MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **72** (2014) 489-500

ISSN 0340 - 6253

The Architecture of DNA Polyhedral Links with Odd Tangles

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(Received April 2, 2014)

Abstract: DNA molecules have been used to build a variety of nanoscale structures and devices like DNA polyhedral links over the past 30 years with some important potential applications. To depict these novel and complex structures, knot theory and topology have been proved useful tools. Here, we present a new method to construct DNA polyhedral links of a given polyhedron based on truncation and topological transformation. This approach can provide a theoretical guideline to the design and prediction of DNA polyhedral links.

1. Introduction

Knot theory [1, 2], an interesting part of topology, has been greatly appreciated for a long time [3-7]. To synthesize intriguing links and knot structures on the molecules level is expected by chemists. In 1991, the dream is realized by Seeman, who synthesized the first DNA polyhedron, a cube [8]. In the following years, more and more DNA polyhedrons were born, such as DNA truncated octahedron [9], octahedron [10], tetrahedron [11], dodecahedron [12, 13] and icosahedrons [14, 15].

The great achievements in the syntheses of DNA polyhedrons not only enrich the DNA structures database, but also bring new challenges in how to describe these structures from a mathematical viewpoint. In this respect, many results have been reported by Qiu and his coworkers. Three models are put forward to describe these DNA nanostructures. The first is '*n*-cross-curve and *m*-twisted double-line covering' [16-19], which uses n-branched curves to cover vertices of a polyhedron and m-twisted double-lines to cover the edges (see Figure 1a). The second is '*n*-branched-curve and *m*-twisted double-line covering' [20-21], which is used to construct DNA polyhedral links with n-degree vertices and m-twisted edges (Figure 1b). The third is called 'Tangle-vertex and single-line covering' [22-23], which constructs polyhedral links based on a four-degree polyhedron by using an even or odd twisted 'tangle' to cover a vertex and using single-line to cover an edge (Figure 1c).

However, all above methods are suitable well for polyhedral links with even tangles. For the odd tangle, these methods do not perform well. So a general strategy, which can be used to construct all kinds of DNA polyhedral links, is proposed.

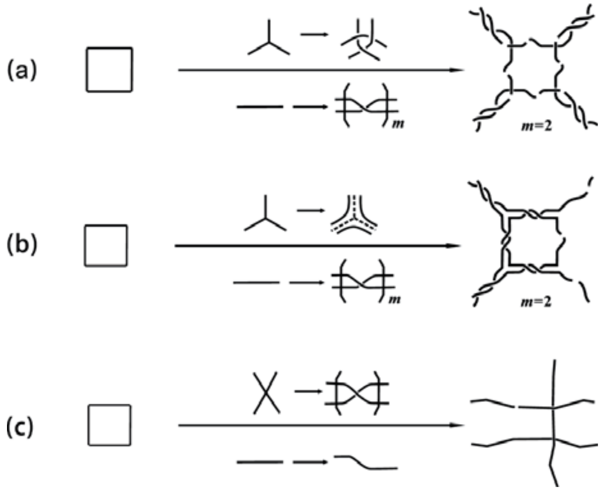

Figure 1. (a) The method of 'n-cross-curve and m-twisted double-line covering'. (b) The method of 'n-branched-curve and m-twisted double-line covering'. (c) The method of 'Tangle-vertex and single-line covering'.

2. Methods

To make the discussion smoothly, we need to clarify some definitions as follows. **Tangle**: A region in the projection plane surrounded by a circle exactly with four emerging arcs {NW, NE, SW, SE}, as shown in Figure 2a. There are two types tangles, one is odd tangle (Figure 2a) and the other is even one (Figure 2b).

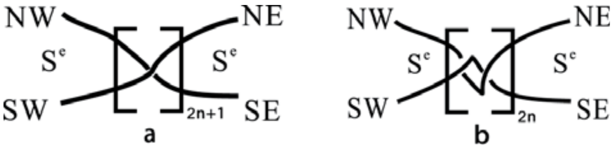

Figure 2. (a) Odd tangles. (b) Even tangles.

Even-to-odd operation: Define the conversion of an even tangle to an odd tangle as the even-to-odd operation that can be achieved by the following process. For a given even tangle (Figure 3a), cutting off its crossover structure in the ring, four separated branches are left (Figure 5b). Then connect the two opposite ends between SW and NE, and between NW and SE (Figure 5c), a crossing will form as an odd tangle (Figure 5d).

