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Extended Goldberg polyhedral links with odd tangles

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Abstract

This paper extends the methodology of the construction of polyhedral links by tangles in knot theory. Building blocks consist of odd tangles which are regions in the projection plane with $2n+1$ half-twist, where n is an integer. Fixing odd tangles at the all vertices of Extend Goldberg polyhedra, and then connect them together will result in many interlocked networks. The solution to the component algorithm of 4-regular polyhedral links has been proposed. Our result shows, by counting the length of central circuits of a polyhedron, the component number of the relating polyhedral link will be presented. Using such topological models, some potential significance in biological and chemical areas is tested to be explored.

1. Introduction

In recent decades, a variety of exotic newcomers whose molecular graphs cannot deform into a plane have been created in Nature [1-3]. DNA and protein molecules are large enough to be flexible that they can form intricate knotted and interlocked topologies. Besides naturally occurring molecular catenanes and knots, some more interesting interlocked 3-dimension structures have been designed in DNA computing [4, 5] and later been synthesized as a chemical challenge [6-12]. The important mathematical tool to address these non-trivial topological entities is knot theory [13, 14], which is the study and quantization of configurations of graphs in Euclidean 3-space (R^3). By reason of the great development in its own right, it has been shown to have applications in researching topological chirality and designing novel topology of chemical molecules [15-21]. The present paper was motivated by the continuing interest of chemists and mathematicians in these amazing constructions.

In knot theory, any four-regular plane graph can be seen as a projection of an alternating link. Jablan has given a unique connection between knots and fullerene or other basic polyhedra [22]. However, we give another relationship between a 4-regular graph and the relating links which are not just one to one. By applying the even tangles to Extended Goldberg polyhedra, many infinite series of links have been generated from each polyhedral graph [23]. Here, the assembling of odd tangles will yield many more complex knotted networks. This work gives a different way for looking the geometrical information of these new polyhedra, and extends our earlier research of the construction of polyhedral links with tangles.

The component number is the basic invariant of knots and links. Another goal of this paper is to determine number of components of links obtained from 4-regular graphs. A polyhedral link is not only a pure mathematical conception, but also provides a new idea to understand some phenomenon in organisms, such as the connection between component numbers and capsomere numbers, knot entanglement and viral crosslinking [24-27]. Additionally, we hope this process would stimulate chemists to set their sights on the design and construction of other interlocked and intertwined molecules of more complex topologies.

2. Odd Tangles as Building Blocks

To provide the necessary background, we begin our account with a simple discussion of some peculiar property of tangle in knot theory. Mile time, some basic concepts and terminology of knot theory are also being depicted.

Tangle *A*. A region in the projection plane surrounded by a circle exactly with four emerging arcs {*NW*, *NE*, *SW*, *SE*}, it is an ideal building block for the construction of compounds possessing various complex knotted topologies. A tangle with a finite sequence *R* left-handed half twist or *R* right-handed half twist will be called *R*-tangle or –*R*-tangle, where *R* is a positive integer and equal to the crossing number. All algebraic knots and links can be obtained from *R*-tangles by applying some tangle operations, such as addition, multiplication and numerator closure. Due to the same character of two strings and twists occur between tangles and double helical DNA or organic intermediate, thereby making the conversion from tangles in topology to real molecular objects in chemistry.

Odd tangles. The tangles can be divided into two types depending on whether *R* is even or odd. When $R = |2n+1|$, n is an integer, the odd tangle is obtained and some examples are shown in Figure 1. Note that as the building blocks, odd tangles have some different properties with even tangles. For examples, the closure of an even tangle will yield a link, whereas the closure of an odd tangle will yield a knot.

Tangle composition. The new tangle operation is tangle composition, which has been proposed for a 4-regular plane graph [23]. It means substituting vertices of graph by tangles and connecting two arcs of tangles along each edge of graph (Figure 2). The following sections of this paper are to determine number of components of links obtained as composition of odd tangles on 4-regular polyhedral graphs.

