MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **62** (2009) 115-130

ISSN 0340 - 6253

A novel molecular design of polyhedral links and their chiral analysis

Xiao-Sheng Cheng[a], Wen-Yuan Qiu[b], He-Ping Zhang[a]

[a] School of Mathematics and Statistics, Lanzhou University, Lanzhou, Gansu 730000, P. R. China

[b] Department of Chemistry, State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou, Gansu 730000, P. R. China

E-mails: wyqiu@lzu.edu.cn; zhanghp@lzu.edu.cn

(Received October 8, 2008)

Abstract

Polyhedral links, interlinked and interlocked architectures, have been proposed for the description and analysis of knotted configurations in DNA and proteins. Qiu *et al.* fabricated cubic polyhedral and carbon nanotube links by the means of three cross curves and double lines covering, and analyzed their chirality by point groups. We present, in this paper, a novel method by replacing three cross curves with branched alternating closed braids to construct a new type of polyhedral links on arbitrary convex polyhedra. We give some conditions to determine the chirality of the polyhedral links in terms of generalized Tutte and Kauffman polynomials. Accordingly, we show that each regular branched closed braid link is chiral. This result shows that the model of bacteriophage HK97 capsid, topologically linked protein catenane, is chiral.

1 Introduction

Since the first two interlocked rings topological catenane [1] was synthesized in 1961, a new field has been opened for searching and synthesizing more topological complex molecules. Particularly, due to the large length and enough flexility of DNA and protein molecules, they can be used as materials to assembly molecular catenanes. Till now, chemists have utilized DNA to address the realization of interlocked molecules with well-defined polyhedral topologies, such as DNA cubes [2, 3] and truncated octahedrons [4], and more recently DNA bipyramids [5], DNA prisms [6], DNA octahedrons [7], DNA dodecahedrons and DNA buckyballs [8]. Moreover, a protein catenane in the shape of a 72-hedron has been discovered in the context of virology [9]. These curious objects provide some topological nontrivial structures that have inspired mathematicians to characterize them by building models [10].

In recent years, a theoretical model of polyhedral and carbon nanotube links, fabricated by Qiu and coworkers [11, 12], which are topological entities with polyhedral and carbon nanotubal shape linking with a collection of finitely separate closed curves, are constructed by using three cross curves and double lines to encode vertices and edges of a polyhedron or carbon nanotube, respectively. Recall that, for the polyhedral shape link, the inspiration for such models comes from the real structures of the protein polyhedral catenanes. By extension, many other constructing methods and possible physico-chemical properties are shown in [13–16]. However, the development of a well-founded scheme for constructing polyhedral catenanes has remained a challenging problem awaiting a satisfactory solution.

Chirality [17] is a geometrical-topological property of many physical systems, and a fundamentally important aspect of chemistry. An object or a system is called chiral if it cannot ambient isotopic to its mirror image. A non-chiral object is called achiral. There exist some topological techniques to prove chirality of knots and links [18–21]. For polyhedral links, but, to date, approaches to detect their chirality are brought forward. Such as present an experienced approach to determining whether the symmetry of a rigid representation is belonged to chiral group, and analyzing whether a molecular structure can be deformed to its mirror image. So we will describe an approach of determining chirality from mathematics for such a survey.

The current paper proposes a novel approach for constructing of polyhedral links by using branched alternating closed braids and double lines to cover every vertex and every edge of a convex polyhedron, respectively. Throughout this paper, the constructed polyhedral links are all alternating. The constructed approach provides a new interpretation for three cross curve covering links, which belong to the family of regular branched closed braid covering links. Furthermore, we shall applying a combinatorial method to analyze the chirality of the model. By using generalized Tutte and Kauffman polynomials, we give sufficient conditions to determine the chirality of the polyhedral links. Accordingly, we show that a polyhedral link each vertex of which is covered by a regular branched closed braid is chiral. This implies bacteriophage HK97 capsid is chiral. We hope that our construction may offer a theoretical guideline for synthesizing of new DNA and protein polyhedra and the chirality criterion for polyhedral links will play an important role in further study of stereochemistry of DNA and protein cage.

2 Prelimaries

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

A polyhedron is a solid in $\mathbf{R}^3$, enclosed by a number of polygons (faces), which, two by two, have a side in common (edges), while three or more polygons join in common vertices.

Let $G = (V, E)$ be a graph with vertex set V and edge set E. We use $n(G)$ to denote the number of vertices of a graph G, $e(G)$ the number of edges, $f(G)$ the number of faces, and $c(G)$ cyclomatic number. Similarly, let $n(P)$ denotes the number of vertices of a polyhedron P, $e(P)$ the number of edges, $f(P)$ the number of faces.

