (the only case excluded from the $k\{p,q\}$ pairs).
3.1 Gemini Trefoils

The first group of cases considered will be toroidal embeddings which contain only opposite-handed trefoil knots—a.k.a. gemini trefoils. It will be proven, via contradiction, that such an embedding cannot be one of a polyhedral graph. Overview:

1. Two toroidal embeddings will be examined, as every other case is symmetric to one of the two:

   (a) $\{2, 3\} \otimes \{2, -3\}$

   (b) $\{2, 3\} \otimes \{3, -2\}$

2. It is assumed that these graphs are polyhedral; thus, Euler’s characteristic formula for planar graphs, $V - E + F = 2$, must hold.

3. The embeddings’ universal covers are employed to reveal that Euler’s formula would, in fact, not hold for these embeddings—the contradiction.

4. Per Kuratowski’s theorem, any graph containing one of these two as a subgraph is non-planar; thus, not polyhedral.

**Lemma 1** There are only two embeddings for the gemini trefoils on the toroidal surface: $\{2, 3\} \otimes \{2, -3\}$ and $\{2, 3\} \otimes \{3, -2\}$. Any other embedding of gemini trefoils is ambient isotopic to one of these two.

A toroidal trefoil knot wraps around one toroidal axis twice, and three times around the other; thus, it is of homotopy type $\{2, 3\}$ or $\{3, 2\}$ or $\{-2, 3\}$—etc. The trefoil knot is chiral; thus, per Kaufmann’s topological invariant, if an achiral embedding contains a trefoil knot, it contains both enantiomers. This raises the question: Which homotopy types represent which enantiomers?—*i.e.:* Which homotopy types are ambient isotopic to one another?
Figure 3.1: A depiction of an ambient isotopy which takes the toroidal knot \(\{2, 3\}\) to \(\{3, 2\}\) [1].

Figure 3.1 depicts an ambient isotopy which takes a \(\{2, 3\}\) knot to a \(\{3, 2\}\) knot, and vice versa. Essentially, the surface is turned inside out, and this interchanges the axes.

In the first step, a ball on the surface, which is disjoint from the knot, is removed from the torus (instead of a hole, a point may also be removed). This hole is then expanded to create the perpendicular ribbons in the second step; the knot is carried with the contracting surface. The ribbon about the major axis is flipped inside-out in the third step, followed by the other ribbon in the fourth step. Finally, the ribbons expand, which brings the surface back to toroidal shape, and the \(\{2, 3\}\) knot has become a \(\{3, 2\}\) knot.

<table>
<thead>
<tr>
<th>({2, 3})</th>
<th>({3, 2})</th>
<th>({2, -3})</th>
<th>({3, -2})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-2, -3)</td>
<td>(-3, -2)</td>
<td>(-2, 3)</td>
<td>(-3, 2)</td>
</tr>
</tbody>
</table>

Figure 3.2: Every torus-knot representation for a trefoil.

In Figure 3.2, every torus-knot representation for a trefoil is given. For any two entries in the same column, the entries are equal by multiplying both numbers negative one. When one of the numbers changes sign, it means that the direction of revolution about the axis has changed. When both revolutions change directions,
they cancel each other out. Therefore, the entries in a column represent the same, exact embedding.

There is a barrier in the middle of the table, which separated the eight embeddings into four. On the left, the \{2, 3\} is next to the \{3, 2\} knot. It was shown that these two are ambient isotopic in Figure 3.1. Therefore, all four entries on the left are ambient isotopic to one another; they will not be embedded together, as the desired pairing are of enantiomers \(i.e.,\) the mirror images, and mirror images are not ambient isotopic for chiral embeddings.

On the right side of the table, \{2, -3\} and \{3, -2\} are next to each another. When the two numbers are swapped like this, the embeddings are ambient isotopic \(\text{see Figure 3.1} \). Therefore, all four embedding on the right are ambient isotopic.

Because the columns have identical embeddings, only one representative is needed for the pairing process. The two knots on the left only need to be embedded with the two on the right, which gives a total of four gemini trefoil embeddings.

\[
\begin{array}{c|c}
\{2, 3\} \otimes \{2, -3\} & \{2, 3\} \otimes \{3, -2\} \\
\{3, 2\} \otimes \{-3, 2\} & \{3, 2\} \otimes \{-2, 3\}
\end{array}
\]

Figure 3.3: All four possible embeddings of gemini trefoils.

In Figure 3.3, all four possible pairing are made. However, in the first column, the first knots listed (\{2, 3\} and \{3, 2\}) are ambient isotopic via axis swapping, and so are \{2, -3\} and \{-3, 2\}. Therefore, if the ambient isotopy in Figure 3.1 is used, the top embedding becomes the bottom, and vice versa. The same holds for the two embeddings on the right. Therefore, Lemma 1 holds.

\(V\) and \(E\) denote the sets of a graph’s vertices and edges, respectively. It is assumed that these embeddings are of polyhedral graphs, so planar embeddings must exist; \(F\) denotes the set of faces of the polyhedra in these planar embeddings. \(V\) will denote \(|V|\), the number of elements in \(V\); similarly, \(E = |E|\) and \(F = |F|\).
Two variables are defined: let $z$ denote the average degree (the number of edges incident to a vertex) of the graph, and let $n$ denote the average face size. That is, for the graph, $G(V,E)$:

$$z := \frac{\sum_{v \in V} \deg(v)}{V} = \frac{2E}{V} \quad \text{and} \quad n := \frac{\sum_{f \in F} \text{edg}(f)}{F} = \frac{2E}{F}$$

**Lemma 2** Let $G$ be a polyhedral graph. Let its average degree size, $z$, be 4. It directly follows, from Euler’s Characteristic Formula, that the average face size, $n$, of $G$ is less than 4.

The examined embeddings are assumed to be of polyhedral graphs, and polyhedral graphs are planar. For this reason, Euler’s characteristic formula for planar graphs must hold: $V - E + F = 2$. The two identities, $z$ and $n$, are substituted into the formula.

$$V - E + F = 2$$
$$\frac{V}{F} - \frac{E}{F} + 1 = \frac{2}{F}$$
$$\frac{n}{z} - \frac{n}{2} + 1 = \frac{2}{F}$$

Because all that has been done above is replacement with equivalent terms, the result above holds for any planar graph.
Figure 3.5: The universal covers for \( \{2, 3\} \otimes \{2, -3\} \) (left) and \( \{2, 3\} \otimes \{3, -2\} \) (right).

