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Stick number of non-paneled knotless spatial graphs

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Abstract. We show that the minimum number of sticks required to construct a non-paneled knotless embedding of K_4 is 8 and of K_5 is 12 or 13. We use our results about K_4 to show that the probability that a random linear embedding of $K_{3,3}$ in a cube is in the form of a Möbius ladder is 0.97380 ± 0.00003, and offer this as a possible explanation for why $K_{3,3}$ subgraphs of metalloproteins occur primarily in this form.

Contents

1. Introduction

Chemists introduced the term *ravel* in 2008 to describe a hypothetical molecular structure whose topological complexity is the result of "an entanglement of edges around a vertex that contains no knots or links" [1]. The first such molecule was synthesized by Feng Li et al. in 2011 [13]. In order to formalize this concept mathematically, spatial graph theorists define an embedding G of an abstractly planar graph in $\mathbb{R}^3$ to be a *ravel* if G is non-planar but contains no non-trivial knots or links. Such embedded graphs are closely related to *almost trivial graphs*, which are abstractly planar graphs with non-planar embeddings such that removing any edge from the embedded graph makes it planar. In fact, any almost trivial graph is a ravel, though the converse is not true. Probably the most famous example of such a graph is Kinoshita's θ-curve [11, 12]. In order to extend the idea

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of a ravel to graphs which are not abstractly planar, we consider embedded graphs which contain no non-trivial knots yet contain at least one cycle which does not bound a disk in the complement of the graph. In particular, we have the following definition.

Definition 1.1. A graph embedded in $\mathbb{R}^3$ is said to be *paneled* if every cycle in the graph bounds a disk whose interior is disjoint from the graph.

A number of significant results have been obtained about paneled graphs. Of particular note, Robertson, Seymour, and Thomas proved that a graph has a linkless embedding if and only if it has a paneled embedding, which in turn occurs if and only if the graph does not contain one of the seven graphs in the Petersen family as a minor [16]. In the same paper, they showed that a given embedding of a graph is paneled if and only if the complement of every subgraph has free fundamental group. In addition, they proved that up to homeomorphism, $K_{3,3}$ and K_5 each have a unique paneled embedding.

A piecewise linear embedding of a knot, link, or graph in $\mathbb{R}^3$ is said to be a *stick* embedding. The *stick number* of a knot or link is the smallest number of sticks that are required to construct it. Numerous results have been obtained about the stick number of knots and links. But the concept of stick number can also be applied to embedded graphs. In particular, we define the *non-paneled knotless stick number* of a graph to be the minimum number of sticks required to create an embedding of the graph which is not paneled and yet contains no knots. For example, Huh and Oh [10] showed that the non-paneled knotless stick number of a θ-graph is 8.

We are interested in the non-paneled knotless stick number of complete graphs. Note that K_3 is paneled if and only if it is knotless, and every embedding of K_n with $n \geq 7$ contains a non-trivial knot [2]. Thus neither K_3 nor K_n with $n \geq 7$ can have a non-paneled knotless stick number. On the other hand, there is a linear embedding of K_6 which contains no knot, and we know from [16] that no embedding of K_6 is paneled. Hence the non-paneled knotless stick number of K_6 is 15 (its number of edges). So the only complete graphs whose non-paneled knotless stick number is unknown are K_4 and K_5.

In Section 2, we show that the non-paneled knotless stick number of K_4 is 9. Then in Section 3, we apply this result to study embeddings of $K_{3,3}$ as subgraphs of metalloproteins, and offer a possible explanation for why such subgraphs seem to occur primarily in the form of a Möbius ladder (i.e., a Möbius strip where the surface is replaced by a ladder with three rungs). Finally, in Section 4, we show that the non-paneled knotless stick number of K_5 is either 12 or 13.

2. Stick number for non-paneled knotless embeddings of K_4

In order to determine the stick number of a non-paneled knotless K_4, we note that the minimum number of sticks of an embedding of K_4 is equal to the number of edges, which is 6. Thus our first step is to show that every 6-stick and 7-stick embedding of K_4 is paneled. Then we will analyze the different cases for an 8-stick embedding — in the first case, the embedding of K_4 has a single edge consisting of three sticks; in the other cases, the embedding has two different edges each composed of two sticks, and these two edges may or may not share a vertex. Our basic strategy is to restrict the number of configurations we need to analyze by noting that if an embedding of K_4 can be isotoped to one that only has 7 sticks by removing one of the degree 2 vertices, then the embedding must be paneled. We use the following definition from [10].

Definition 2.1. Let P be a linear embedding of a graph G. A triangle determined by two adjacent sticks is said to be *reducible* if its interior is disjoint from the edges of P. Otherwise, it is said to be *irreducible.*

Let P be a linear embedding of a graph G with a degree 2 vertex v adjacent to vertices v_1 and v_2. If the triangle determined by the edges $\overline{vv_1}$ and $\overline{vv_2}$ is reducible, then the image of the embedding P is ambient isotopic to one where the 2-stick segment $\overline{v_1vv_2}$ is replaced by a single stick $\overline{v_1v_2}$. Hence, if a non-paneled knotless stick embedding of a graph has a minimum number of sticks, then every triangle determined by the edges incident to a degree 2 vertex must be irreducible. We utilize this property to restrict the possible configurations of non-paneled embeddings of K_4.

Lemma 2.2. *A non-paneled stick embedding of K_4 must contain at least 8 sticks.*

Proof. An embedding of K_4 which has only 6 sticks is a linear embedding, which is paneled because it necessarily has the form of a tetrahedron.

