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Fabrication of a family of pyramidal links and their genus

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Abstract

The model of polyhedral links has been applied to explain DNA and protein cages from mathematics. Recently, a type of polyhedral links has been constructed by the means of branched alternating closed braids and double lines. In this paper, as a special type of the links, pyramidal links $\mathbb{L}(P)$ are fabricated on an pyramid P by 3-cross-curves, n-cross-curve and double-lines covering, where n is the maximum degree of P. We compute the genus of links $\mathbb{L}(P)$ as

$$g(\mathbb{L}(P)) = \begin{cases} n-2, & \text{if } n \text{ is divisible by 3,} \\ n-1, & \text{otherwise.} \end{cases}$$

This result shows that the genus of $\mathbb{L}(P)$ only depends on n, and the complexity of the $\mathbb{L}(P)$ increases with the increase of n.

1 Introduction

Large and flexible macromolecules, such as DNA and polymethylene polyethylene, can form intricate knotted and interlocked topologies which include some more interesting interlocked 3-dimension structures. In recent decades, the DNA tetrahedron [1, 2, 3], DNA cube [4, 5, 6], DNA octahedron [7, 8, 9], DNA dodecahedron

[3, 10], DNA icosahedron [11, 12], DNA buckyball [3], and bacteriophage HK97 capsid have been synthesized and discovered. These interesting DNA polyhedra present tremendous potential in a number of areas, including drug encapsulation and release, regulation of the folding and activity of encaged proteins, as host molecules for nanomaterials and as building blocks for 3D-networks for catalysis and biomolecule crystallization [3]. Thus, these fancy polyhedral structures excited our intensively exploring interesting.

The first topologically linked protein which forms a 72-catenane was discovered in the bacteriophage HK97 capsid in 2000 [13]. From the discover, it can be seen that proteins can form topologically linked architectures. Inspired by this more topologically complex polyhedral catenane, Qiu and co-workers fabricated a family of polyhedral links by the method of the 'three-cross-curve and double-line covering' [14, 15]. Immediately, the model is generalized, and another type of polyhedral links has been constructed by the means of branched alternating closed braids and double lines [16]. Considering these advances in creating polyhedral links [15, 16, 17, 18, 19, 20] and its dual analysis [21, 22], knot theory as a better tool can be used to characterize topologies of these exotic molecular structures.

In knot theory, knot invariants are quantities defined for each knot which is the same for equivalent knots. Thus, they can be used as molecular descriptors to describe the various configurations of large molecules that have non-planar graphs. So far, standard knot invariants include genus, unknotting number, different knot polynomials (Alexander, Conway, Jones, HOMFLYPT, Kauffman...), *etc.* And genus, a topological invariant of a surface, is always used to describe and classify graphs and knots. Apart from its mathematical relevance, genus has a great influence on biology and chemistry. The principle of genus has been lent to guide the molecular design of organic compounds, as well as classify RNA structural motifs [23]. Studies on the genus of knots or links have been brought on more and more attention [24, 25, 26]. It is a splendid molecular descriptor, and can also be used to describe the topological configurations of large molecules. In addition, molecules with genus might constitute interesting targets for a topology-aided chemical design [27, 28, 29].

In this paper, inspired by the bacteriophage HK97 capsid, we extend the method of 'branched alternating closed braids and double lines covering' to pyramids, and finally get some pyramidal links. The resulting structures have not been synthesized yet and might constitute interesting targets for a topology-aided molecular design. Expect for the symmetry analysis, we also investigate the genus and number of components of these links, which provide a new way to detect their complexity. Such mathematical consideration may provide a new guiding principle to topology-aided molecular design in a given surface, and rational evidence for the synthesis in the laboratory.

2 Preliminaries

To provide necessary background, we begin our account with some basic concepts, terminology and denotation.

A knot $K \subset \mathbf{R}^3$ is a subset of points homeomorphic to a circle. A link L of n components is a finite disjoint union of knots: $L = K_1 \cup \cdots \cup K_n$.

