*MATCH*
*Communications in Mathematical and in Computer Chemistry*

MATCH Commun. Math. Comput. Chem. **71** (2014) 185-198

ISSN 0340 - 6253

# Blueprints of DNA Origami Links Constructed with Hamilton Circles

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(Received January 14, 2013)

**Abstract**

DNA origami nanostructures were selected as research subject, a discussion about how two dimensional links assemble into three dimensional links was given and DNA polyhedral links were constructed by a series of Hamilton circles through dual operation. Our results provide further insight into the molecular designing and theoretical characterization of the new DNA nanostructures.

## Introduction

In 1991, Seeman reported his most important paper in Nature which shows how to fold DNA strands into a cube shape artificially [1]. It is a milestone of the DNA nanometer era that based on the special character of DNA that two helical chains of nucleotides held together by the specific hydrogen-bonded base pairs. In the following years, scientists have synthesized various DNA shapes which riches the library of DNA nanostructures [2–7]. In 2006, Rothemund produced some two-dimensional DNA structures with the strategy called "origami" [8], for example, DNA smile faces, five point stars and rectangles [8]. The principle of origami strategy is like this. A long scaffold DNA strand is folded into the desired shape back and forth and some short strands are used to pair with the scaffold at particular

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positions, then a stable DNA geometry is produced. With the stimulus of DNA origami, scientists have made a lot of three and two dimensional DNA structures, for instance, DNA cube [9–10], tetrahedron [11], triangular prism [12] and Mobius band [13] and so on [14–23].

The synthesis of DNA polyhedra have accumulated massive and novel experimental results that need more work to explain them, then a lot of theoretical scientists are attracted and join in this emerging field and have reached great achievements. The methods that calculate components number of DNA polyhedra are reported by N. Jonoska and R. Twarock [24–25]; professor Slavik V. Jablan have discussed the intrinsic properties of DNA structures by graph theory [26–27]; professor Qiu and his group have paid a lot of efforts to describe these structures with polyhedra links [28–31] and proposed many theoretical models to design DNA polyhedra [32–35]. But unfortunately, all these works focused on edges and vertexes of polyhedra to organize their design. Face is a very important element of geometry but it is ignored. As far back as in 1994, Adleman tried to seek Hamilton paths in molecular design to understand how do macromolecular fold with aid of computer experiments [36]. His works inspire us to design DNA nanostructures with origami strategy that begin on a face by Hamilton circles. The idea of this paper is derived from here.

The constructed two dimensional links (2D-links) are nested together as sewing pieces of cloth together with a needle, then a three dimensional links (3D-links) is produced. In this paper, we will not only discuss how to sew 2-D links into 3-D links, but also give a discussion about constructing DNA three dimensional links with Hamilton circles. The results show that any connected plane, curved surface or three-dimensional space, can be constructed by Hamilton circles.

## Assemble 2-D links into 3-D links

For assigned two dimensional links, we can assemble them into a three dimensional links with sewing their common edges together. If the 2-D links are chained together in different ways, the results are not the same. So we divided them into two kinds: direct embedding and embedding with additional rings. Here, for convenience we select 2-D links as shown in figure 1 to discuss. Before the discussion, we must have a common view: for any polyhedron $P$, the number of vertexes, faces and edges are $V$, $F$, $E$ and the component number of the $i$th face $F_i$ is $C_i$.

## Direct embedding

If 2-D links is embedded together directly, then common boundary between two 2-D links will be edge of 3-D links and vertexes are points that some 2-D links gather. For convenience of discussion, all edges and vertexes are topological on a plane shown in figure1. The arcs embedded together maybe on entirely different components or some of them on same one. However, each arc must be part of a component of 2-D links. Here, we must consider the crossing number *n* is even or odd, because the results are different.

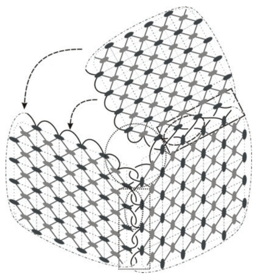

Figure 1: Direct embedding 2-D links into 3-D links.