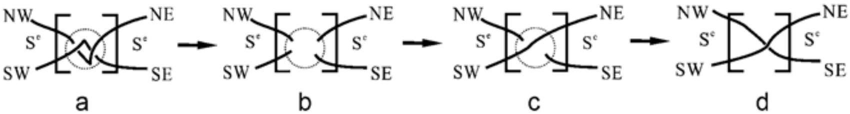

Figure 3. The conversion of the even tangle to the odd one.

Herein, we take a tetrahedron as an example to illustrate the approach for constructing polyhedral links. To realize the goal of constructing all possible DNA polyhedral links by a rational and systematical method, three basic courses are needed.

2.1 Polyhedral link with pure even tangles

Starting from an arbitrary polyhedron, a polyhedral link with pure even tangles could be obtained by truncation and 'tangle-vertex and single-line covering' which provide a concise skeleton for further operations.

Firstly, truncate a tetrahedron to get the according truncated polyhedron which is featured by all vertexes of 4 degrees, namely octahedron. Then, a octahedral link is constructed using the method of 'tangle-vertex and single-line covering' (Figure 1c), via the following two steps: (i) cover all edges of the remaining faces of the original tetrahedron in Figure 4c with single-line curves, and (ii) all component curves tangle with each other to replace all vertices of the octahedron, as shown in Figure 4.

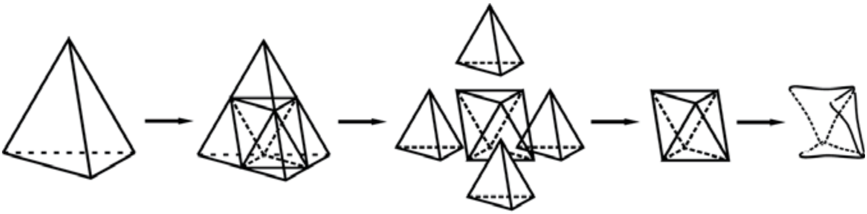

Figure 4. The process for obtaining the octahedral link with even tangles.

2.2 Polyhedral link with odd tangles

Perform 'even-to-odd' operations to the corresponding polyhedral link with pure even tangles to yield polyhedral links consisting of both even and odd tangles. New branches could also be derived from this process and then be assembled into new polyhedral links in according to some principles.

Step 1: Mark all even tangles, and suppose that the polyhedron link with pure even tangles is the first type of truncated polyhedron link, which is named as A (Figure 5a).

Step 2: Apply the 'even-to-odd' operation to the first even tangle 1(Figure 5a.1) to get the first odd tangle which represents the occurrence of the second type of truncated polyhedron link B (Figure 5b). Then select another even tangle adjoining the first odd tangle on the newly constructed branch (Figure 5b.2) to get C (Figure 5c).

This process will merge two small branches into a new one (Figure 5b) which could be used as building blocks to assemble new type of polyhedron links later. Noted there are three different even tangles on C (Figure 5b.3, 4, 5), the 'even-to-odd' operation will give rise to three different links: D (Figure 5d), E (Figure 5e) and F (Figure 5f).

Step 3: Continue this approach until all even tangles are changed into odd tangles.

It should be noted, when applying the 'even-to-odd' operation to an even tangle through which a big branch cross with itself, for instance, the even tangle 4 in Figure 5d, sometimes a new branch similar to trefoil knot would occur (Figure 5h) when it accomplishes odd times of turn or the primitive branch would be split into two small branches (Figure 5k) when it accomplishes even times of turn.