A *Seifert surface* of a knot or link L is a surface S whose boundary is a given knot or link. The surface S is compact, connected, orientable. Seifert, in the 1934's, gave an algorithm which produces such a surface S for a given link diagram L [30]. The algorithm eliminates each knot or link crossing by connecting each of the strands coming into the crossing to the adjacent strand leaving the crossing, as shown in Fig. 1. The resulting strands no longer cross but form instead a set of nonintersecting circles called *Seifert circles*. The Seifert circles of trefoil knot is shown in Fig. 2.

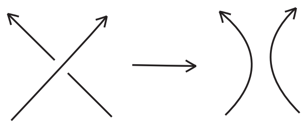


Fig. 1. Eliminate a crossing according to orientation of strands.

Definition 2.1. *[32] The genus of an oriented link L is the minimum genus of any connected orientable surface that spans L. The genus of an unoriented link is the minimum taken over all possible choices of orientation. The genus of a link L denoted by $g(L)$.*

Throughout this paper, we use D to denote an oriented diagram representing a

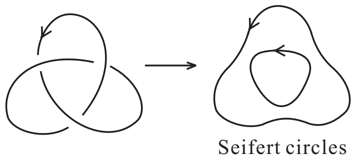


Fig. 2. Seifert circles of the trefoil knot.

given oriented link L, and $s(D)$ the number of Seifert circles of D. The maximal number of Seifert circles of an unoriented diagram L is denoted by $\bar{s}(L)$.

Let $P = (V; E)$ be a polyhedron with vertex set V and edge set E. We use $n(P)$ to denote the number of vertices of P, $f(P)$ the number of faces. $\triangle(P)$ denotes the maximum degree of P.

3 Construction of pyramidal links

According to Ref. [16], we introduced a type of branched alternating closed braids polyhedral links, which is fabricated by the means of branched alternating closed braids and double lines. In [16], $\hat{S}_i$ is denoted by a branched alternating closed braid, which has arbitrary number of strings and crossing number. Here, let $\hat{T}_1$ denote a branched alternating closed braid with the number of string 2 and crossing number n. Let $\hat{T}_2$ denote a branched alternating closed braid with the number of string 2 and crossing number 3. That is, $\hat{T}_1$ and $\hat{T}_2$ are 3-crossing curve and n-crossing curve, respectively, as shown in Fig. 3.

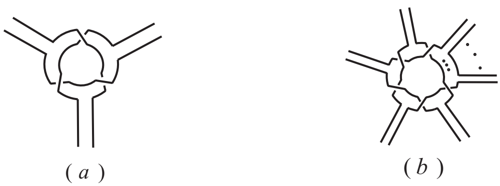


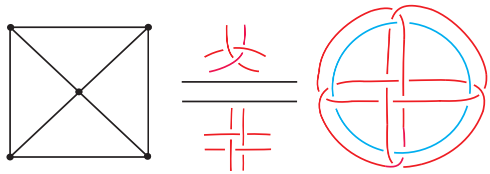
Fig. 3. (a) $\hat{T}_1$: 3-crossing curves. (b) $\hat{T}_2$: n-crossing curve.

As a special case of branched alternating closed braids polyhedral links, pyramidal links are constructed by n-crossing curve, 3-crossing curves and double-lines covering. The construction method is

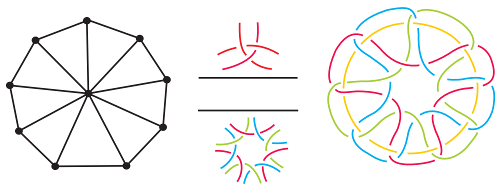
(1) Use an n-crossing curve to cover vertex of a cone of P.

(2) Use n 3-crossing curves to cover others n vertices of P.

For example, a 4-pyramidal link is constructed by a 4-crossing curve, four 3-crossing curves and double lines covering on 4-pyramid, as illustrated in Fig. 4 (a). A 9-pyramidal link is constructed by a 9-crossing curve, nine 3-crossing curves and double lines covering on 9-pyramid, as illustrated in Fig. 4 (b).



(a)



(b)

Fig. 4. (a) Construction of 4-pyramidal link. (b) Construction of 9-pyramidal link.

