

The Braid Index of Complicated DNA Polyhedral Links

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Abstract

The goal of this paper is to determine the braid index of two types of complicated DNA polyhedral links introduced by chemists and biologists in recent years. We shall study it in a more broad context and actually consider so-called Jaeger's links (more general Traldi's links) which contain, as special cases, both four types of simple polyhedral links whose braid indexes have been determined and the above two types of complicated DNA polyhedral links. Denote by $b(L)$ and $c(L)$ the braid index and crossing number of an oriented link L , respectively. Roughly speaking, in this paper, we prove that $b(L) = \frac{c(L)}{2} + 1$ for any link L in a family including Jaeger's links and contained in Traldi's links, which is obtained by combining the MFW inequality and an Ohyaama's result on upper bound of the braid index. Our result may be used to characterize and analyze the structure and complexity of DNA polyhedra and entanglement in biopolymers.

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Introduction

The braid index of links has some applications in chemistry and molecular biology. For example, representing knotted hydrocarbon complexes as closed braids [1] can facilitate the study of their properties. In recent 20 years, many DNA polyhedral links such as DNA cube [2], DNA tetrahedron [3], DNA octahedron [4], DNA truncated octahedron [5], DNA bipyramid [6], DNA dodecahedron [7], DNA icosahedron and buckyballs [8] etc, have been synthesized in laboratories or schemes for synthesizing them have been designed by chemists and biologists. In addition, several novel types of polyhedral links have also been posed by mathematicians as a potential object to be synthesized. For four types of simple polyhedral links, their braid indexes have been determined in [9]. The purpose of this paper is to determine braid index of another two types of more complicated polyhedral links appeared in [8,10,11,12,13] and [14], respectively. We shall study it in a more broad context and actually consider so-called Jaeger's links and more general Traldi's links.

In [15], Jaeger associated to a plane graph an oriented link diagram by replacing each edge of the graph by an oriented clasp as illustrated in (a) of Figure 1. Then he established a relation between the Tutte polynomial [16] of the graph and the HOMFLY polynomial [17,18] of the associated oriented link. Moreover, about one year later, both the construction and the relation were extended by Traldi in [19], Traldi constructed his oriented link diagram based on a plane graph via replacing each edge by one of four types of oriented clasps (a),(b),(c) and (d), as illustrated in Figure 1. By assigning four different weights to edges of the plane graph according to the four types of oriented clasps he built a relation between the weighted dichromatic polynomial [19]

of the graph and the HOMFLY polynomial of the associated oriented link.

Formally, let L be an oriented link, we call L to be a Jaeger's link if L , or its reverse, or its mirror image, or its inverse (i.e. the composition of the reverse and the mirror image), has an oriented diagram which can be obtained from a connected plane graph by replacing each edge of the graph by an oriented clasp (a) in Figure 1. According to the above definition, Jaeger's links will be all alternating. Analogously, we call L to be a Traldi's link if L , or its reverse, has an oriented diagram which can be obtained from a connected plane graph by replacing each edge of the graph by one of four types of oriented clasps in Figure 1. Note that different edges may be replaced by different types of oriented clasps. Traldi's links may not be alternating, say, the link $L8n7$ in the Thistlethwaite Link Table [20]. Clearly, Traldi's links contain Jaeger's links as special cases.

The braid index of an oriented link is the minimum number of strings among all closed braid representatives for the given oriented link. We point out that the braid index depends on orientations of links. See Page 215 of [21]. Let L be an oriented link. We denote by $b(L)$ the braid index of L . It is, in general, very hard to determine this geometric and numerical invariant $b(L)$ [21]. Let $P_L(v,z)$ be the HOMFLY polynomial of the oriented link L . In [22] and [23], Franks, Williams and Morton gave independently a lower bound for the braid index $b(L)$ of an oriented link L in terms of $span_v P_L(v,z)$ as follows:

$$\frac{1}{2} span_v P_L(v,z) + 1 \leq b(L), \quad (1)$$

where $span_v P_L(v,z) = \max \deg_v P_L(v,z) - \min \deg_v P_L(v,z)$, and $\max \deg_v P_L(v,z)$ and $\min \deg_v P_L(v,z)$ denote, respectively, the maximal degree and minimal degree of v in the polynomial $P_L(v,z)$. This inequality (1) is usually called MFW inequality. The MFW inequality was the first known result relating the braid index to the HOMFLY polynomial. To date, we have known that the MFW inequality for many link families is sharp. For example, the inequality is sharp for all torus links, closed positive n -braids with a full twist [22], 2-bridge links [24], alternating fibred links [24] and a certain family of closed positive braids [25]. In this paper we shall prove the sharpness of the MFW inequality for a family of links including Jaeger's links and contained in Traldi's links. We shall make use of the following result obtained by Ohyama in 1993 [26] which states that for a non-splittable oriented link L ,

$$b(L) \leq 1 + \frac{c(L)}{2}, \tag{2}$$

where $c(L)$ is the crossing number of L . In fact, you will see this upper bound and the MFW lower bound coincide for a family of links including Jaeger's links, but do not coincide for general Traldi's links.

