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Topological Aspect of DNA Cages: Genus

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Abstract

DNA cages are kind of artificial polyhedra that are interlinked and interlocked with DNA double-strands. A simple formula to calculate genus of DNA cages is presented here. The formula connects some topological properties of DNA cages, including component number μ, crossing number c and Seifert circle number s. It shows that no matter the way of DNA strands interlinked, the genus is a constant which only depends on the component number of the underlying polyhedral graph. Our study demonstrates that, the genus is an essential topological aspect of DNA polyhedra, which provides a novel classification and a design principle for DNA cages.

Introduction

The points, lines and planes are form languages to express the external spaces of polyhedral structures, which have been studied and celebrated for thousands of years [1]. A great theorem called Euler's polyhedral formula [2, 3], has been used to describe geometry and topology of regular polyhedra.

$$V + F - E = \chi \tag{1}$$

Here, V, F and E are the total numbers of vertices, faces and edges of a polyhedron,

respectively, and χ denotes the Euler characteristic. In algebraic topology, the Euler characteristic is a topological invariants. For an orientable closed surface, the Euler characteristic χ and the genus g meet a basic relationship as follows:

$$\chi = 2 - 2g \tag{2}$$

It is worth noting that an equivalence substitution can be made between Eq. (1) and (2), then the genus of a given polyhedra can be easily gotten by Eq. (3).

$$V + F - E = 2 - 2g \tag{3}$$

In particular, the regular Platonic polyhedra satisfy $V + F - E = 2$, so their genus are zero. Similarly, the genus of a sphere is 0, whereas it is one of a torus.

Genus is always considered as an important topological index of a surface to describe and classify graphs and knots. Researches on the genus of knots and links have deserved more and more attention [4-8], which bring a mathematical concept in geometry to structural biology and chemistry. As a powerful molecular descriptor, genus is also considered to describe the topological configurations of large molecules, such as classify RNA structural motifs and fullerene molecules [9]. Therefore, molecules with higher genus might be novel targets for a topology-aided chemical design [10-13].

In the past 20 years, DNA has been considered as an ideal material to build nanostructures with discrete and periodic patterns due to its complementary base pairing [14]. A series of novel nano-structures have been synthesized in labs, including DNA tetrahedra [15-18], cubes [19, 20], octahedra [21-24], dodecahedra [25, 26] and icosahedra [26, 27], which beyond our imaginations of what is possible in building novel artifacts with biology macromolecules. Each face of these structures is made of a closed, interlocked DNA ring, a double-helix or quadruplex-helix DNA strand decorates each edge, and an immobile multi-arm junction is located at each vertex [14]. Not only interest in their intriguing architectures and topologies is rapidly increasing [28, 29], but also the undetermined problems have led to the birth of a new field of deeper understanding of nature. In order to address these exciting questions, Hu et al. turned to mathematics for help and creatively combined polyhedral links[30-36] and Seifert algorithm[37] together to deduce the new Euler's formula for DNA Polyhedra[10], which

connects the Seifert number s, component number μ and crossing number c, as Eq. (4) shows:

$$s+\mu-c=2 \tag{4}$$

The new Euler's formula can be extended to DNA cages, which embedded in surfaces with higher genus, leading to Eq. (5).

$$s+\mu-c=2-2g \tag{5}$$

So, genus g of DNA cages can be calculated by Eq. (6).

$$g=1+\frac{c-s-\mu}{2} \tag{6}$$

Eq. (6) shows that genus is essential aspect in topology, which opened a door to study DNA cages. On the basis of polyhedral links, the mathematical models for DNA cage, the aim of this paper is using knot theory and Seifert algorithm to investigate the intrinsic topological properties of DNA cages further. We restricted ourselves to some topological indexes, especially genus, and to reveal the relationship in topological transformation between DNA cages. Our research demonstrates that genus would offer a new guiding principle to predict the design of DNA cages.

Method

Polyhedral links are powerful mathematical models to simulate DNA polyhedra, only if DNA stands are regarded as strings without thickness [38]. To make the discussion smoothly, basic mathematical definitions are defined as follows.

Definition 1. A polyhedral link L is an alternating link, which with a projection that has crossings that alternate between over and under as one travel around the link in a fixed direction.

For a given polyhedral graph G, if using tangles to replace its vertices and edges, then an interlinked and interlocked polyhedral link L is obtained. A tetrahedral link (Figure 1b), which belongs to T_{2k} polyhedral links [30, 31], where k denotes the number of full-twists along each edge. Two crossings correspond to a full twist, so in the present example $k=1$.