In terms of linked molecular framework, symmetry plays an important role as a guiding principle for the design of novel molecules. Therefore, here we will discuss the symmetry of the polyhedra P and its corresponding links $\mathbb{L}(P)$. Compare to the polyhedron P, the symmetry of $\mathbb{L}(P)$ loses its mirror symmetry in our construction. For instance, the tetrahedron and n-pyramid ($n \geq 4$) have T_d and D_{nd} symmetry, respectively. However, the tetrahedral links and n-pyramidal links have T and D_n symmetry, respectively.

4 Genus of pyramidal links

Gabai, in 1986, pointed out that if Seifert's algorithm is applied to an alternating diagram, a Seifert surface of minimal genus can be yield. Therefore, Theorem 4.1 and 4.2 provide a computing method of genus of an oriented alternating link.

Theorem 4.1. *[31] Every Seifert surface obtained by applying Seifert's algorithm to alternating diagrams is of minimal genus.*

Theorem 4.2. *[32] The genus of a projection surface F constructed from a connected diagram D satisfies $2g(F) = [1 - s(D) + c(D)] + [1 - \mu(D)]$, where $s(D)$ denotes the number of Seifert circles, $c(D)$ the number of crossing number, $\mu(D)$ the number of component of diagram D.*

Given a link L with n-components, there are 2^n cases based on the orientations of n closed curves involved. Then it has 2^n oriented link diagrams $D_1, D_2, \cdots, D_{2^n}$. By Theorem 4.2, for all oriented link diagrams, it has genus $g(D_1), g(D_2), \cdots, g(D_{2^n})$. According to Definition 2.1 and Theorem 4.2, in order to make genus as small as possible, we must pick the maximum number of Seifert circles from $D_1, D_2, \cdots, D_{2^n}$. Hence, $g(L)$ only depends on the maximum number of Seifert circles.

In $D_1, D_2, \cdots, D_{2^n}$, there exist some oriented diagrams whose numbers of Seifert circles are the same, then we can expurgate those oriented diagrams. Proposition 4.3 gives a method of expurgating.

Given an oriented link diagram D, we can form its reverse $-D$ by reversing the orientations on all of its components. Their numbers of Seifert circles are equal. That is $s(D) = s(-D)$. From this, we have the following proposition immediately.

Proposition 4.3. *Let $L \cup M$ be an oriented link diagram with components $L_1, \ldots, L_p$, $M_1, \ldots, M_q$. Then $s(-L \cup M) = s(L \cup -M)$.*

Given an n-pyramidal link $\mathbb{L}(P)$, its number of components is related to the $\triangle(P)$.

Theorem 4.4. *Let P be an n-pyramid.*

(i) $\mathbb{L}(P)$ is a 4-component link, if n is divisible by 3.

(ii) $\mathbb{L}(P)$ is a 2-component link, otherwise.

Proof: Let n-crossing curve properly embedded in a 3-ball B^3. Then $\partial(B^3)$ meets it transversely in exactly $2n$ points. We label the points from $1, 2, \cdots, 2n$.

(i) If n is divisible by 3, then lines of labeled $\{1, 4, 7, \cdots, 2n-2\}$, $\{2, 5, 8, \cdots, 2n-1\}$, $\{3, 6, 9, \cdots, 2n\}$ consist of three components of $\mathbb{L}(P)$. The unlabeled line is the fourth component.

(ii) If n is not divisible by 3, and each crossing of $\mathbb{D}(P)$ is regarded as a vertex, then the labeled line is an Euler circuit, which is a component of $\mathbb{L}(P)$. The un-labeled line is another component. Therefore, the case has two components. $\square$

In the following part, we will discuss the number of Seifert circles of each oriented link diagram.

Let A be a local region in an n-pyramidal link diagram surrounded by a circle, as illustrated in Fig. 5. Thus A has 4 components and 16 possible choices of orientation. Let A_i denotes the i^{th} possible choices, where $i = 1, 2, \cdots, 2^4$. Therefore, the number of Seifert circles of an oriented n-pyramidal link diagram are obtained by applying Seifert's algorithm to the link diagram for every A_i. Let $\mathbb{D}_i(P)$ denote an oriented n-pyramidal link diagram whose orientation is determined by A_i, $s(\mathbb{D}_i(P))$ the number of Seifert circles of $\mathbb{D}_i(P)$.