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 braid is a set of n strings, all of which are attached to a horizontal bar at the top and at the bottom. Each string always heads downward as we move along any one of the strings from the top bar to the bottom bar. Tying the top ends to the bottom ends of braid b, to form a link, called a closed braid $\hat{b}$, as shown in Figure 1. Let $n(b)$ be the number of strings of braid b.

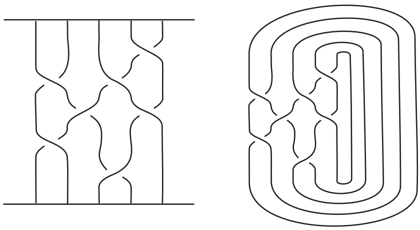

Figure 1. A braid b and it corresponding closed braid $\hat{b}$.

An ordered combination of the σ_i and σ_i^{-1} symbols constitutes a braid word. For example, $\sigma_i^{-1}\sigma_{i+1}^{-1}\sigma_i^{-1}$ is a braid word for the braid illustrated Figure 2(b), where the symbols can be read off the diagram left to right and then top to bottom. For the left of Figure 1, the braid b is denoted to be $\sigma_4\sigma_1\sigma_3\sigma_2^{-1}\sigma_4\sigma_1\sigma_3^{-1}$.

3 Construction of polyhedral links

Our method of constructing polyhedral links is based on the knowledge of closed braid. Using branched alternating closed braids and double lines to cover every vertex and edge of a polyhedron P, respectively. The resulting link is the polyhedral link we

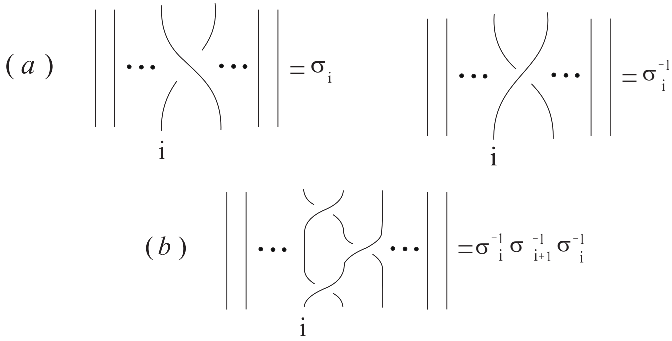

Figure 2. (a)The geometric interpretation of generators $\sigma_1, \sigma_2, \cdots, \sigma_n$. (b) A braid word.

fabricate. Let $\mathbb{L}(P)$ denotes a polyhedral link from our construction. To explain the construction, we first introduce the definition of branched alternating closed braid.

Let

$$J_i = \begin{cases} (\sigma_1\sigma_3\cdots\sigma_{n(J_i)-2}\sigma_2^{-1}\sigma_4^{-1}\cdots\sigma_{n(J_i)-1}^{-1})^{k_i} & \text{if } n(J_i) \text{ } is \text{ } odd \\ (\sigma_1\sigma_3\cdots\sigma_{n(J_i)-1}\sigma_2^{-1}\sigma_4^{-1}\cdots\sigma_{n(J_i)-2}^{-1})^{k_i} & \text{if } n(J_i) \text{ } is \text{ } even \end{cases}$$

or

$$J_i = \begin{cases} (\sigma_1^{-1}\sigma_3^{-1}\cdots\sigma_{n(J_i)-2}^{-1}\sigma_2\sigma_4\cdots\sigma_{n(J_i)-1})^{k_i} & \text{if } n(J_i) \text{ } is \text{ } odd \\ (\sigma_1^{-1}\sigma_3^{-1}\cdots\sigma_{n(J_i)-1}^{-1}\sigma_2\sigma_4\cdots\sigma_{n(J_i)-2})^{k_i} & \text{if } n(J_i) \text{ } is \text{ } even, \end{cases}$$

where $i = 1, 2, \cdots, n(P)$; k_i is crossing number between the 1^{st} and the 2^{st} string of J_i. Then J_i is called k_i-regular alternating braid. So $\hat{J}_i$ is called k_i-regular alternating closed braid, as illustrated in Figure 3.

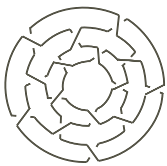

Figure 3. The regular alternating closed braid $\hat{J}_i$ with $k_i = 5$.

If $c[j : j+1] \neq c[k : k+1], j \neq k, \ j, k \in \{1, 2, 3, \cdots, n(J_i) - 1\}$, $c[1 : 2] = k_i$ and $2 \leq c[j : j+1] \leq k_i, \ j = 2, 3, \cdots, n(J_i) - 1$, where $c[j : j+1]$ denotes crossing number between the j^{st} and the $j+1^{st}$ string of an alternating braid J_i, then J_i is called irregular.