Note that many types of polyhedral links are, in fact, Jaeger's links defined above. Four types of simple polyhedral links considered in [9] are actually all Jaeger's links constructed from subdivisions of (convex) polyhedral graphs or their duals. Note that the dual of a polyhedral graph is also a polyhedral graph and Steinitz's theorem states that a polyhedral graph is a 3-connected simple (i.e. no loops and no multiple edges) planar graph. Thus the result in [9] can not be used to deal with general Jaeger's links.

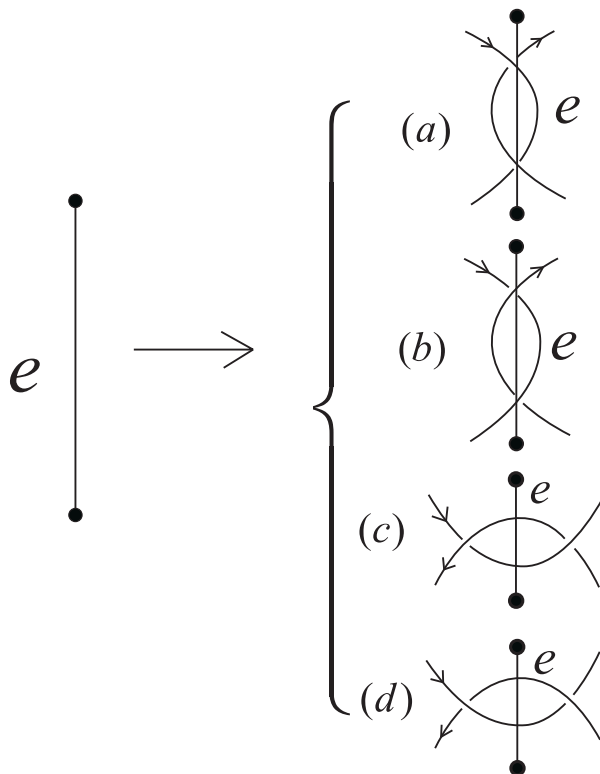


Figure 1. Replace an edge by four types of oriented clasp.
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Roughly speaking, in this paper we prove that $b(L) = \frac{c(L)}{2} + 1$ for any link L in a family including Jaeger's links and contained in Traldi's links and thus extend the result in [9]. This extension enables us to determine the braid index of another two types of more complicated polyhedral links in [8,10] and [14] as well as four types of polyhedral links in [9]. It is probable that our result be used to determine braid indexes of new types of polyhedral links to be synthesized in the future. Our research demonstrates that using the braid index or crossing index to describe the complexity of some polyhedral links are equivalent and it may open a door to characterize, analyze the structure and complexity of DNA polyhedra and entanglement in biopolymers.

Analysis

Before analyzing the braid index of polyhedral links, we give some preliminary knowledge on links, the HOMFLY polynomial, graphs and the dichromatic polynomial.

1. Links

A **knot** is a simple closed curve in $R^3 \subset S^3$, i.e. the image of the embedding of S^1 into R^3 . A **link** L of n components is a disjoint union of n knots: $L = K_1 \cup \dots \cup K_n$. A knot is a link with one component. An oriented link is a link with each of its component assigned an orientation. A **link diagram** is a (regular) projection of a link onto a plane with the under-strand specified by using gaps at each crossing. When the link is oriented, the link diagram will inherit the orientation of the link in a natural way and called oriented link diagram. The **crossing number** or **crossing index** of a link L , denoted by $c(L)$, is the least number of crossings that occur in any diagram of the link. A diagram with fewest number of crossings for a given link is called a **minimal** diagram for the link.

An **n -string braid** b is a set of n strings in a 3-dimensional cube $I \times I \times I$, where $I = [0,1]$, all of which are attached to a horizontal bar at the top $\{\frac{1}{2}\} \times I \times \{1\}$ and at the bottom $\{\frac{1}{2}\} \times I \times \{0\}$ such that each $I \times I \times x$, $x \in S^1$, meets the n strings in exactly n points. A **closed n -string braid** \hat{b} is a set of n strings embedded in $I \times I \times S^1$ such that each $I \times I \times x$, $x \in S^1$, meets the n strings in exactly n points. An example is illustrated in Figure 2.

