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The New Euler's Formula of the Crossed DNA Polyhedral Links

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Abstract: The Euler's formula for polyhedra displays the geometric properties of polyhedral structures, while the new Euler's formula for DNA polyhedra reveals the intrinsic properties of these novel structures, and offers an important tool for the description and study of the DNA polyhedra. In this paper, we focus on the crossed DNA polyhedral links, study their topological properties including the number of Seifert circles and the new Euler's characteristic, and get the expressions of their new Euler's characteristics. The study extends the new Euler's formula to more kinds of DNA polyhedra and provides theoretic foundations to the design and synthesis of more complex DNA polyhedra.

1. Introduction

Elegant polyhedra are fundamental forms of life in nature. The Euler's formula describes polyhedra in the form of $V + F = E + 2$, in which V, F and E denote the numbers of vertices, faces and edges respectively. The synthesis of these polyhedral structures has aroused keen interest of many scientists. For the double helix structure and highly selective base-pairing mechanism, DNA catenanes have been important materials for the synthesis of nanostructures. Since the first rigid DNA nanostructure, DNA cube [1] was synthesized by Seeman in 1991, a variety of DNA polyhedral architectures have been obtained in the laboratories, such as DNA tetrahedron [2-8], DNA octahedron [9-11], DNA dodecahedron [4, 12], DNA icosahedron [13, 14] and so on [15-20]. Meanwhile, these novel polyhedral structures have also attracted some

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theoretic scientists' attention [21-25], and polyhedral links were brought up to describe the topological properties of DNA polyhedra. In the DNA polyhedral links, the two strands on each edge are oriented and opposite in direction, since one strand of the DNA double-helix follows a direction from 5' to 3', and the other from 3' to 5'.

There are mainly three methods to construct the polyhedral links: '*n*-branched-curve and *m*-twisted double-line covering' [26-28], '*n*-cross-curve and *m*-twisted double-line covering' [29-32] and 'cross-curve and single-line covering' [32-34]. The method for '*n*-cross-curve and *m*-twisted double-line covering' is proposed on the basis of the peculiar structure of HK97 capsid [35]. In the polyhedral link constructed by '*n*-cross-curve and *m*-twisted double-line covering', a vertex of degree *n* is replaced by an *n*-cross-curve, and an edge is replaced by an *m*-twisted double-line (Fig. 1 (a)).

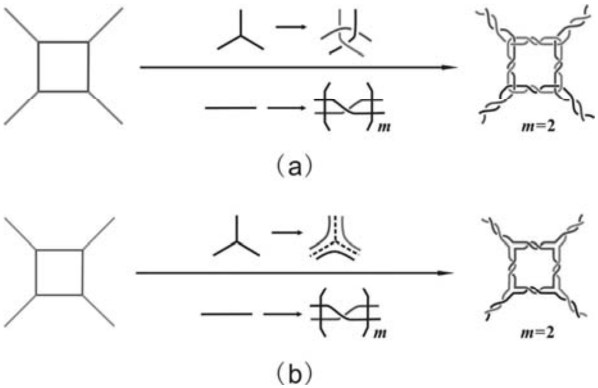


Fig. 1. The method for '*n*-cross-curve and *m*-twisted double-line covering' (a) and '*n*-branched-curve and *m*-twisted double-line covering' (b)

'*N*-branched-curve and *m*-twisted double-line covering' is a method of constructing polyhedral links based on the architecture of the polyhedra. In these polyhedral links, the vertices and the edges of the polyhedron are replaced respectively by *n*-branched curves and *m*-twisted double-lines (Fig. 1 (b)). The new Euler's formula raised by Hu *et al*, $s+\mu=c+2$ [36], can be used to describe these *n*-branched DNA polyhedral links, and provides a new theoretical principle for the description of the novel DNA polyhedral structures. In this formula, s, μ and c are the total numbers of Seifert circles, components and crossings of the DNA polyhedral link, respectively. The number of Seifert circles, which is an important topological invariant of knots and links, is gotten from the Seifert algorithm [37]. Fig. 2 shows how to eliminate the crossing in the planar graph of an oriented knot or link [38] to obtain the nonintersecting circles named Seifert circles. On this basis, Li Wei [39] put forward the concept 'the new Euler's characteristic' to describe the DNA polyhedra, the expression of which is $\lambda = s + \mu - c$. The variables in the formula can be expressed with the number of vertices V, of edges E or of faces F by way of suitable transformations.