We define

$$\hat{S}_i = \hat{J}_i - \{a_1 \cup a_2 \cup \ldots \cup a_{k_i}\},$$

where $a_1, a_2, \ldots, a_{k_i}$ are subarcs of the first string of $\hat{J}_i$. Let $\hat{S}_i$ denotes branched alternating closed braid. If $\hat{J}_i$ is regular, then $\hat{S}_i$ is called regular. The irregular alternating closed braid $\hat{J}_i$ and the branched alternating closed braid $\hat{S}_i$ as illustrated in Figure 4.

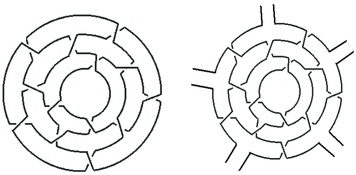

Figure 4. The irregular alternating closed braid $\hat{J}_i$ and the branched alternating closed braid $\hat{S}_i$.

We can construct a new type of polyhedral links on an arbitrary convex polyhedra by the method of $\hat{S}_i$ and double lines covering. Firstly, taking a $\hat{J}_i$ with $c[1:2] = k_i$, using $\hat{S}_i$ to cover a vertex with $d(v_i) = k_i$ of a polyhedron P until every vertex of P is covered in the same way. secondly, using double lines to cover every edge of P. For example, when $n(\hat{J}_i) = 2$, $\hat{S}_i$ is k_i cross curve, as shown in Figure 5. Applying $\hat{S}_i$ and double lines covering on tetrahedron leads to tetrahedral links, as shown in Figure 6. Applying $\hat{S}_i$ and double lines covering on bipyramid leads to bipyramidal links, as shown in Figure 7.

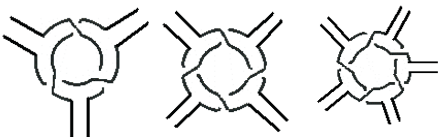

Figure 5. 3–cross–curve, 4–cross–curve and 5-cross-curve.

4 Some conditions for the polyhedral links to be chiral

A connected plane medial graph $M(G)$ is a 4-regular plane graph which can be obtained from a connected non-trivial graph G as shown in Figure 8. A signed graph is a graph with each of its edges labeled with a sign (+1 or -1). According to the sign of the

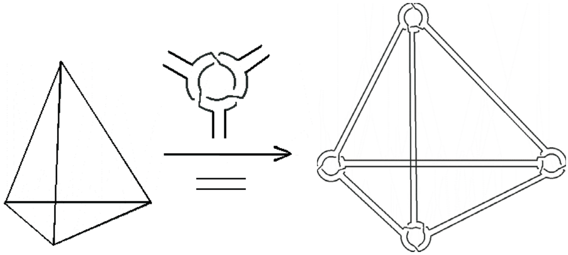

Figure 6. The tetrahedral link obtained by three cross curves and double lines covering.

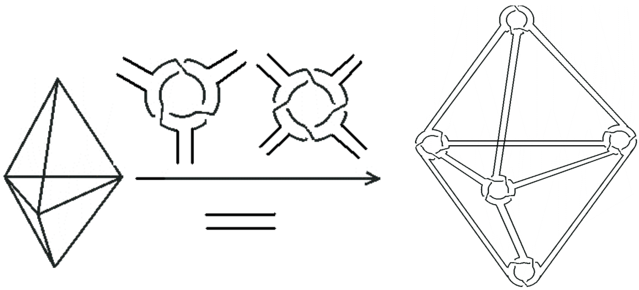

Figure 7. The bipyramidal link obtained by three cross curves, four cross curves and double lines covering.

edge, as shown in Figure 9, we can obtain a knot or link $L(G)$ by converting each vertex of medial graph $M(G)$ into a crossing, as illustrated in Figure 10.

There is a one-to-one correspondence between link diagrams and signed plane graphs via medial construction [22]. Therefore, conversley, given a link diagram L, we first shade every other region of the link diagram so that the infinite outermost region is not shaded, then connect it with a signed plane graph G as follows: put a vertex at the center of each shaded region and connect with an edge any two vertices that are in regions that share a crossing.

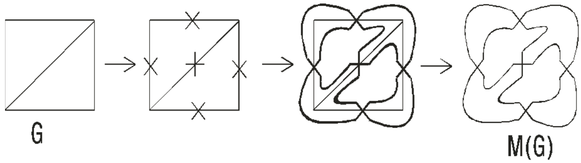

Figure 8. A planar graph G becomes a medial graph $M(G)$.