Definition 2. For any projection of a polyhedral link L, the crossing number, denoted *c(L)*, is the least number of crossings that it just has[10]. It is easy to determine the crossing number

of a polyhedral link because it is the sum of crossings of edges. Thus, the crossing number of example link (Figure 1b) is 12.

Definition 3. The number of closed nonintersecting curves of a polyhedral link L, denoted $\mu(L)$, which is called component number. In figures, components of a polyhedral link always assigned by different colors. So, the component number of the tetrahedral link shown in Figure 1b is 4.

Definition 4. The Seifert circle number of a polyhedral link L, denoted $s(L)$, is the number of Seifert circles generated from an orientable surface with the polyhedral link as its only boundary.

Seifert algorithm, proposed by Herbert Seifert [37] in 1935, to embed surfaces in space with a polyhedral links as boundary component. The result will be a set of circles in the plane, these circles are called Seifert circles. DNA polyhedral links are 'oriented', since DNA polymerization prefers to a direction from 5'(five prime) end to 3'(three prime) end. Due to the helix structure of DNA, intuitively, two kinds of holes in DNA polyhedra will be obtained during the Seifert construction: vertices generate large circles and edges generate small circles. Therefore, the number of Seifert circles of tetrahedral link in Figure 1b is 10, four large circles at vertices and 6 small circles at edges.

Figure 1. The Seifert construction of the T_2-tetrahedral link. a: a tetrahedral graph; b: an oriented tetrahedral link, closed curves with different colors represent components, the arrows indicate the 5' - 3' direction of the DNA backbone; c:The large Seifert circles distributed at vertices and small Seifert circles at edges.

In the context of knot theory, crossing numbers c, component numbers μ and Seifert circle numbers s are three fundamental indexes of polyhedral links. However, topological invariants that used to describe the transformation mechanism of DNA cages are still needed.

Definition 5. Genus of a polyhedral link L is the least genus of any Seifert surface for that polyhedral link. For example, a sphere, which has genus 0.

Definition 6. The least number of edges decorated with odd half-turns of DNA polyhedral links that required transforming a T_{2k} polyhedral link into a link L with components number μ, denoted $\mathrm{O}(L)$.

The component number of a T_{2k} link is equal to face number F. To reduce the component number by 1, one odd half-twisted edge is needed to replace an even half-twisted edge. Figure 2 shows a T_0 (k=0) tetrahedron link with components 4 is transformed to a link contains only one component, so we can conclude Eq. (7).

$$\mathrm{O}(L) = F - \mu \qquad (0 \le \mathrm{O}(L) \le F - 2) \tag{7}$$

The minimum of $\mathrm{O}(L)$ is zero when the link is a T_{2k} link, and take for granted that the maximum is F-1 when links with only one component. However, for DNA cages, each edge must be is antiparallel strands, T_{2k} links cannot be further transformed into links with one component, see Refs. [39], so the maximum of $\mathrm{O}(L)$ is F-2.

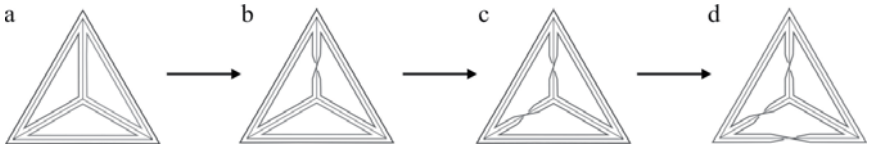

Figure 2. A T_0 tetrahedral link is transformed into other links by adding odd half-twisted edges. a: a T_0 tetrahedral link with four components; b: a tetrahedral link with three components; c: a tetrahedral link with two components; d: a tetrahedral link with only one components.

Results

In DNA polyhedron, each edge is covered by antiparallel DNA strands and each vertex is represented by a branch junction, then DNA cages can be looked as simple T_{2k} polyhedral links.

On the basis of vertices and edges respectively, two sets of Seifert circles will be created if apply the Seifert algorithm to a polyhedral link. Therefore, in the minimal graph, to compute the number of Seifert circles, vertex and edge building blocks of a polyhedral link must be considered separately.

