# When graph theory meets knot theory

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ABSTRACT. Since the early 1980s, graph theory has been a favorite topic for undergraduate research due to its accessibility and breadth of applications. By the early 1990s, knot theory was recognized as another such area of mathematics, in large part due to C. Adams' text, <u>The Knot Book</u>. In this paper, we discuss the intersection of these two fields and provide a survey of current work in this area, much of which involved undergraduates. We will present several new directions one could consider for undergraduate work or one's own work.

## 1. Introduction

This survey considers three current areas of study that combine the fields of graph theory and knot theory. Recall that a graph consists of a set of vertices and a set of edges that connect them. A spatial embedding of a graph is, informally, a way to place the graph in space. Historically, mathematicians have studied various graph embedding problems, such as classifying what graphs can be embedded in the plane (which is nicely stated in Kuratowski's Theorem [25]), and for non-planar graphs, what is the fewest number of crossings in a planar drawing (which is a difficult question for general graphs and still the subject of ongoing research, see [23] for example). A fairly recent development has been the investigation of graphs that have non-trivial links and knots in every spatial embedding. We say that a graph is *intrinsically linked* if it contains a pair of cycles that form a non-splittable link in every spatial embedding. Similarly, we say that a graph is *intrinsically knotted* if it contains a cycle that forms a non-trivial knot in every spatial embedding. Conway, Gordon [9], and Sachs [31] showed the complete graph on six vertices,  $K_6$ , is intrinsically linked. We refer the reader to a very accessible proof of this result in Section 8.1 of The Knot Book [1]. Conway and Gordon further showed that  $K_7$ is intrinsically knotted. These results have spawned a significant amount of work, including the complete classification of minor-minimal examples for intrinsically linked graphs by Robertson, Seymour, and Thomas [30]. After the completion of this classification, work has turned to finding graphs in which every embedding has a more complex structure such as finding other minor-minimal intrinsically knotted graphs [17], [16], graphs with cycles with high linking number in every

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spatial embedding [14], as well as graphs with complex linking patterns [11] (see Section 2 for a bit more on what this means).

Recall that a natural generalization of an intrinsically linked graph is an intrinsically *n*-linked graph, for an integer  $n \geq 2$ . A graph is *intrinsically n*-linked if there exists a non-split *n*-component link in every spatial embedding. In Section 2, we will try to survey known results about intrinsically 3-linked graphs, and we present a few less-technical proofs. In particular, we discuss Flapan, Naimi and Pommersheim's [13] result that  $K_{10}$  is the smallest complete graph that is intrinsically 3-linked. We also talk about other examples of intrinsically 3-linked graphs that are minor-minimal or possibly minor-minimal.

In Section 3, we restrict our attention to embeddings of graphs with straight edges. Conway and Gordon's work guarantees a 2-component link in any embedding of  $K_6$  and a knot in any embedding of  $K_7$ , but says nothing of the number of such embeddings. Due to the restrictive nature of straight-edge embeddings, we can determine the possible *number* of links and knots in such embeddings. Theorem 3.1 and 3.2 characterize the number of 2-component links in  $K_6$  and  $K_7$ . Table 1 characterizes the number of stick knots occurring in a large class of straight-edge embeddings of  $K_7$ . This work is of interest to molecular chemists who are trying to synthesize topologically complex molecules. One could imagine that the vertices of these graphs represent atoms and the edges are the bonds of a molecule.

In Section 4, we expand the work of Conway and Gordon by showing in Theorem 4.1 [4] that every  $K_n$   $(n \ge 7)$  contains a knotted Hamiltonian cycle in every spatial embedding.

While we make every effort to explain the machinery necessary for the following results in each section, we refer the reader to <u>The Knot Book</u> [1] and <u>Introduction to Graph Theory</u> [7]. A number of open questions will be posed throughout the sections. For easy reference, the questions will be listed again in Section 5.

## 2. Intrinsically 3-linked graphs

We start this section with a quick introduction to the linking number. Recall that given of a link of two components,  $L_1$  and  $L_2$  (two disjoint circles embedded in space), one computes the linking number of the link by examining a projection (with over and under-crossing information) of the link. Choose an orientation for each component of the link. At each crossing between two components, one of the pictures in Figure 1 will hold. We count +1 for each crossing of the first type (where you can rotate the over-strand counter-clockwise to line up with the under-strand) and -1 for each crossing of the second type. To get the linking number,  $lk(L_1, L_2)$ , take the sum of +1s and -1s and divide by 2. One can show that the absolute value of the linking number is independent of projection, and of chosen orientations (see [1] for further explanation). Note that if  $lk(L_1, L_2) \neq 0$ , then the associated link is non-split. The converse does not hold. That is, there are non-split links with linking number 0 (the Whitehead link is a famous example, see again [1]). Any linking numbers we use will be the ordinary linking number, taken mod 2.

In this section, we survey the known results about intrinsically 3-linked graphs, and we present a few results. Before doing so, we introduce some more terminology. Recall that a graph H is said to be a *minor* of the graph G if H can be obtained from G by a sequence of edge deletions, edge contractions and/or vertex deletions.



FIGURE 1. Computing the linking number.

A graph G is said to be *minor-minimal* with respect to a property, if G has the property, but no minor of G has the property. It follows from the result of Robertson and Seymour [29] that there are only finitely many minor-minimal intrinsically *n*-linked graphs, and since having a n-linkless embedding is preserved by minors (see [26], [13]), a graph is intrinsically *n*-linked if and only if it contains a member of a finite list (not yet determined) of graphs as a minor.