In the universal covers above, vertices of the same color are equivalent, which means that they represent the same vertex on the torus. In each of the two universal covers, four copies of the tori are shown; in a torus’ actual universal cover, the copies of the torus tile the infinite plane. The differently colored edges differentiate the two knots. It is clear, from the universal cover, that every vertex has a degree of 4. This means that the average degree, \( z \), must be 4. The substitution of \( z = 4 \) is used below:

\[
\frac{n}{4} - \frac{n}{2} + 1 = \frac{2}{F} \\
n = 4 - \frac{8}{F}
\]

This result (Lemma 2) holds for any planar graph with an average degree of 4. For this reason, it will be used in the next chapter, as well.

**Lemma 3** Let \( \gamma \) be an embedding consisting only of two gemini trefoils on a single torus; then \( \gamma \) is an embedding of a non-planar graph.

The above equation, together with the fact that \( F \) is non-negative, imply that \( n < 4 \). However, for \( n \) to be less than 4, there must be at least one cycle of less than 4 edges; yet, in the universal covers, not a single, such cycle exists.
This contradiction means that Euler’s equation does not hold for this graph; i.e., it is non-planar. Planarity is one of the three qualities of polyhedral graphs; thus, neither of these two graphs are polyhedral.

**Lemma 4** Let \( \gamma \) be a toroidal embedding of a graph, \( G \). As a subembedding, \( \gamma \) contains gemini trefoils. Then, \( G \) is not polyhedral.

The above proved that the two example embeddings cannot be of polyhedral graphs; however, can an embedding be created with these two gemini trefoils, such that its corresponding graph is planar? Kuratowski’s theorem states that a graph is non-planar if, and only if, it contains one of the graphs, \( K_5 \) or \( K_{3,3} \). In the following universal covers of \( \{2,3\} \otimes \{2,-3\} \), vertices are grouped to show that \( K_5 \) and \( K_{3,3} \) are both contained as subgraphs.

![Figure 3.6: The vertices are grouped to reveal \( K_5 \) (left) and \( K_{3,3} \) (right) as subgraphs of \( \{2,3\} \otimes \{2,-3\} \).](image)

Both of the embeddings must contain either \( K_5 \) or \( K_{3,3} \), per Kuratowski’s theorem. Because the non-planarity was proven using Euler’s characteristic formula for planar graphs, and the contradiction was that there wasn’t a cycle of 3 edges, one might wonder if adding enough 3-edge cycles could bring balance to this formula.

However, none of the original vertices or edges can be removed. In other words, any toroidal embedding of a graph which contains gemini trefoils must contain one of these two embeddings as a subembedding. As a result, \( K_5 \) or \( K_{3,3} \) is part of the underlying graph of this embedding, and it is non-planar. The non-planarity is a
result of the gemini trefoils, themselves. As a result, no achiral, toroidal embedding which contains a trefoil knot may be the graph of a polyhedron.

### 3.2 $k\{p, q\}$ Pairs

This proof, via contradiction, will be similar to that of the gemini trefoils':

1. Again, two cases will cover all possible scenarios. However, this time, the two cases will be examined separately. They are:
   
   - (a) $k\{p, q\} \otimes k\{p, -q\}$
   - (b) $k\{p, q\} \otimes k\{-q, p\}$

2. The universal cover will be constructed, which will show that $z$ is always 4, like the trefoil cases.

3. Because $z = 4$, in order to be polyhedral, the average face size, $n$, must be less than 4.

4. The universal cover and the Euclidean metric will be employed to show that this restriction does not hold—the contradiction.

**Lemma 5** Let $p$ and $q$ be co-prime integers, and let $k$ be a natural number. Let $G$ be a graph whose toroidal embedding, $\gamma$, consists of only a gemini $k\{p, q\}$ pair. Then $\gamma$ is ambient isotopic to one of two embeddings: $k\{p, q\} \otimes k\{p, -q\}$ or $k\{p, q\} \otimes k\{-q, p\}$.

Lemma 5 holds because all of the possible cases can be constructed as the gemini trefoil cases were in Figure 3.3. Again, there are only four embeddings, but, because they can be written analogously to the four cases in Figure 3.3, the same ambient isotopy (Figure 3.1) narrows it down to just the two cases in the lemma.
3.2.1 \( k\{p, q\} \otimes k\{p, -q\} \)

For the examination of the first case, the universal cover will be constructed using \( k\{p, q\} = 1\{3, 5\} = \{3, 5\} \); this specific case will help visualize the general one. The embedding is \( \{3, 5\} \otimes \{3, -5\} \). Because it will not adversely affect reasoning, for the duration of this paper, it is assumed that \( p \) and \( q \) are positive, and that \( p < q \). It is noted that \( k \) only takes positive values because it is the number of copies of the same knot which form the link. Reminder: \( p \) and \( q \) are co-prime.

To repeat: The purpose of the universal cover is that it will reveal (a) the constant vertex degree of 4, and (b) the metric-length of the edges (a constant). The metric-length of the edges will be used to calculate, without construction, the minimum number of edges to get from one vertex to a copy of itself in the universal cover (this number represents the number of edges in a polygonal face). While the construction is a bit tedious, it culminates in extremely quick and general calculations.

![Diagram](image.png)

Figure 3.7: A universal cover containing only the equivalent corner vertex, and two whole tori visible [10].

**Lemma 6** In the universal cover for the torus link \( k\{p, q\} \), the link is represented by the set of lines

\[
\left\{ y = \frac{q}{p}x - \frac{a}{p} : a \in \mathbb{Z} \right\}
\]
Toroidal links are of the form $k \{p, q\}$: $\{p, q\}$ represents a knot which revolves $p$ many times about the major axis, and $q$ many times about the minor axis; $k$ is the number of $\{p, q\}$ knots embedded on the same torus, forming a link. To begin, $p$ is assumed to be less than $q$, and $k = 1$.

The universal cover is tiled with equivalent unit squares. They each represent the torus, in its entirety. The toroidal knots will be assumed to have constant curvature. This makes the constructions and calculations easier, without interfering with reasoning.

Constant curvature on the torus means that there is a constant ratio between the revolution speeds. For example: with a $\{2, 3\}$ knot, for every 2 revolutions about the major axis, the minor axis is revolved about 3 times. Constant curvature means that, as the knot is drawn, for every 2 degrees it rotates about the major axis, it will rotate 3 degrees about the minor axis. After 4 degrees about the major axis, the knot has rotated 6 degrees about the minor axis; after 8 degrees about the major, 12 about the minor. After 720 degrees (two full revolutions) about the major axis, 1080 degrees have revolved about the minor axis (three full revolutions). Thus, a $\{p, q\}$ knot will revolve about the major axis $p$ degrees for every $q$ degrees about the minor axis.