According to the Ref. [10], each vertex generates a Seifert circle. Thus, Seifert circles derived from vertices s_v can be calculated by Eq. (8), where V denotes the vertex number of a polyhedron.

$$s_v = V \tag{8}$$

Here, suppose a polyhedral link L with μ components, the number of required odd half-twisted edges is $\mathrm{O}(L)$, crossing number of an odd half-twisted edge is $2k$+1 and of an even half-twisted edges is $2k$. Therefore, the Seifert circle number s_e is sum of Seifert circles derived from odd and even half-twisted edges. As shown in Figure 3, there will generate $2k$-1 Seifert circles if the edge with 2k anti-parallel half-twists. Similarly, for $2k$+1 half-twists, $2k$ Seifert circles will be generated.

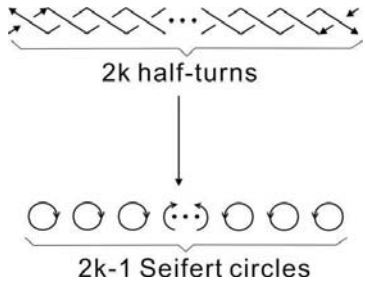

Figure 3. A 2k anti-parallel half-twisted edge will generate 2k-1 Seifert circles.

Thus, the number of Seifert circles derived from odd half-twisted edges s_{odd} can be computed by Eq. (9):

$$s_{odd} = 2k\mathrm{O}(L) \tag{9}$$

The total number of edges is E, so the number of edges with even half-twists is $E - \mathrm{O}(L)$. Therefore, the number of Seifert circles derived from even half-twisted edge s_{even} can be computed by Eq. (10):

$$s_{even} = (2k-1)(E - \mathrm{O}(L)) \tag{10}$$

Therefore, each Seifert circle is corresponded to each half-turn on edges and each central cavity of vertexes of a polyhedral link. As a result, the total number of Seifert circles s is sum of s_{odd}, s_{even} and s_v:

$$\begin{aligned} s &= s_{odd} + s_{even} + s_v \\ &= 2kE - E + \mathrm{O}(L) + V \end{aligned} \tag{11}$$

Moreover, each face corresponds to one cyclic strand because of each edge is decorated with even half-turns of DNA. However, according to definition 5 and Eq. (7), the introduction of odd half-twisted edges will reduce component number. Therefore, the number of these closed DNA strands, is calculated by:

$$\mu = F - \mathrm{O}(L) \qquad (2 \le \mathrm{O}(L) \le F) \tag{12}$$

where F denotes the face number of a polyhedron. And besides, crossing number c is expressed as a function of edge number E:

$$\begin{aligned} c &= (2k+1)\mathrm{O}(L) + 2k(E - \mathrm{O}(L)) \\ &= 2kE + \mathrm{O}(L) \end{aligned} \tag{13}$$

To substitute s, μ and c into Eq. (5), yields:

$$2 - 2g = 2 - \mathrm{O}(L) \tag{14}$$

Thus, genus of DNA cages can be calculated by Eq. (15):

$$g = \frac{\mathrm{O}(L)}{2} \qquad (0 \le \mathrm{O}(L) \le F - 2) \tag{15}$$

Eq. (15) suggests that genus of a DNA polyhedral link is only determined by the number of odd half-twisted edges $\mathrm{O}(L)$. For a given DNA polyhedral link with μ component, $\mathrm{O}(L)$ can be easily be calculated by Eq. (7). In other words, genus of a DNA polyhedral link depends on component number. The Eq. (15) is not only a capable equation to calculate genus of DNA cages but also an indicator for designing more complex DNA polyhedra. Obviously, for any T_{2k} polyhedral link, $\mathrm{O}(L)$ is 0, so the genus is zero.

Here, we use tetrahedral links and dodecahedral links shown in Figure 4 as examples for further understanding of Eq. (15). In Figure 4a, b, c, the components number are 2, so the least number of odd half-twisted edges they needed are 2, thus, the genus of them are 1. As examples of contrast, the genus of all cases in Figure 4 are calculated by Eq. (6) and (15), respectively, the results are listed in Table 1. For tetrahedral links with 2 components, the genus of them are all 1 no matter which Eq. is used.