Suppose that there exists a non-paneled stick embedding of K_4 which has only 7 sticks. Then precisely one of the edges is composed of 2 sticks. We can think of the stick graph as a linear embedding of a graph with five vertices one of which has degree 2. Label the vertices v_1, v_2, v_3, v_4, v_5, where v_2 is the vertex of degree 2 and is adjacent to v_1 and v_3. The triangle $\langle v_1, v_2, v_3\rangle$ must be irreducible, since otherwise the embedding would be isotopic to an embedding with only 6 sticks which we saw is paneled. Thus the edge $\overline{v_4v_5}$ must pierce the triangle $\langle v_1, v_2, v_3\rangle$ as illustrated in Figure 1.

But now adding back the linear segments connecting vertices v_1 and v_3 to vertices v_4 and v_5 (illustrated with dotted segments in Figure 1) yields an embedding of K_4 that is isotopic to a paneled one, contradicting the assumption that our embedding is not paneled. □

The following lemmas deal with the three combinatorially distinct types of 8-stick embeddings of K_4.

Lemma 2.3. *An 8-stick embedding of K_4 with a single edge consisting of 3 sticks is either paneled or contains a knot.*

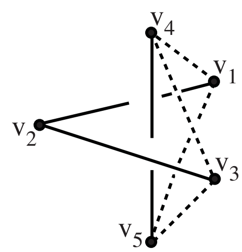

FIGURE 1. Even though the triangle $\langle v_1, v_2, v_3\rangle$ is pierced by $\overline{v_4v_5}$, this embedding is paneled.

Proof. We consider an 8-stick embedding of K_4 as a graph on 6 vertices. We denote the vertices of K_4 by v_1, v_2, v_3, v_4, where the edge between v_3 and v_4 has 3 sticks with intermediate degree 2 vertices v_5 and v_6, so that the edge from v_3 to v_4 is the path $\overline{v_3v_5v_6v_4}$.

We saw in Lemma 2.2 that the stick number of a non-paneled K_4 is at least 8. Thus if the embedding of K_4 is non-paneled, then the triangles $\langle v_4, v_6, v_5\rangle$ and $\langle v_3, v_5, v_6\rangle$ must be irreducible. Without loss of generality, either $\overline{v_1v_2}$ or $\overline{v_2v_3}$ pierces the triangle $\langle v_4, v_6, v_5\rangle$. In either case, up to an affine transformation, we may assume that the piercing edge is orthogonal to the triangle $\langle v_4, v_6, v_5\rangle$, which lies in the horizontal plane.

Case 1: $\overline{v_2v_3}$ pierces $\langle v_4, v_6, v_5\rangle$ and $\overline{v_1v_2}$ does not pierce $\langle v_4, v_6, v_5\rangle$.

In order for the triangle $\langle v_3, v_5, v_6\rangle$ to be irreducible, $\overline{v_1v_4}$ must intersect the triangle. There are two subcases according to whether $\overline{v_1v_4}$ goes in front or behind $\overline{v_2v_3}$. In the first subcase the embedding contains a knot, while in the second subcase the embedding is paneled (see Figure 2).

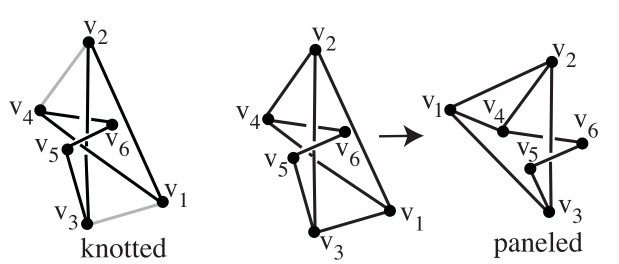

FIGURE 2. If $\overline{v_2v_3}$ pierces $\langle v_4, v_6, v_5\rangle$ and $\overline{v_1v_2}$ does not, the embedding either contains a knot or is paneled.

Case 2: Both $\overline{v_1v_2}$ and $\overline{v_2v_3}$ pierce $\langle v_4, v_6, v_5\rangle$

As in Case 1, there are two subcases according to whether $\overline{v_1v_4}$ goes in front or behind $\overline{v_2v_3}$. However, both embeddings are isotopic to the same paneled embedding as illustrated in Figure 3.

Case 3: $\overline{v_1v_2}$ pierces $\langle v_4, v_6, v_5\rangle$ and $\overline{v_2v_3}$ does not pierce $\langle v_4, v_6, v_5\rangle$.

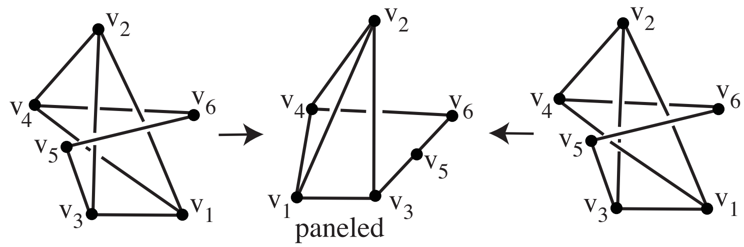

FIGURE 3. If both $\overline{v_1v_2}$ and $\overline{v_2v_3}$ pierce $\overline{v_4v_6v_5}$, the embedding is paneled.

In this case, the irreducibility of the triangle $\langle v_3, v_5, v_6\rangle$ implies that, up to symmetry, either $\overline{v_1v_4}$ or $\overline{v_1v_2}$ pierces it. If $\overline{v_1v_4}$ pierces $\langle v_3, v_5, v_6\rangle$, then (since $\overline{v_1v_2}$ is orthogonal to $\langle v_4, v_6, v_5\rangle$) so must $\overline{v_1v_2}$. Hence we obtain the paneled embedding in Figure 4.