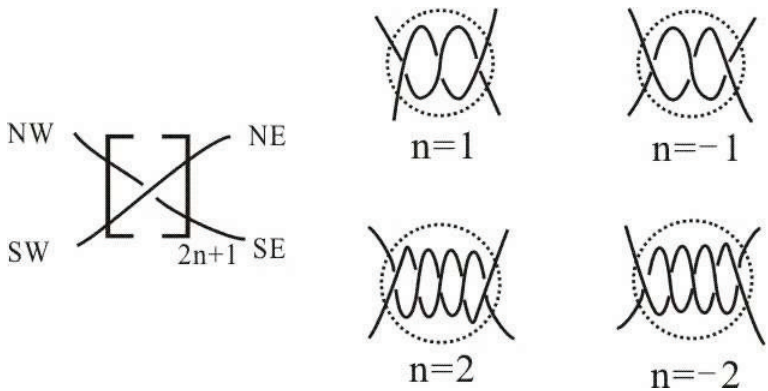

Figure 1. Odd tangles obtained by 2n+1 half-twists

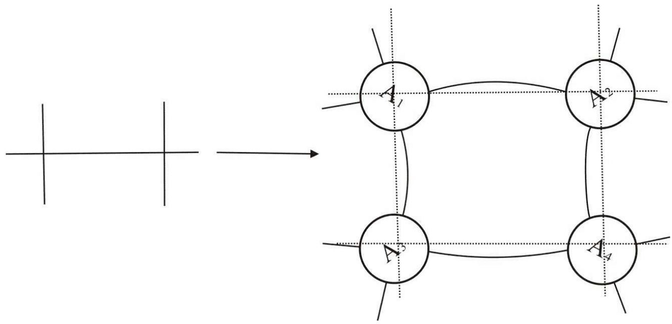

Figure 2. The operation of tangle composition on a 4-regular graph

A graph in which all vertices are 4-valent is called a 4-regular graph. Among the graphs corresponding to the polyhedra, the octahedron graph is the smallest 4-regular. The resulting of using the odd tangles to replace the vertices of some 4-regular polyhedral graph is easy to show some alternating links. As examples in Figure 3(a), the borromean link will be obtained by applying unit tangles to octahedral graph, because no pair of rings is linked. In Figure 3(b), the resulting structures of $2n+1(n>0)$ tangles is similar to DNA borromean link which was obtained by Seeman [28], the only difference is in that the signs of the three outer nodes are opposite to those of the three inner nodes in DNA borromean link.

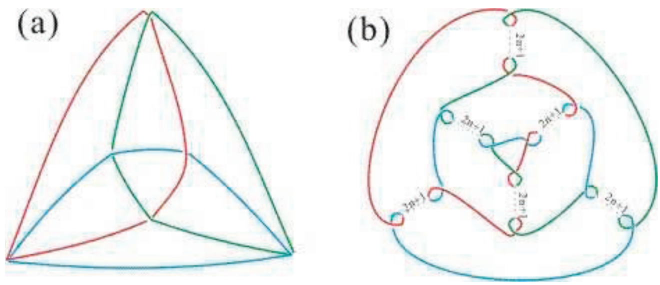

Figure 3. Borromean links obtained by replace vertices of octahedral graph by (a) 1 and (b) 2n+1 tangles

3. Component Algorithm

Definition 1. For a 4-regular polyhedron graph G, a central circuit ***CC*** is a walk without repeated edges and every edge of ***CC*** is the opposite neighbor of its preceding edge [29, 30].

Note that, after applying the tangles of odd numbers to a 4-rugular polyhedral graph, many series of alternating polyhedral links L whose components correspond to its *central circuits* are obtained. As a result, each vertices relates to an odd tangle with $2n+1$ crossings, thus, the number of crossings is a multiple of vertices number V by $2n+1$, but the number of components is little difficult to count. Additionally, the number of half-twist n could be any integers, thus, the mapping between polyhedron and their links is one-to-many.

