KNOT THEORY:

HISTORY AND APPLICATIONS WITH A CONNECTION TO GRAPH THEORY

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Mitchel Todd Keller

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ABSTRACT

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This honors thesis introduces some fundamental ideas of knot theory in a way that is accessible to nonmathematicians. It summarizes some of the major historical developments in the mathematical theory of knots, beginning with Thomson and Tait and ending with some of the important results of the late 20^{th} century. A few important examples of ways in which knot theory can be used to model real-world phenomena are discussed, including the importance of topology to the pharmaceutical industry. It concludes by using chain complexes of based, finitely-generated Z-modules to study the Laplacians of signed plane graphs and to extend a theorem of Lien and Watkins [14] regarding the Goeritz equivalence of the signed Laplacians of a signed plane graph and its dual by showing that it is possible to use only (±1)diagonal forms instead of the (0, ±1)-diagonal forms used by Lien and Watkins.

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CHAPTER 1. INTRODUCTION

The first thing that most people think of upon hearing the word "knot" is probably a troublesome tangle in a piece of string or perhaps the contortion of shoelaces that prevents shoes from falling off. In mathematics, such messes are not knots, however, since they have loose ends floating around. If we take the two loose ends and glue them together, then we have what mathematicians will agree to call a knot. Of course we really cannot define a knot as "a tangled piece of string with its ends glued together" and hope to do any serious mathematics using this definition. First of all, a piece of string has thickness and exists in the real world, a place mathematicians are notorious for abhorring, so we must introduce some abstraction here. (Really, we must; otherwise mathematicians in the United States might start arguing with those in France over how thick the string should be and if the measurements should be in imperial units or metric units.)

We do not want to be *too* abstract here, since the nonmathematical reader should be able to read at least Chapters 2 and 3 without suffering a severe migraine. However, there is some mathematical jargon that will be unavoidable in presenting the concrete definition of "knot" that we desire. First of all, we need to think about the space in which knots live. Certainly they don't live on a straight line, since there's the whole issue of the glued-together ends. An important aspect of knots is, for lack of a better word, their knottedness; that is, there are places where the string goes over or under itself. Thus, we cannot work with knots (other than a knot that's not really knotted) that lie in the Cartesian plane familiar to anyone who has taken a high school algebra class. However, a three-dimensional space akin to the one in which we live, which mathematicians denote by \mathbb{R}^3 , will work just fine for studying knots. (Now the topologists scream and demand that we use S^3 instead of \mathbb{R}^3 , but today we will just ignore them.)

Fine, so we know where knots live, but that has not gotten us any closer to having a definition of a knot. We have already mentioned the problem of thickness and how allowing it could escalate into World War III, so perhaps it is best to begin by freeing our knots of thickness. One of the first things that we learned in geometry was that lines have no thickness, so it seems natural to put this property to use. Since we need to have endpoints to glue together, we might try to bring a line segment such as [0, 1] into play. (There we go with notation again. What is [0, 1]? It consists of all the points lying between 0 and 1, including those two numbers. By all the points we really mean all the points between them $-1/2, 1/\sqrt{2}, 1/\pi$, etc.) Perhaps a knot could be a continuous mapping f of [0, 1] into \mathbb{R}^3 such that f(0) = f(1) and if f(x) = f(y), but $x \neq y$, then we have that one of x and y is 0 and the other is 1. This seems plausible; it essentially gives us a way to trace out the knot in three-dimensional space and does not introduce any thickness. There is a problem with this idea, however, since it would allow us to have a "knot" with infinitely many twisted portions in it, which fails to fit in with our intuitive idea of a knot as being a piece of string with its ends glued together. If we sacrifice this intuitive idea in forming our abstraction, we make it far more difficult, if not impossible, to relate our abstract model to the real world. Therefore, we cannot use this definition. Instead, we will use the definition given in [15].

We first must explain the notion of a *closed polygonal curve* in \mathbb{R}^3 . Suppose that p and q are two different points in \mathbb{R}^3 . Then let [p, q] denote the honest-to-goodness line segment between p and q. Now suppose that we have an ordered list of distinct points (p_1, p_2, \ldots, p_n) from \mathbb{R}^3 . Then the union of all of the line segments $[p_1, p_2]$, $[p_2, p_3], \ldots, [p_{n-1}, p_n], [p_n, p_1]$ is what we will call a *closed polygonal curve*. (The word *closed* is used to indicate that we start at p_1 and come back to p_1 by including $[p_n, p_1]$.) Perhaps an example would be in order. Figure 1 shows two closed polygonal



Figure 1. Closed polygonal curves (p, q, r, s) and (p, r, q, s)

curves based on the same set of four points but in different orders. This illustrates the fact that a single set of points can define multiple closed polygonal curves. We might now rush to define a knot as a closed polygonal curve in \mathbb{R}^3 , but Figure 1 also points out a problem with using such a definition. In the curve (p, r, q, s), we have the line segments [p, r] and [q, s] intersecting at a point other than our four distinguished points. This would not fit within our abstraction of our intuitive knot, since a piece of string cannot pass through itself. Thus, we will require a special type of closed polygonal curve called a *simple* closed polygonal curve. This is a closed polygonal curve in which each line segment intersects exactly two other line segments and does so only at their endpoints. With this in hand, we are finally ready to give a definition of a knot.

Definition 1.1. A *knot* is a simple closed polygonal curve in \mathbb{R}^3 .

Seems like we went through a lot of effort to come up with this definition, but having done things properly here has given us a taste of the worrying that we must do (and we have omitted a great deal of the optional worrying that the biggest worriers will do) when using mathematics to model a real-world entity. If we fail to impose enough restrictions on the mathematical model, we can find ourselves dealing with a model that admits objects that cannot exist in the real world. Now we can put all of this worrying behind us and remain content that we have a solid idea of what a knot



Figure 2. Trefoil and figure-8 knots

is. From now on, we will generally not draw our knots as simple closed polygonal curves, but rather as smooth curves such as can be seen in Figure 2, where we show the trefoil knot and the figure-8 knot. (This does not violate our definition, as we can use many very small straight line segments to produce a drawing that appears smooth.) In our figures, we will use a break in the drawing to indicate the portion of the knot that is passing under another portion of the knot. Such a representation of a knot will be called a projection or diagram.

A few additional bits of knot theory jargon will be useful for reading the remainder of this thesis. First, a *link* is a generalization of a knot in which there may be multiple distinct simple closed polygonal curves, referred to as components, that link around each other. A knot then becomes a link with one component, so sometimes we will usually use "link" in a sense that includes knots. A knot is said to be *alternating* if it has a projection in which the crossings alternate between over and under as the knot is traced out. (The trefoil and figure-8 knots are both alternating, but the knot pictured in Figure 3 is not.) Finally, just as with the integers, we have an idea of a *prime* knot. Intuitively a knot is prime if it does not consist of two knots tied in the same piece of string. Figure 3 shows a composite knot (*i.e.*, one that is not prime) consisting of two trefoils connected (or "added") together.

From here we will proceed to explore the historical development of the mathematical theory of knots. Since much of the early history of knot theory was motivated



Figure 3. A composite knot

by applications it will be difficult to avoid any reference to applications of knot theory in this process. However, discussion of modern applications of knot theory will be reserved for Chapter 3, which will also include a look at ways in which graph theory can be used to study knots. We will conclude with some original research conducted by the author.

CHAPTER 2. A BRIEF HISTORY OF KNOT THEORY

2.1. Early work

Human beings have long been interested in the utility of knots. Ancient peoples used knots in ropes as a way to mark the passage of time and keep records, and every good boy scout knows the appropriate knot to tie in any given situation. One might expect that the mathematical theory of knots dates back into antiquity as well, but knots are a rather new arrival on the mathematical scene. The origins of a mathematical theory of knots can be traced back to the German mathematician Carl Friedrich Gauß, who tried to classify closed plane curves with a finite number of self-intersections, which he sometimes called "Tractfiguren". (Think of them like the knot projections in Figure 2, except with letters labeling the crossings creating a crossing sequence in place of the broken lines indicating which strand passes over the other.) According to Epple [7], Gauß' reason for studying the knot-projectionlike Tractfiguren remains unclear. However, we do know that Gauß worked on his Tractfiguren in 1825 and 1844, but only after his death were his results published. He worked out a set of rules for what crossing sequences were admissible for Tractfiguren with at most four crossings, but he soon discovered that his rules did not hold for Tractfiguren with five or more crossings and was never able to write down such a list.

While Gauß may not have taken a long-term active interest in studying what we now recognize as knots, his student Johann Benedikt Listing did. Listing's 1847 *Vorstudien zur Topologie*, in which he first coined the term "topology," included a discussion of mathematical knots and their classification. Listing was interested in developing an algebraic calculus of knot diagrams so that it could easily be determined when two diagrams represented the same knot (for an appropriate definition of "same"). However, the way he couched the problem prevented him from proving any useful results in knot theory, so Listing will remain a minor character in our tale here. (We should note that Listing is anything but a minor character in the overall history of topology, however.)