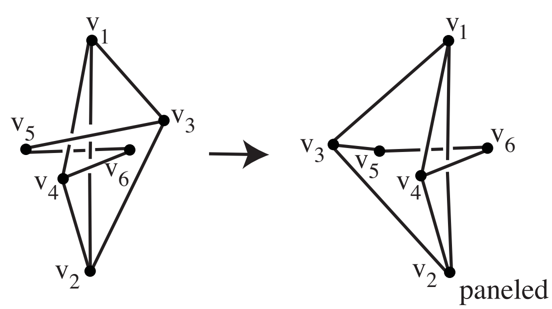

FIGURE 4. If $\overline{v_1v_4}$ pierces $\langle v_3, v_5, v_6\rangle$, then so must $\overline{v_1v_2}$. Hence the embedding is paneled.

Otherwise, $\overline{v_1v_2}$ pierces $\langle v_3, v_5, v_6\rangle$ and $\overline{v_1v_4}$ does not. Now there are two subcases according to whether v_3 is below or above the plane determined by the triangle $\langle v_4, v_6, v_5\rangle$. However, in both subcases the embedding contains a knot, as illustrated in Figure 5. □

Lemma 2.4. *An 8-stick embedding of K_4 with two disjoint edges each consisting of two sticks is either paneled or contains a knot.*

Proof. We again consider an 8-stick embedding of K_4 as a graph on 6 vertices. Label the vertices v_1, v_2, v_3, v_4, v_5, v_6 so that v_2 and v_5 each have degree 2 and are adjacent to v_1, v_3 and v_4, v_6, respectively. Thus there is no edge between v_1 and v_3 and no edge between v_4 and v_6.

Suppose the embedding is non-paneled. Then the triangle $\langle v_1, v_2, v_3\rangle$ must be irreducible, since otherwise the K_4 would be isotopic to a 7-stick embedding, which we saw is necessarily paneled. Thus, without loss of generality,

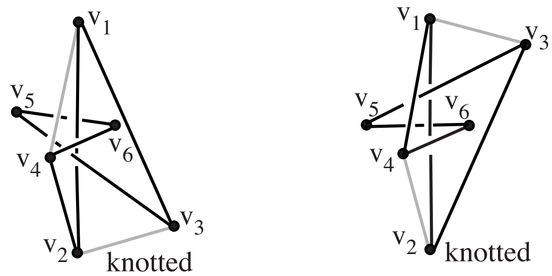

FIGURE 5. If $\overline{v_1v_2}$ pierces $\langle v_3, v_5, v_6\rangle$, then the embedding contains a knot.

the edge $\overline{v_4v_5}$ pierces the triangle $\langle v_1, v_2, v_3\rangle$. Up to an affine transformation, we may further assume that $\overline{v_4v_5}$ is orthogonal to the triangle $\langle v_1, v_2, v_3\rangle$.

Now, the triangle $\langle v_4, v_5, v_6\rangle$ must also be irreducible, since otherwise the embedding would again be isotopic to a 7-stick embedding. So either $\overline{v_1v_2}$ or $\overline{v_2v_3}$ pierces the triangle $\langle v_4, v_5, v_6\rangle$. Up to symmetry, these two cases are the same; so we assume $\overline{v_2v_3}$ pierces the triangle $\langle v_4, v_5, v_6\rangle$.

Note we can always isotope v_6 out of the plane determined by $\langle v_1, v_2, v_3\rangle$. If v_6 is below the plane of $\langle v_1, v_2, v_3\rangle$, then we have to consider the cases where the edge $\overline{v_1v_6}$ is in front of or behind the edge $\overline{v_4v_5}$. However, as we see in Figure 6, both of these cases are paneled.

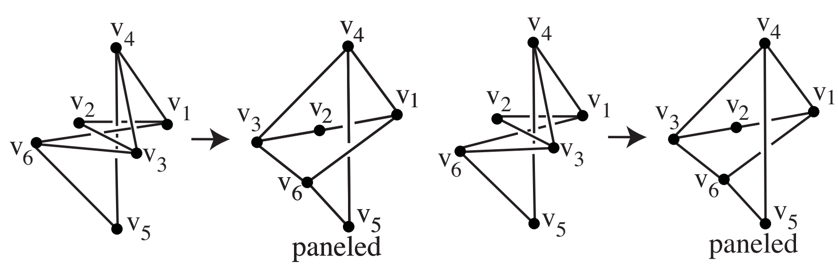

FIGURE 6. If v_6 is below the plane, then the embedding is paneled.

If v_6 is above the plane determined by $\langle v_1, v_2, v_3\rangle$, then we consider whether the edge $\overline{v_1v_6}$ is in front of or behind $\overline{v_4v_5}$ and $\overline{v_3v_4}$. As shown in Figures 7-8, two of the embeddings are paneled and the third contains a knot. □

Lemma 2.5. *An* 8*-stick embedding of* K_4 *such that two adjacent edges consist of two sticks each is either paneled or contains a knot.*

Proof. Again we consider an 8-stick embedding of K_4 as a graph on 6 vertices. We let the degree 3 vertices of K_4 be labeled v_1, v_2, v_3, v_4, the

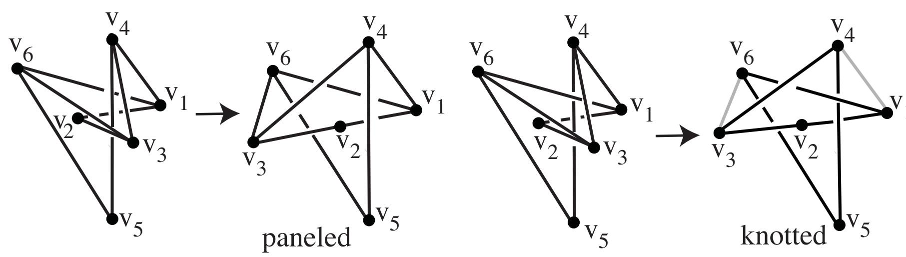

FIGURE 7. Here v_6 is above the plane. If $\overline{v_1v_6}$ is behind $\overline{v_4v_5}$ and $\overline{v_3v_4}$, the embedding is paneled. If $\overline{v_1v_6}$ is in front of $\overline{v_4v_5}$ but behind $\overline{v_3v_4}$, the embedding contains a knot.