It is clear that a closed n -string braid \hat{b} is an oriented link with the convention that we always orient \hat{b} from the top to the bottom. Conversely, Alexander [27], in 1923, showed that every oriented link in S^3 can be represented as a closed n -string braid. The **braid**

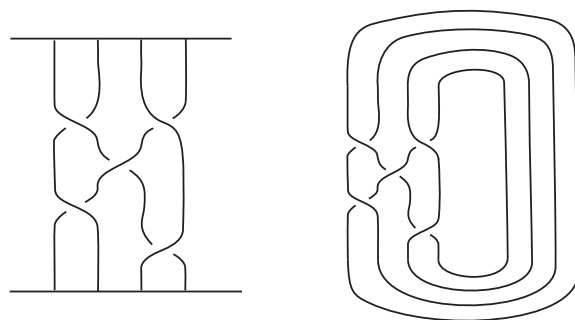


Figure 2. A braid b and its corresponding closed braid \hat{b} .
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index $b(L)$ for an oriented link L is the smallest positive integer n such that L can be represented as a closed n -string braid.

Let L be an oriented link. We denote by L' and L^m the reverse (reversing the orientation of each component of L) and the mirror image of L , respectively. Then it is obvious that $b(L) = b(L') = b(L^m)$.

2. The HOMFLY polynomial

The HOMFLY polynomial is an invariant of oriented links, introduced in [17] and [18] independently. Now we recall the definition of the HOMFLY polynomial. The HOMFLY polynomial of an oriented link L , denoted by $P_L(v, z)$, can be defined by the three following axioms [28].

- (1) $P_L(v, z)$ is invariant under ambient isotopy of L .
- (2) If L is the trivial knot then $P_L(v, z) = 1$.
- (3) It satisfies the skein relation: $v^{-1}P_{L_+}(v, z) - vP_{L_-}(v, z) = zP_{L_0}(v, z)$, where L_+ , L_- and L_0 are link diagrams which are identical except near one crossing where they are as in Figure 3 and are called a skein triple.

It possesses the following basic properties [28], which imply that $span_v P_L(v, z) = span_v P_{L^m}(v, z) = span_v P_{L'}(v, z)$.

- (a) If L' is the reverse of L , then $P_{L'}(v, z) = P_L(v, z)$.
- (b) If L^m is the mirror image of L , then $P_{L^m}(v, z) = P_L(-v^{-1}, z)$.

3. Graphs

Let $G = \langle V(G), E(G) \rangle$ be a graph. We denote by $|V(G)|$ and $|E(G)|$ the numbers of vertices and edges, respectively, of the graph G . A graph G is said to be **connected** if it has a path with two distinct vertices u and v whenever $u, v \in V(G)$ and G is said to be disconnected otherwise. A **component** of a graph G is a subgraph that is connected and is not properly contained in any other connected subgraph of G . We denote by $k(G)$ the number of components of the graph G . An edge e of G is said to be a **bridge** if $k(G - e) > k(G)$. If G has no bridges, G is said to be bridgeless. An edge e of G is said to be a **loop** if its two end-vertices are the same. If G has no loops, G is said to be loopless. The **rank** $r(G)$ and **nullity** $n(G)$ of the graph G is defined to be $|V(G)| - k(G)$ and $|E(G)| - |V(G)| + k(G)$, respectively. It is well known that $r(G)$ and $n(G)$ are exactly the dimensions of cycle space and cut space, respectively, of the graph G and hence, are both non-negative integers. See, for example, [29].

Given a graph G and an edge e of G , we write $G - e$ for the graph obtained from G by deleting the edge e , and G/e for the graph obtained from G by contracting e , i.e. deleting e firstly and then identifying its two endvertices. A **planar** graph is a graph which can be embedded in the plane or equivalently, the sphere S^2 . A specific embedding of a planar graph is called a **plane**

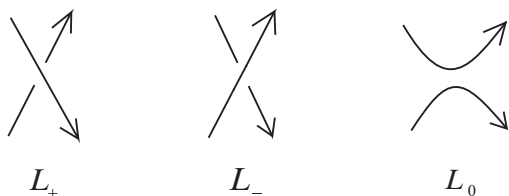


Figure 3. L_+ , L_- and L_0 . doi:10.1371/journal.pone.0048968.g003

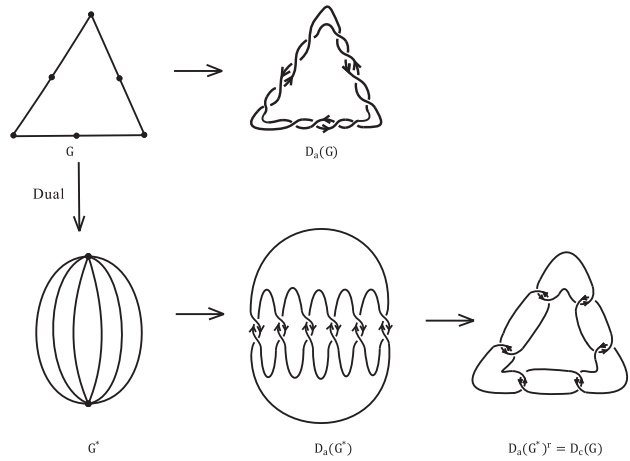


Figure 4. An example. doi:10.1371/journal.pone.0048968.g004

graph. For undefined notations and terminologies on graph theory, we refer the readers to [29].