However, the following algorithm solves the component number problem of a polyhedral link L from a 4-regular graph G: Let us take a starting point on any edge of G and head along the edge in the chosen direction. When arriving to a vertex, continue it straight ahead the edge opposite the entering one. Continuing to apply this rule reiteratively until return to the start point, we will obtain a first central circuit of G and it is a projection of one component of L. After that, we choose a point on another edge which not contained in the first circuit and continuing to apply the same algorithm until all the edges of the graph are exhausted [13].

Definition 2. For a 4-regular polyhedron graph G, the length Lc of a central circuit is the number of its edges, and the symbol of ave (Lc) denotes the average length of central circuit of a polyhedron.

As the definition, *central circuits* cover every edges of polyhedral graph G exactly once, thus the component number Nc of the corresponding link L can be calculated by the following equation:

$$Nc = E \,/\, \text{ave}\,(Lc\,) = \sum_i \varepsilon \sum_i c_i \,/ \sum_i Lc_i \quad (1)$$

Where E denotes the edge number and c_i denotes the ith *central circuit*.

4. Polyhedral links

4.1. Extended Goldberg polyhedra

Now, recall the class of new icosahedral and 4-regular polyhedra [31], whose the number of vertices and edges are decided by two coordinates (h, k), where $0< h \geq k\geq 0$ and the triangulation number $T = h^2+hk+k^2$. An Extended Goldberg polyhedral cage obeys some basic relations：

$$\sum dV_d = 2E,\ 4V = 2E \quad (2)$$

$$\sum Sf_S = 2E,\ 3f_3 + 4f_4 + 5f_5 + 6f_6 = 2E \text{ or } 3f_3 + 5f_5 + 6f_6 = 2E \quad (3)$$

Euler theorem: V-E+F = 2 (4)

Where V_d and fs are the number of vertices of degree d and the number of s-gonal faces, respectively, and (d = 4, $s \geq 3$). In this paper, we will focus on (3, 4) - and (3, 0)-Goldberg polyhedra (Figure 4), which are obtained by adding 3- and 4-gonal or 3-gonal faces on icosahedral fullerene - Goldberg polyhedra.

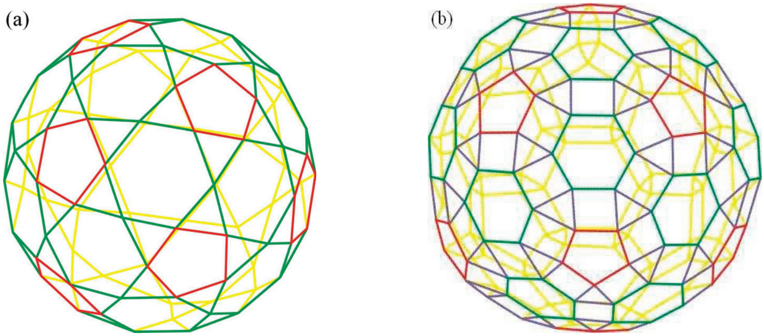

Figure 4. Extended Goldberg polyhedra derived from 32-hedron (C_{60}).
(a) The I_h (3, 0)-92-hedron. (b) The I_h (3, 4)-182-hedron

4.2. (3, 4)-Extended polyhedral links

For a (3, 4)-Extended polyhedral link, the parent polyhedron is a Stretch-Extended Goldberg polyhedron, which have vertices number Vs = 60(h^2+hk+k^2), face number Fs = 60(h^2+hk+k^2) +2, and h^2+hk+k^2 = T. By equation (4), the number of edges Es =120(h^2+hk+k^2) =120T.

In the kind of polyhedra, there are two different types of the *central circuits*, which contain only a pentagon and only a hexagon, defined as 5-circuit and 6-circuit, respectively. Each 5-circuit (Figure 5a) pass through 5 pentagons and 5 quadrangles and the contribution of each polygon to the circuit length is unit one, thus, the length of 5-circuit is L_5 = 10. Each 6-circuit (Figure 5b) pass through 6 triangles and 6 quadrangles, thus, the length of 6-circuit is

L_6 = 12. Additionally, there are exactly 12 pentagons in a polyhedron, so the number of hexagons is Fs-12 = $10(h^2+hk+k^2-1)$. It means that the number of 5-circuits and 6-circuits are N_5 = 12 and N_6 = $10(T-1)$, respectively. Therefore, the ave (Lc) of a Stretch-Extended Goldberg polyhedron can be calculated by equation: $L_5 \times N_5 + L_6 \times N_6 / N_5 + N_6$. The result is $[12\times10+10(T-1)\times12] / [10T+2] = 60T / (5T+1)$. By equation (1), we obtain the component number Nc of (3, 4)-Extended polyhedral links is $10T+2$.