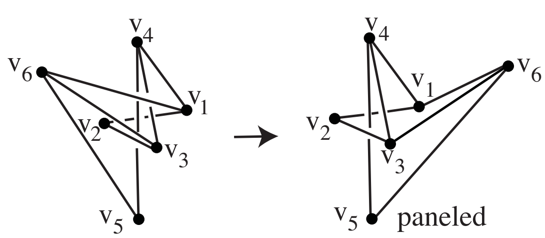

FIGURE 8. If v_6 is above the plane and $\overline{v_1v_6}$ is in front of both $\overline{v_4v_5}$ and $\overline{v_3v_4}$, then the embedding is paneled.

edge between v_1 and v_2 contain vertex v_5, and the edge between v_2 and v_3 contain vertex v_6.

If the embedding is non-paneled, then the triangles $\langle v_1, v_5, v_2\rangle$ and $\langle v_2, v_6, v_3\rangle$ must both be irreducible. Hence one of the edges $\overline{v_3v_4}$ or $\overline{v_3v_6}$ must pierce the triangle $\langle v_1, v_5, v_2\rangle$, and one of the edges $\overline{v_1v_4}$ or $\overline{v_1v_5}$ must pierce the triangle $\langle v_2, v_6, v_3\rangle$. In each case, we may assume that, up to affine transformation, the edge is orthogonal to the triangle it pierces. Thus if only $\overline{v_3v_4}$ pierces the triangle $\langle v_1, v_5, v_2\rangle$, then $\overline{v_1v_4}$ cannot pierce $\langle v_2, v_6, v_3\rangle$; and if $\overline{v_3v_6}$ pierces the triangle $\langle v_1, v_5, v_2\rangle$, then $\overline{v_1v_5}$ cannot pierce $\langle v_2, v_6, v_3\rangle$.

Case 1: Only the edge $\overline{v_3v_4}$ pierces the triangle $\langle v_1, v_5, v_2\rangle$.

The location of v_6 must be such that $\langle v_2, v_6, v_3\rangle$ is pierced by $\overline{v_1v_5}$. Since v_3 is above the plane of $\langle v_1, v_5, v_2\rangle$, this means v_6 must be below the plane of $\langle v_1, v_5, v_2\rangle$. Up to isotopy, this yields the configurations in Figure 9, where the different cases are determined by whether the edge $\overline{v_6v_2}$ is behind both $\overline{v_1v_4}$ and $\overline{v_3v_4}$ (illustrated in the first diagram), is in front of both $\overline{v_1v_4}$ and $\overline{v_3v_4}$ (illlustrated in the third diagram), or passes between $\overline{v_1v_4}$ and $\overline{v_3v_4}$ (illustrated in the fourth diagram). The first and third configurations are isotopic to the second and paneled, and the fourth configuration contains a knot.

Case 2: $\overline{v_3v_6}$ pierces the triangle $\langle v_1, v_5, v_2\rangle$.

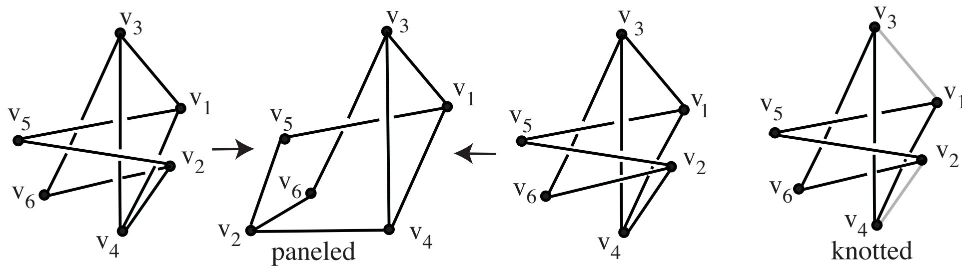

FIGURE 9. $\overline{v_1v_5}$ pierces $\langle v_2, v_6, v_3\rangle$, so $\overline{v_2v_6}$ must pass either behind, in front of, or between $\overline{v_1v_4}$ and $\overline{v_3v_4}$.

In this case, the location of v_4 must be such that $\langle v_2, v_6, v_3\rangle$ is pierced by $\overline{v_1v_4}$. Thus $\overline{v_2v_5}$ must pass either in front of, behind, or between $\overline{v_1v_4}$ and $\overline{v_3v_4}$. If it is in front or behind both $\overline{v_1v_4}$ and $\overline{v_3v_4}$ (illustrated in the first and third diagrams in Figure 10), then the configuration is paneled. If it is between $\overline{v_1v_4}$ and $\overline{v_3v_4}$ (illustrated in the fourth diagram of Figure 10), then the configuration contains a knot. □

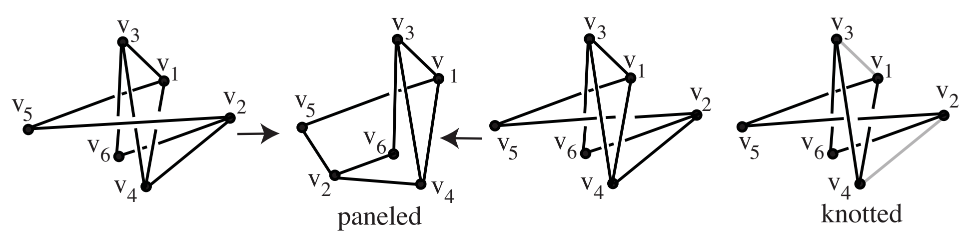

FIGURE 10. $\overline{v_1v_4}$ pierces $\langle v_2, v_6, v_3\rangle$, so $\overline{v_2v_5}$ must pass either in front of, behind, or between $\overline{v_1v_4}$ and $\overline{v_3v_4}$.