In the universal cover, a revolution about one axis means a traversal of one unit in the opposite axis’ direction; e.g.: the straight line from $(0, \frac{1}{2})$ to $(1, \frac{1}{2})$ has revolved about the $y$-axis once, but not at all about the $x$-axis; it has traveled around the $y$-axis, back to the original point, by only moving along the $x$-axis ($(0, \frac{1}{2})$ and $(1, \frac{1}{2})$ are equivalent in the universal cover, so they represent the same point in the torus). Thus, a $\{p, q\}$ knot will traverse $p$ units along the $x$-axis for every $q$ units along the $y$-axis. This is simply a straight line with a slope of $\frac{2}{p}$.

First, only one copy of the torus will be considered: the torus bound by the lines...
\(y = 0, y = 1, x = 0, \) and \(x = 1\). From the definition of the universal cover, it is clear that the corners \((0, 0), (0, 1), (1, 0), \) and \((1, 1)\) are equivalent—i.e.: they represent the same point on the torus—but this depiction makes this clear: Because the left and right boundaries are equivalent, \((0, 0)\) is equivalent to \((1, 0)\), and \((0, 1)\) is equivalent to \((1, 1)\). However, the upper and lower boundaries are also equivalent, so \((0, 0)\) is equivalent to \((0, 1)\), and \((1, 0)\) is equivalent to \((1, 1)\). Therefore, these four points in the plane represent a single point in the torus. These points are important because they are the starting and ending points of the knots in this construction. I.e.: On the toroidal surface, a knot can be traced from a starting point, and path of the knot will lead back to that, exact point; in the universal cover, knots begin and end at points which are distinct in the plane, but which are equivalent in the universal cover.

The example to be constructed is \(\{p, q\} = \{3, 5\}\). Because the slope is \(\frac{q}{p} = \frac{5}{3}\), a positive number, the starting point is \((0, 0)\); its enantiomer, \(\{3, -5\}\), will start at \((0, 1)\), and have a negative slope.

The line with slope \(\frac{q}{p}\) which passes through the point \((0, 0)\) is \(y = \frac{q}{p}x\). Each time the line touches a boundary, it will wrap around to the equivalent point in the opposite boundary. This continuation is illustrated by drawing a new line, with the same slope, shifted one unit in the direction of the opposite boundary. Here, \(y = \frac{5}{3}x\) touches the upper boundary first, so the next line will be shifted one unit down, to continue at the lower boundary.

To shift a function, \(f(x)\), \(v\) units down, \(f(x)\) becomes \(f(x) - v\). To shift a function, \(f(x)\), \(h\) units left, \(f(x)\) becomes \(f(x + h)\).

The starting point of \(y = \frac{5}{3}x\) is \((0, 0)\), and its ending point is \((\frac{3}{5}, 0)\). Because this is a traversal of one unit in the \(y\)-direction, it represents one complete revolution about the \(x\)-axis (which represents the minor axis of the torus). In general, the first \(x\)-revolution will start at \((0, 0)\), and end at \((\frac{2}{q}, 1)\). The knot continues at the lower
boundary, one unit down, at the point \( \left( \frac{3}{5}, 0 \right) = \left( \frac{p}{q}, 0 \right) \), which is equivalent to \( \left( \frac{3}{5}, 1 \right) \) in the universal cover; the equation for this line is \( y = \frac{5}{3}x - 1 = \frac{5}{3}x - \frac{3}{3} = \frac{2}{p}x - \frac{2}{p} \) (it will become apparent why 1 is written as \( \frac{p}{p} \) soon).

The second revolution about the \( x \)-axis begins at \( \left( \frac{p}{q}, 0 \right) = \left( \frac{3}{5}, 0 \right) \) and should have terminated at \( \left( \frac{2p}{q}, 1 \right) = \left( \frac{6}{5}, 1 \right) \) (the point where this second line reaches the upper boundary); however, the line reaches the right boundary before the upper boundary; this is the first revolution about the \( y \)-axis (major toroidal axis). Because the right boundary is reached, the next line will continue the knot at the equivalent point in
the left boundary, and the equation is \( y = \frac{q}{p}(x + 1) - \frac{p}{p} = \frac{q}{p}x - \frac{p-q}{p} = \frac{5}{3}x - \frac{2}{3} \).

Figure 3.10: As described [10].

Sidebar—a brief reminder on modular arithmetic: for integers \( a, b, \) and \( c; \) \( a \equiv b \pmod{c} \) (read: “\( a \) is equivalent to \( b \), modulo \( c \)” or, simply “\( b \), mod \( c \)” ) if, and only if, \( a - b \) is an integer multiple of \( c \); \( c \) is called the modulus; and \( a \) and \( b \) are said to be in the same equivalence class. E.g.: the hours of the day have a modulus of 12, so, 4 hours after 9 a.m., it is 1 p.m.; or, equivalently, in 24-hour time, it is 1300 hours; because \( 13 \equiv 1 \pmod{12} \).

The notation, \( \overline{a}_n \), signifies the equivalence class of the integers equivalent to \( a \), modulo \( n \), which is the set \( \{ \ldots , a - 2n, a - n, a, a + n, a + 2n, \ldots \} \). Any integer in the equivalence class can be the representative; e.g.: \( \overline{1}_{12} \) and \( \overline{13}_{12} \) both represent the same set. When the modulus is understood, the subscript may be omitted. For the modulus, \( n \), there are \( n \)-many, disjoint equivalence classes. End sidebar.

For the \( \{3, 5\} \) knot, the second revolution about the \( x \)-axis begins as \( y = \frac{5}{3}x - \frac{2}{3} \), but is completed by the line \( y = \frac{5}{3}x - \frac{2}{3} \). The only difference in the two equations is the constant at the end. However, these two constants have equivalent numerators, modulo 5; i.e.: \( -2 \equiv 3 \pmod{5} \). After every revolution about the \( x \)-axis, the equation of the next line is the same as the one before it, minus 1. Then, in general, the \( n \)-th
revolution about the $x$-axis is the line $y = \frac{q}{p}x - (n - 1) = \frac{q}{p}x - \frac{(n-1)p}{p}$. When the first revolution about the $y$-axis happens, the first line of the current $x$-revolution is as predicted, but a second line, one unit to the left, will complete the $x$-revolution: $y = \frac{q}{p}(x+1) - \frac{(n-1)p}{p} = \frac{q}{p}x - \frac{(n-1)p-q}{p}$. Because the second equation’s constant’s numerator is the same as the first, minus $q$, they are equivalent, modulo $q$: $(n-1)p-q \equiv (n-1)p \pmod{q}$; this statement holds because the difference between $(n-1)p-q$ and $(n-1)p$ is $-q$, which is an integer multiple of $q$.