If the crossing number *n* is even but not 0, as shown in area *A* of figure 1, the elliptic region *B* and the rest of area *A* are mirror image. As everyone knows, the component number $C_p$ has nothing to do with *n* while n is even. Therefore, $C_p$ is equal to the sum of component numbers of all 2-D links; we can calculate it by formula (1).

$$C_p = \sum_i^F C_i \tag{1}$$

If the crossing number *n* is odd, is shown in area *C* of figure1, the elliptic region *D* and the rest of area *C* are mirror image. We can find that two components belong to two 2-D links are merged into one. Nevertheless, if there are *m* (*m*≥0 and *m* is integer) pairs of arcs on boundary, if *m* is even (include 0), then two components will not merge to one; but if *m* is odd, the number of components will reduce 1. We can calculate $C_p$ by formula (2).

$$C_p = \sum_i^F C_i + \sum C(m) \tag{2}$$

Here, *C(m)* indicates the function that whether two components combined to one. If two components combined to one, *C(m)*= -1; otherwise, *C(m)*=0, and ∑*C(m)* is the total number of reduced components.

## Embedding with additional rings

If we add a series of rings between edges, vertexes as shown in figure 2. The cross between rings and arcs maybe alternate cross, unalternate cross or these two coexist. The crossing number *n* is even or odd will determine that whether $C_p$ reduces. If *n* is even and the number of components will not change. So the components number of polyhedra link can be calculated by formula (3).

$$C_p = \sum_i^F C_i + V + E \tag{3}$$

If we define the number of additional rings $C_+$ satisfies $C_+ = V + E$, then formula (3) can be rewritten to formula (4).

$$C_p = \sum_i^F C_i + C_+ \tag{4}$$

If the number of crossings *n* between additional rings and arcs is even, crossings number between additional rings is all odd, all even or these two coexist, $C_+$ is not equal to the total of *V* and *E* but is determined by *q*, which is the number of odd crossings between each two rings.

$$C_q = \left\{ \begin{array}{ll} -1, & q \text{ is odd} \\ 0, & q \text{ is even} \end{array} \right\} \tag{5}$$

Then, the formula (4) can be revised to formula (6).

$$C_p = \sum_i^F C_i + V + E + C(q) \tag{6}$$

## Construct 3-D origami links by Hamilton circles

Hamilton paths were sought to understand how macromolecule strands fold can be traced back to 1994, Adleman tried to find the Hamilton paths in molecular designing with aid of computer. We are motivated by his work and determine to construct 3-D links by Hamilton circles. Our design idea as follows: start from one face of a polyhedron, cross edges and travel to adjacent faces until all faces are traveled and go back to the starting face to get a loop circuit. Repeat this operation and we will get a series of Hamilton circles, and make them intertwine together and a 3-D link is produced. Then, replace all crossings with tangles and we can get polyhedron origami links. The problem that Hamilton paths travel all faces of polyhedra is similar to the problem that Hamilton paths travel all vertexes of polyhedra. Therefore, we can set up bridge between the two problems through dual operation. The Platonic polyhedral are most beautiful convexes and cube was first synthesized with DNA strands in Seaman's lab. Research about Hamilton paths of Platonic polyhedra is maturity, so in the following we will cite Platonic polyhedra examples to carry out our idea.

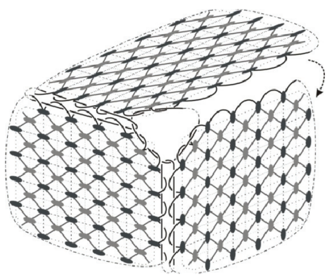

Figure 2: Embedding 2-D links into 3-D links with additional rings.