Theorem 2.6. *There is a* 9*-stick non-paneled knotless embedding of* K_4*, but no such embedding of* K_4 *exists with fewer than* 9 *sticks.*

Proof. It follows from Lemmas 2.2, 2.4, 2.3, and 2.5 that no embedding of K_4 with 8 or fewer sticks can be both non-paneled and knotless.

Huh and Oh [10] created an 8-stick embedding of a θ-graph which is isotopic to Kinoshita's θ-graph, and hence is knotless and non-paneled. The drawing on the left in Figure 11 illustrates a 9-stick embedding of K_4 which is obtained from Huh and Oh's θ-graph by adding an edge joining vertices v_3 and v_4 (illustrated as a dotted segment).

Since this K_4 contains a non-paneled θ-graph, it must be non-paneled. On the right in Figure 11, we illustrate the only cycles with at least 6 sticks which were not in Huh and Oh's θ-graph, both of which are unknotted. No knotted cycle can have fewer than 6 sticks. All of the other cycles in this K_4 are also unknotted since they were contained in Huh and Oh's θ-graph. □

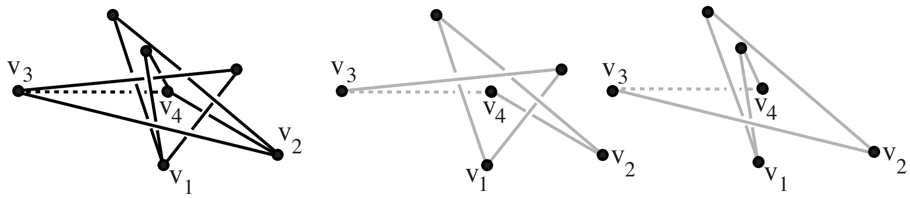

FIGURE 11. A non-paneled knotless 9-stick embedding of K_4.

3. Applications to metalloproteins

Many metalloprotein structures contain one of the graphs $K_{3,3}$ or K_5 and hence are non-planar. For example, nitrogenase is a complex metalloprotein containing a MoFe protein, which itself contains two M-clusters and two P-clusters. Each M-cluster contains $K_{3,3}$, and if we include the protein backbone, each P-cluster also contains $K_{3,3}$. Thus nitrogenase itself contains four separate $K_{3,3}$'s [4].

To understand the topological complexity of such metalloproteins, it is not sufficient to know that the structure contains one or more copies of K_5 or $K_{3,3}$, we need to know how these subgraphs are embedded in $\mathbb{R}^3$. However, looking at proteins as diverse as nitrogenase, cyclotides with a "cysteine knot motif," and nerve growth factor we observe that each of them contains a $K_{3,3}$ whose embedding resembles a Möbius strip as illustrated in Figure 12.

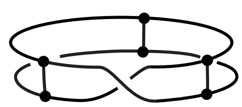

FIGURE 12. An embedding of $K_{3,3}$ is in *Möbius form* if it is isotopic to this embedding or its mirror image.

Definition 3.1. We say an embedding of $K_{3,3}$ in $\mathbb{R}^3$ is in *Möbius form*, if it is isotopic to the embedding illustrated in Figure 12 or its mirror image.

As an example, in Figure 13 on the top left we illustrate part of a nitrogenase molecule that contains a $K_{3,3}$. In order to better see the $K_{3,3}$ subgraph, we progressively remove more of the graph around it. After that, we can easily isotope the $K_{3,3}$ to the form illustrated in Figure 12. The question that we are interested in here is why the Möbius form of $K_{3,3}$ is so prevalent in metalloproteins that contain a $K_{3,3}$.

Note that while the Möbius form is knotless, not every embedding of $K_{3,3}$ which is knotless is necessarily in Möbius form. We illustrate such an embedding in Figure 14. To see that this embedding is knotless, observe that any knot would have to contain at least three crossings. Hence a knot would necessarily contain two of the three edges incident to v. But if we

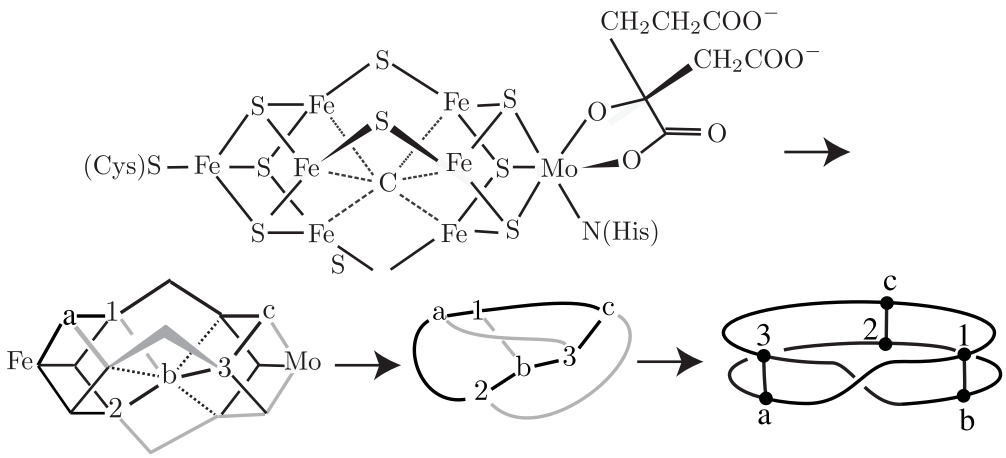

FIGURE 13. One of the $K_{3,3}$'s in the metalloprotein nitrogenase.