4. The dichromatic polynomial

A weighted graph is a graph G together with a function w mapping $E(G)$ into some commutative ring R with unity 1. If e is an edge of the weighted graph G , then $w(e)$ is the weight of the edge e . The dichromatic polynomial for weighted graphs was introduced by Traldi in [19], which is a generalization of the Tutte polynomial for signed graphs introduced by Kauffman in [30]. We point out there are actually several weighted versions of the Tutte polynomial.

The dichromatic polynomial $Q(t, z)$ of a weighted graph G can be defined as

$$Q(t, z) = \sum_{F \subseteq E(G)} \left(\prod_{f \in F} w(f) \right) t^{k\langle F \rangle} z^{n\langle F \rangle}, \quad (3)$$

where the summation is over all edge subsets, F , of G , $k\langle F \rangle$ and $n\langle F \rangle$ are the number of components and the nullity, respectively, of the spanning subgraph $\langle F \rangle$, induced by F , of G . It can also be defined by using the following recursive relations:

- (1) If G is an edgeless graph with $n \geq 1$ vertices $Q(G) = t^n$.
- (2) If e is a loop of G , then $Q(G) = (1 + w(e)z)Q(G - e)$.
- (3) If e is not a loop of G , then $Q(G) = Q(G - e) + w(e)Q(G/e)$.



Figure 5. An alternating Traldi's link upper and lower bounds of whose braid index are not equal. doi:10.1371/journal.pone.0048968.g005

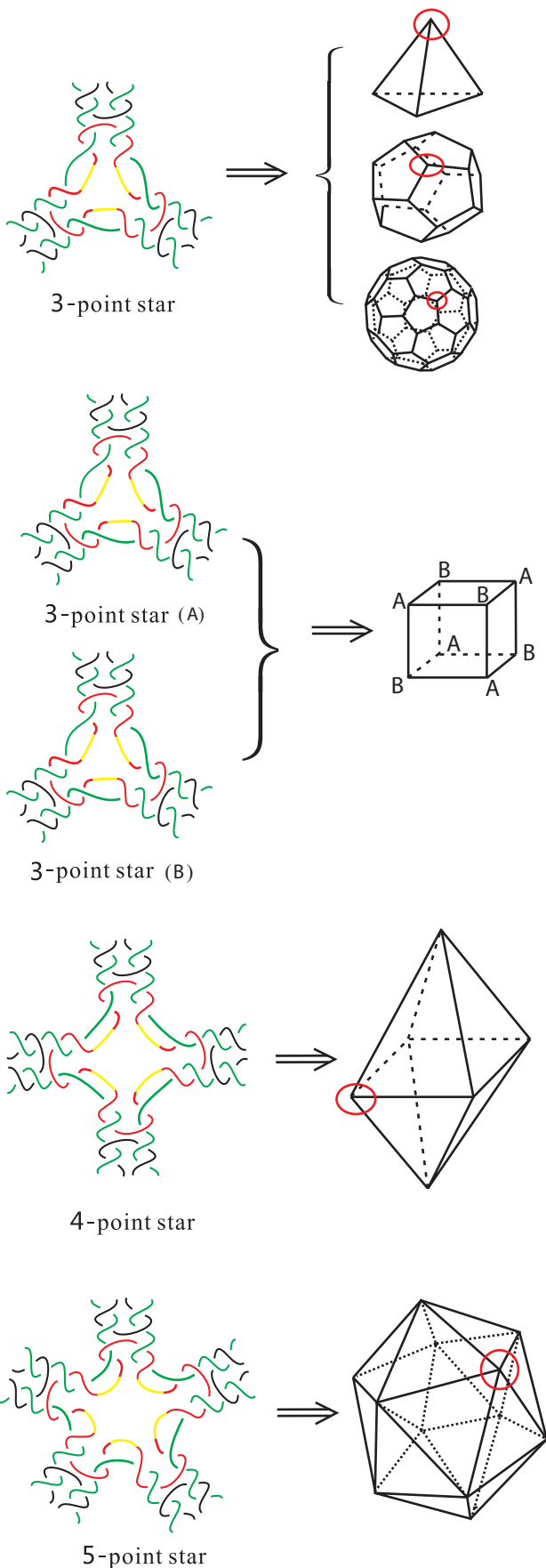


Figure 6. 3-point star motifs: DNA tetrahedron, cube, dodecahedron, buckyball; 4-point star motifs: DNA octahedron; 5-point star motifs: DNA icosahedron.
doi:10.1371/journal.pone.0048968.g006

Just as the Tutte polynomial, it also has a spanning tree expansion and we do not explain it here.

Now we start to analyze the braid index of polyhedral links. We first consider a family of Jaeger’s links.