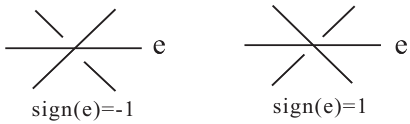

Figure 9. Signs of edges.

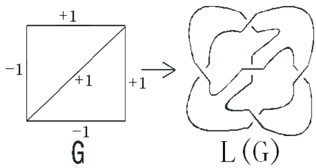

Figure 10. A signed graph G becomes a link $L(G)$.

Definition 4.1. *[23, 24, 25, 26] The Kauffman bracket polynomial* $< L >$ *of a link diagram L is defined by the following three relations:*

(1) $< \bigcirc >= 1$, *where* $\bigcirc$ *denotes the diagram of one component and no crossings.*

(2) $< \bigcirc \sqcup L >= (-A^2 - A^{-2}) < L >$, *where* $\bigcirc \sqcup L$ *denotes the diagram L together with a single component that does not cross itself or L.*

(3) $<$  $>= A <$  $> + A^{-1} <$  $>$.

Definition 4.2. *[22] The generalized Tutte polynomial for a signed graph G is defined by the following properties:*

1. If e is neither an isthmus (i.e., a cut edge) nor a loop in G, then

$$T(G) = A^{-1}T(G-e) + AT(G/e) \qquad sign(e) = +1,$$

$$T(G) = AT(G-e) + A^{-1}T(G/e) \qquad sign(e) = -1,$$

where $G-e$, G/e are obtained from G by deleting and contracting the edge e, respectively.

2. If every edge of G is either an isthmus or a loop and G is connected, then

$$T(G) = X^{i_+ + l_-}Y^{i_- + l_+},$$

where $X = -A^{-3}, Y = -A^3$; $i_+(i_-)$ is the number of the positive (respectively negative) isthmuses; $l_+(l_-)$ is the number of the positive (respectively negative) loops.

3. If G is the disjoint union of graphs G_1 and G_2 , then

$$T(G) = (-A^2 - A^{-2})T(G_1)T(G_2).$$

The relation of Kauffman bracket polynomial and Tutte polynomial is given as follows:

Theorem 4.3. *[22] Let G be a signed plane graph, $L(G)$ be the link diagram associated with G via the medial construction. Then*

$$T(G) =< L(G) > .$$

Theorem 4.4. *[25] If a link L is achiral, then*

$$< L > (A) =< L^* > (A) =< L > (A^{-1}),$$

where link L^* is mirror image of link L.

From Theorem 4.4 we immediately find that the polynomial of an achiral link must be palindromic. Converse-negative proposition of Theorem 4.4 holds. Hence we have the following Theorem:

Theorem 4.5. *If $< L > (A) \neq < L > (A^{-1})$, then link L is chiral.*

According to Theorem 4.5 above, if the sum of degree of maximum and minimum term of Kauffman polynomial of a link diagram L is not equal to zero, then the link L is chial. Hence we can obtain the following conclusions:

Theorem 4.6. *Let G be a signed planar graph from a polyhedral link diagram $\mathbb{L}(P)$, G_i be a signed planar graph from $\hat{J}_i$.*

If $sign(e) = 1, e \in G$, then the maximum degree term and minimum degree term of $< \mathbb{L}(P) >$ are respectively

$$(-1)^{\sum_{i=1}^{n(P)} c(G_i)+f(P)-1} A^{\sum_{i=1}^{n(P)} e(G_i)+2\sum_{i=1}^{n(P)} c(G_i)+2f(P)-2}$$

and

$$(-1)^{-\sum_{i=1}^{n(P)} c(G_i)+\sum_{i=1}^{n(P)} e(G_i)-f(P)+1} A^{2\sum_{i=1}^{n(P)} c(G_i)-3\sum_{i=1}^{n(P)} e(G_i)+2f(P)-2}.$$

If $sign(e) = -1, e \in G$, then the maximum degree term and minimum degree term of $< \mathbb{L}(P) >$ are reverse.

Proof: For each $e \in G$, $sign(e) = 1$ or -1 since $\mathbb{L}(P)$ is alternating. So there are two cases for considering the maximum and minimum degree term of $\mathbb{L}(P)$.

If $sign(e) = 1, e \in G$, then the minimum degree term $< \mathbb{L}(P) >$ comes from spanning tree Γ of graph G. The maximum degree term $< \mathbb{L}(P) >$ comes from graph G^*, where G^* is a graph with one vertex and $\sum_{i=1}^{n(P)} c(G_i) + f(P) - 1$ edges.