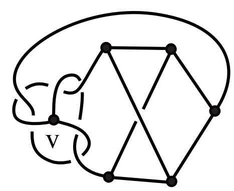

FIGURE 14. An embedding of $K_{3,3}$ which is not in Möbius form yet contains no knot.

remove any one of the three edges containing v, the crossings between the remaining two can be removed.

In order to shed some light on the question as to why the Möbius form of $K_{3,3}$ is prevalent in metalloproteins, we model embeddings of $K_{3,3}$ in a metalloprotein by random linear embeddings of $K_{3,3}$ in a cube and prove the following theorem.

Theorem 3.2. *The probability that a random linear embedding of* $K_{3,3}$ *in a cube is in Möbius form is* 0.97380 ± 0.00003.

As the first step in proving this theorem, we will show that any knotless linear embedding of $K_{3,3}$ is in Möbius form. Then we randomly distribute 6 points in a cube and connect all pairs of points with straight segments to create a random linear embedding of K_6. Finally, we compute the probability that such a K_6 contains a knot and use it to compute the probability that a random linear embedding of $K_{3,3}$ is in Möbius form.

For the first step, we will use the definition and results below.

Definition 3.3. An embedded graph Γ in $\mathbb{R}^3$ is said to be *free* if the fundamental group of the complement of Γ is free, and *totally free* if every subgraph of Γ is free.

Lemma (Robertson, Seymour, and Thomas [16])**.** *An embedded graph is paneled if and only if it is totally free.*

Theorem (Robertson, Seymour, and Thomas [16])**.** *Up to homeomorphism, $K_{3,3}$ and K_5 each have a unique paneled embedding.*

Theorem (Huh and Lee [9])**.** *Every linear embedding of a graph with no more than* 6 *vertices all of degree at least* 3 *is free.*

We now prove the following.

Theorem 3.4. *Every knotless linear embedding of $K_{3,3}$ is isotopic to an embedding in Möbius form.*

Proof. Fix a knotless linear embedding Γ of $K_{3,3}$ in $\mathbb{R}^3$. Observe that if we delete a single edge of Γ we obtain a knotless 8-stick embedding of K_4 with two disjoint edges each consisting of two sticks (see Figure 15). It now follows from Lemma 2.4 that such a K_4 subgraph must be paneled.

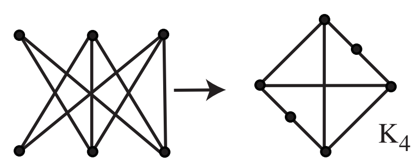

FIGURE 15. If we delete a single edge of $K_{3,3}$ we obtain a K_4.

Thus by the above lemma of Robertson, Seymour, and Thomas [16], every K_4 subgraph of Γ is totally free. Since every proper subgraph of Γ is obtained by removing at least one edge, such a subgraph must be contained in a K_4 subgraph, and hence must be free. Also, we know from Huh and Lee's Theorem [9] that Γ itself is free. Thus Γ is totally free.

By using Robertson, Seymour, and Thomas's Lemma [16] again we see that Γ is paneled. Finally, observe that the form of $K_{3,3}$ in Figure 12 is paneled, and hence by Robertson, Seymour, and Thomas's Uniqueness Theorem [16], Γ must be in Möbius form. □

We are now ready to prove Theorem 3.2, showing that the Möbius form of $K_{3,3}$ is overwhelmingly the most common among random linear embeddings.

Proof of Theorem 3.2. Hughes [6], Huh and Jeon [8], and Nikkuni [14] independently proved that a linear embedding of K_6 contains at most one knot (which is a trefoil knotted 6-cycle), and the embedding contains such a knot if and only if it contains three Hopf links. It was shown in [5] that the probability that a random linear embedding of K_6 in a cube has exactly three Hopf links is $\frac{45q-1}{2}$, where $q = 0.033867 \pm 0.000013$.

Now we randomly distribute 6 vertices in a cube and add linear segments between each pair of vertices to obtain a random linear embedding of K_6. We then remove a pair of disjoint 3-cycles to get a random linear embedding of

$K_{3,3}$. The only way this embedding could contain a knot is if the embedding of K_6 contained a knot and the pair of disjoint 3-cycles that were removed left the knot intact. There are 10 distinct pairs of disjoint 3-cycles in K_6, only one of which shares no edges with a given 6-cycle. It follows that the probability that $K_{3,3}$ is knotted is $\frac{45q-1}{20} = 0.02620 \pm 0.00003$. By using Theorem 3.4 the result follows. □

4. Stick number for non-paneled knotless embeddings of K_5

We have seen that the non-paneled knotless stick number of K_4 is 9. Thus, the remaining case of non-paneled knotless stick embeddings of K_n, is when $n = 5$. In this section, we show that the number of sticks in such an embedding of K_5 is at least 12 and at most 13.

Theorem 4.1. *There are precisely two linear embeddings of K_5 in general position up to affine transformation. Futhermore, all linear embeddings of K_5 are paneled and ambient isotopic.*

Proof. We begin with vertices v_1, v_2, v_3, v_4 in general position in $\mathbb{R}^3$. The solid tetrahedron these vertices determine can be thought of as the intersection of four half-spaces, each defined by the plane containing three of the four vertices. For each such plane, we call the half-space that contains the tetrahedron the *inside* half-space, and the half-space that does not contain the tetrahedron the *outside* half-space.