Assume that A_1, A_2, A_3 and A_4 are such oriented diagrams, as shown in Fig. 6.

Fig. 5. A region A in an n-pyramidal link diagram.

Theorem 4.5. *If $\mathbb{L}(P)$ is a 4-component link, then $\mathbb{D}_i(P)$ has only four different numbers of Seifert circles, and the four situations are uniquely determined by A_1, A_2, A_3, A_4, where $i = 1, 2, \cdots, 16$.*

Proof: Given A an orientation, and suppose that the resulting A is A_1. Reversing the orientation of some components of A will result in different number of Seifert

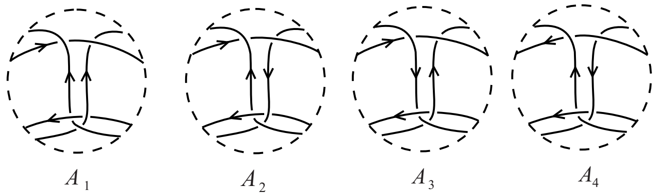


Fig. 6. Four possible orientations of A.

circles (may not change the number). So the reversing has $C(4,1)+C(4,2)=10$, as shown in Fig. 7.

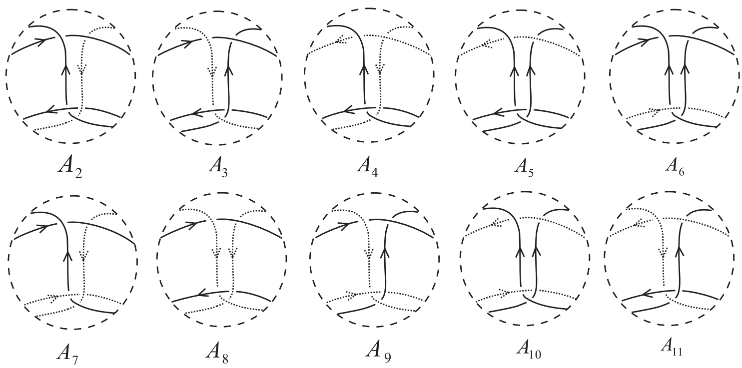


Fig. 7. The numbers of reversing of A_1.

In Fig. 7, by Proposition 4.3, $s(\mathbb{D}_4(P)) = s(\mathbb{D}_9(P))$, we can delete A_4 or A_9. Here we assume that delete A_9. Similarly, $s(\mathbb{D}_8(P)) = s(\mathbb{D}_{10}(P))$, $s(\mathbb{D}_7(P)) = s(\mathbb{D}_{11}(P))$. So, A_{10} and A_{11} are deleted. Therefore, the number of A_i is reduced. So we have only $A_1, A_2, \cdots, A_8$. From above, 16 choices of orientation are reduced to 8. We need to reduce more choices.

For every A_i, it has two neighbors which are denoted by A_i^l and A_i^r, respectively. Let $T_i = \{A_i^l, A_i, A_i^r\}$. If $i=1$, then $A^l = -A_7$, $A^r = A_8$. So, $T_1 = \{-A_7, A_1, A_8\}$. If $i=7$, then $T_7 = \{-A_8, A_7, -A_1\}$. If $i=8$, then $T_8 = \{-A_7, A_8, A_1\}$. Therefore, $s(\mathbb{D}_1(P)) = s(\mathbb{D}_7(P)) = s(\mathbb{D}_8(P))$. From this, we can divide A_1, A_7 and A_8 into a class K_1. Similarly, $s(\mathbb{D}_2(P)) = s(\mathbb{D}_5(P)) = s(\mathbb{D}_6(P))$, then A_2, A_5, A_6 are divided into a class K_2. In addition, $T_3 = \{A_3, A_3, A_3\}$, $T_4 = \{A_4, A_4, A_4\}$. Hence we can divide A_i into four classes: $K_1 = \{A_1, A_7, A_8\}$, $K_2 = \{A_2, A_5, A_6\}$, $K_3 = \{A_3\}$ and $K_4 = \{A_4\}$. So we need only consider A_1, A_2, A_3, A_4. Therefore, 8 choices are reduced to 4.