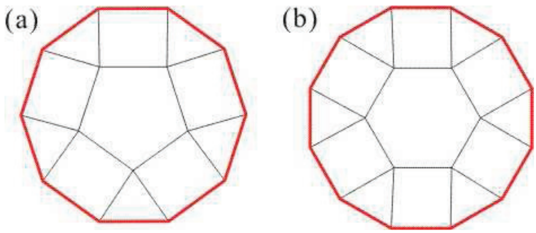

Figure 5. (a) The 5-circuit with length of 10, (b) The 6-circuit with length of 12

These total circuit number, or component number$10T+2$ are magic numbers. Note that the face number of Goldberg polyhedra is $10T+2$, thus, the capsomere number of a spherical virus is also equal to this number. The 5-circuit with length of 10 and 6-circuit with length of 12 have C_5 and C_3 symmetry, hence, these two different circuits may been used to represent pentamers and hexamers of viral capsids, respectively. Note that these circuits have some particular property, such as the crosslinking and the existing of overlapping areas between any adjacent circuits, may present in some complex viral capsids [32].

If $(h, k) = (1, 0)$, then $T = 1$, using odd tangles to cover 60 vertices of I_h (3, 4)-182-hedron, then connect them will result in a series of nested networks with $60(2n+1)$ crossings and 12 components. When $n = 0$, in Figure 6 (a), each vertices of polyhedron transforms into a crossing point of the polyhedral links. Each circuit of length 10 transforms into a component which contains a pentagon of the parent polyhedron, note that the pentagon in the outermost circuit is distributed on the behind of paper. Moreover, any group of two adjacent *central circuits* is interlocked via Hopf links, i.e. no pair of loops can be separated without cutting. When $n = 1$, in Fig 6(b), it is combined in such a way that any two component loops form a 4^1_2 link.

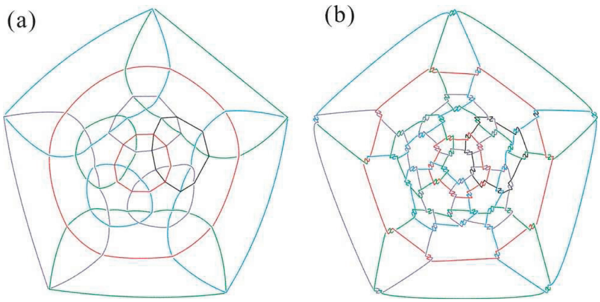

Figure 6. *I* (3, 4)-182-hedral links with 1 and 3- tangles

If $(h, k) = (1, 1)$, then $T= 3$, using odd tangles to cover 180 vertices of I_h (3, 4)-242-hedron, then connect them will result a series of nested networks with $180(2n+1)$ crossings and 32 components. Moreover, any group of two adjacent *central circuits* is interlocked via a link with crossing number of $4n+2$, thus, the absolute value of linking number of such sub-link is $2n+1$. The second example of $n=1$ is shown in Figure 7.