Vertex v_5 cannot be in the plane of any three of the existing vertices, since the vertices are in general position. If vertex v_5 is inside the tetrahedron $\langle v_1, v_2, v_3, v_4\rangle$, then it is in the inside half-space of the planes determined by all of the faces (see Figure 16a). If vertex v_5 is outside the half-space of the face $\langle v_2, v_3, v_4\rangle$ and inside the half-space of the three other faces, then the five vertices are in the configuration of two tetrahedra glued along the face $\langle v_2, v_3, v_4\rangle$ together with the edge $\overline{v_1v_5}$ (see Figure 16b). If vertex v_5 is outside the half-spaces of the faces $\langle v_1, v_2, v_3\rangle$ and $\langle v_1, v_2, v_4\rangle$ and inside the half-spaces of the faces $\langle v_1, v_3, v_4\rangle$ and $\langle v_2, v_3, v_4\rangle$, then the five vertices are in the configuration of two tetrahedra glued along the face $\langle v_3, v_4, v_5\rangle$ together with the edge $\overline{v_1v_2}$ (see Figure 16c, where v_5 is above $\langle v_1, v_2, v_4\rangle$ and in front of $\langle v_1, v_2, v_3\rangle$). If vertex v_5 is outside the half-spaces of the faces $\langle v_1, v_2, v_3\rangle$, $\langle v_1, v_2, v_4\rangle$, and $\langle v_1, v_3, v_4\rangle$ and inside the half-space of the face $\langle v_2, v_3, v_4\rangle$, then vertex v_5 is the point of a cone about vertex v_1. Thus vertex v_1 lies inside tetrahedron $\langle v_2, v_3, v_4, v_5\rangle$ (see Figure 16d). The case where vertex v_5 lies on the outside half-space of all four faces is impossible.

Observe that Figures 16(a) and (d) are equivalent by affine transformation, and Figures 16(b) and (c) are equivalent by affine transformation. Also, all of the embeddings in Figure 16 are paneled and ambient isotopic. □

Note that a linear embedding of K_5 has 10 sticks. We show below that there are no knotless non-paneled 11-stick embeddings of K_5.

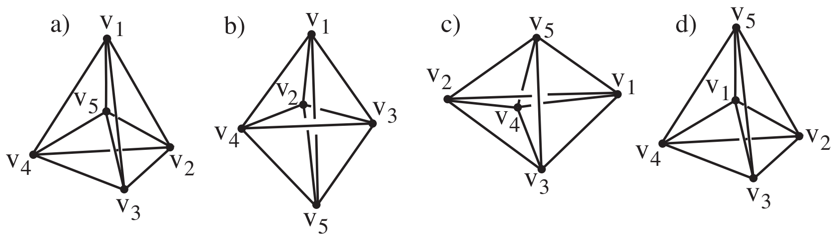

FIGURE 16. These are all the linear embeddings of K_5 up to affine transformation.

Theorem 4.2. *Every* 11*-stick embedding of* K_5 *is either paneled or contains a knot.*

Proof. Suppose that there exists a non-paneled knotless embedding of K_5 with 11 sticks. Then the stick graph is a linear embedding of a graph with six vertices, one of which has degree 2. Label the vertices v, v_1, v_2, v_3, v_4 and v_5, where v is the vertex of degree 2 and is adjacent to v_1 and v_2. The triangle $\langle v_1, v, v_2\rangle$ must be irreducible, since otherwise the embedding would be isotopic to an embedding with only 10 sticks which is paneled by Theorem 4.1. Thus one of the edges $\overline{v_3v_4}$, $\overline{v_4v_5}$, or $\overline{v_3v_5}$ must pass through the triangle $\langle v_1, v, v_2\rangle$. Up to re-labeling and affine transformation, we may assume that the edge $\overline{v_3v_4}$ intersects the triangle $\langle v_1, v, v_2\rangle$ orthogonally. Up to symmetry, we may also assume that v_5 lies above the plane determined by the triangle $\langle v_1, v, v_2\rangle$ and on the same side of the plane determined by $\langle v, v_3, v_4\rangle$ as v_1 is.

We now determine the possible positions of v_5 by orthogonal projection onto the plane determined by $\langle v_1, v, v_2\rangle$. The projection of the vertex v_5 can either lie inside the infinite wedge bounded by the rays $\overrightarrow{v_3v_1}$ and $\overrightarrow{v_3v_2}$ in the projection, or outside of this wedge. Note that in the projection v_3 and v_4 are the same point.

In the case that v_5 is inside the wedge, we obtain an embedding isotopic to Figure 17(a), which is paneled. For the case when v_5 is outside of the wedge, first recall that we assumed v_5 was on the same side of the plane determined by $\langle v, v_3, v_4\rangle$ as v_1. The spatial configurations are now determined by whether $\overline{v_2v_5}$ pierces the triangle $\langle v_1, v_3, v_4\rangle$ and whether $\overline{v_4v_5}$ pierces the triangle $\langle v_1, v, v_2\rangle$.

If $\overline{v_2v_5}$ pierces $\langle v_1, v_3, v_4\rangle$ and $\overline{v_4v_5}$ pierces $\langle v_1, v, v_2\rangle$, we obtain an embedding isotopic to Figure 17(b), which is paneled. If $\overline{v_2v_5}$ does not pierce $\langle v_1, v_3, v_4\rangle$ and $\overline{v_4v_5}$ does pierce $\langle v, v_1, v_2\rangle$, the embedding is isotopic to Figure 17(c), which is paneled. If $\overline{v_2v_5}$ pierces $\langle v_1, v_3, v_4\rangle$ but $\overline{v_4v_5}$ does not pierce $\langle v, v_1, v_2\rangle$, we obtain an embedding isotopic to Figure 17(d), which contains a trefoil knot. Finally, if neither $\overline{v_2v_5}$ pierces $\langle v_1, v_3, v_4\rangle$ nor $\overline{v_4v_5}$ pierces $\langle v, v_1, v_2\rangle$, then the embedding is isotopic to Figure 17(e), which is paneled. □