The first work on knot theory outside of Germany began in Scotland in the late 1860s as the physicist William Thomson (later Lord Kelvin) began looking for a suitable atomic theory. In 1867, Thomson, who was inspired by Hermann von Helmholtz's work on vortex motion and a demonstration by Peter Guthrie Tait exhibiting the properties of vortices using smoke rings, presented a paper to the Royal Society of Edinburgh proposing that atoms were knotted vortices. He recognized that the particular shape of a vortex was not as important as the underlying topological structure, and felt that an understanding of such vortices would lead to a complete understanding of matter. Despite his important role in the development of Thomson's idea, Tait initially felt that Thomson was on the wrong track in trying to apply vortex motion to develop an atomic theory. Rather, Tait felt that vortex motion's principal application would be in the theory of electromagnetism. Despite Tait's initial disinterest, Thomson continued thinking about atoms as vortices, sparking the interest of James Clerk Maxwell.

Maxwell had been doing work in electromagnetism for some time, and was primarily interested in how the theory of knots could be applied in his work. However, he was also open to the idea that knotted vortices could be the fundamental building blocks of matter. He wrote to Tait and Thomson discussing some of his ideas and discoveries. They were very interested in his ideas, particularly his novel use of equations to represent the knots as three-dimensional curves. In that letter, he noted that the trefoil was the simplest knot that was truly knotted that consisted of a single strand and gave equations for the curve. He went on to recognize that a parameter in his equations determined if the trefoil thus produced was right-handed or left-handed (an idea which will be explained in the next chapter) and claimed (without proof) that there was no way to change a right-handed trefoil into a left-handed one or vice versa.

In the fall of 1868, Maxwell began to undertake a serious study of topology. It appears that at this point he had not yet been exposed to Listing's *Vorstudien zur Topologie*, as he proposed some of the same questions regarding knots and links as Listing had [6, p. 333]. Specifically, Maxwell wanted to know when two projections of a link represented the same link in 3-dimensional space. In order to answer the question, he devised a labelling scheme for the crossing points of a link projection and then showed that every that every link diagram must contain a region bounded by fewer than fewer than four arcs, where he defined an arc to be a segment of the projection from one crossing point to the next.

With this result in hand, he worked to determine all of the possibilities for such regions. In the case of a region bounded by one arc, this was simply a twist as shown in Figure 4, which could easily be undone without changing the link. For regions bounded by two arcs, he found two possibilities. Namely, a region created as a strand passed over another strand at two consecutive points or a region created as a strand passed over and then under another. (See Figure 4.) In the first case, the top strand can be moved so that it no longer crosses over the bottom strand without changing the link type; the second however, could not be undone. Surprisingly, the situation gets no more complicated with regions bounded by three arcs, where there are two possible cases as shown in Figure 4. Maxwell explained the situation, writing "[i]n the first case, any one curve can be moved past the intersection of the other two without disturbing them. In the second case this cannot be done and the intersection of two curves is a bar to the motion of the third in that direction." [16, p. 437] Maxwell also considered regions bounded by four or more arcs, but made little progress. In fact, one of his claims in [16, p. 438] (that any region whose boundary was partially right-handed and partially left-handed could be reduced in some way) showed that he did not know of the existence of non-alternating knots.



Figure 4. Regions bounded by fewer than four arcs

Maxwell's pioneering work was a major advance for the theory of knots. He did not prove or even claim (which is surprising considering that during in Maxwell's era, mathematical papers often contained false claims that the authors considered "obvious" and did not bother to prove) that his observations regarding regions bounded by three or fewer arcs were sufficient to transform any projection of a link into any other projection. However, nearly sixty years later the German mathematician Kurt Reidemeister would prove this very fact, and today the diagrammatic "moves" discovered by Maxwell bear Reidemeister's name. This is a prime example of how it is almost always best to be the *second* mathematician to discover something, as the first rarely gets the credit deserved.

2.2. Counting knots

While, as we have remarked earlier, P.G. Tait was initially skeptical of Thomson's vortex theory of atoms, he gradually changed his mind, and by 1876 he had set out to make a complete table of knots (up to a certain number of crossings). By creating a table of knots, Tait hoped that he would develop a table of elements to go with Thomson's atomic theory. Tait's serious investigation of knots began, like Gauß' and Maxwell's, with the development of a way to symbolically encode the crossings of a knot projection. Despite his earlier correspondence with Maxwell, Tait developed his own encoding scheme, which more closely resembled the one developed by Gauß than that of Maxwell. Shortly after beginning his study of knots, Tait delivered a sealed envelope to the Royal Society of Edinburgh on 16 October 1876. Despite his numerous reports to the Royal Society regarding his succeeding investigations of knots, the envelope remained sealed for 111 years and was opened for the first time in 1987.

Tait's envelope contained two conjectures that appeared implicitly in his later work, but were never as explicitly stated as in his sealed paper of 1876. Tait seemed to take the first conjecture, which was cryptically stated as "If the simplest is + -+-+- then irreducible" (as quoted in [6, p. 358]), as an "obvious" theorem in later papers. Today we would interpret Tait's statement as meaning that an alternating knot diagram without nugatory crossings—those that separate two nontrivial distinct portions of the knot—cannot be manipulated to have fewer crossings. For example, the trefoil and figure-8 knot in Figure 2 cannot be drawn with fewer crossings, as they are both depicted as alternating knots without nugatory crossings. Despite Tait's belief in this conjecture, it was first rigorously proved by Murasugi in [18, 19]. Tait was not so sure of his second conjecture, today best known as Tait's flyping conjecture, which is usually stated (as in [11]) as "any two reduced alternating diagrams of a given knot are related via a sequence of flypes," diagrammatic moves such as the one depicted in Figure 5. (We should note that Tait applied the name "twist" to what modern knot theorists call a "flype" and reserved the term "flype" for another move.) Tait's flyping conjecture remained an important open problem in knot theory until Menasco and Thistlethwaite proved it in 1993 (see [17]).

In the course of his efforts to tabulate knots, Tait naturally became interested in knot *invariants*, which are properties of knots that do not depend on a particular projection of the knot. As an example, consider the (minimal) crossing number, which is the smallest number of crossings that any projection of a particular knot



Figure 5. A flype

can contain. While Tait knew of the crossing number, he did not feel that it was the most important invariant to consider. Instead, he tried to establish an invariant that he wanted to call "beknottedness". Today, we cannot give a proper definition of what Tait meant by beknottedness, since he never settled on a definition himself. He did develop ideas that looked promising. However, they only worked for alternating diagrams without nugatory crossings (so-called "reduced diagrams") and the fact that they were invariants of reduced alternating diagrams was not established until Tait's flyping conjecture was proved. The one major positive result that came out of Tait's initial work on knot enumeration was the establishment of the existence of knots that could be deformed from right-handed to left-handed without changing the structure of the knot. He called these knots *amphicheiral*, a term that survives to this day (coexisting with the term *achiral*), and recognized that the figure-8 was amphicheiral. The idea of chirality is important in modern applications of knot theory, and will be discussed in more detail in the next chapter.

Epple reports in [6] that Tait gave up the enumeration of knots for about two weeks in 1877, citing the realization that there were in fact far *fewer* distinct knots than he was prepared to find. He decided that the effort required to complete an enumeration was becoming far too difficult and that the work required would be more combinatorial in nature than he wanted. However, Tait soon read some of Listing's early work on knots and thought that he could make use of Listing's "typesymbol" (as Tait called it), which emphasized the regions of a knot projection over the crossings. This again gave Tait hope of completing an enumeration of knots that would be sufficient for the needs of chemists and physicists. He worked things out to the point of giving a table of knots with crossing number seven. However, he believed that the complexity of the knots he was producing would prevent them from all being stable enough as vortices to represent atoms, meaning that a tabulation of knots with higher crossing numbers would be required. Such a tabulation would require either more efficient methods or a mechanized means of determining if two knot diagrams were the same, an idea that would not be realized for over 100 years.

Between 1877 and 1883. Tait did little work in knot theory. However, he gave an address on topology to the Edinburgh Mathematical Society in late 1883 in which he mentioned the problem of enumerating knots and how it was believed to be "a mere question of skilled labour" (quoted in [6, p. 366]). Tait received a response to his pseudo-advertisement for someone to assist with knot enumeration from the Reverend Thomas Penyngton Kirkman, Rector of Croft, Lancashire, who had spent a significant portion of the previous 30 years considering combinatorial problems involving graphs and hypergraphs (e.g., Kirkman's schoolgirl problem involving how many ways there are for 15 schoolgirls to take daily walks in rows of three so that each girl walks in the same row with each other girl exactly once). Kirkman viewed the knot enumeration problem as a problem of enumerating particular 4-regular planar graphs that could be projections of alternating knots or links and set to work on the problem. However, he and Tait soon got into arguments over whether the enumeration of knot projections was the right way to approach the problem. Kirkman, being a true combinatorialist and not a topologist, felt that twisting moves were not of interest and equivalences via such operations should not be considered.

Kirkman sent his first paper to Tait in May 1884, in which he had enumerated all knot projections up to 10 crossings. Tait then set about doing the work that Kirkman didn't want to do and determined which alternating projections in Kirkman's paper represented the same knot. Their work was combined and presented to the Royal Society of Edinburgh very shortly thereafter. While Tait was not completely mathematically satisfied with the tables in that he had no proof of the inequivalence of each of the knots (lending support to the view that he did not take his flyping conjecture to be true), he was satisfied that there were now enough knots known to provide a "periodic table" for the vortex theory of atoms. (Kirkman did not subscribe to the vortex theory of Tait and Thomson, which may help explain his lack of interest in the topological equivalence of knot projections.)