Graph G yields graph G^* through $\sum_{i=1}^{n(P)} e(G_i) - [\sum_{i=1}^{n(P)} c(G_i) + f(P) - 1]$ operations of contracting edges. Hence, according to definition 4.2, tree Γ contributes the maximum degree term of $< \mathbb{L}(P) >$, which is

$$A^{\sum_{i=1}^{n(P)} e(G_i)-[\sum_{i=1}^{n(P)} c(G_i)+f(P)-1]}(-A^3)^{\sum_{i=1}^{n(P)} c(G_i)+f(P)-1}.$$

That is

$$(-1)^{\sum_{i=1}^{n(P)} c(G_i)+f(P)-1} A^{\sum_{i=1}^{n(P)} e(G_i)+2\sum_{i=1}^{n(P)} c(G_i)+2f(P)-2}.$$

Graph G gives rise to spanning tree Γ by $\sum_{i=1}^{n(P)} c(G_i) + f(P) - 1$ operations of deleting edges. So the minimum degree term of $\mathbb{L}(P)$ is

$$A^{-[\sum_{i=1}^{n(P)} c(G_i)+f(P)-1]}(-A^{-3})^{\sum_{i=1}^{n(P)} e(G_i)-[\sum_{i=1}^{n(P)} c(G_i)+f(P)-1]}.$$

That is

$$(-1)^{-\sum_{i=1}^{n(P)} c(G_i)+\sum_{i=1}^{n(P)} e(G_i)-f(P)+1} A^{2\sum_{i=1}^{n(P)} c(G_i)-3\sum_{i=1}^{n(P)} e(G_i)+2f(P)-2}.$$

If $sign(e) = -1, e \in G$, then the spanning tree Γ of graph G generates maximum degree term. Graph G^*, consisting of one vertex and $\sum_{i=1}^{n(P)} c(G_i)+f(P)-1$ edges, generates minimum degree term.

We can prove, in the same manner, that graph G^* contributes the maximum degree term of $< \mathbb{L}(P) >$, which is

$$(-1)^{-\sum_{i=1}^{n(P)} c(G_i)+\sum_{i=1}^{n(P)} e(G_i)-f(P)+1} A^{2\sum_{i=1}^{n(P)} c(G_i)-3\sum_{i=1}^{n(P)} e(G_i)+2f(P)-2}$$

and

$$(-1)^{\sum_{i=1}^{n(P)} c(G_i)+f(P)-1} A^{\sum_{i=1}^{n(P)} e(G_i)+2\sum_{i=1}^{n(P)} c(G_i)+2f(P)-2}.$$

□

Applying Theorem 4.6, sufficient condition for the polyhedral links to be chiral can be described via the following Theorem and Corollarys.

Theorem 4.7. *If*

$$\sum_{i=1}^{n(P)}[c(G_i)-n(G_i)]+2f(P)+n(P)-2\neq 0, \tag{1}$$

then polyhedral links $\mathbb{L}(P)$ *are chiral.*

Proof: According to Theorem 4.5, this means that

$$\begin{aligned} & (-1)^{-\sum_{i=1}^{n(P)} c(G_i)+\sum_{i=1}^{n(P)} e(G_i)-f(P)+1} A^{2\sum_{i=1}^{n(P)} c(G_i)-3\sum_{i=1}^{n(P)} e(G_i)+2f(P)-2} \\ \neq\ & (-1)^{\sum_{i=1}^{n(P)} c(G_i)+f(P)-1} A^{-[\sum_{i=1}^{n(P)} e(G_i)+2\sum_{i=1}^{n(P)} c(G_i)+2f(P)-2]}. \end{aligned}$$

So

$$2\sum_{i=1}^{n(P)} c(G_i)-3\sum_{i=1}^{n(P)} e(G_i)+2f(P)-2\neq -[\sum_{i=1}^{n(P)} e(G_i)+2\sum_{i=1}^{n(P)} c(G_i)+2f(P)-2].$$

That is

$$2\sum_{i=1}^{n(P)} c(G_i)-\sum_{i=1}^{n(P)} e(G_i)+2f(P)-2\neq 0.$$

However

$$e(G_i)=n(G_i)+c(G_i)-1,$$

therefore

$$\begin{aligned} & 2\sum_{i=1}^{n(P)} c(G_i)-\sum_{i=1}^{n(P)} e(G_i)+2f(P)-2 \\ =\ & 2\sum_{i=1}^{n(P)} c(G_i)-\sum_{i=1}^{n(P)}[n(G_i)+c(G_i)-1]+2f(P)-2 \\ =\ & \sum_{i=1}^{n(P)}[c(G_i)-n(G_i)]+2f(P)+n(P)-2 \\ \neq\ & 0. \end{aligned}$$

Hence, a sufficient condition for the polyhedral links $\mathbb{L}(P)$ to be chiral is

$$\sum_{i=1}^{n(P)}[c(G_i)-n(G_i)]+2f(P)+n(P)-2\neq 0.$$

□

We now have a better result than the above Theorem by converting $c(G_i)$ and $n(G_i)$ to crossing number of $\hat{J}_i$.