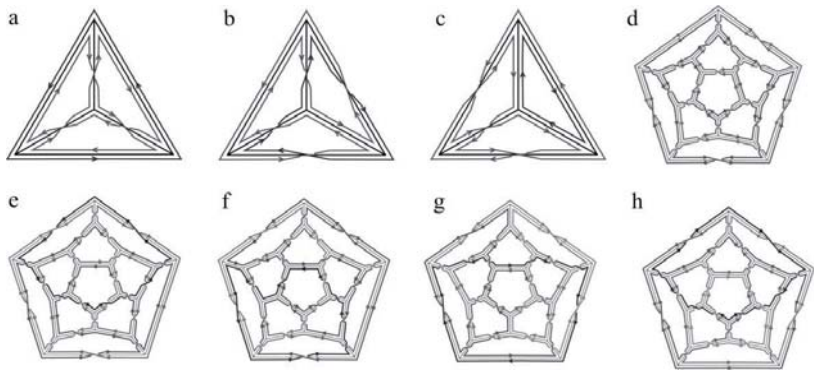

Figure 4. Some polyhedral links.

Table 1. Topological invariants of some polyhedral links shown in figure 4.

	s	c	μ	$\mathrm{O}(L)$	$g=1+\frac{c-s-\mu}{2}$	$g=\frac{\mathrm{O}(L)}{2}$
a	1	3	2	2	1	1
b	2	4	2	2	1	1
c	1	3	2	2	1	1
d	14	24	2	10	5	5
e	14	24	4	8	4	4
f	14	24	4	8	4	4
g	14	24	6	6	3	3
h	14	24	6	6	3	3

Two types of vertex junction have been reported by Jonnska and Twarock [39, 40], uncrossed and crossed vertex. The uncrossed vertex has been discussed in the ahead section, whereas the crossed vertex will be discussed in the following section. Figure 5a shows how to convert a three uncrossed vertex into a crossed one. Two dodecahedral links with one crossed vertex (Figure 5b) and two crossed vertexes (Figure 5c) are shown as examples, whose Seifert circle number s, crossing number c, component number μ and genus g are listed in Table 2.

If a three uncrossed vertex is replaced by a crossed vertex, as shown in Figure 5, the components number is reduced 2, and the number of odd half-twisted edges $\mathrm{O}(L)$ adds 2, so the genus is added by one. Thus, if n uncrossed vertexes are replaced, the change of

parameter $O(L)$ meets Eq. (16):

$$O(L)' = O(L) + 2n \tag{16}$$

Substitute Eq. (16) into Eq. (15), yields:

$$g' = g + n \tag{17}$$

Table 2. Topological invariants for some polyhedral links shown in figure 5.

	s	s'	c	c'	μ	μ'	$O(L)$	$O(L)'$	g	g'
b	14	17	24	27	4	2	8	10	4	5
c	14	20	24	30	6	2	6	10	3	5

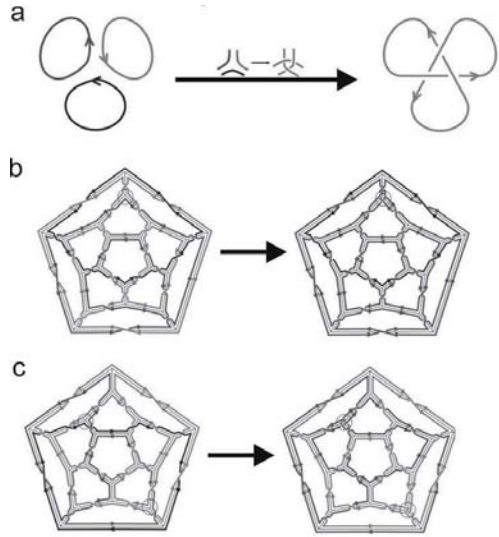

Figure 5. a:The structural change of replacing a uncrossed vertex by a crossed vertex; b:The structural change of replacing one uncrossed vertexes by one crossed vertexes; c: The structural change of replacing two uncrossed vertexes by two crossed vertexes.

On the basics of Eq. (6), the components number reduces 2, the crossings number and the Seifert circle number both add 3. Thus, if n uncrossed vertexes are replaced, the change of parameters is shown as follows:

$$\begin{aligned} \mu' &= \mu - 2n \\ c' &= c + 3n \\ s' &= s + 3n \end{aligned} \tag{18}$$

Then, the genus can be deduced and the result is Eq. (17).

For three degree vertexes, the Eq. (17) suggests that the new genus g' is sum of g and the number of crossed vertex n. However, the new genus of vertexes with even degree will be fractional. For example, if a four degree uncrossed junction is replaced by a crossed junction, then the components number reduces 3, the crossings number and the Seifert circle number add 4, so the genus adds 1.5, according to Eq. (6) and (15).