As Tait prepared to publish the tables prepared through his work on Kirkman's knot projections, he received an enumeration of knots up to 10 crossings from Charles N. Little, a mathematics Ph.D. student of H.A. Newton at Yale University. (His knot tabulation served as his doctoral dissertation, entitled *On Knots, with a Census for Order 10*, which earned him his doctorate in 1885.) Comparing his list with Little's, Tait found one duplication in his list and a duplication and omission in Little's. After correcting his errors, he sent the paper to press. Before publishing the table up to 10 crossings, Tait had received a list of 1581 knot projections of 11-crossing knots from Kirkman, but he decided that the work involved in determining the equivalences of those diagrams was too great and officially retired from knot tabulation in 1885. However, he did suggest that Little make an investigation of the 11-crossing knots. Little did that and more, eventually taking on the much more difficult problem of enumerating non-alternating knots, which only exist for crossing numbers greater than seven. (The problem is so difficult that Tait initially did not believe that such knots existed, and it took until 1930 to rigorously prove that a non-alternating knot exists.

Ironically, there are far more non-alternating knots than alternating knots.) Despite lacking any useful invariants to distinguish non-alternating knots, Little sent a table to Tait in 1899 for communication to the Royal Society that purported to contain a complete table of the 43 distinct non-alternating knots with crossing number 10. The tables of alternating knots made by Tait and Little have withstood the test of time and are now known to be complete and without duplication, truly a remarkable feat. It is also quite surprising that Little's list of non-alternating knots contained only one duplication, which was not identified until 1974!

As time went on, Thomson had become increasingly skeptical of the vortex theory of atoms, and thus Tait's retirement from knot tabulation was the death knell for the theory. Knot theory was just beginning to come into its own as an area of mathematical study with the development of new topological tools that would allow questions about knots and links to be resolved by rigorous proofs. Without these tools, knot enumeration came to a virtual standstill for many decades, the only exception being Mary Gertrude Haseman's 1917 doctoral dissertation at Bryn Mawr College, which was entitled On knots: with a census of the amphicheirals with twelve crossings, and her paper on 14-crossing amphicheirals that appeared the Transactions of the Royal Society of Edinburgh. According to the Mathematics Genealogy Project Haseman studied under Charlotte Angas Scott and James Ryals Conner. Scott was educated at the University of Cambridge in the United Kingdom, and Conner was a student of Frank Morely, who also earned his doctorate from Cambridge, so Haseman would have had exposure to the Scottish tabulating tradition through the influence of her advisors. However, she did not make any use of the new topological techniques that had been developed since Tait gave up tabulation.

After sufficient topological invariants had been developed to rigorously show that the knots in the tables were truly different and not just different projections related by extremely complicated sequences of moves, mathematicians again became interested in tabulating knots. In the 1960s, John H. Conway developed yet another notation for encoding knots and links, and this scheme allowed him to enumerate all links up to 10 crossings. (Without detecting the duplication in Little's list of 10-crossing alternating knots.) He also attempted a tabulation of prime knots up to 11 crossings. According to [11], Conway detected 11 omissions and one duplication in Little's list of 11-crossing alternating knots, but his own list of nonalternating knots had four omissions which were not detected until the late 1970s by Caudron. Hand tabulation came to an end at that time after collaborative work by Bonahon and Siebenmann and independent work by Perko completed the tabulation of 11-crossing knots.

Dowker and Thistlethwaite were the first to computerize knot enumeration. Their work in the early 1980s brought the table of knots up to 13 crossings. Work halted again until the early 1990s when a group of high-school students won time on a Cray supercomputer. They recruited Hoste to help them to enumerate all alternating knots through 14 crossings. In [11], Hoste, Thistlethwaite, and Weeks discuss the techniques they used to complete the tabulation through 16 crossings, finding 1, 701, 936 distinct prime knots. (Their work had a built-in check, as Hoste and Weeks worked together using hyperbolic invariants and Thistlethwaite worked independently using absolutely no hyperbolic invariants.) The computerization of the problem has made knot enumeration considerably easier, but the rapid growth in the number of knots is astonishing. For example, Hoste reports in [10] that a July 2003 tabulation of all prime, alternating knots through 22 crossings performed by S. Rankin, J. Schermann, and O. Smith found 6,217,553,258 knots! That's over six thousand times as many *alternating* knots with between 17 and 22 crossings, inclusive, as there are alternating *and* nonalternating knots with at most 16 crossings.

2.3. Non-enumerative developments

Of course, enumerative knot theory is just one part of the field. The development of topology and knot theory over the past one hundred years has created far too many significant ideas to be discussed in this thesis. However, we will attempt to discuss some of the major advances alluded to earlier and that have an impact on applications of knot theory, which will be discussed in the following chapter.

Poincaré's development of the fundamental group was a significant advance in the study of topology, as it created a way for the more-established tools of abstract algebra to be used by those studying the young field of topology. The first use of the fundamental group to study the complement of a knot (meaning what is left of a space after deleting the knot) occurred in 1905, when the Austrian mathematician Wilhelm Wirtinger, whose work was actually motivated by the study of algebraic functions of a single complex variable, showed rigorously for the first time that the trefoil knot was really knotted. This advance, which was made by showing that the fundamental group of the trefoil is the symmetric group on three elements, confirmed that Tait, Kirkman, and Little had not wasted their time creating tables of knots. Soon Wirtinger realized that his method of showing that the trefoil was knotted could be easily generalized to construct the fundamental group of an arbitrary link. This presentation of the fundamental group is now known as the Wirtinger presentation.

Max Dehn, a German mathematician who studied under Hilbert, became interested in the theory of knots as he worked to prove the Poincaré conjecture. Of course, Dehn did not prove the Poincaré conjecture, but he did develop another algorithm (distinct from Wirtinger's) for constructing the fundamental group of the complement of a link. Using this, Dehn showed (modulo a flaw in the proof of a lemma that was later resolved) that a knot is nontrivial if and only if its fundamental group is nonabelian. He went on to show that a trefoil knot and its mirror image (formed by changing all of the overcrossings to undercrossings and vice versa) are topologically distinct, confirming what Maxwell had claimed nearly fifty years earlier. The work of Dehn and his colleagues came to a halt with the outbreak of World War I, and it would not be until after the war that any significant work in knot theory resumed.

In the 1920s, James W. Alexander at Princeton and Kurt Reidemeister in Vienna took up the study of knots. Unlike Wirtinger and Dehn, whose interest in knots was secondary to solving other problems in which they were interested, Alexander and Reidemeister actually were interested in studying the properties of knots themselves. Taking completely different approaches (Alexander via homology groups and Reidemeister via fundamental groups) they arrived at the same knot invariants. Alexander later went on to develop a polynomial invariant of knots (the Alexander polynomial), and Reidemeister showed that all projections of a link were related by a sequence of the three moves shown in Figure 6. (Note the similarities with Maxwell's observations discussed earlier.) Again the outbreak of war disrupted the study of knots, as Reidemeister lost his professorship in Königsberg in 1933 for being "politically unreliable" [7]. The Nazis also disrupted collaborations by other German mathematicians as they fired Jewish mathematicians and moved others around to fill their positions. Alexander and others not in German-controlled areas went to work on war-related problems and left knot theory behind, at least temporarily.

After the war, Princeton again became a center for knot-theoretical research in the United States, as Reidemeister and others came to stay at the Institute for Advanced Study. (Reidemeister would not re-establish a group of students interested in knot theory in Germany until he took a position in Göttingen in 1955.) The leader of post-war knot theory in the United States was Ralph H. Fox at Princeton. Fox felt that the classical definitions of knots (such as the one given in chapter 1) caused knot theory to be too disconnected from the rest of topology. He proposed to replace



Figure 6. Reidemeister moves

the polygonal curves by an appropriate topologically-defined set of curves and that \mathbb{R}^3 should be replaced by other compact 3-manifolds. Fox essentially succeeded in reshaping the foundations of knot theory, providing greater access to the tools of topology for those studying knots. Thus, his work led to a number of new geometric knot invariants.

In the 1970s, J.H. Conway was doing more than simply tabulating knots as discussed in the previous section. He devised a new way to calculate the Alexander polynomial using an algorithm on knot diagrams. In fact, his work actually led to a refinement of the Alexander polynomial that is often called the Conway polynomial. A major breakthrough in knot theory occurred in 1984 when Vaughan Jones developed a new polynomial invariant of knots (the Jones polynomial) as he conducted research on von Neumann algebras. The Jones polynomial was a significant improvement over the earlier polynomial invariants as it was able to distinguish many knots from their mirror images. In 1990, Jones' work earned him a Fields medal, arguably the most prestigious award for mathematical research.

We could write pages about the new polynomial invariants that have been developed since 1984 alone, but then our story would require far more of a mathematical background than has been required to this point. Furthermore, not enough time has passed to reflect upon which developments will have seriously lasting significance in order to determine what is most important. Thus, we will leave the history of knot theory here and will proceed to consider some interesting applications of knot theory to other fields.