Let G be a connected plane graph. Let $D_a(G)$ be the oriented link diagram constructed based on G by covering each edge of G with oriented clasp (a) in Figure 1. Oriented link diagrams $D_b(G), D_c(G)$ and $D_d(G)$ can be defined similarly. Let $D_{a,d}(G)$ be the oriented link diagram constructed based on G by covering some edges of G with oriented clasp (a) and other edges with oriented clasp (d) in Figure 1. Oriented link diagrams $D_{b,c}(G)$ can be defined similarly. Note that $D_{a,d}(G)$ (resp. $D_{b,c}(G)$) contains $D_a(G), D_d(G)$ (resp. $D_b(G), D_c(G)$) as special cases. More generally, $D_{a,b,c,d}(G)$ is defined to be the oriented link diagram obtained from G by covering each edge with one of four types of clasps (a), (b), (c) and (d). In [19], Traldi obtained the following general formula.

Theorem 1. Let G be a plane graph. Let $D(G) = D_{a,b,c,d}(G)$ be the Traldi’s oriented link diagram. Let the weight of the edge replaced by oriented clasp (a), (b), (c) and (d) be $\frac{v}{z}$, $-\frac{1}{vz}$, $\frac{z}{v}$ and $-vz$, respectively. Then

$$P_{D(G)}(v,z) = \frac{z}{v^{-1}-v} (vz)^a \left(-\frac{z}{v}\right)^b v^{2c-2d} Q_G\left(\frac{v^{-1}-v}{z}, \frac{v^{-1}-v}{z}\right), \quad (4)$$

where a, b, c and d are numbers of edges of G which are replaced by oriented clasp (a), (b), (c) and (d), respectively.

The following theorem is a main theoretical tool for determining the braid index of polyhedral links.

Theorem 2. Let G be a connected bridgeless and loopless plane graph. Let $L_{a,d}(G)$ (resp. $L_{b,c}(G)$) be the oriented link that $D_{a,d}(G)$ (resp. $D_{b,c}(G)$) represents. Then

$$b(L_{a,d}(G)) = |E(G)| + 1 = \frac{c(L_{a,d}(G))}{2} + 1, \quad (5)$$

$$b(L_{b,c}(G)) = |E(G)| + 1 = \frac{c(L_{b,c}(G))}{2} + 1. \quad (6)$$

Proof. Note that $L_{b,c}(G)$ is the mirror image of some $L_{a,d}(G)$ and taking the mirror image does not change the braid index and the crossing index. It suffices for us to prove Eq. (5). When G is bridgeless and loopless, it is not hard to observe that $D_{a,d}(G)$ is a connected alternating oriented link diagram without nugatory crossings. According to the famous result [31,32,33] due to Kauffman, Murasugi and Thistlethwaite: A connected alternating link diagram without nugatory crossings is minimal, we obtain that

$$c(L_{a,d}(G)) = 2|E(G)|, \quad (7)$$

where $L_{a,d}(G)$ is the link that the link diagram $D_{a,d}(G)$ represents. In addition, by a result [34] due to Menasco that states that a link with an alternating diagram will be non-splittable if and only if the diagram is connected, we know that $L_{a,d}(G)$ is non-splittable. Thus, by Eq. (2), we have

$$b(L_{a,d}(G)) \leq |E(G)| + 1. \tag{8}$$

Now we consider the lower bound of $b(L_{a,d}(G))$. For the oriented link $L_{a,d}(G)$, as a special case of Theorem 1, we obtain

$$\begin{aligned} P_{L_{a,d}(G)}(v,z) &= \frac{z}{v^{-1}-v} (vz)^a v^{-2d} Q_G\left(\frac{v^{-1}-v}{z}, \frac{v^{-1}-v}{z}\right)_{w_a=vz, w_d=-vz} \\ &= \left(\frac{z}{v^{-1}-v}\right)^{a-2d} z^a \sum_{F \subseteq E(G)} \left(\prod_{f \in F} w(f)\right) \left(\frac{v^{-1}-v}{z}\right)^{k\langle F \rangle} \left(\frac{v^{-1}-v}{z}\right)^{n\langle F \rangle} \\ &= \left(\frac{z}{v^{-1}-v}\right)^{a-2d} z^a \sum_{F \subseteq E(G)} \left(\prod_{f \in F} w(f)\right) \left(\frac{v^{-1}-v}{z}\right)^{|F|-|V(G)|+2k\langle F \rangle} \\ &= \left(\frac{z}{v^{-1}-v}\right)^{a-2d} z^a \sum_{F \subseteq E(G)} \left(\left(\frac{v}{z}\right)^{a(F)} (-vz)^{d(F)}\right) \left(\frac{v^{-1}-v}{z}\right)^{|F|-|V(G)|+2k\langle F \rangle} \tag{9} \\ &= v^{a-2d} z^a \sum_{F \subseteq E(G)} (-1)^{d(F)} v^{|F|} z^{d(F)-a(F)} \left(\frac{v^{-1}-v}{z}\right)^{|F|-|V(G)|+2k\langle F \rangle-1} \\ &= \sum_{F \subseteq E(G)} (-1)^{d(F)} v^{a-2d+|V(G)|-2k\langle F \rangle+1} (1-v^2)^{|F|-|V(G)|+2k\langle F \rangle-1} \\ &\quad z^{a+d(F)-a(F)-|F|+|V(G)|-2k\langle F \rangle+1}, \end{aligned}$$

where $a(F)$ and $d(F)$ are numbers of edges in F covered by clasps of types (a) and (d) , respectively. It is clear that $a(F) + d(F) = |F|$.