The study of intrinsically 3-linked graphs first appeared briefly in a student paper [19], where the authors showed a 3-component linkless embedding of  $K_{3,3,3}$ . Soon after that paper was written, the first author spoke with Erica Flapan about the problem of finding intrinsically 3-linked graphs. She became interested in determining the lowest value of n such that  $K_n$  is intrinsically n-linked. The first author had the more modest goal of finding an intrinsically 3-linked graph. As a result of this conversation, we formulated the following pasting type lemma, which first appeared in [12], and is easily proven. Recall that if the cycles  $C_2$  and  $C_3$ intersect along an arc, then we may form a new cycle,  $C_2 + C_3$  by using the edges that are only in  $C_2$  or only in  $C_3$ .

LEMMA 2.1. If  $C_1, C_2$ , and  $C_3$  are cycles in an embedded graph,  $C_1$  disjoint from  $C_2$  and  $C_3$ , and  $C_2 \cap C_3$  is an arc, then  $lk(C_1, C_2) + lk(C_1, C_3) = lk(C_1, C_2 + C_3)$ .

#### This leads to:

LEMMA 2.2. [12] Let G be a spatially embedded graph that contains simple closed curves  $C_1, C_2, C_3$  and  $C_4$ . Suppose that  $C_1$  and  $C_4$  are disjoint from each other and both are disjoint from  $C_2$  and  $C_3$ , and  $C_2 \cap C_3$  is an arc. If  $lk(C_1, C_2) = 1$ and  $lk(C_3, C_4) = 1$ , then G contains a non-split 3-component link.

PROOF. If  $lk(C_1, C_3) = 1$  or if  $lk(C_2, C_3) = 1$ , then  $C_1, C_2$  and  $C_3$  form a non-split 3-component link. Similarly, if  $lk(C_1, C_4) = 1$ , then  $C_1, C_3$  and  $C_4$  form a non-split 3-component link. Finally, if  $lk(C_1, C_4) = lk(C_2, C_4) = lk(C_1, C_3) =$  $lk(C_1, C_4) = 0$ , then by Lemma 2.1,  $lk(C_1, C_2 + C_3) = lk(C_1, C_2) + lk(C_1, C_3) = 1$ and  $lk(C_4, C_2 + C_3) = lk(C_4, C_2) + lk(C_4, C_3) = 1$ . Thus  $C_1, C_2 + C_3, C_4$  forms a non-split 3-component link.

One can use this Lemma to show that various graphs are intrinsically 3-linked. For example (see [13]), let J be the graph obtained by pasting two copies of  $K_{4,4}$ along an edge (see Figure 2). Sachs [32] showed that for every spatial embedding of  $K_{4,4}$ , every edge of the graph is contained in a cycle that is non-split linked to



FIGURE 2. The graph J.

another cycle. Consider an arbitrary embedding of J. In one copy of  $K_{4,4}$  there are a pair of cycles with non-zero linking number, call them  $C_1$  and  $C_2$ , and by Sachs' result, we may assume one of the cycles, say  $C_2$ , uses the edge shared by the two copies of  $K_{4,4}$ . In the other copy of  $K_{4,4}$ , there are another pair of cycles with non-zero linking number, call them  $C_3$  and  $C_4$ , and again, we may assume that one of the cycles, say  $C_3$ , uses the shared edge. Thus by Lemma 2.2, there is a 3-component link in this embedding of J. It follows that J is intrinsically 3-linked. It is not known if J is minor-minimal with respect to this property. At the time the paper was being written, the authors of [13] believed that J is either minor-minimal, or the graph obtained from removing the shared edge from J is minor-minimal with respect to being intrinsically 3-linked, though a proof of this was never written down.

The fact that J is intrinsically 3-linked was later generalized in [5] to include the graph obtained from two copies of  $K_7$  pasted along an edge, as well as the graph obtained from  $K_{4,4}$  and  $K_7$  pasted along an edge. We quickly sketch a proof here. We first need the following lemma:

LEMMA 2.3. [5] Let G be a spatial embedding of  $K_7$ , then every edge of G is in a non-split linked cycle.

PROOF. First embed  $K_7$ , then consider an edge  $e_1 = (v_1, v_2)$  in  $K_7$ . The vertices of  $G - v_2$  induce a  $K_6$ . Then vertex  $v_1$  is in a linked cycle in this embedded  $K_6$ , say  $(v_1, v_3, v_4)$  is linked to cycle C. By Lemma 2.2,  $lk((v_1, v_3, v_4), C) = lk((v_1, v_3, v_2), C) + lk((v_1, v_2, v_3, v_4), C)$ , and thus  $e_1$  is in a linked cycle.  $\Box$ 

The proof of the following result is similar to the proof that J is intrinsically 3-linked.

THEOREM 2.1. [5] Let G be a graph formed by identifying an edge of a graph  $G_1$  with an edge from another graph  $G_2$ , where  $G_1$  and  $G_2$  are either  $K_7$  or  $K_{4,4}$ . Then every such G is intrinsically 3-linked.

At this time, we do not know whether the graphs described by this theorem are minor-minimal or not. Before we go further, we review one important definition. Let a, b, and c be vertices of a graph G such that edges (a, b), (a, c) and (b, c) exist. Then a  $\triangle - Y$  exchange on a triangle (a, b, c) of graph G is as follows. Vertex v is added to G, edges (a, b), (a, c) and (b, c) are deleted, and edges (a, v), (b, v) and

(c, v) are added. Given the graph G in Figure 3, the illustration in the Figure depicts the result of  $\triangle - Y$  expansion on triangle *abc*. A  $Y - \triangle$  exchange is the reverse operation.



FIGURE 3. A graph G and the results of a  $\Delta$ -Y exchange.