CHAPTER 3. KNOT THEORY IN THE REAL WORLD

Pure mathematicians often take pride in doing work that is of purely theoretical importance, and this author will readily admit to often appreciating a beautiful mathematical result as just that without any thought as to practical applications of the idea. Sometimes, however, the real-world applications of a mathematical result jump out and smack a mathematician alongside the head so hard that they cannot be ignored. Knot theory is one area of what is traditionally considered pure mathematics in which such occurrences are fairly common. In the previous chapter, we saw how the early development of knot theory was motivated almost entirely by the idea of understanding the basic building blocks of matter, and we mentioned how the topic of amphicheiral knots kept appearing without any real discussion of what an amphicheiral knot actually is. The anticipated moment is almost here, but first we're going to take a bit of a detour to discuss a way to use graph theory to look at knots and links.

3.1. Using graphs to study knots

In the previous chapter we saw how knot theory is an area of mathematics that is best described as topological due to the importance of equivalence of knots under deformations; however, it also has a strong combinatorial aspect when considering the idea of counting knots and constructing tables of knots. Thus it is not surprising that combinatorialists have developed techniques to look at knots using tools to which they are more accustomed. Furthermore, theorems regarding knots have been used to prove theorems about graphs, such as the theorem of Lien and Watkins [14] that we extend in the next chapter. This section will serve as a brief introduction to the idea of turning knots into graphs and vice versa and will discuss how Reidemeister moves are then done on these graphs.

Formally, a graph G = (V, E) is a pair of (multi)sets. We say that V is the

set of vertices and E is the (multi)set of edges, consisting of one- and two-element subsets of V. Informally, a graph is a set of points (vertices) and line segments (edges) connecting those points. Graph theorists can never seem to agree if more than edge should be permitted between two vertices or if an edge should be permitted to go from a vertex back to itself, but we will need those features in our graphs, so the formal definition given above permits them. Such graphs are sometimes called multigraphs or pseudographs, but we will stick with the term graph here. Figure 7 shows some examples of graphs.



Figure 7. A few graphs

One of the interesting (and topological) properties of a graph is planarity. We say that a graph is *planar* if it can be embedded in the plane with edges meeting only at vertices. Of the graphs above, the one labelled K_3 is planar, as is K_4 . A hasty look at G_1 might suggest that G_1 is not planar, as two of its edges cross in the middle of the square but there is no vertex there. However, G_1 is *isomorphic* to K_4 , as they both contain precisely four vertices and all the possible edges between them. Thus, G_1 is planar, although the way it is drawn is not a planar embedding. The graphs K_5 and $K_{3,3}$ are not planar. In fact, they are the simplest nonplanar graphs and it is a well-known theorem attributed to Kuratowski but first proved by Pontryagin that every nonplanar graph contains a graph equivalent one of these graphs, for a suitable definition of "equivalent". In this thesis, we will be concerned entirely with planar graphs, as we will establish a one-to-one correspondence between planar graphs (with a sign of + or - assigned to each edge) and knot diagrams. First, however, we will need to discuss checkerboard colorings of knot diagrams.

Given a knot diagram, it divides the plane into a number of regions. We begin by coloring the outer, unbounded region white. We then cross over any strand of the knot diagram and color the region into which we entered black. Next we cross into a bordering region and color it white. The process of crossing strands and alternating colors continues until all the regions have been colored black or white. (While it might not seem likely at first, this process really does create a well-defined coloring.) Figure 8 shows a checkerboard coloring of a trefoil knot.



Figure 8. Checkerboard coloring

Once we have created a checkerboard coloring, we are set to construct a graph, which we will call the *medial graph* of the knot diagram. To do this, we first place a vertex in each of the black regions. (Our choice of the black regions is arbitrary. The graph constructed by using the white regions is just as useful, and in fact is the planar dual of the medial graph we will construct.) Next, we must add edges to our graph. We add an edge between two vertices if and only if there is a crossing that "connects" the regions to which the vertices correspond. Finally, we assign each edge a sign based on the slope of the overstrand encountered as one "walks along" the edge. (Figure 9 gives examples of the two types of crossings.) Medial graphs for a trefoil and figure-8 knot are shown in Figure 10. The fact that the signs are all the same in the medial graphs for these knots is not a fluke. Rather, it is due to the fact that the knots are drawn as alternating knots, so all the crossings have the same type.



Figure 9. Crossings



Figure 10. Medial graphs of the trefoil and figure-8 knots

In order to determine if two medial graphs represent the same knot, we need to understand how to perform Reidemeister moves on the graphs. This is as simple as drawing the graph corresponding to each move in Figure 6. Of course, the coloring with which we are working influences how the move affects the graph, so the type I and II moves have two graphical possibilities as shown in Figure 11. For the type IIII move, the dual starting position to the one depicted below is essentially the same (up to signs) as the ending position, so a single drawing conveys the needed information.



Figure 11. Reidemeister moves on medial graphs

Before leaving the world of abstraction for some discussion of concrete applications, we should make a few observations. First, our construction of the medial graph guarantees that it will always result in planar graph. (More specifically, we get a specific planar embedding of a graph.) Second, we can reverse our process of constructing the medial graph by drawing appropriate crossings on a signed plane graph and then adding strands to create the regions the vertices represent. Thus, there is a one-to-one correspondence between link diagrams and signed plane graphs.

3.2. Chirality

The much-anticipated moment has arrived for us to discuss the importance of chirality. The root of the word *chiral* is the Greek word *cheir* meaning "hand", and handedness is what chirality is all about. Human beings know that our left hands are physically different from our right hands. No amount of twisting or turning will make one look like the other to the point that they cannot be distinguished, even by an outside observer who cannot see the body to which they are attached. (Of course, we are not claiming that we can always remember which to call "left" and which to call "right". That is an entirely different issue.) There is, however, one way in which we can look at a right hand and think that it is a left hand—by looking at it in the mirror. Thus, we say that our hands are *mirror images* of each other.

Much like hands, there is a way to consider the mirror image of a knot projection, which is formed by changing all the crossings in the projection so that the overstrand becomes the understrand and vice versa. (In terms of a graph-theoretic approach, we change the sign of every edge to its opposite.) As an example, Figure 12 shows a trefoil knot and its mirror image. Looking at these two knots, it seems reasonable to say that they are different knots, as J.C. Maxwell claimed roughly 140 years ago. However, it is far from trivial to *prove* that there is no deformation transforming one to the other, since such a proof requires that it be shown that *no one* can perform such a deformation, not just that one mathematician can find no way to do it. (A proof using one of the many knot polynomials developed in the last twenty years is not all that difficult, but those polynomials are very sophisticated tools in themselves.) Knots, such as the trefoil, that can be distinguishable from their mirror images are called *chiral*. Those that are (topologically) indistinguishable from their mirror images (if such knots even exist) are called *achiral* or *amphicheiral*.



Figure 12. Left- and right-handed trefoils

In keeping with our handedness analogy, we can in fact designate one trefoil as left-handed and the other as right-handed in a straightforward manner. To do this, we need to *orient* the knots, in effect providing a direction in which we trace out the knot. (The arrows on the knot projections in Figure 12 provide an orientation for each.) The trefoil on the right in Figure 12 is a right-handed trefoil because if we look at any crossing and think of grasping the overstrand with our thumb pointing in the direction of the orientation, our fingers curl and point in the direction of the orientation of the understrand. For the other trefoil, we note that our fingers curl the opposite direction of the orientation when using our right hand, but doing the same thing with our left hand again leads to consistency with the knot's orientation. We should note that if we reverse the orientation of a knot we will still reach the same conclusion as to if it is right-handed or left-handed, which is important. Otherwise, we'd have another circumstance in which World War III might arise as mathematicians fought over which way to orient a knot is the "correct" way.

One might hastily claim that *all* knots are distinct from their mirror images. Of course, it is foolish to make conjectures after considering only one example, so let's move up one level in complexity and consider the figure-8 knot in Figure 13. At first glance, we have no reason to expect that this knot can be deformed into its mirror image. However, we can in fact make such a deformation. One sequence of Reidemeister moves affecting such a transformation is shown in Figure 14. (Here we show only the graphs at each stage, but our discussion in the previous section explains how to reconstruct knot projections at each stage if desired.)

Now we know that there are chiral knots and achiral knots, but so far we have yet to say anything that might indicate that such distinctions matter to anyone other than a pure mathematician. After all, this chapter is supposed to be about real-world applications. Although it might not seem like it from the discussion above, chirality



Figure 13. Figure-8 knot



Figure 14. A demonstration of the achirality of the figure-8 knot

is an issue of great interest to many nonmathematicians. (No, not just in that it is good to have a right hand and a left hand that are distinct.) Knots appear in nature more often than one might think, and the chirality (or lack thereof) of such knots is often important. One area in which such questions often arise is chemistry, where the difference between a right-handed and a left-handed molecule can coincide with the difference between helpful and harmful. More discussion of molecules that are actually knotted will follow in a later section, but for now we will spend a moment on the consequences of chirality of unknotted molecules, as it will present a simpler arena for discussion.