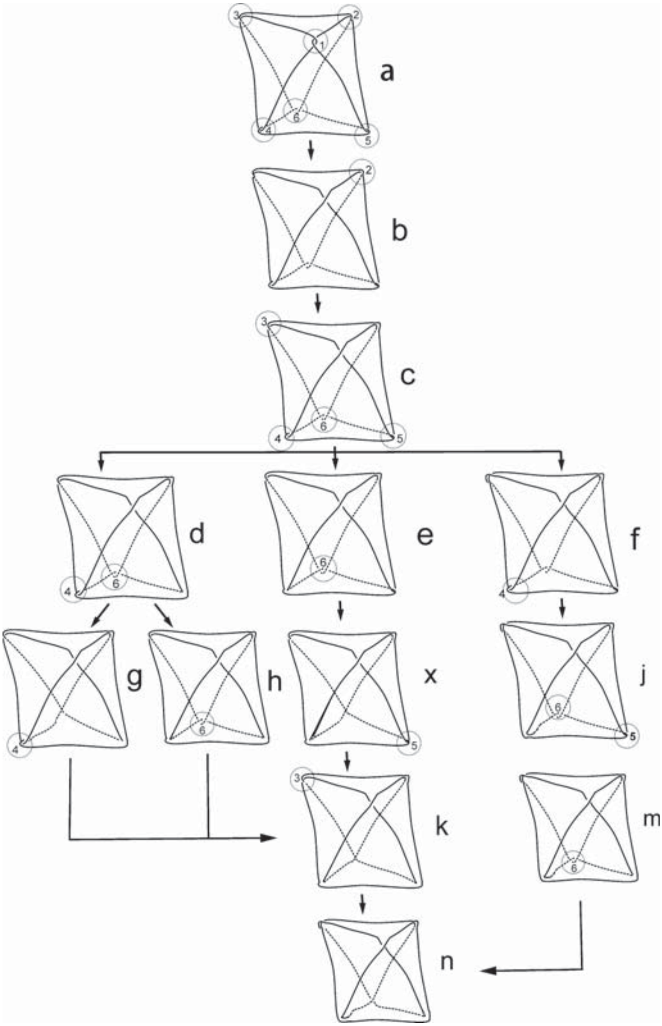

Figure 5. The procedures of 'even-to-odd' operation applied to the octahedral links.

Step 4: The above procedures could be took as the first circulation. Then start from tangle 2 and continue the procedures of step 3 and 4 to accomplish another circulation. Repeat the *process until all tangles carry on the same circulations.*

Sometimes, to know which symmetry group the polyhedron belongs to will significantly facilitate the arduous work. For instance, in the case of octahedron, because of the symmetry, all tangles are on a prevalent position and only one circulation is necessary.

Step 5: Use new branches obtained to assemble other structures.

Three principles should be followed in the process:

(1) Every branch must be connected by pure odd tangles.

(2) All different branches should only be connected by even tangles.

(3) The combinations of branches could cover the polyhedron.

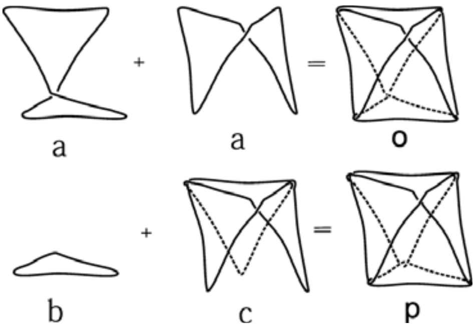

Figure 6. The combinations of new branches to get new polyhedral links.

There are only two combinations satisfying the three principles in this case. It is noted that the new branches (Figure 6a, 6c) are derived from octahedral link B (Figure 5b) and from octahedral link F (Figure 5f), respectively.

Step 6: Check all octahedral links and delete the repeating ones, and all possible structures will be obtained.

For example, the link P (Figure 7p) assembled in step 5 is actually topologically equivalent to link F (Figure 7f) obtained in step 3, so only one structure should be kept.

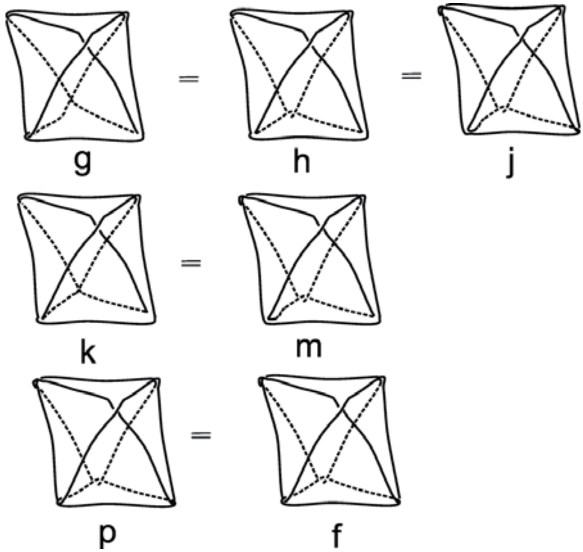

Figure 7. The repeating links in the above procedure

2.3 Topological transformation to target DNA polyhedral links.

All corresponding truncated polyhedral links will be topologically deformed into the target DNA polyhedral links. Actually, the approach is dependent on the polyhedral links of truncated polyhedron, i.e., a polyhedral link of truncated polyhedron will result in an according DNA polyhedral link of target polyhedron. The edges are pulled to the center of the faces following the directions of the arrows shown in Figure 8b. In this way the four faces in the octahedral link are transformed into three-branched vertices, while the six vertexes are transformed into twisted double-lines, and the octahedral link is transformed into the branched DNA tetrahedral link (Figure 8).