The beginning and ending points of the $x$-revolutions have a similar pattern: For the $\{3, 5\}$ knot, the first $x$-revolution begins at $(0,0)$ and ends at $(\frac{3}{5}, 1)$. The second $x$-revolution begins at $(\frac{3}{5}, 0)$ and ends at $(\frac{1}{5}, 1)$. This second $x$-revolution requires two equations, so the end-point comes from the second of these; the first equation reaches the upper boundary at $(\frac{23}{5}, 1) = (\frac{6}{5}, 1)$. The pattern is in the numerators of the $x$-values: they are equivalent, modulo 5 (i.e.: $6 \equiv 1 \pmod{5}$).

In the current construction, the first revolution about the $y$-axis has occurred, and it happened during the $n$-th, $x$-axial revolution. After this $n$-th revolution has finished, the $(n+1)$-th, $x$-axial revolution begins. The last line drawn has touched the upper boundary, so the next line must continue at the lower boundary. Therefore, the equation for this line is the same as the one before it, minus 1: $y = \frac{q}{p}x - \frac{(n-1)p-q-1}{p} = \frac{2}{p}x - \frac{np-q}{p} = \frac{5}{3}x - \frac{1}{3}$. The first pattern would have called for the constant at the end to be (negative sign ignored) $\frac{np}{p}$. Again, the numerators are equivalent, modulo $q$: $np - q \equiv np \pmod{q}$.

The next equation’s constant (negative sign ignored) will be $(n+1)p - q$, which is equivalent to $(n+1)p$, modulo $q$; and this pattern will continue until the second $y$-axis revolution occurs (for $\{3, 5\}$, the next $y$-axis revolution occurs during the fourth $x$-axial revolution). Assume this happens during the $(n+m)$-th, $x$-axial revolution (where the first $y$-axial revolution occurred during the $n$-th $x$-axial revolution). In
the current pattern, the first equation is \( y = \frac{q}{p} x - \frac{(n+m-1)p-q}{p} = \frac{5}{3} x - \frac{3-5}{3} = \frac{5}{3} x - \frac{4}{3} \). After the right boundary is reached, the new line is begun 1 unit to the left, so \( y = \frac{q}{p} (x + 1) - \frac{(m+n-1)p-q}{p} = \frac{q}{p} x - \frac{(m+n-1)p-2q}{p} = \frac{5}{3} x - \frac{1}{3} \). Again, the two equations involved have numerators which are equivalent, modulo \( q \); in fact, these two numerators are equivalent to the original pattern’s numerator as well, modulo \( q \); i.e.: \((m+n-1)p-q \equiv (m+n-1)p \pmod{q}\) and \((m+n-1)p-2q \equiv (m+n-1)p \pmod{q}\). For the \( \{3,5\} \) knot, these three numerators are 9, 4, and \(-1\), which are all equivalent, modulo 5.

In fact, because the first line’s constant is 0, then, will either have \( 1 = \frac{2}{p} \) subtracted (when an \( x \)-axial revolution has occurred), or \( \frac{2}{p} \) subtracted (for \( y \)-axial revolutions), the constant will always be a ratio of an integer over \( p \); i.e.: the line beginning the \( n \)-th \( x \)-axial revolution, after \( m \) \( y \)-axial revolutions have occurred, is \( y = \frac{q}{p} x - \frac{(n-1)p-(m-1)q}{p} \).

Thus, for the \( n \)-th \( x \)-axial revolution, this integral numerator will always be \( (n-1)p \), or equivalent to \( (n-1)p \), modulo \( q \); this is because subtracting an integral multiple of \( q \) from an integer generates a number in the same equivalence class.

These constants are the lines’ \( y \)-intercepts, and this torus’ left boundary is the \( y \)-axis. This means that, when the constant is positive, the line enters the torus from the left, and only from \( y \)-values which are an integer over \( p \). There are, at most, \( p \) many of these points \( \left( \frac{0}{p}, \ldots, \frac{p-1}{p} \right); \frac{p}{p} = 1 \) is the \( y \)-intercept of a tangent line).

Because these lines have a positive slope, they will enter the torus from the left, or from the bottom of the torus. The bottom of the torus is the line \( y = 0 \); thus, the \( x \)-value of the entering point is the solution to \( y = \frac{q}{p} x - \frac{(n-1)p-(m-1)q}{p} = 0 \). Thus, \( x = \frac{(n-1)p-(m-1)q}{q} \). The numerator is the same as the constant’s, so it is an integer equivalent to \( (n-1)p \), modulo \( q \). Because \( n \) is the number of the current \( x \)-axial revolution, the solution to \( y = 0 \) is also the starting point of said revolution. There are \( q \) such points \( \left( \frac{0}{q}, \frac{1}{q}, \ldots, \frac{q-1}{q} \right); \) the line through \( \frac{2}{q} \) is tangent to this torus). Because \( p \) and
q are co-prime, the multiples of p span the equivalence classes of q, and do no repeat until each class is represented. E.g.: for \{3, 5\}, the multiples of 3, \{0, 3, 6, 9, 12\}, each represent a different equivalence class, modulo 5: \{0 = 0, 3 = 3, 6 = 1, 9 = 4, 12 = 2\}. As in the manner in this example, the equivalence classes of q can be represented by the multiples of p, but \(np\) is not necessarily equal to \(n\).

In short, this means is that (1) each x-revolution will begin at a unique point type of point (for the n-th revolution, the numerator of the x-value must be equivalent to \((n - 1)p\), modulo q, and the denominator is q); and (2) that there are q-many such points in the lower boundary, which is precisely how many one would hope for, since the construction calls for q-many revolutions about the x-axis.

The initial point for the n-th x-axial revolution has been described, but what about the final point? For said revolution, numerator of the constant (or constants) describing the line (or lines) will be equivalent to \((n - 1)p\), modulo q. The final point is at the upper boundary, which is \(y = 1\); so the x value of this point is the solution to \(y = \frac{q}{p}x - \frac{a}{p} = 1\), where \(a \equiv (n - 1)p \pmod q\). Then \(x = \frac{a + p}{q}\). Because \(a \equiv (n - 1)p \pmod q\), \(a + p \equiv np \pmod q\).