When considering unknotted molecules, our method of distinguishing between right- and left-handedness will not work. However, chemists do have a means for determining if a chiral molecule is right-handed or left-handed and call two chiral molecules that are mirror images of one another *enantiomers*. To determine if an enantiomer is right- or left-handed, they pass a beam of polarized light through a sample. If the sample consists of molecules that all have the same chirality, the light will be bent to the right or left. If the light bends to the left, the enantiomer is called *levo*, usually abbreviated by the letter L. Conversely, if the light bends to the right, we call the enantiomer *dextro*, denoted by the letter D. A mixture containing both enantiomers of a chiral molecule is called a *racemic* mixture, while a compound containing only one enantiomer is said to be *optically pure*.

As a good example of a chiral molecule, consider limonene, which has chemical formula $C_{10}H_{16}$. Both enantiomers of limonene have a citrus scent. However, the Dlimonene molecule has a pleasing orange scent, while L-Limonene has a lemon scent that is usually described as harsh, piney, and turpentine-like. Based on the differences between limonene enantiomers, we can reasonably assume that molecular chirality is of interest to the makers of household cleaning products. If that were the only way in molecular chirality were interesting, however, there is no way that molecular topology would have become a course at North Dakota State University or Erica Flapan would have written [8]. The real importance of molecular chirality comes in not in making household cleaners smell good but rather in ensuring that pharmaceuticals are safe for human use.

A prime example of the problems that can arise when patients are given a racemic mixture is the drug Thalidomide, which was prescribed to pregnant women in the 1960s as a treatment for morning sickness. The drug did successfully reduce problems of morning sickness. However, it also caused horrible birth defects. As it turns out, the left-handed enantiomer was making the expectant mother feel better, while the right-handed enantiomer was causing severe damage to the fetus. In the years since the Thalidomide disaster, pharmaceutical companies have had to consider the chirality of their drug molecules to ensure that the undesirable side effects of one enantiomer do not outweigh the benefits of the other. (Of course, in most cases one enantiomer passes harmlessly through the body while the other provides positive treatment.)

The articles [20] and [21] provide an interesting look at how drug chirality has become big business in recent years. Rouhi reports that in 2001, 36% of the worldwide sales of formulated pharmaceutical products belonged to single-enantiomer drugs, up from 34% in 2000 and 32% in 1999. Developing new chiral drugs has been an important part of this growth, but it is also attributable to the use of chirality to extend the profitable life of existing drugs. As an example, consider the antiulcer drug Prilosec, produced and marketed by AstraZeneca. Prilosec was approved by the Food and Drug Administration (FDA) in 1995 as a racemic mixture. However, only the levo enantiomer is pharmacologically active, so AstraZeneca later filed for a patent on the levo molecule alone, providing extended protection for when the patent on the racemic mixture expired in 2002. They then introduced their "new" antiulcer drug Nexium, which was no different from Prilosec in function except that the optic purity of Nexium allows half the dose to provide the same effect. Another means of extending the commercial life of a pharmaceutical that some companies have used is to combine an older drug, such as montelukast, with a newer drug, such as laratidine. Both are used in fighting asthma, but montelukast's patent expires after laratidine's, providing a longer period of exclusivity to the manufacturers.

One company has actually made its name on drug chirality. Sepracor has been

examining other companies' drugs for years and testing to determine if both enantiomers are pharmacologically active or if an optically pure drug would be more effective. In the latter case, they file a patent on the effective enantiomer and offer the drug's original manufacturer a license for that molecule. This was the case with Eli Lilly's Prozac, in which only the L-enantiomer is active. However, not all drug companies are receptive to such offers, so then Sepracor proceeds to get FDA approval on its own and licenses another company to produce and market the drug. For example, Schering Corporation, which manufactures the racemic asthma drug albuterol marketed as Preventil, was not interested in Sepracor's offer for a license on optically pure levalbuterol, which they had determined to be more effective and lacking in the aggravating side-effects of racemic albuterol. Sepracor took the drug to market as Xopenex in 1999 for adults and 2002 for children, and it has been a big success.

3.3. Knot strength

Now that we've seen that topology is an important tool for chemists, we turn to a brief look at real physical knots and their strength. In [4], the authors used high-speed photography to study the strength of knots tied in monofilament fishing lines and cooked spaghetti. Here we will provide a brief summary of their results.

The authors began by looking at overhand and figure-8 knots tied in fishing line. (The overhand knot is the open-ended version of the trefoil knot.) To compare their strength, they tied an overhand knot and a figure-8 knot on the same strand of fishing line and pulled evenly on both ends. They found that the overhand knot always broke before the figure-8 knot. They conducted further experiments that showed that the overhand knot is weaker than any other knot up to 7 crossings. They were unable to create a complete ranking of all the knots tested, however, as the knots with more than four crossings failed to consistently pull into a single tight configuration as the overhand and figure-8 knots did. After concluding that overhand knots break more easily than figure-8 knots, the next natural question was to determine where a knot was most likely to break. This is where the spaghetti enters the picture, as the fishing line was so thin that it would completely break between exposures of the high-speed camera, necessitating a thicker "rope."

One immediate difference that was encountered when using spaghetti instead of monofilament is that the overhand knot was no longer always the first to break. However, the authors attributed that to the likelihood of imperfections in the structure of the noodle, as the overhand knot continued to break first in about 70 percent of cases. The theoretical model of knotted string that the authors were investigating predicted that the spaghetti would break at the point of highest curvature. (The easiest way to picture the curvature of a smooth curve at a point is by trying to fit a circle into the curve so that it is tangent at that point. The curvature is then the reciprocal of the radius of the circle. Thus, the more the curve curves, the smaller the circle is that can be fit, and the larger the curvature is.) They speculated that such a point would be the breaking point as the outer surface of the "string" would be stretched the most at that point and the inner surface would be greatly compressed. When actually examining where the breakage occurred, however, they found that the spaghetti broke at the entrance of the knot but at the outside instead of inside where the point of highest curvature was located. (It is worth noting that the real breaking point was a point of high curvature, just not the maximizing point.) A reasonable explanation for this difference between the theoretical model and the physical reality is the friction involved in the tightening of the knot. The authors speculate that at the breaking point the friction has become so great that the spaghetti is no longer able to move against itself, and thus breaks.

3.4. Other applications

We have of course only touched the surface of how knot theory is applicable in the "real world." Biologists are also interested in knot theory for its applicability to the study of DNA, which can be examined by considering the knot structures into which it is twisted. Living creatures have also been seen turning themselves into knots, as is the case with the hagfish, which knots itself up for hygenic purposes, defensive reasons, and to get food. The interested reader should refer to [3] as a starting point for further examples of physical knots.

CHAPTER 4. SIGNED GRAPH LAPLACIANS

Algebraic invariants derived from knot diagrams and medial diagrams have long been studied. Most of these studies have focused on the abstract graph theoretic properties while ignoring the plane embedding. However, Whitney showed in [23] that only 3-connected graphs have unique embeddings in the plane, giving some importance to the particular embedding. In this chapter, we wish to study invariants which incorporate information from the plane embedding. We do this by constructing a chain complex corresponding to a signed plane graph and then examining the properties of its Laplacians.

4.1. Graphs and Chain Complexes

In this chapter we permit graphs with multiple edges between a single pair of vertices but disallow self-loops and vertices of degree one (i.e., vertices adjacent to only one other vertex). We make the second restriction to prevent small technical problems when dealing with the dual graph, since vertices of degree one create loops in the dual. See [22] for definitions and concepts from graph theory.

Fix an orientation for S^2 and let $G \subset S^2$ be a signed plane graph. Let G have ordered vertex set $V = \{v_1, v_2, \ldots, v_n\}$, ordered edge set $E = \{e_1, e_2, \ldots, e_m\}$, and ordered face set $F = \{f_1, f_2, \ldots, f_r\}$. (By the Euler characteristic, we have that r = 2 - n + m.) The chosen orientation of S^2 induces an orientation on F, but we choose an arbitrary orientation for each edge in E, making G a signed plane digraph. When considering the oriented edges, we will refer to them as $\vec{e_i}$.

Definition 4.1. Given an S^2 embedding of a signed digraph $G \subset S^2$, we can construct the *chain complex corresponding to* G (denoted $\mathcal{C}[G]$), a complex of free \mathbb{Z} -modules of finite rank, as follows:

$$0 \longrightarrow C_2 \xrightarrow{\partial_2} C_1 \xrightarrow{\partial_1} C_0 \longrightarrow 0$$

where C_0 is the free Z-module on the vertices of G, C_1 is the free Z-module on the edges of G, and C_2 is the free Z-module on the faces of G. If $\vec{e} = (v_i, v_j) \in C_1$ (where our convention is that \vec{e} is oriented from v_i to v_j), then $\partial_1(\vec{e}) = v_j - v_i$. Similarly, if $f \in C_2$, we define $\partial_2(f)$ to be the sum of the edges on the boundary of f with coefficient +1 if the orientation of the edge agrees with the induced orientation of fand coefficient -1 if it disagrees. When a particular ordered basis is important, we will denote the complex as $\mathcal{C}_{\mathcal{B}}[G]$, with \mathcal{B}_0 , \mathcal{B}_1 , and \mathcal{B}_2 as the bases of C_0 , C_1 , and C_2 , respectively.