Corollary 4.8. *If*

$$\sum_{i=1}^{n(P)} n(\hat{J}_i)+\frac{1}{2}\sum_{i=x(P)+1}^{n(P)} k_i+2f(P)+x(P)>\frac{1}{2}\sum_{i=1}^{n(P)} k_i n(\hat{J}_i)+n(P)+2, \tag{2}$$

then the polyhedral links $\mathbb{L}(P)$ are chiral, where $x(P)$ denotes the number of i such that $n(\hat{J}_i)$ is even.

Proof: The cyclomatic number of graph G_i from $\hat{J}_i$ is

$$c(G_i)=\begin{cases}\sum_{j=1}^{\frac{n(\hat{J}_i)}{2}-1} c[n(\hat{J}_i)-2j:n(\hat{J}_i)-2j+1]+1 & \text{if } n(\hat{J}_i) \textit{ is even}\\ \sum_{j=1}^{\frac{n(\hat{J}_i)-1}{2}} c[n(\hat{J}_i)-2j+1:n(\hat{J}_i)-2j+2] & \text{if } n(\hat{J}_i) \textit{ is odd,}\end{cases}$$

.

The number of vertices of graph G_i is

$$n(G_i)=\begin{cases}\sum_{j=1}^{\frac{n(\hat{J}_i)}{2}} c[n(\hat{J}_i)-2j+1:n(\hat{J}_i)-2j+2] & \text{if } n(\hat{J}_i) \textit{ is even}\\ \sum_{j=1}^{\frac{n(\hat{J}_i)-1}{2}} c[n(\hat{J}_i)-2j:n(\hat{J}_i)-2j+1]+1 & \text{if } n(\hat{J}_i) \textit{ is odd.}\end{cases}$$

According to $\sum_{i=1}^{n(P)}[c(G_i)-n(G_i)]+2f(P)+n(P)-2$, in order to make it as small as possible, we want to pick a $\hat{J}_i$ where $c(G_i)$ is small but $n(G_i)$ is large. So, the $\hat{J}_i$ is such an alternating closed braid.

If $n(\hat{J}_i)$ is even, then

$$c[n(\hat{J}_i)-2j:n(\hat{J}_i)-2j+1]=2,\ j=1,2,\cdots,\frac{n(\hat{J}_i)}{2}-1,$$

$$c[n(\hat{J}_i)-2j+1:n(\hat{J}_i)-2j+2]=k_i,\ j=1,2,\cdots,\frac{n(\hat{J}_i)}{2}.$$

If $n(\hat{J}_i)$ is odd, then

$$c[n(\hat{J}_i)-2j+1:n(\hat{J}_i)-2j+2]=2,\ j=1,2,\cdots,\frac{n(\hat{J}_i)-1}{2},$$

$$c[n(\hat{J}_i)-2j:n(\hat{J}_i)-2j+1]=k_i,\ j=1,2,\cdots,\frac{n(\hat{J}_i)-1}{2}.$$

Therefore

$$\begin{aligned}
&\sum_{i=1}^{n(P)}[c(G_i)-n(G_i)]+2f(P)+n(P)-2\\
=&\sum_{i=1}^{x(P)}[c(G_i)-n(G_i)]+\sum_{i=x(P)+1}^{n(P)}[c(G_i)-n(G_i)]+2f(P)+n(P)-2\\
\geq&\sum_{i=1}^{x(P)}[(2-k_i)(\frac{n(\hat{J}_i)}{2}-1)-k_i+1]+\sum_{i=x(P)+1}^{n(P)}[(2-k_i)\frac{n(\hat{J}_i)-1}{2}-1]\\
=&\sum_{i=1}^{n(P)}n(\hat{J}_i)-\frac{1}{2}\sum_{i=1}^{n(P)}k_in(\hat{J}_i)+\frac{1}{2}\sum_{i=x(P)+1}^{n(P)}k_i+2f(P)+x(P)-n(P)-2.
\end{aligned}$$