Now we compute the highest and lowest degrees in v of Eq. (9). Note that the power of $1-v^2$ is $|F|-|V(G)|+2k\langle F \rangle-1 = n\langle F \rangle + k\langle F \rangle - 1 \geq 0$. Thus we have

$$\begin{aligned} \max \deg_v P_{L_{a,d}(G)}(v,z) &= \max_F \{(a-2d+|V(G)|-2k\langle F \rangle+1) \\ &\quad + 2(|F|-|V(G)|+2k\langle F \rangle-1)\} \\ &= \max_F \{a-2d+|V(G)|-1+2n\langle F \rangle\} \\ &= a-2d+|V(G)|-1+2n\langle E(G) \rangle \\ &= a-2d+|V(G)|-1+2|E(G)|-2|V(G)|+2 \\ &= a-2d+2|E(G)|-|V(G)|+1. \end{aligned}$$

The third equation holds since $n\langle F \rangle$ attains maximality if and only if $F = E(G)$ because of G is bridgeless. Similarly, we have

$$\begin{aligned} \min \deg_v P_{L_{a,d}(G)}(v,z) &= \min_F \{a-2d+|V(G)|-2k\langle F \rangle+1\} \\ &= a-2d+|V(G)|-2k\langle \emptyset \rangle+1 \\ &= a-2d-|V(G)|+1. \end{aligned}$$

The second equation holds since $k\langle F \rangle$ attains maximality if and only if $F = \emptyset$ since G is loopless. Thus,

$$\begin{aligned} \text{span}_v P_{L_{a,d}(G)}(v,z) &= \max \deg_v P_{L_{a,d}(G)}(v,z) - \min \deg_v P_{L_{a,d}(G)}(v,z) \\ &= (a-2d+2|E(G)|-|V(G)|+1) - (a-2d-|V(G)|+1) \\ &= 2|E(G)|. \end{aligned}$$

Hence, by Eq. (1), we obtain

$$b(L_{a,d}(G)) \geq |E(G)| + 1. \tag{10}$$

Combining Eq. (8) with Eq. (10), we show that Eq. (5) holds. \square

Corollary. (1). Let G be a connected bridgeless plane graph. Then

$$b(L_a(G)) = |E(G)| + 1 = \frac{c(L_a(G))}{2} + 1, \tag{11}$$

$$b(L_b(G)) = |E(G)| + 1 = \frac{c(L_b(G))}{2} + 1. \tag{12}$$

(2). Let G be a connected loopless plane graph. Then

$$b(L_c(G)) = |E(G)| + 1 = \frac{c(L_c(G))}{2} + 1, \tag{13}$$

$$b(L_d(G)) = |E(G)| + 1 = \frac{c(L_d(G))}{2} + 1. \tag{14}$$

As a result,

$$b(L) = \frac{c(L)}{2} + 1 \tag{15}$$

for any Jaeger's link L .

Proof. By checking the proof of Theorem 2, we find that the condition "loopless" is actually not necessary for the special case $L_a(G)$. Hence, Eq. (11) holds. Eq. (12) follows from Eq. (11) and the fact $L_b(G) = L_a^m(G)$. Let G be a connected loopless plane graph and G^* be the planar dual of G . Then G^* is connected and

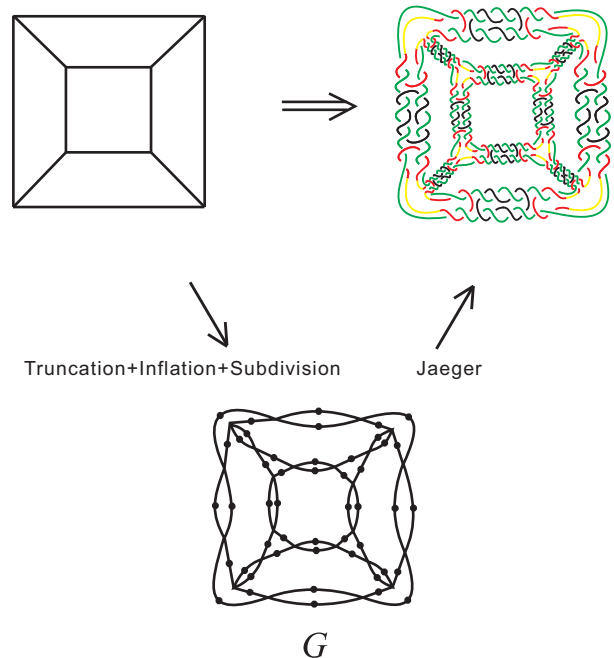


Figure 7. Planar form of double crossover DNA cube and its associated plane graph G .