Discussion

For a polyhedral link, its geometrical and topological characters can be described by many topological invariants, such as genus, component number, crossing number and so on. However, for a DNA cages, chemists have particular preference over genus g and component number μ. Genus not only denotes the number of holes going through the surface, but also can signify the number of tunnels in DNA cages that used to deliver drug. Component number, the most basic factors needs to be considered in synthesizing. So, it is very important to reveal the essential relationship between them.

The majority of DNA polyhedra can be described by T_{2k} polyhedral links, which not contain edges with odd half-twists, so the genus of them are 0. The results suggested that all synthesized DNA cages can be topological transformed to a surface, which is homeomorphic to a sphere. In practices, genus is not a purely mathematical definition any more, but be considered as a heuristic indicator to design novel structures [11].

A series of theoretical work about constructing dodecahedral DNA cages in all possibility have been reported by Jonnska and Twarock [39, 40]. Our study shows that genus is only determined by the number of odd half-twisted edges. All these pave a brand new way to design novel polyhedral architectures with g>0 for DNA and macromolecules. For example, a DNA octahedral cage with genus 3 has been designed, see Ref. [10]. Through the reverse synthetic method, g is 3 means $\mathrm{O}(L)$ is 6, then components number μ is 2. There are two methods to design a DNA octahedra with two components, one is using six odd half-twisted edges to replace even half-twisted edges (see Figure 6a); the other is to replace two uncrossed vertexes by crossed ones (see Figure 6b).

In addition, Eq. (15) is also appropriate to characterize the recombinase regulation and controlling mechanisms for DNA polyhedra. Recombinase can cut two segments and interchange the ends of DNA, which can lead to the inversion or the deletion or insertion of a DNA segment [41]. It means that the component number of polyhedral links will be added or reduced one while each recombination. In Figure 6c and d, the recombination of a dodecahedral link reduce the component number by one. The genus of the dodecahedral link (Figure 6d) is still 5, which is mysterious according to Eq. (15). However, $O(L)$ is not changed in the recombination process, so the genus remains 5.

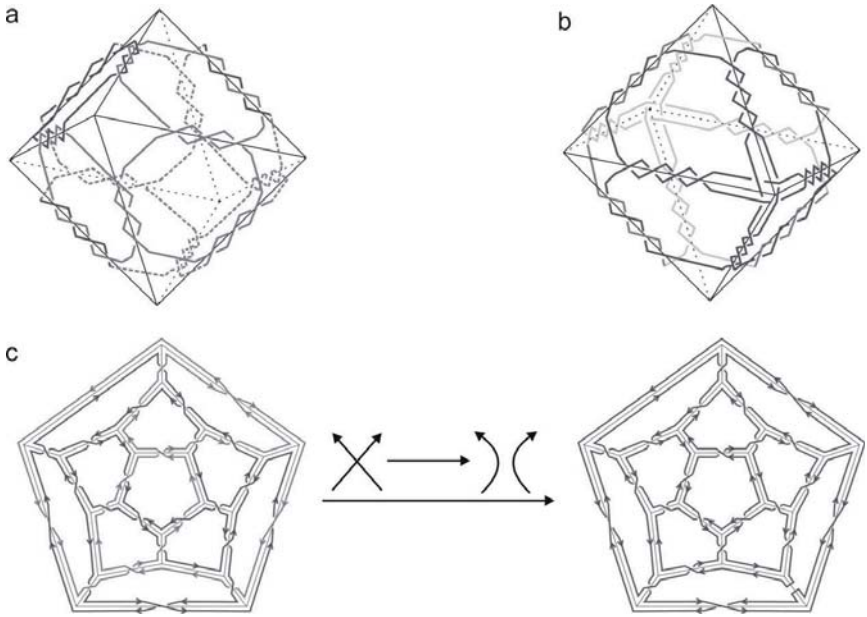

Figure 6. Two applications of the new genus's formula. a: using six odd half-twisted edges to replace the even half-twisted edges; b: replacing of two uncrossed junctions by crossed ones c: The recombination of a dodecahedral link.

Conclusion

In this paper, we have defined a novel topological invariant $O(L)$ based on the number of odd half-twisted edges. It can be used to describe the dynamical properties of DNA cages, particular the addition and deletion of crossings. In addition, genus is an essential aspect in topology of DNA cages, which reveals the relation of these structures with their embedding

surfaces. Accordingly, our study of genus of DNA cages could give a new clue for the classification and guiding principle for the molecular design of novel nanostructures.

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