According to Theorem 4.7, when

$$\sum_{i=1}^{n(P)}n(\hat{J}_i)-\frac{1}{2}\sum_{i=1}^{n(P)}k_in(\hat{J}_i)+\frac{1}{2}\sum_{i=x(P)+1}^{n(P)}k_i+2f(P)+x(P)-n(P)-2>0,$$

that is

$$\sum_{i=1}^{n(P)}n(\hat{J}_i)+\frac{1}{2}\sum_{i=x(P)+1}^{n(P)}k_i+2f(P)+x(P)>\frac{1}{2}\sum_{i=1}^{n(P)}k_in(\hat{J}_i)+n(P)+2,$$

the polyhedral links are chiral. □

Corollary 4.9. *If $\hat{J}_i$ is regular, then polyhedral links $\mathbb{L}(P)$ are chiral, where $i=1,2,\ldots,n(P)$.*

Proof: From Theorem 4.7, we immediately yield

$$
\begin{aligned}
& \sum_{i=1}^{n(P)}[c(G_i)-n(G_i)]+2f(P)+n(P)-2 \\
= & \sum_{i=1}^{x(P)}[c(G_i)-n(G_i)]+\sum_{i=x(P)+1}^{n(P)}[c(G_i)-n(G_i)]+2f(P)+n(P)-2 \\
= & -\sum_{i=1}^{x(P)}(k_i-1)-[n(P)-x(P)]+2f(P)+n(P)-2 \\
= & -\sum_{i=1}^{x(P)}(k_i-1)+x(P)+2f(P)-2 \\
= & -\sum_{i=1}^{x(P)}(k_i-1)+x(P)+2e(P)-2n(P)+2 \\
= & -\sum_{i=1}^{x(P)}(k_i-1)+x(P)+\sum_{i=1}^{n(P)}k_i-2n(P)+2 \\
= & \sum_{i=x(P)+1}^{n(P)} k_i+2x(P)-2n(P)+2 \\
\geq & \ 3[n(P)-x(P)]+2x(P)-2n(P)+2 \\
= & \ n(P)-x(P)+2>0.
\end{aligned}
$$

Hence the polyhedral links $\mathbb{L}(G)$ are chiral. □

Note: A necessary condition of Theorem 4.7 and its Corollary 4.8 is not necessarily hold. For example, for a tetrahedra, when

$$
\begin{cases} n(\hat{J}_i)=4, n(\hat{J}_4)=3 & i=1,2,3 \\ k_j=3 & j=1,2,3,4. \end{cases}
$$

The tetrahedral link we construct as shown in Figure 11.

The tetrahedral link is chiral, because $<\mathbb{L}(P)>=-A^{60}+15A^{56}+\ldots+9A^{-56}-A^{-60}$ is not palindromic. However, according to Theorem 4.7, we have

$$
2\sum_{i=1}^{n(P)}[c(G_i)-n(G_i)]+2f(P)+n(P)-2=-3\times 3-1+10=0.
$$

Hence the necessary condition is not necessarily true.

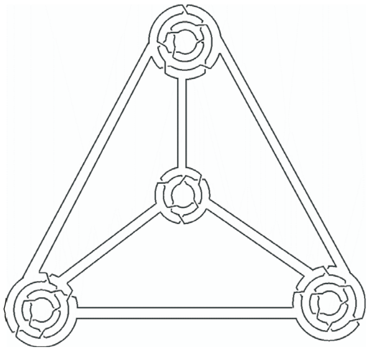

Figure 11. Polyhedral link with chirality dissatisfy formula 1 and 2.

5 Conclusions

We have presented a novel method for the fabrication of polyhedral links to explain some characteristic of DNA and protein polyhedral catenanes, as well as, have obtained three sufficient conditions for the polyhedral links to be chiral. The novel method is a generalization of three cross curves and double lines covering, which in fact can be applied to an arbitrary 3-regular convex polyhedron. For a 72-hedron, when $n(\hat{J}_i) = 2$, $k_i = 3$, then $\hat{J}_i$ is a 3-regular alternating closed braid and $\hat{S}_i$ is a three cross curve, the polyhedral link with 12 pentameric and 60 hexameric rings is obtained. Interestingly, we find that the structure can be used to model the novel folding fashion of HK97 capsid proteins.