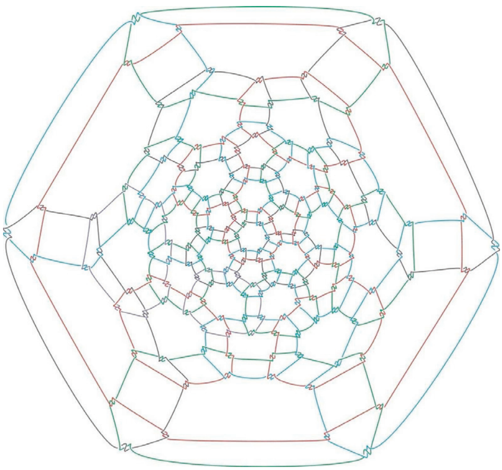

Fig. 7. *I* (3, 4)-242-hedral links with 3-tangles

4.3. (3, 0)-Extended polyhedral links

For a (3, 0)-Extended Goldberg polyhedral link, the parent polyhedron is a Rotate-Extended Goldberg polyhedron, which vertices number is $V_R = 30(h^2+hk+k^2)$, face number is $F_R = 30(h^2+hk+k^2)+2$, and $h^2+hk+k^2 = T$. By equation (4), the number of edges $E_R = 120(h^2+hk+k^2) = 60T$.

For each polyhedron, all of the *central circuits* have the same length; it means that the length of *CC* is an invariant for one of these kinds of polyhedra. Considered as a circle cutting polyhedral surface, each *CC* partitions all 12 pentagons into two equal segments, which are five in the interior and another five in the exterior regions.

When $T = 1$, then the I_h (3, 0)-92-hedron is obtained. Any *central circuits* pass through 5 pentagons and the remaining pentagon having no contribution to the circuit length is contained in the inner central position of a *CC*. Additionally, for a *CC*, there is a triangle between two pentagons, thus each circuit also passes 5 triangles and the length of central circuit is 10. By using our above method, the link with $30(2n+1)$ crossings and 60/10 = 6 components have been obtained, the cases of n = 0 and 1 are shown in Figure 8. Note that, each loop is intersecting with any other loops to form a closely interlocked network, and with the increase of *T,* the length of loop will increase too. For all Extended Goldberg polyhedra, the accounting of loops number becomes more complicated. However, in the following special two cases, the components number can be obtained by discussion of the length of *central circuits*. We give some examples to elucidate our method and algorithm for calculating the component number.

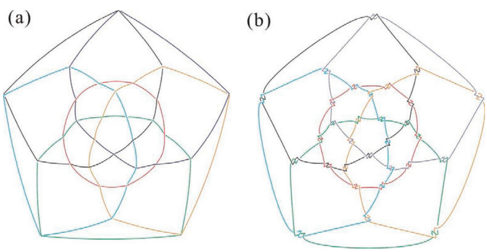

Figure 8. *I* (3, 0)-92-hedral links with 1 and 3-tangles

In the first type polyhedra, the face number are $F_n = f_5+f_6+f_3 = 12+10(a^2+2a)+20(a+1)^2$, then the edge number $E = [5\times12+6\times10(a^2+2a)+3\times20(a+1)^2] / 2 = 60(a+1)^2$ are given by equation (3), and the vertices number $V = 30(a+1)^2$ are given by equation (2), where a denotes a natural number. In this case, each *CC* pass through 5 pentagons, 5a hexagons and 5(a+1) triangles. Hence, the average length is also the length of all circuits is 10(a+1), then the component number $Nc = 60(a+1)^2/10(a+1) = 6(a+1)$.

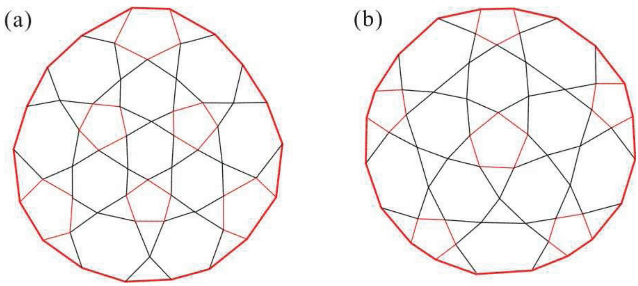

Figure 9. Two type of patches which are bounded by central circuits with different lengths.
(a) A patch of I(3,0)-122-hedron with border of 5 hexagons, 5 pentagons and 10 triangles.
(b) A patch of I (3, 0)-92-hedron with border of 6 hexagons, 3 pentagons and 9 triangles.