In [13], the authors were able to find a minor-minimal intrinsically (n + 1)linked graph G(n), for every integer n > 2. By showing that J is not obtainable from G(2) by a sequence of  $\Delta - Y$  and  $Y - \Delta$  moves, they also showed that the set of all minor-minimal intrinsically 3-linked graphs cannot be obtained from one of the graphs in the set by a sequence of  $\Delta - Y$  and  $Y - \Delta$  moves-unlike the set of minor-minimal intrinsically linked graphs which can all be obtained from  $K_6$  by  $\Delta - Y$  and  $Y - \Delta$  moves.

In [12], Flapan, Naimi and Pommersheim were able to determine that  $K_{10}$  was intrinsically 3-linked. By exhibiting a 3-linkless embedding of  $K_9$ , they also established that n = 10 is the smallest n for which  $K_n$  is intrinsically 3-linked. In order to prove their result for  $K_{10}$ , the authors used a careful examination of linking patterns of triangles in spatial embeddings of  $K_9$ , as well as Lemma 2.2. We will briefly discuss those patterns here.

A 4-pattern within an embedded graph, G, consists of a 3-cycle, B, that is linked with four other 3-cycles that can be described as follows. For vertices q,r in G, each 3-cycle linked to B is of the form (q, r, x) where x is one of any four vertices of G other than B, q, and r (see Figure 4).

A 6-pattern within an embedded graph, G, consists of a 3-cycle, B, that is linked with six other 3-cycles that can be described as follows. For vertices p,q,r in G, each 3-cycle linked to B is either of the form (p,q,x) or (p,r,x) where x is one of any three vertices of G other than B, p, q, and r (see Figure 4). We may now state the following Lemma. The proof of this lemma is somewhat technical, so we refer the reader to the original source for a proof.



FIGURE 4. A possible 4-pattern on the left, and a possible 6-pattern on the right

LEMMA 2.4. [12] There exists an embedding of  $K_9$  without any 3-component links. For any embedding of  $K_9$  every linked 3-cycle is in a 4-pattern, a 6-pattern, or a 3-component link.

More recently, O'Donnol [27] has used a clever examination of linking patterns in complete bipartite graphs to show that every embedding of  $K_{2n+1,2n+1}$  contains a non-split link of *n*-components. O'Donnol further showed that for  $n \ge 5$ ,  $K_{4n+1}$ is intrinsically *n*-linked. Even more recently, Drummund-Cole and O'Donnol [10] improved this result by showing that for every n > 1, every embedding of  $K\lfloor \frac{7}{2}n \rfloor$ contains a non-split link of *n*-components. It would be a good project to determine if this is the best one can do for low values of *n*. In particular, is 17 the fewest vertices of an intrinsically 5-linked graph (this number could be as low as 15)? For n = 4, 14 is currently the fewest number of vertices need to guarantee  $K_n$  is intrinsically 4 linked, but this number could be as low as 12. Drummund-Cole and O'Donnol further showed that there exists a function f(n) such that  $\lim_{n\to\infty} \frac{f(n)}{n} = 3$ and, for every n,  $K_{f(n)}$  is intrinsically linked. As 3 vertices are the fewest possible for a link component, this asymptotic result is the best possible.

The quest for finding a complete set of minor-minimal intrinsically 3-linked graphs is still very much alive-there remains much work to be done. In [13], there are two families of intrinsically 3- linked graphs presented. As we mentioned earlier in the paper, one is the single member family consisting of the triangle-free graph J (or possibly some minor of J. If this minor had a 3-cycle, then the family would be more than one member). The other family consists of the graph G(2) described in [13], as well as the other two graphs that can be obtained from G(2) by  $Y - \Delta$ exchanges (one can readily argue that they are intrinsically 3-linked, using the same arguments given in [13]). Moreover, since G(2) is minor-minimal intrinsically 3linked, so are these graphs. This follows from the following lemma, which makes for a good exercise in graph theory. The curious and/or frustrated reader can look up the proof online if they are interested. LEMMA 2.5. [28], [6] Let P be a graph property that is preserved by  $\Delta - Y$  exchanges, and let G' be a graph obtained from G by a sequence of  $\Delta - Y$  moves. If G has property P, and if G' is minor-minimal with property P, then G is also minor-minimal with property P.

The graph J, the graph obtained by pasting two copies of  $K_7$  along an edge, and the graph obtained by pasting an edge of  $K_7$  to an edge of  $K_{4,4}$  may also lead to new families of minor-minimal intrinsically 3-linked graphs-we just do not know yet if these graphs are themselves minor-minimal, or if they can be pared down.

As we mentioned earlier, the authors in [12] showed that  $K_{10}$  is intrinsically 3-linked. Bowlin and the first author [5] later showed, using techniques similar to those used in [12], that the subgraph obtained from  $K_{10}$  by removing 4 edges incident to a common vertex is also intrinsically 3-linked; they also showed that the subgraph obtained from  $K_{10}$  by removing two non-adjacent edges is also intrinsically 3-linked. They were not able to prove that these graphs are minor-minimal (the first author strongly suspects at least the former is). If they were, then by  $\Delta - Y$ exchanges, they would yield two new families of graphs for our set. Finally, Bowlin and Foisy showed that any graph obtained by joining two graphs from the Petersen family by a 6-cycle that has vertices that alternate between copies of the two graphs is intrinsically 3-linked:

THEOREM 2.2. [5] Let G be a graph containing two disjoint graphs from the Petersen family,  $G_1$  and  $G_2$ , as subgraphs. If there are edges between the two subgraphs  $G_1$  and  $G_2$  such that the edges form a 6-cycle with vertices that alternate between  $G_1$  and  $G_2$ , then G is intrinsically 3-linked.