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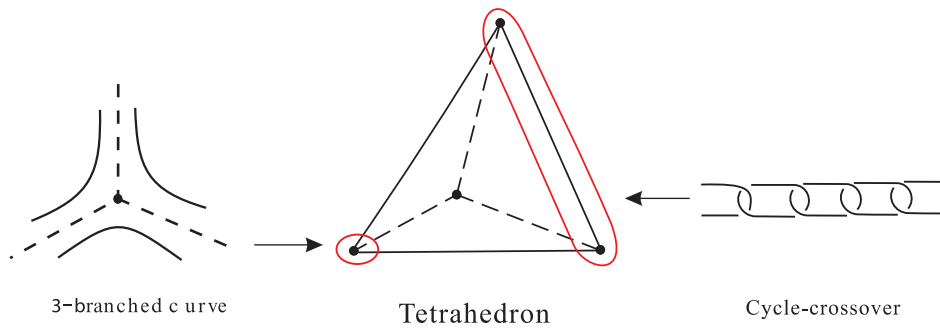


Figure 8. 3-branched curve, cycle-crossover and the construction of cycle-crossover tetrahedral link.
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bridgeless. Note that $L_c(G) = L'_a(G^*)$ (see Figure 4 for an example) and $L_d(G) = L^m_a(G^*)$ and reversing orientations do not change braid index and crossing index. Hence, Eqs. (13) and (14) hold. By the definition of a Jaeger's link L , we know that there is a connected plane graph G such that L is equivalent to one of the four links: $L_a(G)$, $L^m_a(G)$, $L'_a(G)$ and $L^{mr}_a(G) = L^m_a(G)$. It will suffice to prove that $b(L_a(G)) = \frac{c(L_d(G))}{2} + 1$ for any connected plane graph G . Firstly, $b(L_a(G)) = |E(G)| + 1 = \frac{c(L_d(G))}{2} + 1$ for any connected bridgeless plane graph G . Secondly, if G has bridges, let G' be the connected plane graph obtained from G by contracting all bridges of G . Note that $L_a(G)$ is equivalent to $L_a(G')$ via untwisting oriented clasps covering bridges. Hence, we have $b(L_a(G)) = b(L_a(G')) = \frac{c(L_d(G'))}{2} + 1 = \frac{c(L_d(G))}{2} + 1$. □

Remark. Eq. (15) generalizes Theorem 4.3 in [9] from subdivisions of polyhedral graphs to any connected plane graphs.

To conclude the section, we point out that the braid index of general Traldi's links (even for alternating Traldi's links) can not be determined similarly since the upper and lower bounds are not always equal in general. An example of alternating Traldi's links, denoted by L , is shown in Figure 5 which is constructed from a theta graph by replacing edges e_1, e_2 by oriented clasp (a) and e_3 by clasp (c). On the one hand, by using the software KnotGTK, we obtain

$$P_L(v, z) = z^{-1}(-v^5 + v^3) + z(-v^5 + 3v^3) + z^3v^3 \quad (16)$$

and hence, $\text{span}_v P_L(v, z) = 2$. On the other hand, we have $c(L) = 4$. Therefore,

$$2 = \frac{\text{span}_v P_L(v, z)}{2} + 1 \leq b(L) \leq \frac{c(L)}{2} + 1 = 3. \quad (17)$$

Results

It is obvious that by the Corollary the braid index of four types of polyhedral links (see Fig. 2 of [9]) can be determined. In this section, we determine the braid index of two types of complicated DNA polyhedral links. However, braid indexes of these two new types of polyhedral links can not be obtained by the previous result in [9]. You will see these new types of polyhedral links are all alternating and hence their crossing numbers are easily obtained. By the Corollary, in order to obtain the braid index, we only need

to show that these links are Jaeger's links, and equivalently to find their associated plane graphs. Note that two strands of DNA have antiparallel orientations which are consistent with Jaeger's orientations. For simplicity, we do not draw orientations in the following any more.

1. Double crossover DNA polyhedral links

Recent years, in [8,10,11,12,13], the authors, in laboratory, designed and synthesized some fancy double crossover DNA polyhedra, such as DNA tetrahedron, cube, octahedron, dodecahedron, icosahedron and buckyball, by covering each vertex of degree n of the polyhedron by " n -point star motif (tiles)" and through sticky-end association between the tiles. The " n -point star motif" has an n -fold rotational symmetry and consists of $2n + 1$ single strands: a long repetitive central DNA strand (colored red and yellow), n identical medium DNA strands (colored green) and n identical short DNA strands (colored black). The colored yellow part at the center of the motif represents n unpaired DNA single-strands whose lengths can be adjusted to change bending degree of the whole structure. See Figure 6.