If a = 1, using odd tangles to cover 120 vertices of I_h (3, 0)-122-hedron, then connect them will result a series of nested networks with 120(2n+1) crossings. Thanks to the invariability of circuit length, we are only demanded to calculate the length of any one of *central circuits*, then the component number of links will be obtained. Using a diagram (Figure 9a) to show the patch of polyhedral graph, this is bounded by one of the *central circuits*. Each pentagon and hexagon occurs five times, and each triangle occurs ten times on a circuit, so the length of *CC* is 20. Furthermore, the component number is 12 and each pair of adjacent loops in the embedding has a linking number of 2n+1. The example of n = 1 is shown in Figure 10.

In the second type polyhedra, the face number are $F_n = f_5+f_6+f_3=12+10(a^2+a) +20(a^2+a+1)$, then the edge number $E = 60(a^2+a+1)$, and the vertices number are $V = 30(a^2+a+1)$. In this case, each *CC* pass through 3 pentagons, 3(a+1) hexagons and 3(a+2) triangles. Hence, the average length is $6(a+2)$, then the component number are $Nc = 10(a^2+a+1)/(a+2)$. If $a = 1$, using odd tangles to cover 90 vertices of I_h (3, 0)-92-hedron, then connect them will result a series of nested networks with $90(2n+1)$ crossings. The length of the *CC* is 18, which pass 3 pentagons, 6 hexagons and 9 triangles (Figure 9b). Therefore, the component number is 10 and the linking number of each pair of adjacent loops in the embedding is $2n+1$ too. The example of $n = 1$ is shown in Figure11.

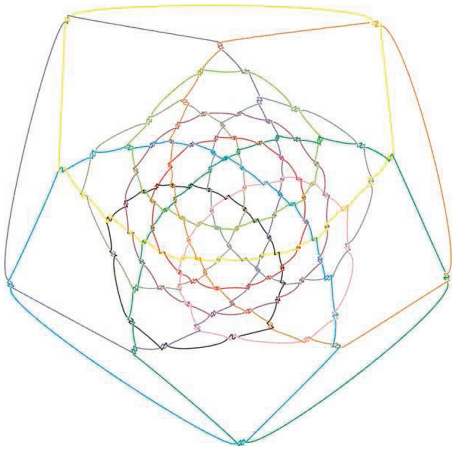

Figure 10. I (3, 0)-122-hedral links with 3-tangles

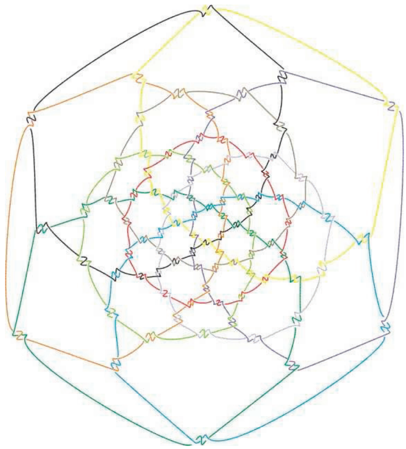

Figure 11. I (3, 0)-92-hedral links with 3-tangles

5. Conclusion

As the increase of the number of tangle *n*, each link will take place a series of topological transformation and thus more polyhedral links will be gained. In summary, the polyhedral links constructed by even tangles are some simple knotted structures, which contain 5-rings and 6-rings such small cycles, but the odd tangles correspond to some warp and weft interwoven networks here, and sets up a new relationship between a 4-regular graph and its corresponding links. Therefore, these structures become more complex and the properties of links depend on the topology of polyhedra. The investigation of the component algorithm proves that the component numbers of our constructions are even. In fact, Corinne Cerf [33] proved that every oriented alternating link with an even number of components is topologically chiral. After given an orientation, the chirality of these links is another important property, which has been discussed in paper [23].

Knotted networks, of substantial interest to bio-chemistry, have been realized in laboratory and nature. Therefore, the helical structure of metallo-organic intermediate and giant DNA strands may induce the formation of these mathematically rich entities. It also can be used to probe the possibility of crosslinking form for general types of viruses.

Acknowledgements

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