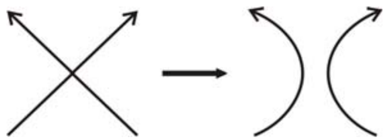


Fig. 2. The operation of eliminating the crossing

In this paper we will do our research on the DNA polyhedral links constructed by the way of 'n-cross-curve and m-twisted double-line covering', *i.e.* 'the crossed DNA polyhedral links' hereinafter, and try to find the law of the number of Seifert circles and the new Euler's characteristic, hoping to provide a theoretical basis for the synthesis of DNA polyhedra.

2. Topological properties of the crossed DNA polyhedral links

In order to facilitate the discussion, we divide all the polyhedra into two based on the degrees of the vertices identical or not, then construct the DNA polyhedral links by the way of 'n-cross-curve and m-twisted double-line covering', and study their numbers of Seifert circles and the new Euler's characteristics.

2.1. The crossed DNA polyhedral links with vertices of the same degree

The polyhedra with vertices of the same degree satisfy Euler's formula:

$$V + F - E = 2 \tag{1}$$

And

$$nV = 2E \tag{2}$$

where n, V, F and E denote respectively the degree of the vertices and numbers of vertices, faces and edges of the polyhedra. The value of n will be 3, 4 or 5.

The crossed DNA polyhedral links are constructed on the basis of these polyhedra. The architectures of the vertices in the polyhedra and in the DNA polyhedral links are shown in Fig. 3. After orienting and applying the Seifert construction to these vertices, we can see that each vertex gives rise to one Seifert circle, which is represented by a loop in Fig. 3, no matter what the degree is (There will be two situations when the degree of the vertex is even, as discussed in the latter part).

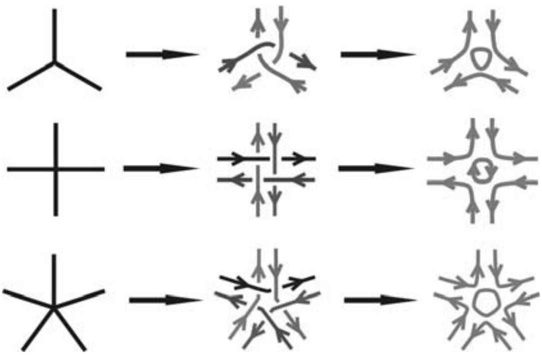


Fig. 3. Architectures of the vertices in the polyhedra, the crossed DNA polyhedral links and the Seifert structures

Then the crossed DNA polyhedral links are divided into two parts: the polyhedral links without twists on the edges and the polyhedral links with twists on each edge. We will not discuss the polyhedral links with twists on some of the edges in this paper for simplicity.

(1) When there are no twists on the edges, there are no Seifert circles derived from them. In this case, there is respectively one Seifert circle corresponding to each vertex and each face in DNA polyhedral links. So the number of Seifert circles s_v derived from vertices is:

$$s_v = V \tag{3}$$

where V denotes the vertex number of a polyhedron. And the number of Seifert circles s_f derived from faces is:

$$s_f = F \tag{4}$$

where F denotes the face number of a polyhedron. Therefore, the total number of Seifert circles s can be expressed as:

$$s = s_v + s_f = V + F \tag{5}$$

There are no crossings apart from n crossings in each n-degree vertex, so the crossing number is given by:

$$c = c_v = nV \tag{6}$$

where n denotes the degree of vertices. Thus we can obtain:

$$s - c = V + F - nV \tag{7}$$

The simultaneous equations of Eq. (1) and (2) will yield:

$$F = 2 - V + nV/2 \tag{8}$$

Substitution of Eq. (8) into Eq. (7) yields:

$$s - c = 2 - nV/2 \tag{9}$$

Then the new Euler's characteristic λ can be calculated by:

$$\lambda = s + \mu - c = \mu + 2 - nV/2 \tag{10}$$

On account of the relationship among n, V, E and F, the new Euler's characteristic can also be expressed as:

$$\lambda = \mu + 2 - E = \mu + 4 - V - F \tag{11}$$

(2) When there are twists on the edges, we can learn from Fig. 4, which shows a DNA tetrahedral link with twists on the edges, that each vertex corresponds to two Seifert circles. So the number of Seifert circles s_v derived from vertices is:

$$s_v = 2V \tag{12}$$

When there are k crossings on the edge, *i.e.* k half-twists, there will be k-1 Seifert circles yielded (Fig. 5). In other words, the number of Seifert circles is always 1 less than the crossing number on each edge. So the number of Seifert circles s_e derived from edges is E less than the crossing number of edges c_e, given by:

$$s_e = c_e - E \tag{13}$$

where E denotes the edge number of a polyhedron. There are n crossings in each n-degree vertex. So the crossing number of vertices c_v is:

$$c_v = nV \tag{14}$$

Then we can get the following equation:

$$s - c = (s_v + s_e) - (c_v + c_e) = 2V - nV - E \tag{15}$$

The new Euler's characteristic can be calculated by:

$$\lambda = s + \mu - c = \mu + (2 - 3n/2)V = \mu + 6 - V - 3F \tag{16}$$

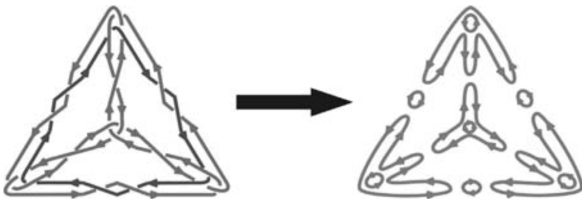


Fig. 4. A DNA tetrahedral link with twists on the edges and its Seifert construction

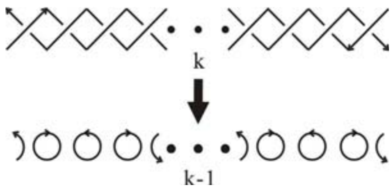


Fig. 5. The Seifert construction of an edge in DNA polyhedral links

2.2. The crossed DNA polyhedral links with vertices of different degrees

When the degrees of the vertices in a polyhedron are different, we get:

$$3V_3 + 4V_4 + 5V_5 + \cdots + nV_n = 2E \tag{17}$$

$$V_3 + V_4 + V_5 + \cdots + V_n = V \tag{18}$$

where V_n denotes the number of n-degree vertices in the polyhedron.

(1) When there are no twists on the edges, there are no crossings apart from n crossings in each n-degree vertex. Meanwhile, each vertex and each face of a DNA polyhedral link correspond to a Seifert circle. So the crossing number c and the number of Seifert circles s are

given by:

$$c = 3V_3 + 4V_4 + 5V_5 + \cdots + nV_n = 2E \tag{19}$$

$$s = V + F \tag{20}$$

Therefore, we can get:

$$s - c = V + F - 2E = 2 - E = 4 - V - F \tag{21}$$

So the new Euler's characteristic can be calculated by:

$$\lambda = s + \mu - c = \mu + 4 - V - F \tag{22}$$

(2) When there are twists on the edges, the number of Seifert circles s_v derived from vertices is given by:

$$s_v = 2V \tag{23}$$

The number of Seifert circles s_e derived from the edges and the crossing number of edges c_e have the relationship expressed as:

$$s_e = c_e - E \tag{24}$$

The crossing number of vertices c_v is:

$$c_v = 3V_3 + 4V_4 + 5V_5 + \cdots + nV_n = 2E \tag{25}$$

Therefore, we can obtain:

$$s - c = (s_v + s_e) - (c_v + c_e) = 2V - 3E = 6 - V - 3F \tag{26}$$

So the new Euler's characteristic is given by:

$$\lambda = s + \mu - c = \mu + 6 - V - 3F \tag{27}$$

As we can see from the preceding discussion, the new Euler's characteristic can be expressed as $\lambda = \mu + 6 - V - 3F$ when there are twists on the edges, and as $\lambda = \mu + 4 - V - F$ when there are not, no matter what the degrees of the vertices are. Three variables V, F and μ are contained in the two expressions. Thus the new Euler's characteristic of any crossed DNA polyhedral link can be figured out if the values of these variables are known. However, the component number μ of a complicated crossed DNA polyhedral link is often not easy to tell. Therefore, we will take three-crossed DNA polyhedral links and four-crossed DNA polyhedral links for example to show that how to use the expressions we have obtained to calculate their new Euler's characteristics, and meanwhile, give more detailed discussions about their respective component number μ, hoping to get the more specific expression of the new Euler's characteristic.

3. The three-crossed DNA polyhedral links

The three-crossed DNA polyhedral links are constructed on the basis of three-polyhedra, in which all the vertices are of three degrees. These links are divided into three according to the twist number on the edges. We will study on their component numbers and the new Euler's characteristics respectively.