We point out in Figure 6 the tiles are a little different in the ends of tiles from the actual assemblies of such DNA polyhedra. For

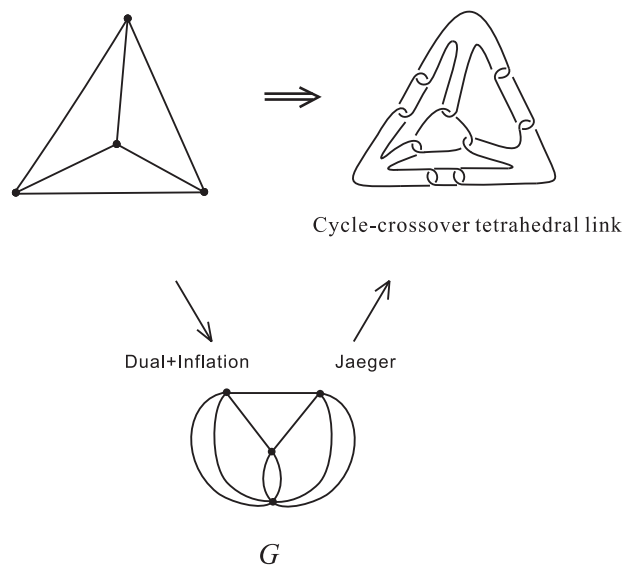


Figure 9. Planar form of cycle-crossover DNA tetrahedron and its associated plane graph G .
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actual assemblies, we refer the reader to Fig. 1 of [8] for DNA tetrahedron, dodecahedron and buckyball, Fig. 4 of [11] for DNA cube, Fig. 1 of [13] for DNA octahedron and Fig. 4(f) of [10] and Fig. 1 of [12] for DNA icosahedron. However, one will obtain the same polyhedral links based on our drawings as actual assemblies, and hence do not affect the analysis of their braid indexes.

Now we take double crossover DNA cube as an example to show double crossover DNA polyhedra are all Jaeger's links. The planar form of double crossover DNA cube link and its associated plane graph are shown in Figure 7 (upper and right) and (lower), respectively. In general, the associated plane graph G can be obtained from the polyhedron P by the following steps:

Step 1: Truncating the polyhedron P , i.e. cutting each corner of the polyhedron P , we obtain a polyhedral graph Q .

Step 2: Inflating edges of Q corresponding to edges of P , i.e. converting a single edge into two parallel edges, we obtain a plane graph H .

Step 3: Subdividing each edge of H by inserting a vertex, we obtain the associated graph G .

Let P be a polyhedron with m edges. Then, by simple calculation, the associated plane graph G has $8m$ edges and thus the braid index of the corresponding double crossover DNA polyhedral link is $8m + 1$.

2. Cycle-crossover polyhedral links

This type of polyhedral links was introduced in [14], designed as a potential object for synthesising, which can be constructed from a polyhedron by replacing each edge of the polyhedron by a "cycle-crossover" and replacing each vertex of degree n by an n -branched curve. See Figure 8. The planar form of the cycle-crossover cube link is shown in Figure 9 (upper and right) and its associated plane graph is shown in Figure 9 (lower).

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In general, cycle-crossover polyhedral links are all Jaeger's links. The associated plane graph G can be obtained from the polyhedron P by the following steps:

Step 1: Computing the planar dual of P , we obtain a plane graph H

Step 2: Inflating edges of H , i.e. converting a single edge into several parallel edges, we obtain the associated graph G .

In this case suppose that the total lengths of cycle-crossovers used to construct cycle-crossover polyhedral links are m . Then the associated plane graph G has m edges and thus the braid index of the corresponding cycle-crossover DNA polyhedral link is $m + 1$.

Discussion

Firstly, note that the two associated plane graphs in Figures 7 and 9 are both not subdivisions of polyhedral graphs and for both types of polyhedral links. This means that the method used in [9] can not be used here. Secondly, it is easy to find that the braid index of two types of complicated polyhedral links does not depend on the structure of the polyhedron. Thirdly, as the referee points out that there are two types of DNA cube: 4 turns and 4.5 turns. See Figure 4 and Figure 1, respectively, of [11], we only consider the 4-turn DNA cube in this paper. It deserves to study the braid index of 5-turn DNA cube and more general 5-turn DNA polyhedra. Finally, in fact Theorem 2 is more powerful than it has been used, and hence may be used to determine the braid index of more complicated polyhedral links in the future.

Author Contributions

Conceived and designed the experiments: XSC XJ. Performed the experiments: XSC XJ. Analyzed the data: XSC XJ. Contributed reagents/materials/analysis tools: XSC XJ. Wrote the paper: XSC XJ.