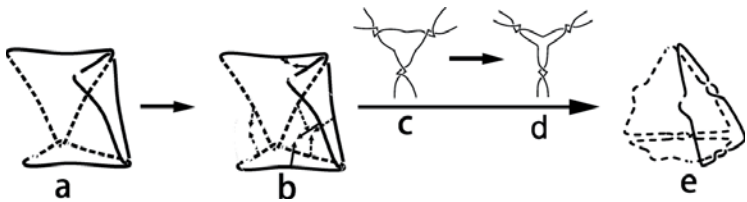

Figure 8. The topological transformation of the tetrahedron link.

Finally, all octahedral links and according DNA tetrahedral links could be given as illustrated in Figure 9. Every DNA tetrahedral link in the bracket is deformed from the octahedral link on its left side topologically.

3. Validity and application

This method could produce all possible DNA polyhedral links. If there is a DNA polyhedral link could not be derived from this method, when it agrees with the principles in step 5, which means it is assembled by the pure odd branches through even tangles, all we need to consider is the pure odd branches. If not, select one odd tangle of this DNA polyhedron and change it into an even tangle. Actually, it is the reverse of the even-to-odd operation which is part of the construction process in step 4 or 5. Continue this procedure one by one until all odd tangles become even tangles. This process can also be applied to the pure odd branches of the DNA polyhedral links obtained by combination in step 5. Because there is only one link connected by pure even tangles, reversing the process will derive the original DNA polyhedral link, so it could be obtained by our method. Thereby this method will generate all possible DNA polyhedral links.

Recently, a simple formula called new Euler's formula, $s + \mu - c = 2$, which connects the numbers of Seifert circles s, components μ, and crossings c, has been proposed by Hu[24]. Baesd on that, a new invariant called new Euler's characteristic, $\lambda = s + \mu - c$, was derived and explored explicitly by Li[25].

The new invariant unites several features of the DNA polyhedral link and has the potential to reveal the intrinsic properties of DNA polyhedrons. As an example, the smaller the new Euler's characteristic is, the more asymmetric the related DNA polyhedral link is. However, the difficulty to caculate the new Euler's characteristic is that there is no efficient way to compute the number of components μ. Our method could give all possible DNA polyhedral links, and inclusively, the number of components μ, which will finally resolve the problem of the computation of the new Euler's characteristics.

4. Simplified methods

The above process to get all types of DNA polyhedral links is very complex, however, if only one special type of structure is needed, the method could be simplified.