Subsequently, we will discuss that $\mathbb{L}(P_n)$ do produce different number of Seifert circles for A_i, where $i = 1, 2, 3, 4$.

Let $\mathbb{D}(P_n) = \mathbb{D}(P_{n-3}) \oplus W_i$, where W_i denotes a set of curve in sectorial region shown in Fig. 8. $\mathbb{D}(P_{n-3})$ can be obtained by identifying a, a', b, b' and c, c' respectively after deleting W_i. Applied Seifert's algorithm to W_i, as illustrated in Fig. 9, we have

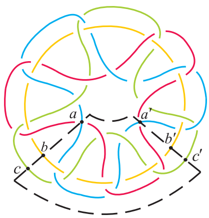


Fig. 8. $\mathbb{D}(P_{n-3})$ can be obtained by identifying a, a', b, b' and c, c' respectively after deleting W_i.

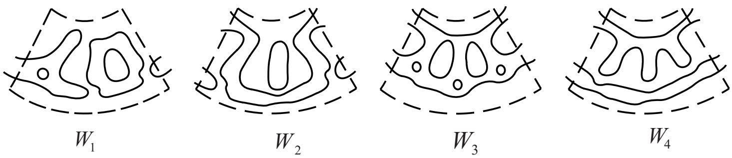


Fig. 9. Some Seifert curves are obtained by applying Seifert's algorithm to W_i, respectively.

(i) if $i = 1$, then $s(\mathbb{D}(P_n)) = s(\mathbb{D}(P_{n-3})) + 4$.

(ii) if $i = 2$, then $s(\mathbb{D}(P_n)) = s(\mathbb{D}(P_{n-3})) + 2$.

(iii) if $i = 3$, then $s(\mathbb{D}(P_n)) = s(\mathbb{D}(P_{n-3})) + 6$.

(iv) if $i = 4$, then $s(\mathbb{D}(P_n)) = s(\mathbb{D}(P_{n-3}))$.

Therefore, we obtain $s(\mathbb{D}_i(P)) \neq s(\mathbb{D}_j(P))$, where $i, j = 1, 2, 3, 4,\ i \neq j$. From this, $\mathbb{D}_i(P)$ has only four different numbers of Seifert circles, which are uniquely determined by A_1, A_2, A_3, A_4, where $i = 1, 2, \cdots, 16$. □

Theorem 4.5 reduced the possible choice of orientation from 16 to 4. Then we can find the maximum number of Seifert circles from the 4 possible choices. The following theorem indicates that the maximum number of Seifert circles only depends on the maximum degree of P.

Theorem 4.6. *Let P_n be an n-pyramid. Then $\bar{s}(\mathbb{L}(P_n)) = 2n + 2$.*

Proof: If $\mathbb{L}(P_n)$ is a 2-component link and each crossing of $\mathbb{D}(P)$ is regarded as a vertex, then the labeled line is an Euler circuit. Thus the orientation of every two neighboring labeled lines is different. This means that $s(\mathbb{L}(P_n)) = 4$ or $n(P_n) + f(P_n)$. Therefore, $\bar{s}(\mathbb{L}(P_n)) = 2n(P_n) = 2n + 2$.

If $\mathbb{L}(P_n)$ is a 4-component link, then in $i = 4$, the recursive formula will produce the maximum number of Seifert circles. From this, we have

$$\begin{aligned} s(\mathbb{D}(P_n)) &= s(\mathbb{D}(P_{n-3})) + 6 \\ &= \cdots \\ &= s(\mathbb{D}(P_0)) + 2n. \end{aligned}$$

However, $\mathbb{D}(P_0)$ is an alternating closed braid with the number of string 2 and crossing number n. Thus $\mathbb{D}(P_0)$ is a knot or link, and the numbers of Seifert circles are equal to 2 by applying Seifert's algorithm to $\mathbb{D}(P_0)$. Therefore, we have

$$\bar{s}(\mathbb{D}(P_n)) = 2n + 2.$$

□

Up to now, the maximal number of Seifert circles of $\mathbb{L}(P)$ has been obtained. By Theorem 4.2, we can obtain the genus of $\mathbb{L}(P)$.