From $\mathcal{C}[G]$, we also construct its dual $\mathcal{C}^*[G]$, which has modules $C_i^* = \text{Hom}(C_i, \mathbb{Z})$ and coboundary maps $\delta_i : C_i^* \to C_{i+1}^*$. The dual complex is shown in the following diagram.

$$0 \longleftarrow C_2^* \xleftarrow{\delta_1} C_1^* \xleftarrow{\delta_0} C_0^* \longleftarrow 0$$

A bilinear form \langle , \rangle on C_1 is a mapping $C_1 \times C_1 \to \mathbb{Z}$ that is linear in each variable. That is,

$$\begin{array}{lll} \langle cx+y,z\rangle &=& c\langle x,z\rangle+\langle y,z\rangle\\ \langle x,cy+z\rangle &=& c\langle x,y\rangle+\langle x,z\rangle. \end{array}$$

We say that \langle , \rangle is symmetric if $\langle x, y \rangle = \langle y, x \rangle$. The matrix of \langle , \rangle is $A = (\langle e_i, e_j \rangle)$, where $\{e_i\}$ is an ordered basis. (Note that a change of basis corresponds to congruence of A, i.e., $A \longmapsto P^t A P$, where $P\{e_i\} = \{e_i\}$.) If A has integer entries, we call \langle , \rangle unimodular if det $A = \pm 1$. (When the entries come from another ring, we require that det A be a unit.) Equivalently, \langle , \rangle is unimodular if the adjoint

$$\operatorname{Ad}\langle , \rangle : C_1 \longrightarrow \operatorname{Hom}(C_1, \mathbb{Z}) \cong C_1^*$$

 $e \longmapsto (f \mapsto \langle e, f \rangle_1)$

is an isomorphism.

Example 4.2. For C[G], there are two common symmetric bilinear forms that we wish to consider on C_1 .

a. The standard "dot product" on C_1 is defined by declaring the edges with chosen orientation $\{\vec{e}_i\}$ to be an orthonormal basis. Then

$$\langle \vec{e}_i, \vec{e}_j \rangle_1 = \delta_{ij},$$

where δ_{ij} is the Kronecker delta.

b. If G is a signed graph, we set

$$\langle \vec{e}_i, \vec{e}_j \rangle_{1,\varepsilon} = \operatorname{sign}(\vec{e}_i) \delta_{ij}.$$

Note that the matrices of both these products are diagonal with all entries ± 1 , making them unimodular. Therefore Ad $\langle , \rangle_{1(,\varepsilon)}$ is an isomorphism, and we have proved the following lemma.

Lemma 4.3. As \mathbb{Z} -modules, C_1 and C_1^* are isomorphic.

While the adjoint specifies an identification between C_1 and C_1^* , it is by no means a canonical isomorphism.

Definition 4.4. Given a signed plane digraph $G \subset S^2$, the dual signed plane digraph of G (denoted \widehat{G}) is constructed by

- a. choosing a vertex set $\widehat{V} = \{\widehat{v}_1, \widehat{v}_2, \dots, \widehat{v}_r\}$ for \widehat{G} in one-to-one correspondence with F;
- b. choosing a face set $\widehat{F} = (\widehat{f}_1, \widehat{f}_2, \dots, \widehat{f}_n)$ in one-to-one correspondence with V;

c. putting the edge set \widehat{E} of \widehat{G} in one-to-one correspondence with E such that an edge $\widehat{e} \in \widehat{E}$ has the opposite sign of the corresponding edge $e \in E$ and is oriented from the vertex corresponding to the face whose orientation disagrees with that of e to the vertex corresponding to the face whose orientation agrees with that of e.

Note that the chain complex of the dual of G is (with reordering) the dual of the chain complex of G (i.e., $\mathcal{C}[\widehat{G}] \cong \mathcal{C}^*[G]$).

Notation. We let ε_i denote $\langle e_i, e_i \rangle_{\varepsilon}$ for $e_i \in C_1$ and ε_i^* denote $\langle e_i^*, e_i^* \rangle_{\varepsilon}$ for $e_i^* \in C_1^*$. (Notice that, since the dual modules correspond to the edge sets of dual signed graphs, $\varepsilon_i^* = -\varepsilon_i$.)

4.2. Laplacians

Now we define the Laplacians both of a graph and of a chain complex, and then show the connections between the two of them.

Definition 4.5. The Laplacian matrix $L_0(G)$ of a graph G is

$$L_0(G) = D(G) - A(G),$$

where $D(G) = \text{diag}(d_G(v_1), d_G(v_2), \dots, d_G(v_n))$, the diagonal matrix of vertex degrees and A(G) is the adjacency matrix of the graph G. The signed Laplacian matrix of a graph is

$$L_{\varepsilon}(G) = \sum_{\substack{e \in E(G)\\\partial e = \{i,j\}}} \varepsilon_{ij} (E_{ii} - E_{ij} - E_{ji} + E_{jj}),$$

where E_{st} is the $n \times n$ matrix with exactly one nonzero entry in position (s, t) and ε_{ij} is +1 or -1, depending on the sign of the edge in question. (Note that the reference to G will be omitted when the context is clear.) For the dual graph \widehat{G} , we will denote $L_{\varepsilon}(\widehat{G})$ by $\widehat{L}_{\varepsilon}$.

Since we have defined a chain complex corresponding to a graph, we consider now its combinatorial Laplacians and then show their relations to the graph Laplacians of definition 4.5.

Definition 4.6. Given a chain complex $C = \{C_i, \partial_i\}$ where each module is endowed with a bilinear form that makes its basis orthonormal, its *combinatorial Laplacians* $\Delta_i : C_i \to C_i$ are

$$\Delta_{i} = (\mathrm{Ad}\langle \,,\,\rangle_{i})^{-1} \delta_{i-1} \,\mathrm{Ad}\langle \,,\,\rangle_{i-1} \partial_{i} + \partial_{i+1} (\mathrm{Ad}\langle \,,\,\rangle_{i+1})^{-1} \delta_{i} \,\mathrm{Ad}\langle \,,\,\rangle_{i}$$

If we use $\operatorname{Ad}\langle , \rangle_{1,\varepsilon}$ to identify C_1 and C_1^* , we write $\Delta_{i,\varepsilon}$.

Lemma 4.7. Let G be a signed graph (with fixed but arbitrary edge orientation) embedded in S^2 and with corresponding chain complex C[G]. Then

a.
$$\Delta_0 = \partial_1(\mathrm{Ad}\langle , \rangle_1)^{-1} \delta_0 \mathrm{Ad}\langle , \rangle_0 = L_0(G),$$

b.
$$\Delta_{0,\varepsilon} = \partial_1(\operatorname{Ad}\langle , \rangle_{1,\varepsilon})^{-1} \delta_0 \operatorname{Ad}\langle , \rangle_0 = L_{\varepsilon}(G),$$

c.
$$\Delta_{2,\varepsilon} = \operatorname{Ad}\langle , \rangle_2 \delta_2 \operatorname{Ad}\langle , \rangle_{1,\varepsilon} \partial_1 = \widehat{L}_{\varepsilon}(G).$$

Proof. As a matrix, ∂_1 is a rank $C_0 \times \text{rank } C_1$ matrix with rows corresponding to the vertices of G and columns corresponding to the edges of G, so it has a +1 and a -1 in every column, and $\delta_0 = \partial_1^t$. We commonly refer to ∂_1 as the oriented vertex-edge incidence matrix of G. Similarly, δ_1 is the oriented vertex-edge incidence matrix of \hat{G} , and $\partial_2 = \delta_1^t$.

Since $\operatorname{Ad}\langle , \rangle_i$ is simply represented by the identity matrix, we can see that the first statement is proved in [2, p. 27]. Let $Q = \partial_1(\operatorname{Ad}\langle , \rangle_{1,\varepsilon})^{-1}\delta_0\operatorname{Ad}\langle , \rangle_0$ and denote its *ij*-th entry by q_{ij} . First consider a diagonal entry q_{ii} . It is the inner product of row *i* of ∂_1 with column *i* in $(\operatorname{Ad}\langle , \rangle_{1,\varepsilon})^{-1}\delta_0$. These two vectors have nonzero entries

in the same locations, since they correspond to the same vertex and $\operatorname{Ad}\langle , \rangle_{1,\varepsilon}$ only multiplies entries by ±1. Then for all $j, 1 \leq j \leq m$, we have three possibilities. First, the *j*-th entry is zero, and contributes nothing to q_{ii} . Second, $\varepsilon_j = +1$, so *j*-th entries of the vectors are both either +1 or -1, and 1 is added to q_{ii} . Finally, $\varepsilon_j = -1$, so one of the vectors has +1 as its *j*-th entry and the other has -1, meaning that -1 is added to q_{ii} . Therefore $q_{ii} = \sum_{j=1}^{m} \varepsilon_j$.