Therefore, for the n-th x-axial revolution, the x-values are both rational numbers, with a denominator of q. The initial point’s numerator is equivalent to \((n - 1)p\), modulo q, and the final point’s numerator is equivalent to np, modulo q. As with the lower boundary, the upper boundary has precisely q-many such points: \(\frac{1}{q}, \frac{3}{q}, \ldots, \frac{q}{q} = 1\).

Let \(A := \{-p - 1, -(p - 2), \ldots, q - 2, q - 1\}\), which is a subset of the integers. Let \(L := \{y = \frac{q}{p}x - \frac{a}{p} : a \in A\}\), a set of parallel lines in the universal cover. L is the set of all lines of slope \(\frac{q}{p}\), with y-intercepts which are ratios of an integer over p, such that the line passes through the torus being considered. In these equations, if \(a\) were \(-p\) or q, the line would be tangential to the torus, so they are not of interest.
It was just deduced that, $L_{(p,q)}$, the lines which represent the \{p, q\} knot in the universal cover, are precisely of this form. Therefore, $L_{(p,q)}$ is a subset of $L$ (written: $L_{(p,q)} \subseteq L$). If $L$ can be shown to be a subset of $L_{(p,q)}$, then the sets are equal.

Let $y = \frac{q}{p}x - \frac{a}{p}$ be a line in $L$. This $a$ is in one of the equivalence classes of $q$, which are \{0, 1, \ldots, q-1\}. As was stated above, an equivalent representation of these equivalence classes is \{0p, 1p, 2p, \ldots, (q-1)p\}. Assume $a \equiv (n - 1)p \pmod{q}$, which implies that the only $x$-axial revolution it can be a part of is the $n$-th.

If this line enters the torus from the lower boundary, then it begins the $n$-th $x$-axial revolution. Because there is no other point on the lower boundary with a numerator equivalent to $(n - 1)p$, modulo $q$, this is the only line which can begin this revolution, so it must be in $L_{(p,q)}$.

If this line enters the torus from the left boundary, then it intercepts the upper boundary, $y = 1$, at $x = \frac{a+np}{q}$. Because it was assumed that $a \equiv (n - 1)p \pmod{q}$, $a + p \equiv np \pmod{q}$. Because there is no other rational point on the upper boundary with a denominator of $q$ and a numerator equivalent to $np$, modulo $q$, this is the only line which can complete the revolution, so it must be in $L_{(p,q)}$.

Thus, $L \subseteq L_{(p,q)}$, which means that $L$ and $L_{(p,q)}$ are equal.

![Figure 3.11: As described][10]
The only way that this series of lines describes a simple, closed curve is if it intersects with itself at the beginning point, and only at the beginning point. With the way these lines have been constructed, the final line has an $a$ value equivalent to $(q - 1)p$, modulo $q$ (before the equivalence classes repeat, at $\overline{qq}$). This final line intercepts the upper boundary, $y = 1$, at $y = \frac{2}{p}x - \frac{a}{p} = 1$, so $x = \frac{a + p}{q}$. It is known that $a \equiv (q - 1)p \pmod{q}$, so $a + p \equiv qp \pmod{q}$, which is equivalent to 0, modulo $q$. This means that the numerator of the $x$-value of this point is equivalent to 0. Because the denominator is $q$, the $x$-value, itself, is equivalent to 0. The $y$ value is 1, which is equivalent to 0, as well. Thus, this point is equivalent to $(0, 0)$ in the universal cover, which is the beginning point.

This curve has revolved about the $x$-axis $q$ many times before self intersection. This curve does not self-intersect because it is represented, in the universal cover, by parallel lines, which never intersect (unless they are the same line). Additionally, as these lines pass through other tori, they will not intersect or disrupt the $\{p, q\}$ knots within them, but will form a part of said $\{p, q\}$ knot. This is because every $\{p, q\}$ segment has the same slope, so to have a common point means to be the same, exact line.

The last question is whether the knot has revolved about the $y$-axis $p$ many times. It was already deduced that there are $p$ many lines begun on the left boundary, each of which begins a $y$-axial revolution. The knot terminates at the point $(1, 1)$, which is equivalent to $(0, 0)$, which serves, simultaneously, as an end to an $x$-axial revolution (because $y = 1$) and a $y$-axial revolution (because $x = 1$). Thus, precisely $p$ many revolutions have occurred about the $y$ axis, and a $\{p, q\}$ knot has been constructed.

During the construction, it was calculated that there are $p$-many, equally-spaced intersections of the $\{p, q\}$ knot with the left boundary (and right boundary, since the two are equivalent), and $q$-many, equally-spaced intersections of the knot with the
lower boundary (and the equivalent upper boundary). These are \( p+q-1 \) points—(0,0) is on both boundaries—on these two boundaries, which is \( 2(p+q-1) \) points in total.

This means that, for a quicker construction, one may take a unit square, mark off the corners, and draw out the \( p-1 \) middle points per left and right boundary, and \( q-1 \) middle points per upper and lower boundary, and then connect them in the only logical way: the two points closest (0,1), then the next two points, and so on. *I.e.*: connect \( (0, \frac{p-1}{p}) \) to \( \left( \frac{1}{q}, 1 \right) \), then \( (0, \frac{p-2}{p}) \) to \( \left( \frac{2}{q}, 1 \right) \), and so on.

One restriction here is that \( p < q \), so what happens when the opposite is true? In the gemini trefoils section, a graphic showed how a \{2,3\} knot could be continuously deformed into a \{3,2\} knot. This deformation—an ambient isotopy—swaps the number of revolutions about each toroidal axis. In fact, the two axes have switched places. In the universal cover, this is tantamount to swapping the \( x- \) and \( y- \)axes, which is the reflection of the plane about the line \( y = x \). Thus, the same construction method works, but the argument is slightly different.

The other restriction is that both \( p \) and \( q \) are positive. After the construction of a \( \{p,q\} \) knot (\( p \) and \( q \) are still assumed to be positive), make one of them negative. If the knot is begun at (0,1), rather than at (1,1), the same boundary points are used, but the lines now run down as they run right.