Theorem 4.7. *Let P be an n-pyramid, then*

(i) $g(\mathbb{L}(P))$ is $n - 2$, if n is divisible by 3.

(ii) $g(\mathbb{L}(P))$ is $n - 1$, otherwise.

Proof: According to Theorem 4.2,

(i) If n is divisible by 3, then

$$\begin{aligned} 2g(\mathbb{L}(P)) &= 2 - \bar{s}(\mathbb{L}(P)) + c(\mathbb{L}(P)) - \mu(\mathbb{L}(P)) \\ &= 2 - 2(n+1) + 4n - 4 \\ &= 2n - 4. \end{aligned}$$

That is

$$g(\mathbb{L}(P)) = n - 2.$$

(ii) If n is not divisible by 3, then

$$\begin{aligned} 2g(\mathbb{L}(P)) &= 2 - \bar{s}(\mathbb{L}(P)) + c(\mathbb{L}(P)) - \mu(\mathbb{L}(P)) \\ &= 2 - 2(n+1) + 4n - 2 \\ &= 2n - 2. \end{aligned} \tag{1}$$

That is

$$g(\mathbb{L}(P)) = n - 1.$$

□

Here, we give some examples for the genus of the family of n-pyramidal links in the following table.

Table 1

	n	whether n divisible by 3 or not	genus
Tetrahedral link	3	Yes	1
4-prism link	4	No	3
5-prism link	5	No	4
6-prism link	6	Yes	4
7-prism link	7	No	6
8-prism link	8	No	7
9-prism link	9	Yes	7

According to the above table, if $|\triangle(P_1)| = 3k - 1$, $|\triangle(P_2)| = 3k$, $k \geq 2$, then $g(\mathbb{L}(P_1)) = g(\mathbb{L}(P_2))$. For examples, the genus of the 5-prism link and 6-prism link are the same, the genus of the 8-prism link and 9-prism link are also the same.

5 Discussion and conclusion

We have constructed a type of n-pyramidal links by the method of 'n-crossing curve, n-crossing curves and double lines covering'. Although the structures of these pyramidal links have not been synthesized, they might constitute interesting targets for a topology-aided molecular design.

The genus of pyramidal link is first given on the basis of what surface they embed into. Research on the genus has provided a new way to detect the complexity of these links. As a result, the pyramidal links with greater genus are more complex. For instance, the 4-pyramidal link is more complex than the 3-pyramidal link. But the genus of the 5-pyramidal link and the 6-pyramidal link are equal. In terms of genus we can not judge which link is more complex. Thus, the number of components of a link is another index of judging the complexity of those pyramidal links with the same genus: the greater number of components is, the more complex link is. Accordingly, the 6-pyramidal link is more complex than the 5-pyramidal link. Due to our discussion, the complexity of pyramidal links $\mathbb{L}(P)$ increases with the increase of n.

The consideration of the correspondence between links and their surfaces is also of chemical importance. The 3-pyramidal protein catenane or the $(3k+1)$-pyramidal protein catenane can be designed in a surface with genus one or $3k$, respectively, where $k = 1, 2, \cdots$. For a surface with genus $3k + 1$, the $(3k + 2)$-pyramidal protein catenane and the $(3k + 3)$-pyramidal protein catenane can be designed, where $k = 1, 2, \cdots$. As a general observation, there are at most two pyramidal catenanes can be designed for a given surface, which provides a new guiding principle to topology-aided molecular design in a given surface and a rational evidence for the synthesis in the laboratory. For examples, aside from 3-pyramidal protein catenane, every pyramidal protein catenanes can not be synthesized in a surface with genus one. The 5-pyramidal protein catenane and the 6-pyramidal protein catenane can be synthesized in a given surface with genus 4.

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