The proof of this theorem requires the use of the following lemma, whose proof is similar to the proof of Lemma 2.2:

LEMMA 2.6. [5] In an embedded graph with mutually disjoint simple closed curves,  $C_1, C_2, C_3$ , and  $C_4$ , and two disjoint paths  $x_1$  and  $x_2$  such that  $x_1$  and  $x_2$  begin in  $C_2$  and end in  $C_3$ , if  $lk(C_1, C_2) = lk(C_3, C_4) = 1$  then the embedding contains a non-split 3-component link.

PROOF (of Theorem 2.2). Let  $\{a_1, a_2, a_3, b_1, b_2, b_3\}$  be the set of vertices that make up the 6-cycle described in the statement of the theorem, where  $\{a_1, a_2, a_3\}$ are in  $G_1$  and  $\{b_1, b_2, b_3\}$  are in  $G_2$ . Embed G. By the pigeonhole principle, at least two vertices in the set  $\{a_1, a_2, a_3\}$  are in a linked cycle within the embedded  $G_1$ (without loss of generality,  $a_1$  and  $a_2$ ), and likewise we may assume that the vertices  $b_1$  and  $b_2$  are in a linked cycle in  $G_2$ . Because of the edges between  $\{a_1, a_2, a_3\}$  and  $\{b_1, b_2, b_3\}$ , we know that there are two disjoint edges between the sets  $\{a_1, a_2\}$  and  $\{b_1, b_2\}$ . By Lemma 2.6, a 3-component link is present in the embedding.

We shall henceforth call a 6-cycle as in the statement of Theorem 2.2 an alternating 6-cycle. We suspect that many of the graphs obtained by joining Petersen graphs by an alternating 6-cycle are minor-minimal with respect to being intrinsically 3-linked. For example, consider two copies of  $K_6$  joined by an alternating 6-cycle, which we will denote by S. We examine the embedding pictured in Figure 5. In the embedded shown, in the  $K_6$  on the left, the only linked cycles are (a, c, e) and (b, d, f). Similarly, for the  $K_6$  on the right, only (A, C, E) is linked with (B, D, F). The only 3-component link in this embedding is (b, d, f), (a, e, c, A, E, C), (B, D, F). If we remove any one of the edges (c, A), (d, f)



FIGURE 5. The graph S is minor-minimal.



FIGURE 6. Removing edge (a, c) results in a 3-linkless embedding.

or (a, e), then the resulting graph has a 3-linkless embedding. If we contract any one of the edges (b, B), (a, b), (d, e), (a, e), then the resulting embedding is 3-linkless.

It remains to show that removing an edge in the class of (a, c) results in a graph with a 3-linkless embedding. This can be seen by examining the embedding depicted in Figure 6 (note that the vertices have been re-labelled slightly).

It will take some time and effort to enumerate exactly what graphs are in the family of all Petersen graphs joined by an alternating 6-cycle. There is, up to isomorphism, only one way to connect copies of  $K_6$ , but for all of the other graphs in the Petersen family, there are multiple ways to connect them. Perhaps Lemma 2.5 might be helpful in efficiently demonstrating that some of these graphs are minor-minimal.

Up to this point in time, all of the minor-minimal intrinsically 3-linked graphs have been shown to be intrinsically 3-linked by using some sort of analogy to Lemma 2.1. For such graphs, the guaranteed 3-link contains at least one cycle that was pasted together from two smaller cycles. (Though it is interesting that Drummund-Cole and O'Donnol [10] have recently shown that every embedding of  $K_{14}$  contains a 3-link of triangles.) Recently some students worked on a related problem, and their work might suggest that there will be some minor-minimal intrinsically 3linked graphs that cannot be proven to be intrinsically 3-linked using an analogy to Lemma 2.1. We briefly describe this work now.

An  $S^1$  embedding of a graph G is an injective map of the vertices of G into  $S^1$ . A *0-sphere* in an  $S^1$  embedding of a graph G is composed of any two vertices that are the endpoints of a simple path in G. We denote a 0-sphere by writing the endpoints of the associated path as an ordered pair. Just as a pair of disjoint cycles forms a link in a spatial embedding, a pair of disjoint 0-spheres (with disjoint underlying paths) forms a link in an  $S^1$  embedding. A link (a, b) and (c, d) is said to be *split* if a and b lie on the same component of  $S^1 - \{c, d\}$ . Thus the link is *non-split* if a and b lie on different components of  $S^1 - \{c, d\}$ . For  $S^1$  embeddings, the mod 2 linking number of two 0-spheres (a, b) and (c, d), denoted lk((a, b), (c, d)), is 0 if and only if (a, b) and (c, d) are split linked and is 1 if and only if (a, b) and (c,d) are non-split linked. An  $S^1$  *n-link* in an  $S^1$  embedding of a graph G is a set of n disjoint 0-spheres in the embedding of G. An n-link in an  $S^1$  embedding is said to be *split* if there are two points, x and y, on the circle such that both components of  $S^1 - \{x, y\}$  contains at least one vertex involved in the *n*-link and every 0-sphere in the link lies entirely on one component of  $S^1 - \{x, y\}$ . Just as some graphs are intrinsically linked in space, some graphs are intrinsically  $S^1$  linked. A graph is intrinsically  $S^1$  linked if every  $S^1$  embedding contains a non-split link. It was shown by Cicotta et al. that the complete minor-minimal set of intrinsically  $S^1$  linked graphs is  $K_4$  and  $K_{3,2}$  [8]. A graph is said to be intrinsically  $S^1$  *n*-linked if every  $S^1$  embedding of the graph contains a non-split *n*-link.