3.1. The three-crossed DNA polyhedral links without twists on the edges

Two kinds of three-crossed DNA polyhedral links without twists on the edges are shown in Fig. 6. Each face of the polyhedron is replaced by a strand in the corresponding link, and the strands are interlocked at the vertices of the link. As a result, the component number of the link equals to the face number of the corresponding polyhedron, given by:

$$\mu = F \tag{28}$$

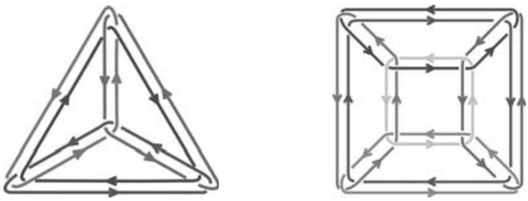
Substitution of Eq. (28) into Eq. (11) gives the expression of the new Euler's characteristic:

$$\lambda = s + \mu - c = 4 - V \tag{29}$$

And this expression is adequate for all the crossed DNA polyhedral links without twists on the edges that satisfy Eq. (28). Combining the formula $s + \mu - c = 2 - 2g$ [40] for knots and links, we can get the expression of the genus g:

$$g = V/2 - 1 \tag{30}$$

The vertex number V of the tetrahedron is 4, so the new Euler's characteristic λ of the crossed DNA tetrahedral link without twists (Fig. 6 (a)) is 0, and the genus g is 1. Then λ of the crossed DNA hexahedral link without twists (Fig. 6 (b)) is -4, and the genus g is 3.



(a) (b)

Fig. 6. A crossed DNA tetrahedral link (a) and a crossed DNA hexahedral link (b)

3.2. The three-crossed DNA polyhedral links with even half-twists on each edge

The orientations of the strands in the DNA polyhedral links will not change when even half-twists are added to the edges. Therefore, the component number μ will not change either, given by:

$$\mu = F \tag{31}$$

The three-polyhedron satisfies Eq. (1), and the vertex degree n in Eq. (2) equals to 3, so we get:

$$3V = 2E \tag{32}$$

Rearranging Eq. (32) gives:

$$E = 3V / 2 \tag{33}$$

Substitution of Eq. (33) into Eq. (1) yields:

$$F = V / 2 + 2 \tag{34}$$

Substitution of Eq. (31) and Eq. (34) into Eq. (16) gives the expression of the new Euler's characteristic of this kind of DNA polyhedral links:

$$\lambda = s + \mu - c = 2 - 2V \tag{35}$$

The genus is given by:

$$g = V \tag{36}$$

So the new Euler's characteristic of the crossed DNA tetrahedral link shown in Fig. 7 is -6, and the genus is 4.

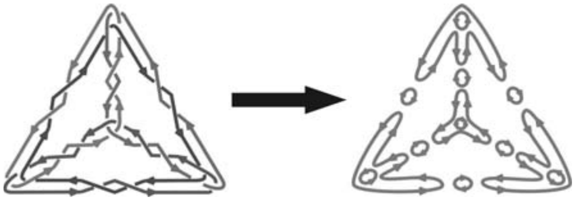


Fig. 7. A crossed DNA tetrahedral link with even half-twists and its Seifert construction

3.3. The three-crossed DNA polyhedral links with odd half-twists on some or all of the edges

For some of these three-crossed polyhedral links, there is no orientation that gets the two strands on each edge opposite in direction. Accordingly, these links are not actually the DNA polyhedral links. For three-crossed DNA polyhedral links that have odd half-twists on some or all of the edges (Fig. 4), however, there is still not a simple equation to express the component number. So we can but substitute $n=3$ into Eq. (16) and get the expression of the new Euler's characteristic, given by:

$$\lambda = s+\mu-c = \mu-5V/2 \tag{37}$$

4. The four-crossed DNA polyhedral links

The octahedral link is taken for example to study on the number of Seifert circles and the new Euler's characteristic of the four-crossed DNA polyhedral links.