## Construct Platonic origami polyhedra links

### Tetrahedron origami links

We all know that tetrahedron is a self-dual polyhedron, so we can discuss the Hamilton paths that travel all its vertexes instead of that travel all faces. For tetrahedron, we can find several different Hamilton circles that travel all vertexes, see full lines in figure 3a, b. But all vertexes are same for they do not distinguish from symmetry, so the Hamilton circles also can be coincided with symmetry operation which is shown by full line and dot dash line in figure 3c. All Hamilton circles in figure 3c are on a plan. Two different Hamilton circles that travel all faces cross one common edge, this means that two Hamilton circles share one edge in the dual graph of tetrahedron.

First, a bunch of parallel Hamilton circles are used to travel all faces of tetrahedral only once as shown in figure 3c. All these Hamilton circles compose a “Cluster”. The circles in a cluster are not inserted with each other, namely they are parallel. A Hamilton cluster can be found in figure 3c that covers all faces of tetrahedron entirely. If two clusters of Hamilton circles inserted with each other, which leads to a series of points with degree 4. Replace all 4 degree points with tangles and a tetrahedron link is gotten.

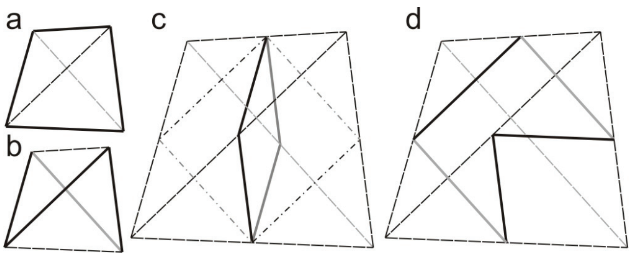


Figure 3: Construct tetrahedron origami links (gray indicates inner, black indicates outer).

The component number $C_p$ of tetrahedron links has no reference to $E$, $V$ and tangle number. It is determined by two factors: the number of Hamilton circles $C_i$ ($i$ can be 1 or 2) and the parity of tangles. As discussed in the preceding section, $C_p$ is a constant if tangles with even crossings, but the Hamilton circles are changed and more badly the preconditions of Hamilton circles are not available. The number of tangles $T$ that replace all 4 degree points can be figured out by formula (7).

$$T=2\times C_1\times C_2 \tag{7}$$

Here, 2 means that two Hamilton circles in two clusters that inserted with each other are sure to have 2 points with 4 degree and therefore they must be replaced by 2 tangles. If the crossing number of *ith* tangle is $k_i$, then no matter tangles are same or not that the total number of crossings $N$ can be calculated by formula (8).

$$N = \sum_{i}^{n} k_i \tag{8}$$

## Hexahedron and octahedron links

To analysis Hamilton circles that travel all faces of hexahedra, we need begin at its dual polyhedra, octahedra. Based on different edges, the Hamilton circles that travel all vertexes of a octahedron can be divided into two parts as follows:

The first is that any two edges adjacent which Hamilton circles travel with no chirality are belong to one triangle（find in figure 4a）. Rotate with the fourth axis and there will be four cases, one of them is shown with full lines in figure 4a. As our definition, there is one “Family” with four “Clusters”. In the second Hamilton circles, two adjacent edges that travel two vertexes (as shown in figure 4b, c) are not edges of any triangle but a square, we definite these vertexes as “Singular-points”. The Hamilton circles in the left of figure 4b and c are enantiomer, each of them is a “Sub-family”.

If a cluster of paralleled Hamilton circles are used to cover all faces, then we can transform vertexes traveling of octahedra to be faces traveling of hexahedra. To ensure to form vertex covering, other different clusters must be added to. There are two methods to add clusters in the first kind. One is a cluster of Hamilton circles are used and some other circles are needed too. Then crossings are produced and cover the full hexahedron, for example, in the middle of figure 4a, circles shown with single point lines are introduced in hexahedron. All these introduced circles form two “Clusters” satisfying rotation symmetry which belong to a “Family”. Four clusters of Hamilton circles with four axes are needed in the other method. Two parallel paths from a cluster and two from another cluster form one group and travel two edges with two rotational axes of hexahedron. Then, six groups cover all edges of hexahedron to ensure that the centers of faces with same density of crossing. However, only two clusters with two rotational symmetries are needed to make crossings that cover the whole hexahedron (in the middle of figure 4b). In the end, all crossings are 4 degree, so hexahedra links can be got by replacing crossings with tangles of 4 degree.