The students easily proved the following analog of Lemma 2.1:

LEMMA 2.7. [6] Given 0-spheres (a, b), (c, d), (c, e), and (d, e) in an  $S^1$  embedding of graph G,  $lk_2((a, b), (c, e)) = lk_2((a, b), (c, d)) + lk_2((a, b), (d, e)).$ 

They also proved the following analog of Theorem 2.1:

THEOREM 2.3. [6] Let G be a graph formed by pasting together graphs A and B, where A and B are each either a  $K_4$  or  $K_{3,2}$ , at a vertex. The graph G is intrinsically  $S^1$  3-linked.

They went on to find 28 minor-minimal intrinsically  $S^1$  3-linked graphs, 6 of which were shown to be intrinsically  $S^1$  3-linked using Lemma 2.7. The other 22 graphs were shown to be intrinsically  $S^1$  3-linked by using other ad hoc methods (it is possible to analyze such graphs by using combinatorics and case checking since there are only finitely many non-equivalent  $S^1$ embedding classes of a given graph). By comparison, all of the intrinsically 3-linked graphs in space have been shown to be intrinsically 3-linked by using some sort of analogy to Lemma 2.7. The work in [6] is thus interesting because it suggests that the intrinsically 3-linked graphs thus far discovered may only be the tip of the iceburg. It is also interesting because it provides a more tractable analogous problem. Hopefully, someone will soon prove that the 28 graphs (or possibly a superset) forms the complete set of minor-minimal intrinsically  $S^1$  3-linked graphs.

In summary, the quest for a complete minor-minimal set of intrinsically 3-linked graphs is going to require some time-consuming methodical work, as well as some breakthroughs. We thus feel it is well-suited to eager and persistent students who have fresh ideas.

We briefly mention some other related results that might be of interest. One could also look for graphs that contain, in every spatial embedding, multi-component

links with various patterns. The authors in [13] were also able to show the existence of an "n-necklace" (a link  $L_1 \cup L_2 \cup ... \cup L_n$ , such that for each i = 1, ..., n - 1,  $L_i \cup L_{i+1}$  is non-split and  $L_n \cup L_1$  is non-split) in every embedding of the graph they call F(n). Flapan, Mellor and Naimi [11] came up with a powerful generalization of this result to show that, given any n and  $\alpha$ , every embedding of any sufficiently large complete graph in  $\mathbb{R}^3$  contains an oriented link with components  $Q_1, ..., Q_n$  such that, for every  $i \neq j$ ,  $|lk(Q_i, Q_j)| \geq \alpha$ . The first author [15] has also shown the existence of a graph that, for every spatial embedding, contains either a 3-component link or a knotted cycle, but it has a knotless embedding and a 3-component linkless embedding.

Finally, we mention one more related open question.

QUESTION 2.1. What is the smallest n, such that, for every straight edge embedding of  $K_n$ , there is a non-split link of 3 components?

We know n is at most 10, but could be 9.

#### 3. Links and knots in straight-edge embeddings of graphs.

In this section, we consider complete graphs composed of straight edges or sticks. A *stick knot* is a knot formed out of rigid straight sticks. Molecular chemists are interested in this type of knot because at the molecular level, molecules are more like rigid sticks than flexible rope, Figure 7. With this application in mind, the following two questions were posed at a knot theory workshop in 2004:

- (1) Does there exist a straight-edge embedding of  $K_6$  with 9 (3-3) links?
- (2) Given a straight-edge embedding of  $K_7$ , how many and what types of knots occur?



FIGURE 7. The trefoil knot and a knotted molecule

The first question was motivated by Conway-Gordon and Sachs' proof that  $K_6$  is intrinsically linked. Any three vertices and adjoining edges form a 3-cycle. In  $K_6$  there are 10 disjoint pairs of 3-cycles. If the edges were allowed to bend and stretch, one could place the vertices and edges of  $K_6$  in space such that all 10 pairs of triangles were linked. But what would happen to the number of links if the edges had to remain straight as in a molecular bond? Due to the techniques used in their

proof, it was known that the number of linked pairs had to be odd. Hence, the question asked if the maximum 9 pairs could be attained.

In regards to the second question,  $K_7$  has 360 Hamiltonian cycles consisting of 7 edges. It is well known that only two non-trivial knots, the trefoil and the figure-8, can be made with 7 sticks. The minimum number of sticks needed to make a knot is 6 and this only occurs for the trefoil. So, to answer the second question, one must not only consider the Hamiltonian cycles on  $K_7$ , but all cycles of length 6 as well.



In 2004 a student of the second author, C. Hughes, showed that any straightedge embedding of  $K_6$  contains either 1 or 3 disjoint 2-component links, thus answering the first question [20]. To do this, she considered the four distinct convex polyhedra that form straight-edge embeddings of  $K_6$  [34] (see Figure 8–11). It was shown that Figures 8 and 9 are ambient isotopic to Figure 10 (note the isotopies preserve the linearity of the edges). Through a series of geometric arguments, Hughes then showed Figure 10 has one 2-linked component and Figure 11 has three distinct 2-linked components, again up to ambient isotopy that preserves the linearity of the edges. Interestingly, in 2007 Huh and Jeon independently showed these same results as well as proving Figure 11 is the only straight-edge embedding of  $K_6$  that contains a knot, a single trefoil [21].

THEOREM 3.1. A straight-edge embedding of  $K_6$  has either one or three 2component links. In 2006, the second author and P. Arbisi extended the work of Hughes, Huh, and Jeon by classifying all the 2-component links in certain straight-edge embeddings of  $K_7$ . This was a challenging task as there are five distinct embeddings of  $K_7$  that form convex polyhedra. In addition, unlike  $K_6$  that has 10 pairs of disjoint 3-cycles,  $K_7$  has 70 pairs of disjoint 3-cycles. With one extra vertex, there is now the possibility of 3-cyles linking with 4-cycles. There are 35 such pairs.