Fig. 8 shows a crossed DNA octahedral link without twists on the edges. When orienting the link, we find out that after the orientation of the transverse strands a_1 and a_2 in the vertex module (Fig. 9) is confirmed, there are two possibilities for the orientation of the longitudinal strands b_1 and b_2 (Fig. 10). Moreover, the two orientations will lead to different Seifert structures, shown in Fig. 10. The difference between two vertices in Fig. 10 is that four crossings in (a) are counted as -1s [41] while crossings in (b) are counted as +1s. Not only the four-degree vertex, but all the even-degree vertices will have two orientations respectively, as the six-degree vertices and the eight-degree vertices shown in Fig. 11. The crossed DNA octahedral link is made up of three pairs of strands. Owing to the two orientations of each pair of strands, there are $2^3 = 8$ possibilities for the orientation of the link, shown in Fig. 12. Actually, 2, 3 and 5 in Fig. 12 are identical, so are 4, 6 and 7. Therefore there are four kinds of crossed DNA octahedral links, and their numbers of Seifert circles *s*, new Euler's characteristics λ and genera *g* are listed in Tab. 1.

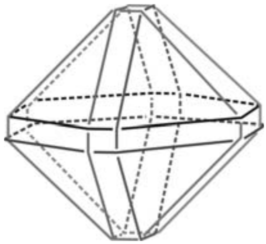


Fig. 8. A crossed DNA octahedral link without twists on the edges

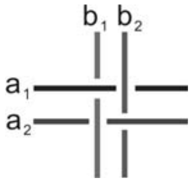
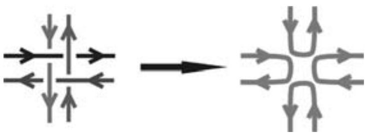


Fig. 9. The vertex module of four-crossed polyhedral links



(a)

(b)

Fig. 10. Two orientations of the four-crossed vertex

Fig. 11. The six-degree vertices (a) and the eight-degree vertices (b)

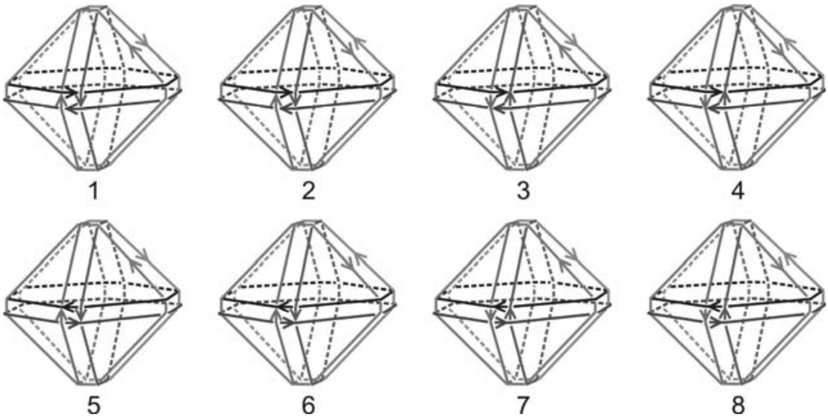


Fig. 12. Eight possibilities for the orientation of the crossed DNA octahedral link

Tab. 1. The values of s, λ and g of the four kinds of crossed DNA octahedral links

Number	s	λ	g
1	14	-4	3
2	8	-10	6
4	8	-10	6
8	14	-4	3

From Fig. 12 and Tab. 1 we can find out that the links 2 and 4 have some crossings counted as -1s and the other crossings counted as +1s, and their new Euler's characteristics and genera are respectively -10 and 6; while the links 1 and 8 have all the crossings counted as +1s, and their new Euler's characteristics and genera are respectively -4 and 3. Moreover, a polyhedral link and its chiral isomer are opposite in signs of crossings (Fig. 13), yet have the same new Euler's characteristics. Then we can conclude that the link with the identical sign of all the crossings has the maximum λ and the minimum g. Referring to the genus of an oriented link L, which is defined as the minimum genus of any connected orientable surface that spans L [40], we define the new Euler's characteristic of the DNA polyhedral links as the maximum of any orientation that generates DNA polyhedral links. So the new Euler's characteristic of the crossed DNA octahedral link is -4 and the genus is 3.