Only one, complete torus has been constructed. What about the torus just above it, bound by \( y = 1 \) and \( y = 2 \)? All of the same lines can be used, just shifted up one unit. *I.e.*: the family of lines is now \( \left\{ y = \frac{2}{p} x - \frac{a}{p} : a \in A - p \right\} \). The notation \( A - p \) means the set \( \{a - p : a \in A\} = \{-(p-1) - p, -(p-2) - p, \ldots, q - 2 - p, q - 1 - p\} \).

Some of these lines are in the original torus, but since their \( y \)-intercepts are integers over \( p \), they overlap with the original lines; *i.e.*: they don’t fall somewhere in between and interfere with the first construction.

For the torus bound by \( x = 0, x = 1, y = v, \) and \( y = v + 1 \), the family of lines
is \( \{ y = \frac{2}{p}x - \frac{a}{p} : a \in A - vp \} \). Thus, for the tori which are only shifted upward (or downward) from the original, the \( y \)-intercepts are still integers over \( p \).

What if the torus were only shifted horizontally, instead? For the torus bound by \( x = 1 \) and \( x = 2 \), the family of lines is shifted one unit to the right, which is \( \{ y = \frac{2}{p}x - \frac{a}{p} : a \in A + q \} \). Again, the \( y \)-intercepts are integers over \( p \), and the overlap of lines which are in the first torus and this one is only of equality; \( i.e.: \) no line from the first torus interferes with the second torus’ knot, and vice versa.

For the torus bound by \( x = h \), \( x = h + 1 \), \( y = 0 \), and \( y = 1 \), the family of equations is \( \{ y = \frac{2}{p}x - \frac{a}{p} : a \in A +hq \} \). Each value of \( a \) is still an integer.

The last step is to consider a torus which is simultaneously shifted \( v \) units up, and \( h \) units to the right. This means, precisely, to shift the lines of the first torus’ \( \{ p, q \} \) knot \( v \) units up and \( h \) units to the right. The lines, then, are \( \{ y = \frac{2}{p}x - \frac{a}{p} : a \in A -vp +hq \} \). Each \( a \) is still an integer, which means that these lines don’t interfere with any other torus.

With this information, it is clear that, for the knot, \( \{ p, q \} \), for any co-prime \( p \) and \( q \), positive or negative, the universal cover consists of the lines \( \{ y = \frac{2}{p}x - \frac{a}{p} : a \in Z \} \), and Lemma 6 is proved.

Another way to follow a knot is to follow one, single line from any point, until it reaches an equivalent point in the universal cover. The easiest such line to consider is, when \( pq > 0 \), \( y = \frac{2}{p}x \), from \((0, 0)\), to \((p, q)\). When \( pq < 0 \), since the slope is negative, the ideal line to follow is \( y = \frac{2}{p}x + q \), from \((0, q)\) to \((p, 0)\).

**Lemma 7** In the graph which is embedded to form only a gemini \( k\{ p, q \} \) pair, the only vertex degree is 4. As a result, the average vertex degree, \( z \), is 4.

For each embedding, two knots, which are ambient isotopic to the other’s mirror image, are embedded together. In the universal cover, this means that one will consist
of parallel lines which have a positive slope, and the other of lines with negative slope. The points of intersection, then, will always be of two lines which represent different knots, and only two lines (a third line would mean that one of the knots is self-intersecting, which was shown to never be the case).

![Figure 3.12: The universal cover of \(\{3, 5\} \otimes \{3, -5\}\) [10].](image)

These intersections generate the vertices of the graph, and each vertex is of degree 4, which is one of the two points which was sought to be proven. The second bit of information is the metric edge-length.

**Lemma 8** For a \(k\{p, q\} \otimes k\{p, -q\}\) embedding, in the universal cover, every edge can be constructed to be of the same metric length.

For the embedding \(k\{p, q\} \otimes k\{p, -q\} = \{3, 5\} \otimes \{3, -5\}\), the knot \(\{3, 5\}\) is represented by the line segment from \((0,0)\) to \((3,5)\), while the \(\{3, -5\}\) knot is represented by the line segment from the point \((0,5)\) to \((3,0)\).

What is examined is the number of times the second knot’s representative line segment is divided by the complete array of \(\{3, 5\}\) knots. This array is evenly spaced, and there are \(2 \times k \times p \times q = 2 \times 1 \times 3 \times 5 = 30\) many lines. Thus, the Euclidean metric maybe be used to find the length of the entire \(\{p, -q\} = \{3, -5\}\) knot, and every edge-length is equal to \(1/(2kpq)\)-th of that value.
This is a symmetric embedding; \( i.e. \), every edge-length is the same, for either link/knot. Figure 3.13 has an entire \( \{3, -5\} \) knot evenly divided by the lines which represent the \( \{3, 5\} \) knot.

![Figure 3.13: As described [10].](image)

From the universal cover, it can be seen that, as is the case with the gemini trefoils, the average degree, \( z \), is 4. This means that the calculations for the gemini trefoils still hold for the average face size: specifically, \( n \) must be less than 4. Again, for this to hold true of one of these embeddings, at least one cycle of less than 4 edges must be exist.

From the universal cover, it can also be seen that the null-homotopic cycles are all composed of at least four edges. The non-null-homotopic cycles, which go to translationally distinct vertices, can be measured by using the Euclidean length of
the edges, thus: Should a cycle’s endpoints be connected by the vector \((\alpha, \beta)\), it must take \(M\) many steps in the \((p, q)\) direction, and \(N\) many steps in the \((p, -q)\) direction, because these are the only directions the edges move in; \(i.e.\):

\[
(\alpha, \beta) = M \left( \frac{(p, q)}{2kpq} \right) + N \left( \frac{(p, -q)}{2kpq} \right)
\]

To explain the division of the vectors by \(2kpq\): The steps which comprise \(M\) are in the direction of the vector \((p, q)\), and are \(1/(2kpq)\)-th of the total length of said vector; a similar statement can be said of the steps of \(N\).

\[
= \left( \frac{M + N}{2kq}, \frac{M - N}{2kp} \right)
\]

\[
2k(|\alpha q|, |\beta p|) = (|M + N|, |M - N|)
\]

By using the triangle equality, one has that:

\[
\begin{align*}
|M| + |N| & \geq |M + N| = 2k|\alpha q| \\
|M| + |N| & \geq |M - N| = 2k|\beta p|
\end{align*}
\]

Thus:

\[
|M| + |N| \geq 2k \max(|\alpha q|, |\beta p|)
\]

The vector \((\alpha, \beta)\) cannot be \((0, 0)\) (it must go to distinct vertices), and \(\alpha\) and \(\beta\) are integers (the two vertices connected by this vector are, in the universal cover, equivalent). Thus, at least one of \(|\alpha q|\) and \(|\beta p|\) is 1 or greater. The variable \(k\) can be examined in two cases: it is either greater than 1, or exactly 1.