FIGURE 15.  $K_7^4$  [3,4,4,4,5,5,5] FIGURE 16.

5] FIGURE 16.  $K_7^5$  [4,4,4,4,4,5,5]

While Hughes was able to argue that three of the embeddings of  $K_6$  were equivalent under ambient isotopies that preserve linearity of edges, this was not readily apparent with  $K_7$ . Instead, the second author and Arbisi focused on the 5 distinct straight-edge embeddings of  $K_7$  that form convex polyhedra [34](see Figures 12–16). In order to distinguish the five embeddings, the figures are labeled with the *external* degree of each vertex. That is, the number associated with each vertex represents the number of edges on the hull that are incident to it. For the remainder of the section, when we refer to the degree of a vertex, we actually mean the number of edges from the hull incident to that vertex, unless otherwise stated.

THEOREM 3.2. The minimum number of linked components in any straight-edge embedding of  $K_7$  which forms a convex polyhedron of seven vertices is twenty-one, and the maximum number of linked components in  $K_7$  is forty-eight. Specifically, we have the following:

	$K_7^1$	$K_{7}^{2}$		$K_{7}^{3}$		$K_{7}^{4}$				$K_{7}^{5}$		
(3-3)	7	7	9	7	9	9	11	13	15	13	15	17
(3-4)	14	14	18	14	18	18	22	23,26	27,30	23,26	27,30	31

The main method employed for the results in Theorem 3.2 was to consider a specific embedding of  $K_7$ , systematically remove a vertex and its adjoining edges, then determine which version of  $K_6$  remained:  $K_6^1$  (Figure 10) with one (3-3) link or  $K_6^2$  (Figure 11) with three (3-3) links.  $K_7^1-K_7^3$  were relatively straight-forward. If a vertex was removed that was not of external degree of 6, then the resulting embedding of  $K_6$  had only one (3,3) link ( $K_6^1$ ). Removing the degree 6 vertex was a bit more challenging and would result in either  $K_6^1$  or  $K_6^2$ , depending on the arrangement of the internal edges in the given embedding of  $K_7$ . This resulted in a varying number of links for  $K_7^2$  and  $K_7^3$ .

Without any degree 6 vertices,  $K_7^4$  and  $K_7^5$  were considerably more challenging. Thankfully, we were able to determine the arrangement of the vertices in various embeddings of  $K_7^4$  and  $K_7^5$  via Steinitz's Theorem which states that a graph G is isomorphic to the vertex-edge graph of a 3-D polyhedron if and only if G is planar and 3-connected. However, we were still finding some inconsistencies in these two embeddings compared to the previous three. Specifically, the number of (3,4) links was not always twice the number of (3,3) links as with the prior cases. This lead us to the following results.

PROPOSITION 3.1. In a straight-edge embedding of  $K_7$ , every 3-cycle is contained in 0, 2, or 4 (3,3) links.

To see why this is true, consider a 3-cycle, A, in a straight-edge embedding of  $K_7$ . Either A is contained in a link or not. Suppose that A is contained in a (3,3) link. The four vertices not contained in A form a straight-edge embedding of  $K_4$ . There are only two possible ways that A will link with one of the faces of the tetrahedron, please see Figure 17.



FIGURE 17. The two ways a 3-cycle can appear in a link.

Figure 17(b) is particularly interesting as such a linking will create 4 (3,3) links, but only 1 (3,4) linking. In contrast, Figure 17(a) creates 2 (3,3) links and 2 (3,4) links. The reason that  $K_7^4$  and  $K_7^5$  were more challenging cases is due to the following.

PROPOSITION 3.2. In a straight-edge embedding of  $K_7$ , only  $K_7^4$  or  $K_7^5$  can have a 4-link tetrahedron.

There are obvious directions in which this work could continue. For the problem under consideration, each embedding of  $K_7$  formed a convex polyhedron with seven vertices. What about an embedding of  $K_7$  which forms a convex polyhedron with 4 vertices? That is, four of the vertices form the hull of the polyhedron and the other three vertices are internal. It seems reasonable that such embeddings are isomorphic to one of the five cases with seven external vertices, but this is not obvious. Moreover, as the number of vertices increases, it seems that one could construct an example of an embedding of a complete graph on n vertices where at least one of the vertices is internal and can not be passed to the hull of the embedding via ambient isotopies that preserve the linearity of the edges. Recently the second author and his student, R. Grotheer, constructed a subgraph of  $K_9$  with one internal vertex that can not be passed to the surface of the hull via ambient isotopies that preserve the linearity of the edges [18]. So one may ask, given a straight-edge embedding G of  $K_n$ ,  $7 \le n \le 8$ , with  $4 \le k \le 8$  external vertices and m = n - k internal vertices, is G always isomorphic to an embedding of  $K_n$  with n external vertices?

Another direction of study is to consider  $K_n$ ,  $n \ge 7$ . While  $K_6$  has only 10 disjoint triangle pairs to consider,  $K_7$  has 70, and  $K_8$  has 280. Moreover, with  $K_6$  there were only (3-3) links.  $K_7$  introduced (3-4) links and for  $K_8$ , one would have to consider (3-3), (3-4), (3-5), and (4-4) links. Whereas there were only 5 distinct convex polyhedral embeddings of  $K_7$ , it is well known there are 14 for  $K_8$  (see, for example [34]). So, given a straight-edge embedding of  $K_n$ , how many (k, m) links does it contain, where  $3 \le k \le n-3$  and  $3 \le m \le n-k$ ? Clearly this is an ambitious question. Possibly a more attainable question is the following: Given a straight-edge embedding of  $K_n$ , what is an upper or lower bound for the number of (k,m) links it contains,  $3 \le k \le n-3$  and  $3 \le m \le n-k$ ?