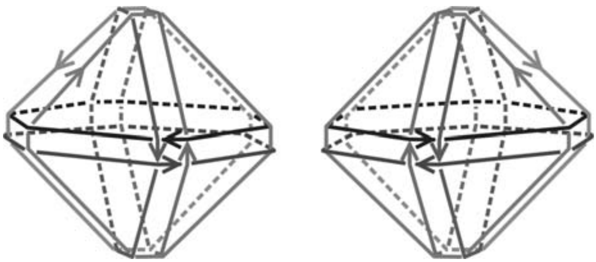


Fig. 13. A crossed DNA octahedral link (Right, the link 1 in Fig. 12) and its chiral isomer (Left)

Substitution of $n=4$ into Eq. (10) and Eq. (16) yields the expressions for the new Euler's characteristic of four-crossed DNA polyhedral links. When there are no twists on the edges:

$$\lambda = s + \mu - c = \mu - 2V + 2 \tag{38}$$

When there are twists on the edges:

$$\lambda = s + \mu - c = \mu - 4V \tag{39}$$

Unlike the three-crossed DNA polyhedral links, there is not a simple equation to calculate the component numbers of all the four-crossed DNA polyhedral links. However, there are expressions to express the component numbers of some four-crossed DNA polyhedral links which follow specific growth laws. For example, the component number of a (3, 4)-Extended polyhedral link which is proposed by Hu *et al* [34] can be expressed as $Nc = 10T + 2$ (The triangulation number $T = h^2 + hk + k^2$). The link is constructed on the basis of the (3, 4)-Extended polyhedron, of which all the vertices are of four degrees. Therefore, we can construct a four-crossed DNA polyhedral link on the basis of this polyhedron, shown in Fig. 14. The component number of the link that we constructed is twice as much as the component number of the corresponding (3, 4)-Extended polyhedral link, given by:

$$\mu = 2Nc = 20T + 4 \tag{40}$$

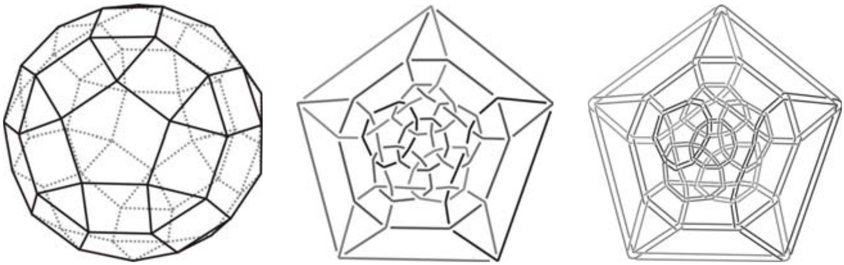
For the (3, 4)-Extended polyhedron, the following relationship holds:

$$V = 60T \tag{41}$$

So the new Euler's characteristic of the four-crossed DNA polyhedral link that we constructed can be expressed as:

$$\lambda = \mu - 2V + 2 = 6 - 100T \tag{42}$$

The triangulation number T of the I_h (3, 4)-62-hedron shown in Fig. 14(a) is 1, so the new Euler's characteristic of the four-crossed 62-hedral link shown in Fig. 14(c) is -94.



(a) (b) (c)

Fig. 14. I_h (3, 4)-62-hedron (a), I_h (3, 4)-62-hedral link (b) and four-crossed 62-hedral link (c)

5. Conclusions

In this paper, we have studied on the topological properties of the crossed DNA polyhedral links, gotten the expressions of the new Euler's characteristic, and taken the three-crossed and four-crossed DNA polyhedral links for example to show how to use the expressions to calculate the new Euler's characteristic. The results are as follows.

1. The new Euler's characteristic of the crossed DNA polyhedral link is given by: (1) $\lambda = \mu + 4 - V - F$ when there are no twists on the edges; (2) $\lambda = \mu + 6 - V - 3F$ when there are twists on the edges.

2. The new Euler's characteristic of the three-crossed DNA polyhedral link is given by: (1) $\lambda = 4 - V$ when there are no twists on the edges; (2) $\lambda = 2 - 2V$ when there are even twists on the edges; (3) $\lambda = \mu - 5V/2$ when there are odd half-twists on some or all of the edges.

3. The new Euler's characteristic of the four-crossed DNA polyhedral link is given by: (1) $\lambda = \mu - 2V + 2$ when there are no twists on the edges; (2) $\lambda = \mu - 4V$ when there are twists on the edges.

The new Euler's characteristic unites several features of the DNA polyhedral link, reveals the intrinsic property of DNA polyhedra, and has been an important tool to describe the elegant DNA polyhedral structures. In this paper, the definition of the new Euler's characteristic of the DNA polyhedral links has been expounded more explicitly. Our study is hoped to promote the research and synthesis of new DNA polyhedra.

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