It is reiterated now that, in order for one of these embeddings to be planar, the average face size, \(n\), must be less than 4. For that to hold true, a cycle of less than four edges must exist. In the following calculations, a cycle’s length, in edges, is
represented by $|M| + |N|$, and the contradiction comes when $|M| + |N|$ is shown always to be $4$ or greater.

From the above facts, one can see that, should $k$ be greater than $1$, $2k$ is at least $4$. Again, at least one of $|\alpha q|$ and $|\beta p|$ is $1$ or greater. $|M| + |N|$, which is the number of edges in the cycle, is at least four. Thus, there is no cycle composed of less than $4$ edges, when $k > 1$.

The second case is when $k$ is exactly $1$. In this event, $p$ and $q$ are at least $2$; otherwise, the embedding is the Hopf link (which is examined last). This is enough information to imply that $|M| + |N| \geq 4$. Again, there is no cycle less than $4$ edges in length.

As with the gemini trefoils, Euler’s formula for planar graphs does not hold. Any embedding of the form $k\{p, q\} \otimes k\{p, -q\}$ is non-planar; thus, non-polyhedral.

By Kuratowski’s theorem, no embedding containing any such embedding as a sub-embedding may be of a planar graph.

### 3.2.2 $k\{p, q\} \otimes k\{-q, p\}$

The approach for this case is very similar to the first. However, the vectors, $(p, q)$ and $(p, -q)$, could be arranged to be the diagonals of a rectangle, which made the area of examination very intuitive (namely, said rectangle). For this case, a broader view must be taken. However, the work already done for the first case proves to be extremely useful.

Again, let $k\{p, q\} = 1\{3, 5\}$. As with the first case, the aim is to segment the blue line, which represents the $k\{-q, p\}$ knot, to derive the Euclidean edge-lengths. The construction for the $k\{p, q\}$ knot remains the same; a line segment representing the $k\{-q, p\}$ knot replaces the line segment which represented the $k\{p, -q\}$ knot.

The vector representing this knot is $(-q, p) = (-5, 3)$, and is begun at $(0, p) =$
Figure 3.14: As described [10].

(0, 3) so that it begins on the y-axis and ends on the x-axis, for ease in observation. To evenly divide this line, $q = 5$ tori must be examined along the x-axis and $p = 3$ many along the y-axis. However, rather than construct all of the lines required for this (as was done the first time), one may simply calculate them.

In the lower-left, a single unit-square is outlined. It contains $5 = kq$ many lines. To calculate this number in general, one may divide the number of lines from the bottom in the first construction, $kpq$, by the number of tori at the bottom, $p$, which is $\frac{kpq}{p} = kq$ many lines. This number, $kq$, can then be multiplied by the number of tori which are now at the bottom, $q$, and the product is $(kq)(q) = kq^2$. Thus, $kq^2$ many lines segment the blue line, from the bottom.

The lines coming from the bottom have been accounted for. From the left, the number of lines may again be observed, $3 = kp$; or calculated. In the original construction, there are $kpq$ lines coming from the left, and $q$ many tori, so $\frac{kpq}{q} = kp$ many lines per torus. In this construction, there are $p$ many tori on the left, so $(kp)(p) = kp^2$ many lines coming from the left.

In total, the blue line, which represents the knot $k\{−q,p\}$, is segmented evenly $kq^2 + kp^2 = k(p^2 + q^2)$ many times. Thus, every edge (blue or red, as the embedding
is symmetric), is \(1/[k(p^2 + q^2)]\)-th the length of the vector representing its knot.

There are no null-homotopic cycles of less than 4 edges. Again, the non-null-homotopic cycles lengths can be calculated using the Euclidean metric:

\[
M \frac{(p, q)}{k(p^2 + q^2)} + N \frac{(-q, p)}{k(p^2 + q^2)} = (\alpha, \beta)
\]

This can be converted into a matrix representation:

\[
\frac{1}{k(p^2 + q^2)} \begin{pmatrix} p & -q \\ q & p \end{pmatrix} \begin{pmatrix} M \\ N \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}
\]

Then rearranged to:

\[
\begin{pmatrix} M \\ N \end{pmatrix} = k(p^2 + q^2) \begin{pmatrix} \frac{p}{\sqrt{p^2 + q^2}} & \frac{q}{\sqrt{p^2 + q^2}} \\ \frac{-q}{\sqrt{p^2 + q^2}} & \frac{p}{\sqrt{p^2 + q^2}} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}
\]

If a matrix, \(A\), exists such that it is square and it’s transposition equals its inverse, \(A^T = A^{-1}\), then it is called a rotation matrix. This is desirable because rotation matrices do not affect vector lengths; thus, they are omissible in such calculations.

To turn this square matrix into a rotation, one may factor out \(\frac{1}{\sqrt{p^2 + q^2}}\):

\[
\begin{pmatrix} M \\ N \end{pmatrix} = k\sqrt{p^2 + q^2} \begin{pmatrix} \frac{p}{\sqrt{p^2 + q^2}} & \frac{q}{\sqrt{p^2 + q^2}} \\ \frac{-q}{\sqrt{p^2 + q^2}} & \frac{p}{\sqrt{p^2 + q^2}} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}
\]
Thus, when the lengths of these two vectors are taken:

\[
\| \begin{pmatrix} M \\ N \end{pmatrix} \| = k \sqrt{p^2 + q^2} \begin{pmatrix} \frac{p}{\sqrt{p^2 + q^2}} & \frac{q}{\sqrt{p^2 + q^2}} \\ \frac{-q}{\sqrt{p^2 + q^2}} & \frac{p}{\sqrt{p^2 + q^2}} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}
\]

The column vectors are turned back into row vectors; the scalar is taken out; and the rotation matrix may be omitted:

\[
||(M, N)|| = \left| k \sqrt{p^2 + q^2} \right| ||(\alpha, \beta)||
\]

The actual length of the vector \((M, N)\) isn’t of importance, but, rather, the value of \(|M| + |N|\), the cycle length. Therefore, the left-hand side of this equation may be analyzed:

\[
||(M, N)|| = \sqrt{M^2 + N^2} = \sqrt{|M|^2 + |N|^2}
\]