We now turn our attention to the second question posed at the knot theory workshop: Given a straight-edge embedding of  $K_7$ , how many and what types of knots occur? Using the insight gained from the work with Arbisi, the second author and R. Grotheer were able enumerate all the possible stick knots in the straightedge embeddings of  $K_7$ , Figure 12–16[18]. There are only two types of knots that can be made with 7 or fewer sticks: the trefoil requires 6 and the figure-8 requires 7.

Table 1 summarizes the findings. We counted the number of cycles possible for each embedding that had 0 though 6 internal edges. Next, we partitioned the problem according to the number of internal edges used in a cycle and then found the number of cycles that would occur in such embeddings. Curiously,  $K_7^1$  has only one knot. Also,  $K_7^5$  was the only embedding that had a figure-8 knot, the rest were all trefoils.

This work extends naturally to our next topic, knotted Hamiltonian cycles in spatial embeddings of graphs.

Internal Edges	$C_{\mathcal{Y}cles}$	$K_{nots}$	$C_{\mathcal{Y}cles}$	$K_{nots}$	$C_{\mathcal{Y}cles}$	$K_{nots}$	$C_{ycles}$	$K_{nots}$	$C_{ycles}$	$K_{nots}$
0	14	0	18	0	17	0	24	0	30	0
1	80	0	72	0	92	0	96	0	90	0
2	164	0	174	0	143	0	123	0	120	0
3	88	1	78	1, 3	91	0, 1	90	2, 3	90	1, 2, 3, 4, 5
4	14	0	18	0,2	16	0, 1, 2	24	0,1	20	2, 4
5	0	0	0	0	1	0, 1	3	0	10	1, 5
6	0	0	0	0	0	0	0	0	0	0
	$K_7^1$		$K_{7}^{2}$			$K_{7}^{3}$	$K_7^4$		$K_{7}^{5}$	

TABLE 1. The number of knots appearing in a straight-edge embedding of  $K_7$ .

## 4. Knotted Hamiltonian Cycles in Spatial Embeddings of Graphs.

Conway and Gordon's beautiful proof that  $K_7$  is intrinsically knotted also shows that  $K_7$  has a knotted Hamiltonian cycle in every spatial embedding. What other graphs have this quality? As Kohara and Suzuki [24] point out, of the graphs obtained from  $K_7$  by  $\Delta - Y$  exchanges, all except the graph they call  $C_{14}$  are known to have embeddings without Hamiltonian knots. In a beautiful paper[33], Shimabara later showed that  $K_{5,5}$  also has a knotted Hamiltonian cycle in every spatial embedding.

In [4], the authors show that every embedding of  $K_n$ , for  $n \ge 7$  contains a knotted Hamiltonian cycle. Here we will present the proof of this result (for background on Arf invariant, see [1] and [22]).

LEMMA 4.1. [4] In every spatial embedding of  $K_7$ , there exists an edge of  $K_7$  that is contained in an odd number of Hamiltonian cycles with non-zero Arf invariant.

PROOF. Consider an arbitrary embedding of  $K_7$ . By Conway-Gordon's result [9], the sum of the Arf invariants of all Hamiltonian cycles in an arbitrary embedding of  $K_7$  must be odd. Thus, in the given embedding there must be an odd number of Hamiltonian cycles with non-zero Arf invariant. Let's say the number of such cycles is 2n + 1. Now, if we count up the edges of such cycles, we get that a grand total of 7(2n + 1) edges (counting multiplicities) are in a cycle with non-zero Arf invariant. On the other hand, if we number the edges of  $K_7$  as  $e_1, \ldots e_{21}$ , and let  $n_i$ ,  $i = 1, 2, \ldots, 21$  stand for the number of Hamiltonian cycles with nonzero Arf invariant that contain  $e_i$ , then we must have that  $\sum_{i=1}^{21} n_i = 7(2n + 1)$ , thus  $\sum_{i=1}^{21} n_i$  must be odd. It follows that at least one of the  $n_i$  must be odd, and our lemma is proven.

THEOREM 4.1. [4] Every  $K_n$ , for  $n \ge 7$  contains a knotted Hamiltonian cycle in every spatial embedding.

**PROOF.** We will prove the theorem for  $K_8$ . The proof for general *n* is similar. Embed  $K_8$ . Consider the embedding of the subgraph  $G_7$  induced by seven vertices of  $K_8$ , and let v denote the eighth vertex, and let  $G_7$  denote the subgraph on 7 vertices. By the previous lemma, the embedded  $G_7$  contains an edge that is contained in an odd number of Hamiltonian cycles with non-zero Arf invariant; we denote this edge e, and let  $w_1$  and  $w_2$  denote the vertices of e. Now, we ignore the edge e, and consider the subdivided  $K_7$  that results from replacing e with the edges  $(v, w_1)$  and  $(v, w_2)$ . We denote this subdivided  $K_7$  by  $G'_7$ . Ignoring the degree 2 vertex v, the embedded  $G'_7$  must have an odd number of Hamiltonian cycles with non-zero Arf invariant. Since there was an odd number of Hamiltonian cycles of  $G_7$  through the edge e with non-zero Arf invariant, there is an even number of Hamiltonian cycles in  $G_7$  that do not contain e and with non-zero Arf invariant. The Hamiltonian cycles of  $G_7$  not containing e are exactly the same as the Hamiltonian cycles in  $G'_7$ not containing the edges  $(v, w_1)$  and  $(v, w_2)$ . Thus, in the embedding of  $G'_7$ , there must be an odd number of Hamiltonian cycles through the edges  $(v, w_1)$  and  $(v, w_2)$ with non-zero Arf invariant. Such a cycle is a Hamiltonian cycle in  $K_8$ . Thus, in the original embedded  $K_8$ , there must be a knotted Hamiltonian cycle.  $\square$ 