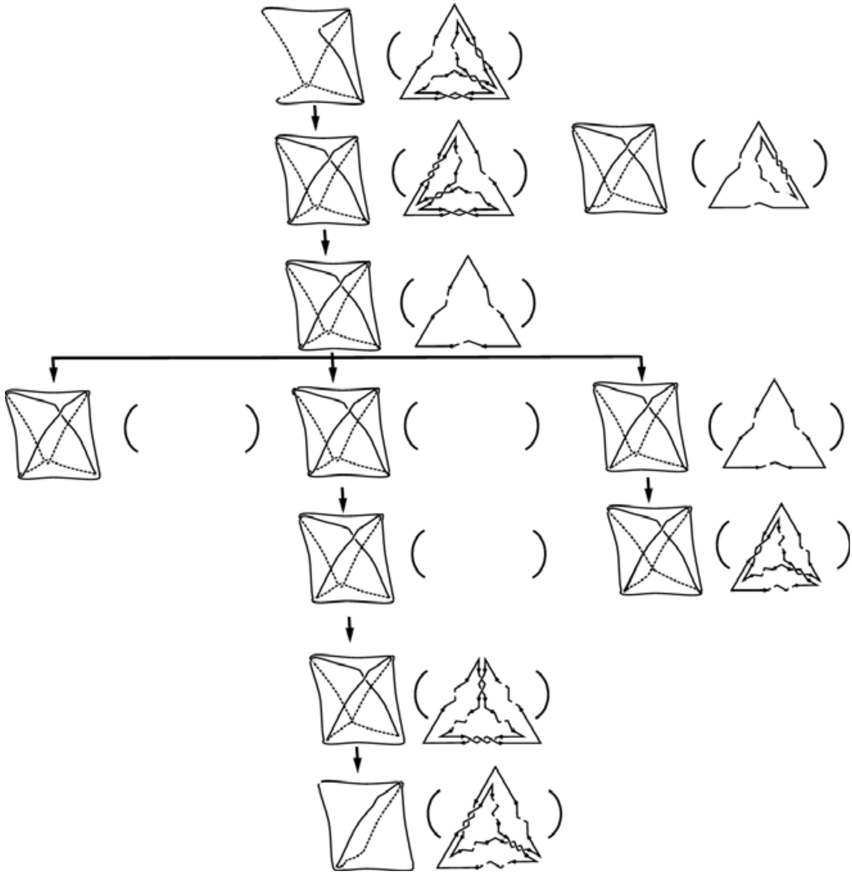

Figure 9. All octahedral links and according DNA tetrahedral links

4.1 Single branch growth method

If only one branch is taken into account, which means only one big circle is generated step by step by applying 'even-to-odd' operation on the DNA polyhedral link constructed by pure even tangles, the method can be simplified. The example of DNA octahedral links is illustrated in Figure 10. The key of this approach is that, when the big branch emerges more and more small branches, it will connect with itself via an even tangle (Figure 10e), which should be retained to avoid the occurrence of the complicated cleavage of the big circle.

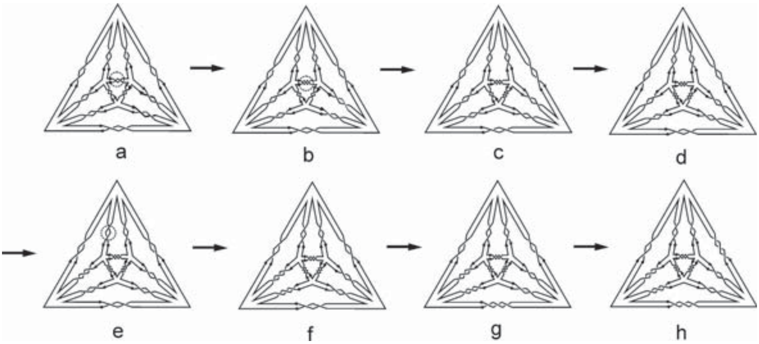

Figure 10. DNA octahedral links obtained by single branch growth method.

4.2 Pure odd tangles method

The construction of one special DNA polyhedral link connected by pure odd tangles can be very easy. Take a cube as an example. Based on its truncated polyhedral link, perform 'even-to-odd' operation on an even tangle (Figure 11c.1) to get an odd tangle (Figure 11d.1) and continue to proceed in the same direction (Figure 11c.1→2→3→4→5→6) until returning to the starting point, then the first circle would be obtained. After that, pick up another even tangle in another branch and apply the same rule to the adjoining even tangles, followed by topological deformation, the target DNA polyhedron will be obtained.

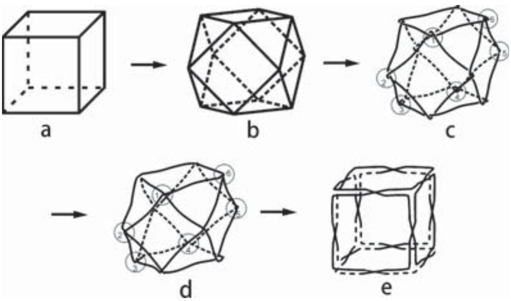

Figure 11. The process of pure odd tangles method applied to a cube.

5. Conclusions

In summary, our research has presented a general method to resolve the problem of the design of DNA polyhedral links especially polyhedron with odd tangles by the following steps: (1) Truncate a polyhedron and use ‘tangle-vertex and single-line covering’ method to get a pure even tangles polyhedral link; (2) Apply 'even-to-odd' operations to the corresponding polyhedral link to yield polyhedral links consisting of both even and odd tangle, then use new branches obtained to assemble other structures and delete the repeating ones; (3) Transform all corresponding truncated polyhedral links into the target DNA polyhedral links. We hope our work not only could help chemists to synthesize novel structures but also could provide a new perspective for the theoretical research in the field of knot and topology.

Acknowledgements: This work was supported by grants from the National Natural Science Foundation of China (Nos. 20973085 and 21173104) and Specialized Research Fund for the Doctoral Program of Higher Education of China (No. 20090211110006).

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