If the broken-lines are replaced by straight lines, there will be some novel results (shown in the right of figure 4a, b). In the first family, four clusters with four rotational axes are needed, each Hamilton circle of a cluster is on an identical plane and all these planes are parallel with each other. But the area that every cluster can cover is limited, for example, the Hamilton circles that figured by heavy lines can only exist in the area between double dot lines. Areas covered by the four clusters interlap with each other, and then all 4 degree crossings cover all faces precisely. The hexahedra links can be made by replacing crossings with 4 degree tangles. For the second family, although four clusters Hamilton circles with four axes are needed to construct links as well in the same sub-family, there are still some differences, as shown in the left of figure 4b. Firstly segmental arcs in any Hamilton circle that traveling faces of a hexahedron are not in identical plane. Second, Hamilton circles travel adjacent edges of face with four axes are corresponding to singular points of octahedra. However, these faces will be covered by 6 degree tangles[33] to construct links.

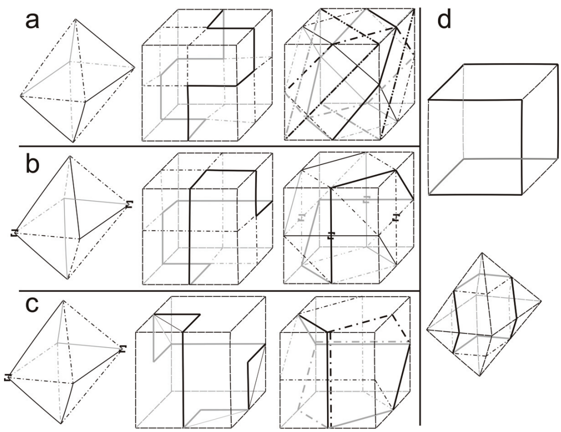


Figure 4: Building 3-D links of hexahedron and octahedron.

If employ four clusters from the different sub-family to construct links, there should be that the two of them are adopted from one sub-family and satisfy with two rotational axes, as well as the remains. At the same time, the faces corresponding singular-points must be coincident otherwise there are no crossings on the other two faces. After then on the faces, one cluster of a sub-family is parallel to one from the other sub-family and intersectant with the other one from the latter.

It is easier to construct octahedron links（in figure 4d）. There is only one family of Hamilton circles in constructing octahedron links because there is one kind of Hamilton circles covering vertexes of hexahedron. That is still only needed two clusters with two axes to construct links.

## The feasibility of constructing dodecahedron and icosahedron origami links

For dodecahedra and icosahedra, not only “cluster” and “family” are more complexity, but also the situations of Hamilton circles are more. So, we give feasibility analysis about constructing here.

The research about Hamilton circles of icosahedra is a troublesome problem. In view of that the Hamiltonian path problem is an N-P complete problem. Here, we use the enumeration method and the results are shown in figure 5a. The Hamilton circles of an icosahedron are so complex that we use its plane to have a discussion. In figure 5a, different Hamilton circles family are figured by full lines and dot dash lines.

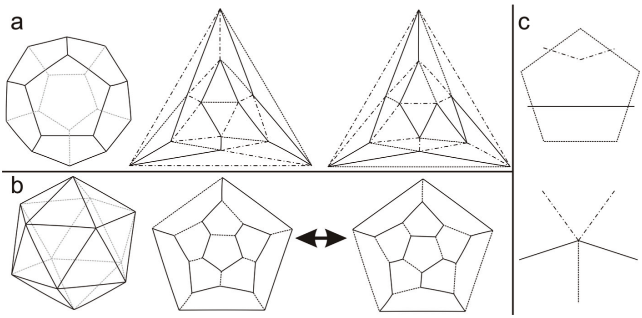


Figure 5: Origami links schemes of dodecahedron and icosahedron.