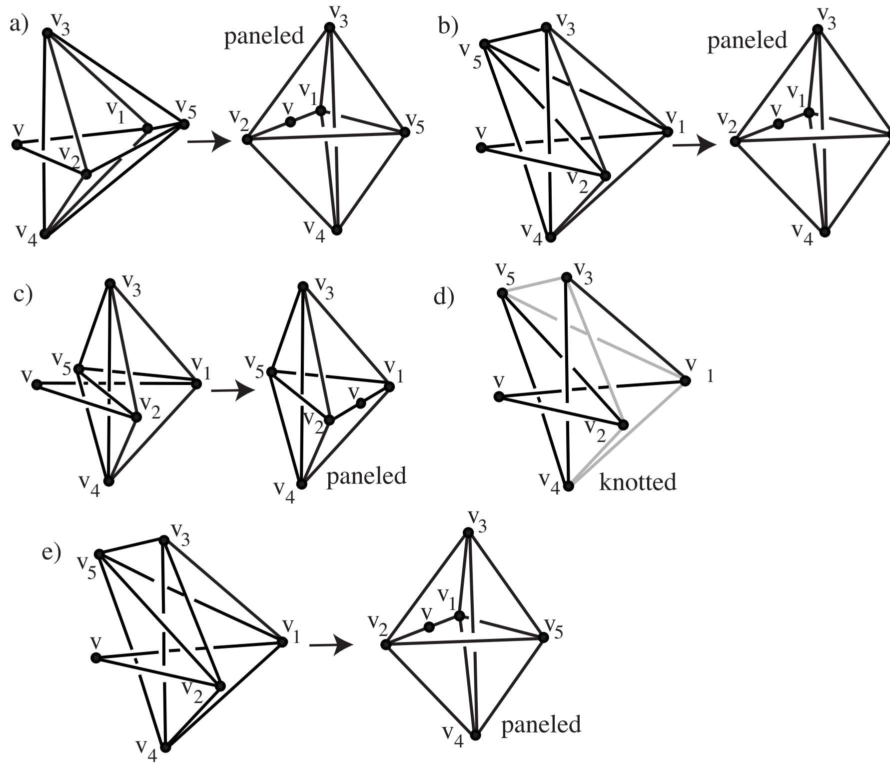

FIGURE 17. Since the triangle $\overline{vv_1v_2}$ and the edge $\overline{v_3v_4}$ are orthogonal, there are only five positions for v_5 up to symmetry and affine transformation.

In Figure 18, we illustrate a non-paneled knotless embedding of K_5 constructed with 13 sticks. Observe that if we remove v_5 and its incident edges as well as the edge $\overline{v_1v_2}$, we obtain the 8-stick Kinoshita's θ-curve, illustrated on the right. Since a Kinoshita's θ-curve is non-paneled, this embedding of K_5 cannot be paneled.

In order to determine if our embedding contains a knot, we only need to consider loops with at least 6 sticks. Such a loop must contain vertex v_4. Hence, up to symmetry and affine transformation, it has the form of one of the grey loops in Figure 19, depending on whether or not it contains the edge $\overline{v_4v_5}$. Since both of these loops are unknotted, this embedding is knotless. This example together with Theorem 4.2 shows that the stick number of a non-paneled, knotless embedding of K_5 is either 12 or 13.

It remains an open question whether it is possible to have a paneled knotless embedding of K_5 with 12 sticks. The analysis of embeddings of K_5 constructed with 12 sticks has considerably more cases than the analysis of K_4 embeddings with 8 sticks. For example, in each of the cases of Lemma 2.3, for K_5 we would have to consider all possible positions of an additional

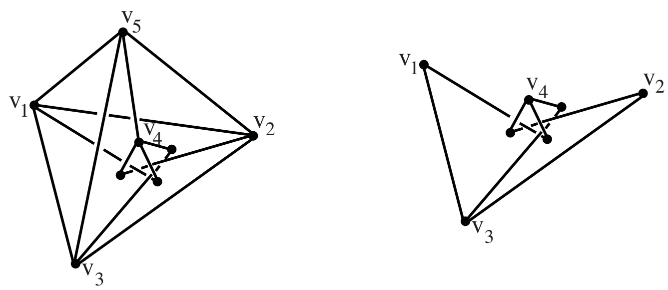

FIGURE 18. A 13-stick embedding of K_5 which contains the 8-stick Kinoshita's θ-curve on the right.

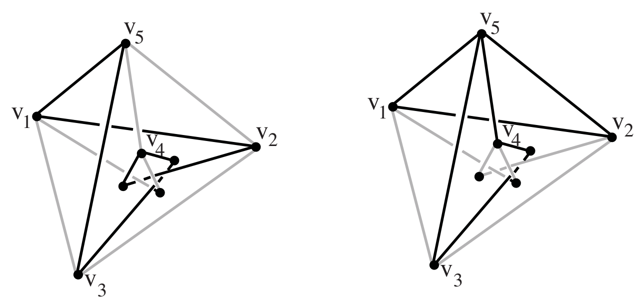

FIGURE 19. Up to symmetry and affine transformation, the grey loops are the only loops in our K_5 with at least 6 sticks.

vertex v_7 connected to each of v_1, v_2, v_3, and v_4. Moreover, we must consider the cases where the edge piercing $\langle v_3, v_5, v_6\rangle$ or $\langle v_4, v_6, v_5\rangle$ contains v_7. Each case in each of Lemmas 2.3–2.5 will have a corresponding increase in complexity.

Alternatively, a matroid approach [7, 15] can be used to determine all 12-stick embeddings of K_5 with the known census of affine point configurations [3]. Eliminating all reducible and knotted embeddings still results in a few thousand cases, only a small number of which can be easily isotoped to a reducible embedding. In order to extend this approach to systematically identify the isotopy types of embeddings of K_5 consisting of 12 sticks, one would need a more general method for determining isotopies of an embedding of a non-complete graph that could change the combinatorial type of the affine point configuration.

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