2\(|M||N|\), a definitely positive term, may be added inside the square root to yield:

\[
\sqrt{|M|^2 + |N|^2} \leq \sqrt{|M|^2 + 2|M||N| + |N|^2} = \sqrt{(|M| + |N|)^2} = |M| + |N|
\]

The result is that:

\[
||(M, N)|| \leq |M| + |N|
\]

This can be applied to the main calculation, and one has that:

\[
|M| + |N| \geq ||(M, N)|| = k \sqrt{p^2 + q^2} ||(\alpha, \beta)||
\]
The restrictions on \((\alpha, \beta)\) are that it can’t equal \((0, 0)\) (this would make the cycle null-homotopic), and that \(\alpha\) and \(\beta\) must be integers (the vector must connect equivalent points in the universal cover). Thus, the length of this vector is at least 1—i.e., \(||(\alpha, \beta)|| \geq 1||\) so, to simplify analysis, \(||(\alpha, \beta)||\) can be omitted, and the following holds:

\[
|M| + |N| \geq k\sqrt{p^2 + q^2}
\]

Again, for planarity to hold, the average face size, \(n\), must be less than 4. This means that a cycle of less than 4 edges must exist. The fact that no such cycle exists (i.e., \(|M| + |N|\) is strictly greater than 3) is the contradiction to be proven. Therefore, the right-hand side can be evaluated to show that its minimum value is greater than 3. Again, \(k\) can be analyzed in two parts: either \(k > 1\) or \(k = 1\).

If \(k\) is assumed to be greater than 1, then the smallest possible \(k\) is 2, and the smallest \((k, p, q)\) triple is \((2, 1, 2)\) (along with other similar triples, such as \((2, 2, 1)\)). Any such triple in the above inequality would yield that \(|M| + |N| \geq 2\sqrt{5} \approx 4.47\). Thus, any embedding with \(k \geq 2\) has no cycle of less than 4 edges. It follows that all such embeddings are non-planar; thus, not polyhedral.

If \(k\) is assumed to be 1, then, aside from gemini trefoils (already proven non-polyhedral), the \((k, p, q)\) triple which yields the smallest value in \(k\sqrt{p^2 + q^2}\) is \((1, 3, 4)\); the result is that \(|M| + |N| \geq 1\sqrt{25} = 5\). Thus, these \(k = 1\) embeddings are also non-planar, which implies non-polyhedral.

With this, it is proven that \(n\) cannot be less than 4. As a result, all embeddings of type \(k\{p, q\} \otimes k\{-q, p\}\) are non-planar; thus, not polyhedral. Per Kuratowski’s Theorem, it follows that no planar (specifically, polyhedral) embedding can contain one of these embeddings as a sub-embedding.
3.3 Hopf Links

The final case is that of toroidal Hopf links. To reiterate: polyhedral graphs are simple, 3-connected, and planar.

Again, simplicity means that there is, at most, one edge between any two vertices; and that no edge may go from a vertex to itself. To meet the criteria for simplicity, these Hopf links must be composed of at least three vertices, apiece.

Again, $k$-connectedness means that no less than $k$ many vertices must be removed, along with the corresponding edges, to make the graph no longer connected. To meet the criteria for 3-connectedness, these links must have at least three disjoint edges going from one link to the other, which will make the Hopf link take the form of a twisted ladder (the link would be the rails, and the edges just described would be the rungs).

However, J. Simon proved that twisted ladders with 3 or more rungs are chiral [15]. The embedding can be made achiral in one of two ways: (i) Its enantiomer can be embedded with it on the torus, or (ii) a rung (or some rungs) can be added to the already-existing rails so that the two enantiomers share the same two rails.

![Three-runged twisted ladder](image)

Figure 3.15: The three-runged twisted ladder, which is chiral [15].

The first case, of two separate enantiomers, would yield the embedding and universal cover in Figure 3.16.

This universal cover shows that the average degree, $z$, would be 4; again, the
average face size, \( n \), would have to be less than 4. It is clear that no cycle of less than 4 edges exists, so this embedding cannot be of a planar graph. As a result that graph could not be polyhedral, either.

The second case, in which the rails are shared, requires the addition of at least one rung. To prove that this would result in a non-planar graph, one may construct a planar embedding of the graph, and find a contradiction there.

![Figure 3.16: Two separate Hopf links, with the universal cover](image)

Above, on the left, the first enantiomer is embedded in the plane. The rails’ vertices are labeled, and their order gives the orientation (clockwise, for both rails). Because the rails in the first enantiomer have the same orientation, their orientations must differ in the second enantiomer.

To this end, the outer rail keeps the same orientation, but the inner rail is changed.
to counterclockwise; the arrangement of the vertices must coincide with these orientations. For maximum flexibility, six new vertices are used (hence: $a', 1'$, etc.), though not all may be necessary. The contradiction comes when one tries to draw the rungs—there is no way to do so without creating a crossing. This edge-crossing means that the underlying graph is non-planar; thus, not polyhedral.
Chapter 4

Additional Research

The inspiration for this thesis topic came from the paper All toroidal embeddings of polyhedral graphs in 3-space are chiral, by T. Castle et al. Unfortunately, the proof within this paper left out details which the inexperienced would have benefitted from. One of the aims of this thesis work was to delve into and explore those details.

Although the paper deals with the toroidal knots and graphs—topological objects—they already had in mind a real-world use of the information. To repeat: whether a molecule is chiral or not is useful information, but there is no direct, general method for determining whether or not one is. Should a molecule fit this mold, it could immediately be determined to be chiral.

Another aim of this thesis work became to find such molecular examples. This proved to be a difficult and, ultimately, fruitless undertaking.

KnotPlot and Avogadro were two of the software applications used to explore molecules. However, in order for atoms to bend into these sorts of complex forms, they need to be quite large. Although Avogadro can display these large molecules, it cannot manipulate them or otherwise help to determine if there is a knot within.

KnotPlot has manipulative functionality, but could not accept molecules with
enough atoms to contort into topologically interesting shapes.

Another effort was to use the school’s academic search engine to scour for toroidal molecules, which gave some results. However, for a molecule to even be considered, it must be 3-connected (to be polyhedral), or have a 3-connected subgraph, but one was not found.

Perhaps an interesting route would be to use theoretical molecular energy calculating software to compare the energies of similar toroidal molecules, such that the only difference in a pair would be the presence of a knot. Additionally, these same molecules could have the same structure(s) added to see which would stay more stable—the one with or without the knot.
Bibliography