Here, we can search Hamilton links by some rules as follows:

1. First, calculate the number edges in a Hamilton circle which share a vertex and in a triangle;

2. If 1 is available, we need to estimate that all triangles share edges, share vertexes or disjoint.
3. If 2 is available, the number of continuous triangles with common edges need to be calculated.

A preliminary judgment can be made by the above methods. If all these are fulfilled, its chirality cannot be determined until by symmetry operation. In middle and right of figure 5a, we can find many families of Hamilton circles. The areas between full lines, between dot dashed lines indicate different Hamilton families.

The families of enumerated Hamilton circles will form crossings with 4 degree, replace them by tangles and then get 3-D links. However, the folding of Hamilton circles is a complex system because each face of an icosahedron is a pentagon, see figure5. Any cluster of Hamilton circles cannot cover the whole of a pentagon. We can conclude that there are two cases of travelling a vertex from travelling vertexes of its dual graph: a Hamilton circle travels edges which share a common vertex is continuous or discontinuous, they are figured in figure 5c with full lines and dot dashed lines, respectively. Therefore, the number of cluster must greater than 2 for constructing dodecahedron links. We conjecture the number is 4 at least.

The Hamilton circles that travel all faces of an icosahedron are easier for its dual polyhedron dodecahedron only has one family of Hamilton circles. Meanwhile, each face of an icosahedron is a triangle. The two intersected Hamilton circles cover all faces and replace them with tangles, we will get links.

The formulas of tetrahedron origami links also satisfy other Platonic polyhedra origami links. If the number of Hamilton circles that construct links is even and greater than 2, we can make two clusters as a group to compute and then summate them.

## Discussion

For any polyhedron $P$, its dual polyhedron $P^*$ can be got by dual algorithm. But whether Hamilton circles can travel all vertexes of $P^*$, there is no effective methods to proof. For polyhedra with such Hamilton circles, it can be construct by this method. The polyhedra without such Hamilton circles cannot be constructed directly, but we can make a modification as follows: in the plane of $P^*$, there is a Hamilton circle that travels the most vertexes as a big circle and construct a series of rings intersect with the big circle based on the rest of vertexes not with repeat edges. The idea has been used in constructing hexahedron links, but the chosen big circle is Hamilton circle.

From above and previous work [33], for any connected area, no matter it is plane, curve or 3-dimensional, it can be covered by a dot matrix or a series of regular points and finally we can get a *2*-regular graph. Then, utilizing the Eulerian graph theorem[37], Hamilton circles and tangles, an origami links can be obtained ultimately.

## Conclusion

In this paper, we are focus on how to fold 2-D links into 3-D links. First, we discuss about constructing polyhedra links with two dimensional links by direct embedding and embedding with additional rings, then we calculated the number of components number $C_p$ and the number of crossings $n$.

Second, we build a bridge between Hamilton circles travel vertexes and faces by dual operation. Then we constructed tetrahedral, hexahedra and octahedra origami links with Hamilton circles and give a feasibility analysis about constructing dodecahedra and icosahedra origami links.

Third, we gave a further discussion about producing origami links by Hamilton circles. For any connected graph, the corresponding links can be constructed if its dual graph has Hamilton circles; otherwise, the corresponding links can be produced through a series of modification.

Although our discussions of how 2-D links were transformed into the origami polyhedra origami links is preliminary, the problem still needs a lot of in-depth research. We hope that the results can provide some theoretical support for the design and synthesis of DNA polyhedron.

*Acknowledgments*: This work was supported by grants from The National Natural Science Foundation of China (Nos.20973085; 10831001; and 21173104) and Specialized Research Fund for the Doctoral Program of Higher Education of China (No. 20090211110006).

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