We note here that Susan Beckhardt [3], a student at Union College, has been able to adapt Conway and Gordon's proof for  $K_7$  to prove that  $K_8$  has a knotted Hamiltonian cycle in every spatial embedding. She was not able to extend her result to  $K_9$ . We also note here that the proof of Theorem 4.1 can be used to show that every edge of  $K_9$  is contained in at least two knotted Hamiltonian cycles in every spatial embedding of  $K_9$ . This can be seen by removing an edge, call it e, from  $K_9$ . The vertices disjoint from e induce a  $K_7$  subgraph. In an arbitrary embedding of  $K_9$ , consider the embedded sub- $K_7$ . One of its edges must lie in an odd number of Hamiltonian cycles with non-zero Arf invariant. We denote this edge f. The edges e and f are connected by 4 different edges, which we shall denote  $e_1, e_2, e_3, e_4$ . Without loss of generality,  $e_1$  and  $e_2$  share no vertex, and neither do  $e_3$  and  $e_4$ . If we replace the edge f with the 4- (vertex) path  $(e_1, e, e_2)$ , then there is a knotted Hamiltonian cycle through the 4-path. Similarly, there is a knotted Hamiltonian cycle through the 4-path  $(e_3, e, e_4)$ . Thus, there are at least two different knotted Hamiltonian cycles through the edge e. One can use an analogous argument to show that every 3-path in  $K_{10}$  is contained in at least two knotted Hamiltonian cycles in every spatial embedding, and in general, every (n-7)-path in  $K_n$  is contained in at least two knotted Hamiltonian cycles in every spatial embedding, for  $n \geq 9$ .

This reasoning allows us to estimate a minimum number of knotted Hamiltonian cycles in every spatial embedding of  $K_n$  for n > 8. One need only compute the number of paths of length (n - 7), then multiply by 2 and divide by n (because every Hamiltonian cycle in  $K_n$  contains exactly n paths of length (n - 7)). To get double the number of paths of length (n - 7) in  $K_n$ , one merely computes n(n - 1)(n - 2)....(8). Dividing by n gives our lower bound:

THEOREM 4.2. [4] For n > 8, the minimum number of knotted Hamiltonian cycles in every embedding of  $K_n$  is at least (n-1)(n-2)...(9)(8).

QUESTION 4.1. Can the lower bound on the number of knotted Hamiltonian cycles in every spatial embedding of  $K_n$  given in Theorem 4.2 be improved?

The lower bound of at least 1 Hamiltonian knotted cycle in every spatial embedding of  $K_8$  was improved to 3 in [4], using techniques of Shimabara [33]. This leads to the open question of what is the minimum number of knotted Hamiltonian cycles in every spatial embedding of  $K_8$  (by a result in [4], it's either 3, 9, 15, or 21). Every straight edge embedding? Finally, we bring up the question of whether or not every spatial embedding of  $K_{3,3,1,1}$  contains a knotted Hamiltonian cycle? Kohara and Suzuki [24] show an embedding of  $K_{3,3,1,1}$  with exactly one knotted Hamiltonian cycle in the form of a trefoil knot, and they show another embedding of  $K_{3,3,1,1}$  with exactly two knotted Hamiltonian cycles, each in the form of a trefoil. Foisy's proof [17] that  $K_{3,3,1,1}$  is intrinsically knotted does not prove that there exists a knotted Hamiltonian cycle in every spatial embedding. It is also unknown at this time if  $K_{3,3,1,1}$  contains a knotted Hamiltonian cycle in every straight-edge embedding.

#### 5. Questions and Acknowledgments

We conclude with a listing of the open questions presented in the article.

QUESTION 5.1. Determine the complete set of minor-minimal intrinsically 3linked graphs. Are the subgraphs of  $K_{10}$  described in [5] minor-minimal intrinsically 3-linked?

QUESTION 5.2. Is  $K_{14}$  the smallest complete graph that contains a 3-link of triangles in every spatial embedding [10]? (At this point,  $K_{10}$  has not been ruled out.)

QUESTION 5.3. What is the smallest n, such that, for every straight edge embedding of  $K_n$ , there is a non-split link of 3 components? (n is at most 10, but could be 9.)

QUESTION 5.4. Given a straight-edge embedding G of  $K_n$ ,  $7 \le n \le 8$ , with  $4 \le k \le 8$  external vertices and m = n - k internal vertices, is G always isomorphic to an embedding of  $K_n$  with n external vertices?

QUESTION 5.5. Given a straight-edge embedding of  $K_n$ , how many (k, m) links does it contain, where  $3 \le k \le n-3$  and  $3 \le m \le n-k$ ?

Clearly this is an ambitious question. Possibly a more attainable question is the following:

QUESTION 5.6. Given a straight-edge embedding of  $K_n$ , what is an upper or lower bound for the number of (k,m) links it contains,  $3 \le k \le n-3$  and  $3 \le m \le n-k$ ?

QUESTION 5.7. What is the minimum number of knotted Hamiltonian cycles in every spatial embedding of  $K_8$  (from [4], it's either 3, 9, 15, or 21)? Every straight edge embedding?

QUESTION 5.8. Does every spatial embedding of  $K_{3,3,1,1}$  contain a knotted Hamiltonian cycle? Every straight-edge embedding?

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