Next consider an off-diagonal entry q_{ij} of Q, which is the inner product of row i of ∂_1 and column j of δ_0 . This row-column pair corresponds to different vertices, so the vectors only have non-zero entries in the k-th position if v_i and v_j are the endpoints of e_k . If $\varepsilon_k = +1$ (i.e., e_k is a positive edge), then one of the vectors has a +1 in the k-th position and the other has a -1. Therefore, -1 is added to q_{ij} . If $\varepsilon_k = -1$ (i.e., e_k is a negative edge), then both vectors have either a +1 or a -1 in the k-th position. Hence, +1 is added to q_{ij} . Thus $q_{ij} = \sum (-\varepsilon_k)$, where the sum is taken over all edges between v_i and v_j . This matches with the definition of $L_{\varepsilon}(G)$.

The third statement is proved in the same manner as the second. \Box

Much attention has been given to $L_0(G)$ and (to a lesser degree) $L_{\varepsilon}(G)$. Despite this interest, the literature contains very little about Δ_1 . Two major reasons for this are that graphs with fixed plane embeddings have been little studied and that the one-Laplacian involves a non-canonical choice of edge orientation. However, the following lemma can easily be proven.

Lemma 4.8. Let G be a bipartite graph with n vertices and m edges with bipartition V_1 and V_2 . Choose an orientation such that the edges of G are all directed from V_1 to V_2 .

a. Then in C[G], we have $(\mathrm{Ad}\langle , \rangle_1)^{-1}\delta_0 \mathrm{Ad}\langle , \rangle_0\partial_1 = 2I_m + A(G^{\#})$, where $A(G^{\#})$ is the adjacency matrix of the line graph of G.

b. If G is planar, we also have $\partial_2(\operatorname{Ad}\langle\,,\,\rangle_2)^{-1}\delta_1\operatorname{Ad}\langle\,,\,\rangle_1 = 2I_m + A(\widehat{G}^{\#}).$

4.3. Goeritz Equivalence

In [9], Goeritz introduced the following equivalence relation on bilinear forms.

Definition 4.9. Let B_1 and B_2 be two bilinear forms on finitely generated free \mathbb{Z} modules M_1 and M_2 , respectively. Then B_1 is *Goeritz equivalent* to B_2 (denoted $B_1 \sim_G B_2$) if $(M_1, B_1 \oplus D_1)$ is isomorphic to $(M_2, B_2 \oplus D_2)$, where the D_i forms have
a basis in which the form is diagonal with entries in $\{0, \pm 1\}$.

Here we define a second, slightly stronger relation as well.

Definition 4.10. Let B_1 and B_2 be two bilinear forms on finitely generated free \mathbb{Z} modules M_1 and M_2 , respectively. Then B_1 is super-Goeritz equivalent to B_2 (denoted $B_1 \sim_{SG} B_2$) if $(M_1, B_1 \oplus D_1)$ is isomorphic to $(M_2, B_2 \oplus D_2)$, where the D_i forms
have a basis in which the form is diagonal with entries in $\{\pm 1\}$.

While the Laplacians are usually thought of as automorphisms or operators, we can use them to define bilinear forms on the modules of the chain complex corresponding to a graph.

Definition 4.11. Let C[G] be the chain complex corresponding a signed plane graph G. For each module C_i , define $B_{i,\varepsilon}(x,y)$ to be $\langle x, \Delta_{i,\varepsilon}y \rangle_{i,\varepsilon}$ for vectors x and y.

The following theorem is equivalent to the theorem Lien and Watkins proved in [14]. Here we have stated the theorem in terms of bilinear forms instead of using matrix terminology.

Theorem 4.12. Let G be a signed plane graph with chain complex C[G]. Then $(C_2, B_{2,\varepsilon}) \sim_G (C_0, B_{0,\varepsilon}).$

Before proceeding, we need to define an idea from module theory and prove two statements about it. **Definition 4.13.** Let M be a finitely-generated free \mathbb{Z} -module with bilinear form B. Then the *left radical of* B, denoted Rad B, is

$$\{u \in M \mid B(u, M) = \{0\}\}.$$

Note that $\operatorname{Rad} B = \{0\}$ if and only if $\operatorname{Ad} B$ is injective. Also, a vector \vec{r} is in the radical of a form with matrix B if and only if $\vec{r} \cdot B = \vec{0}$.

Lemma 4.14. Let M and N be finitely-generated free \mathbb{Z} -modules and let

$$\Phi:(M,B_M)\to(N,B_N)$$

be an isomorphism of modules with a bilinear form. Then

$$(M/\operatorname{Rad} B_M, B'_M) \cong (N/\operatorname{Rad} B_N, B'_N),$$

where $B'_M(\overline{x}, \overline{y}) = B_M(x, y)$ is well-defined by the definition of the radical.

Proof. First note that Φ preserves the bilinear form, and thus Φ maps $\operatorname{Rad} B_M$ to $\operatorname{Rad} B_N$. Let

$$\overline{\Phi}: (M/\operatorname{Rad} B_M, B'_M) \to (N/\operatorname{Rad} B_N, B'_N).$$

We claim that $\overline{\Phi}$ is an isomorphism. First, to check that $\overline{\Phi}$ is well-defined, we must show that $\Phi(m) - \Phi(m+r) \in \operatorname{Rad} B_N$ when $r \in \operatorname{Rad} B_M$. We have that

$$B_{N}(\Phi(m) - \Phi(m+r), n) = B_{N}(\Phi(m) - \Phi(m) - \Phi(r), \Phi(m'))$$

= $-B_{N}(\Phi(r), \Phi(m'))$
= $-B_{M}(r, m')$
= 0,

since $r \in \operatorname{Rad} B_M$. Hence $\Phi(m) - \Phi(m+r) \in \operatorname{Rad} B_N$, and $\overline{\Phi}$ is well-defined.

Next we check that $\overline{\Phi}$ is injective. Let $\overline{x}, \overline{y} \in M/\operatorname{Rad} B_M$ and suppose that $\overline{\Phi}(\overline{x}) = \overline{\Phi}(\overline{y})$. Then $\overline{\Phi}(\overline{x}) - \overline{\Phi}(\overline{y}) = \overline{0}$, so $\Phi(x) - \Phi(y) \in \operatorname{Rad} B_N$. Let $z = \Phi(x) - \Phi(y)$ and set $z = \Phi(w), w \in M$, since Φ is an isomorphism. Since Φ preserves radicals, we must have that $w \in \operatorname{Rad} B_M$. Now observe that

$$\Phi(x) - \Phi(y) - \Phi(w) = 0$$

$$\Rightarrow \Phi(x - y - w) = 0$$

$$\Rightarrow x - y - w = 0$$

$$\Rightarrow x - w = y$$

$$\Rightarrow \overline{x} = \overline{y},$$

since $w \in \operatorname{Rad} B_M$.

Finally we check that $\overline{\Phi}$ is surjective. Let \overline{n} be an arbitrary equivalence class in $N/\operatorname{Rad} B_N$. Then members of \overline{n} are of the form n + r, $r \in \operatorname{Rad} B_N$. Using Φ^{-1} , we have

$$\Phi^{-1}(n+r) = \Phi^{-1}(n) + \Phi^{-1}(r) = m + r',$$

for some $m, r' \in M$. However, r' must be in $\operatorname{Rad} B_M$, since Φ preserves radicals. Hence $m + r' \in M / \operatorname{Rad} B_M$ as required. Therefore $\overline{\Phi}$ is an isomorphism.

Lemma 4.15. The radical respects the direct sum. That is, if B_i and D_i are bilinear forms,

$$\operatorname{Rad}(B_i \oplus D_i) = \operatorname{Rad}(B_i) \oplus \operatorname{Rad}(D_i).$$

Proof. Let $M = \begin{pmatrix} B_i & O \\ O & D_i \end{pmatrix}$ be the matrix of $B_i \oplus D_i$ and let us assume that B_i is an $n \times n$ matrix and D_i is an $m \times m$ matrix. Let $\vec{s} = (r_1, \ldots, r_n)$ and $\vec{t} = (r_{n+1}, \ldots, r_{n+m})$ and consider $\vec{r} = \vec{s} \oplus \vec{t} \in \text{Rad}(C_i \oplus D_i)$. Then $\vec{r} \cdot M$ is necessarily $\vec{0}$. The first n entries of $\vec{r} \cdot M$ depend only on \vec{s} and B_i , so $\vec{s} \cdot B_i = \vec{0}$. Hence $\vec{s} \in \text{Rad}(B_i)$. The last m entries of $\vec{r} \cdot M$ depend similarly only on \vec{t} and D_i , meaning that $\vec{t} \cdot D_i = \vec{0}$. Thus $\vec{t} \in \text{Rad}(D_i)$. Therefore an element of $\text{Rad}(B_i \oplus D_i)$ is formed from an element of $\text{Rad}(B_i)$ and an element of $\text{Rad}(D_i)$. Reversing the argument proves the opposite inclusion.

Now we are in a position to state and prove the following theorem.

Theorem 4.16. If G is a signed plane graph with chain complex $\mathcal{C}[G]$, then

$$(C_2/\operatorname{Rad} B_{2,\varepsilon}, B'_{2,\varepsilon}) \sim_{SG} (C_0/\operatorname{Rad} B_{0,\varepsilon}, B'_{0,\varepsilon}),$$

where the $B'_{i,\varepsilon}$'s are bilinear forms on the quotient modules.