To distinguish the two forms of chirality, which are often designated right-handed or left-handed. Chemists refer to mirror-image molecules as L-configuration and D-configuration. Such as sugars are almost belong to D-configuration, but amino acids are almost belong to L-configuration. Theorem 4.7 is a fundamental formula for determining chirality of polyhedral links. Corollary 4.8 establishes a strong condition for the chirality of polyhedral links, which is basically relied on the string number and crossing number of the fist and second string of every closed braid. Corollary 4.9 emphasize that each polyhedral link which is covered by regular branched alternating closed braids is chiral. The Corollary have the better function of theory direction in practice. For the above model of 72-hedral link, it is chiral obtained by Corollary 4.8. On the other hand, each $\hat{J}_i$, which corresponding $\hat{S}_i$ is the building block of 72-hedral link, is 3-regular. So the chirality of the link can also be determinant from Corollary 4.9. This means HK97 capsid proteins is chiral, which can be confirmed by tilt experiment.

Acknowledgements
This work was supported by grants from The National Natural Science Foundation of China (No. 10831001 and 90203012).

References

[1] H. L. Frisch, E. J. Wassermann, Chemical topology, *J. Am. Chem. Soc.* **83** (1961) 3789–3795.

[2] J. Chen, N. C. Seeman, Synthesis from DNA of a molecule with the connectivity of a cube, *Nature* **350** (1991) 631–633.

[3] N. C. Seeman, DNA in a material world, *Nature* **421** (2003) 427–431.

[4] Y. Zhang, N. C. Seeman, Construction of a DNA-truncated octahedron, *J. Am. Chem. Soc.* **116** (1994) 1661–1669.

[5] C. M. Erben, R. P. Goodman, A. J. Turberfield, A self-assembled DNA bipyramid, *J. Am. Chem. Soc.* **129** (2007) 6992–6993.

[6] F. A. Aldaye, H. F. Sleiman, Modular access to structurally switchable 3D discrete DNA assemblies, *J. Am. Chem. Soc.* **129** (2007) 13376–13376.

[7] F.F. Andersen, B. Knudsen, et al., Assembly and structural analysis of a covalently closed nano-scale DNA cage, *Nucleic Acids Res.* **36** (2008) 1113–1119.

[8] Y. He, T. Ye, M. Su, C. Zhang, A. E. Ribbe, W. Jiang, C. d. Mao, Hierarchical self-assembly of DNA into symmetric supramolecular polyhedra, *Nature* **452** (2008) 198–202.

[9] R. L. Duda, Protein chainmail: catenated protein in viral capsids, *Cell* **94** (1998) 55–60.

[10] N.Jonoska, R. Twarock, Blueprints for dodecahedral DNA cages, *J. Phys. A: Math. Theor.* **41** (2008) 304043.

[11] W. Y. Qiu, X. D. Zhai, Molecular design of Goldberg polyhedral links, *J. Mol. Struct. (THEOCHEM)* **756** (2005) 163–166.

[12] Y. M. Yang, W. Y. Qiu, Molecular design and mathematical analysis of carbon nanotube Links, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 635–646.

[13] W. Y. Qiu, X. D. Zhai, Y.Y. Qiu, Architecture of platonic and Archimedean polyhedral links, *Sci. China Ser. B-Chem.* **51** (2008) 13–18.

[14] G. Hu, W. Y. Qiu, Extended Goldberg polyhedral links with even tangles, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 737–752.

[15] G. Hu, W. Y. Qiu, Extended Goldberg polyhedral links with even tangles, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 753–766.

[16] G. Hu, X. D. Zhai, D. Lu, W. Y. Qiu, The architecture of Platonic polyhedral links, *J. Math. Chem.* (2008) (DOI 10.1007/s10910-008-9487-z).

[17] P. G. Mezey, Chirality measures and graph representations, *Comput. Math. Appl.* **34** (1997) 105–112.

[18] C. Liang, K. Mislow, A left-right classification of topologically chiral knots, *J. Math. Chem.* **15** (1994) 35–62.

[19] C. Liang, K. Mislow, Topological chirality and achirality of links, *J. Math. Chem.* **18** (1995) 1–24.

[20] C. Liang, K. Mislow, Specification of chirality for links and knots, *J. Math. Chem.* **19** (1996) 241–263.

[21] E. Flapan, *When topology meets chemistry-a topological look at molecular chirality*, Cambridge University Press, Cambridge, 2000.

[22] L. H. Kauffman, A Tutte polynomial for signed graphs, *Discrete Appl. Math.* **25** (1989) 105–127.

[23] L. H. Kauffman, State models and the Jones polynomial, *Topology* **26** (1987) 395–407.

[24] L. H. Kauffman, Statistical mechanics and the Jones polynomial, *AMS Contemp. Math. Series* **78** (1989) 263–297.

[25] L. H. Kauffman, New invariants in knot theory, *Amer. Math. Monthly* **95** (1988) 195–242.

[26] L. H. Kauffman, On Knots, *Ann. of Math. Study* **115** Princeton University Press, Princeton, NJ (1987).