Proof. By theorem 4.12, $(C_2, B_{2,\varepsilon}) \sim_G (C_0, B_{0,\varepsilon})$. That is, there exist $(0, \pm 1)$ -diagonal forms D_2, D_0 with

$$B_{2,\varepsilon} \oplus D_2 \cong B_{0,\varepsilon} \oplus D_0.$$

Lemma 4.14 implies that

$$(B_{2,\varepsilon} \oplus D_2)/\operatorname{Rad}(B_{2,\varepsilon} \oplus D_2) \cong (B_{0,\varepsilon} \oplus D_0)/\operatorname{Rad}(B_{0,\varepsilon} \oplus D_0).$$

By lemma 4.15, we have $\operatorname{Rad}(B_i \oplus D_i) = \operatorname{Rad}(B_i) \oplus \operatorname{Rad}(D_i)$. Now $D'_i \cong D_i / \operatorname{Rad}(D_i)$ is a (± 1) -diagonal form. Hence

$$(B_i \oplus D_i) / \operatorname{Rad}(B_i \oplus D_i) \cong B_i / \operatorname{Rad}(B_i) \oplus D_i / \operatorname{Rad}(D_i)$$

 $\cong B_i / \operatorname{Rad}(B_i) \oplus D'_i.$

Therefore the conclusion on super-Goeritz equivalence holds.



Figure 15. One diagram of the knot 8_{20} .



Figure 16. Labelled version of $M(8_{20})$.

4.4. Example

Consider the knot 8_{20} , which is illustrated with its medial graph in figure 15. Let $G = M(8_{20})$ as labelled in figure 16.

Now we can construct $\mathcal{C}[G]$ and examine its boundary maps.

$$\partial_2 = \begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 1 \\ -1 & 0 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 & 0 \end{pmatrix} = \delta_1^t$$

$$\partial_{1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & 1 \\ 0 & 0 & -1 & -1 & 1 & 1 & 0 & 0 \end{pmatrix} = \delta_{0}^{t}$$

Using the formulas of lemma 4.7, we can easily compute the following Laplacians.

$$L_{0} = \begin{pmatrix} 2 & -1 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & -1 \\ 0 & -1 & 3 & -1 & -1 \\ -1 & 0 & -1 & 4 & -2 \\ 0 & -1 & -1 & -2 & 4 \end{pmatrix}, \quad L_{\varepsilon} = \begin{pmatrix} -2 & 1 & 0 & 1 & 0 \\ 1 & 1 & -1 & 0 & -1 \\ 0 & -1 & 1 & 1 & -1 \\ 1 & 0 & 1 & -4 & 2 \\ 0 & -1 & -1 & 2 & 0 \end{pmatrix}$$

$$\widehat{L}_{\varepsilon} = \begin{pmatrix} 2 & -2 & 1 & -1 & 0 \\ -2 & 2 & 1 & 0 & -1 \\ 1 & 1 & -3 & 1 & 0 \\ -1 & 0 & 1 & 1 & -1 \\ 0 & -1 & 0 & -1 & 2 \end{pmatrix},$$

It is clear that the vector (1, 1, 1, 1, 1) spans the radical of L_0 , L_{ε} , and \hat{L}_{ε} . Finally, we compute Δ_1 and $\Delta_{1,\varepsilon}$. Notice that $\Delta_{1,\varepsilon}$ is not a symmetric matrix. The loss of symmetry between entries a_{ij} and a_{ji} occurs if \vec{e}_i and \vec{e}_j are nonadjacent edges with opposite signs. Then $a_{ij} = -a_{ji}$. However, we note that $\Delta_{1,\varepsilon}$ is a self-adjoint matrix with respect to the form $\langle , \rangle_{1,\varepsilon}$; that is, $\langle x, \Delta_{1,\varepsilon}(y) \rangle_{1,\varepsilon} = \langle \Delta_{1,\varepsilon}(x), y \rangle_{1,\varepsilon}$. Considering matrices, this is simply $B_{1,\varepsilon}\Delta_{1,\varepsilon} = \Delta_{1,\varepsilon}^t B_{1,\varepsilon}$.

$$\Delta_{1} = \begin{pmatrix} 4 & 0 & 0 & 0 & 1 & 0 & 1 & 1 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 4 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 & 4 & 1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 & 4 & 0 & -1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 4 & 0 \\ 1 & 1 & 0 & 1 & 0 & -1 & 0 & 4 \end{pmatrix}$$
$$\Delta_{1,\varepsilon} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 1 & 3 \\ 0 & 0 & -2 & 2 & 0 & 0 & 0 & 1 \\ 0 & -2 & 0 & 2 & -1 & 0 & 0 & 0 \\ 0 & 2 & 2 & 0 & 0 & -1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & -3 & -1 & 2 \\ 0 & 0 & 0 & 1 & -3 & 0 & -2 & 1 \\ 1 & 0 & 0 & 0 & -1 & -2 & 0 & 2 \\ 3 & -1 & 0 & -1 & 2 & 1 & 2 & 0 \end{pmatrix}$$

4.5. Further Problems and Questions

The preparation of this paper has lead to many more questions than it has answered, and some of the more prominent ones are included below.

Question 1. Is the super-Goeritz class of $(C_1, B_{1,\varepsilon})$ preserved under Reidemeister moves?

We expect the answer to question 1 to be "yes," since the work of Goeritz [9] and Kneser and Puppe [12] showed that the super-Goeritz classes of $(C_0, B_{0,\varepsilon})$ and $(C_2, B_{2,\varepsilon})$ of *knot* diagrams are preserved under Reidemeister moves. Kyle [13] noticed that only Goeritz equivalence is preserved under Reidemeister moves on *link* diagrams.

Question 2. Study the relationship between $(C_1, B_{1,\varepsilon})$ and

$$(C_2 / \operatorname{Rad} B_{2,\varepsilon}, B'_{2,\varepsilon}) \oplus (C_0 / \operatorname{Rad} B_{0,\varepsilon}, B'_{0,\varepsilon})$$

Note that the Laplacian of the one-chains has no radical. In Appendix 4.6, we show that, if we extend to rational coefficients for the one-chains, there is a duality with the one-cochains and a basis of the rational vector space of one-chains for which the associated Laplacian is a direct sum.

Question 3. Which based chain complexes arise from link diagrams?

This is such a simple question, but it is unlikely that it has a simple answer. An answer to this question will be a set of necessary and sufficient conditions for a chain complex to represent a plane graph.

The zero-Laplacian contains information on the critical group of a graph. This finite abelian group (defined in [1]) of order equal to the determinant of a principal submatrix of the zero-Laplacian formed by deleting a single row and corresponding column. This is the knot invariant discovered by Goeritz. A potential problem is to study the analogous critical group on the one-chain group $C_1(G)$.

4.6. Rational One-Laplacian

The ordered edge set is not the only possible basis for C_1 , and considering an alternative basis puts Δ_1 into a nicer form. However, we must extend the coefficients to include the rational numbers, making $\mathcal{C}[G]$ a chain complex of vector spaces over \mathbb{Q} , and choose yet a third duality isomorphism between C_1 and C_1^* . **Definition 4.17.** Let G be a graph with chain complex C[G]. The rational face-star basis for C_1 is the ordered basis

$$\mathcal{B}'_1 = (\partial_2(f_1), \partial_2(f_2), \dots, \partial_2(f_{r-1}), \delta_0(v_1), \delta_0(v_2), \dots, \delta_0(v_{n-1})).$$

Letting \mathcal{B}'_0 and \mathcal{B}'_2 be the standard vertex and face bases allows us to denote this modified complex by $\mathcal{C}_{\mathcal{B}'}[G]$.

Using the rational face-star basis, the map ∂_2 takes the form

$\left(1\right)$	0		0	-1
0	1		0	-1
:	:	·	÷	:
0	0		1	-1
0	0		0	0
:	÷		÷	:
$\int 0$	0	•••	0	0)

since the first r-1 f_i 's now map to basis elements and $\partial_2(f_r)$ can be expressed as $(-1)\sum_{i=1}^{r-1}\partial_2(f_i)$ because $\sum f_i$ is a 2-cycle representing the generator of $H_2(S^2) \cong \mathbb{Z}$. Since the image of ∂_2 is the kernel of ∂_1 , we also see that ∂_1 takes the form

$$\left(\begin{array}{cccc} 0 & \cdots & 0 & \\ \vdots & & \vdots & M \\ 0 & \cdots & 0 & \end{array}\right),$$

where M is an $n \times (n-1)$ matrix.

The third duality isomorphism is defined by declaring the rational face-star basis to be an orthonormal basis for C_1 and using that fact to identify C_1 and C_1^* , it is clear that $(\mathrm{Ad}\langle , \rangle_1)^{-1} \delta_0 \mathrm{Ad}\langle , \rangle_0 \partial_1$ is an $m \times m$ matrix with all entries 0 except for the $(n-1) \times (n-1)$ submatrix in the lower right corner, and $\partial_2 (\mathrm{Ad}\langle , \rangle_2)^{-1} \delta_1 \mathrm{Ad}\langle , \rangle_1$ is an $m \times m$ matrix with all entries 0 except for the $(r-1) \times (r-1)$ submatrix in the upper left corner. Therefore, Δ_1 is in block form for this choice of orthonormal basis.

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