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The keeping and reversal of chirality for dual links

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Abstract

A new method for understanding the construction of dual links has been developed on the basis of medial graph in graph theory and tangle in knot theory. The method defines two types of oriented 4-valent plane graph: G_e and G_o, whose vertices are covered by *E-tangles* and *O-tangles*, respectively. The result shows that there are two types of dual links: *E-dual links* and *O-dual links,* which have many differences in topological properties, especially their chiral rule. In our paper, we show that dual links can be constructed by oriented 4-valent plant graphs and tangles. This research puts forward the definition of dual links and the methodology for the construction of dual links. Dual links open a new approach for the research of links, and the methodology may also be used to direct the synthesis of chiral molecules.

1. Introduction

Duality is a fundamental concept that underlies almost all natural phenomena. Roughly speaking, duality is the product of the interaction that takes place between the paired components of an elementary system [1, 2]. In physics, duality is used to describe theoretical models that appear to be different, nevertheless can be shown to describe exactly the same physics, and are divided into "trivial" and "nontrivial" [3]. Moreover, duality is also introduced into the research of string theory, and shows that all five string theories, together with M-theory, are dual to one another [4]. In geometry, duality defines a kind of relationship between two polyhedra. According to the duality principle, for each polyhedron, there is another polyhedron whose faces and vertices occupy complementary locations [5]. In graph theory, duality is more universal. Given a plane graph G, the 4-valent plane graph $Med(G)$ is defined as the graph as having vertices the edges of G with two vertices adjacent if and only if they share a vertex and belong to a common face. If $Med(G) = Med(G*)$, then G and $G*$ are dual [6].

Knot theory [7-9] is the area of topology that studies mathematical knots. The recognition problem of knot theory is to determine whether two knots are equivalent or not. Many knot invariants are put forward to solve basic problem, such as bridge number, linking number, HOMFLY polynomial, etc. A table of link and link invariants introduce information of them. Duality is a pervasive and important concept in (modern) mathematics. However, duality of links is never noticed in knot theory. In the paper, a method of constructed dual links is put forward, which is based on median graph in graph theory and tangle in knot theory. Two types of oriented 4-valent plane graph: G_e and G_o are defined, and tangles are divided into *E-tangles* and *O-tangles*. *E-tangles* cover vertices of G_e, which can construct *E-dual links*, and *O-tangles* cover vertices of G_o, which can construct *O-dual links*. The duality of link offers new thought for researching and classifying of links.

At the same time, the chirality of dual links has been studied in this paper because of its importance in chemistry, biology and knot theory. The synthesis and the discovery of many chiral compounds [10] and icosahedral virus capsids [11] show the importance of chirality. Knots and links are the mathematical form of big molecule [12-18], the theoretical research has gotten many fruits [19-27], and therefore, the research of chirality of dual links is necessary. The result shows that chrial rule of *E-dual links* and *O-dual links* are different, and the chiral rule shows that the same components have different chiral results after different manipulations. With this chiral rule, our research can direct the synthesis of chiral molecule, and help understand this kind of structure.

2. Tangles as Building Blocks

Tangles are building blocks of constructing dual links. A tangle is a portion of link diagram from which four arcs emerge pointing in the compass directions *NW, NE, SW,* and *SE* (Figure 1(a)). In this paper, according to the number of half twist, we class tangles into two types: *E-tangles* with even crossings (Figure 1(b)), and *O-tangles* with odd crossings (Figure 1(c)). Figure 2 shows two important manipulations: reflection and 90°-rotation. If reflect a tangle in a mirror that is perpendicular to the projection plane on the *NW-SE* line, it is known as reflection (Figure 2(a)), and if rotate a tangle 90° around an axis that is perpendicular to the projection plane on the intersection of *NW-SE* and *SW-NE* line, it is known as 90°-rotation (Figure 2(b)).

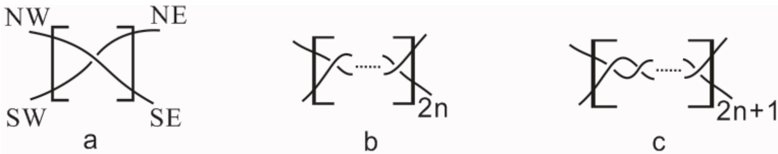

Figure 1. The classification of tangles

Figure 2. Two operations of tangles

Tangle composition is a new manipulation which bases on any 4-valent plant graph. If all 4-valent vertices of a plant graph are covered by tangles, and four arcs of tangles superpose the four edges coming out from the same vertex, then, connecting the arc of a tangle to the arc of another tangle along edge, the process is denoted by tangle composition (Figure 3).

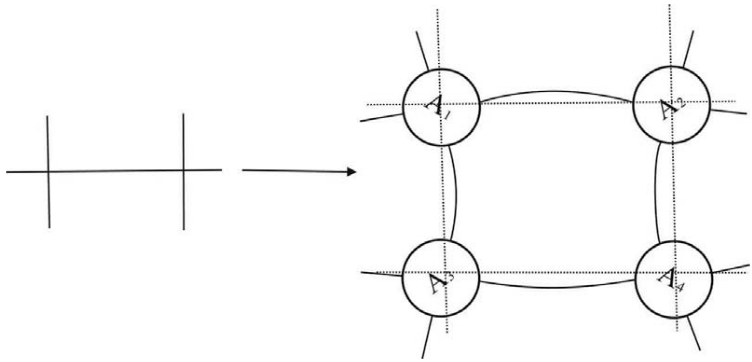

Figure 3. The operation of tangle composition

3. Definition

Four regions of a projection plane come together at a crossing. The over-strand counterclockwise rotates, passing over two of the regions which are labeled with an *A* and the remaining two regions with a *B*. If we split open a channel between the two regions labeled *A*, and call this an *A-split* (Figure 4(Ⅰ)). For two interlaced links, if their *all-A-split* states are complementary, we denote the pair of links by dual links (Figure 4(Ⅱ)). It means that the *all-A-split* state of one is the *all-B-split* state of the other and vice versa.

Let *G* be a 4-valent plant graph, and is denoted by C_1, C_2 a bipartition of the face-set of *G*. Such that no two adjacent faces of *G* own the same signature. We denote the oriented graph by G_e (Figure 5(a)), the edges of which are oriented so that the faces of C_1 are on the right of an incident edge. And the dual links which are constructed by G_e and vertices cover of *E-tangles* are denoted by *E-dual links*.

On the other hand, all edges of *G* attribute to a set of central circuit *CC***.** A clockwise orientation is selected on each *CC* of *G*, and we denote the oriented graph by G_o (Figure 5(b)). The dual links which are constructed by G_o and vertices cover of *O-tangles* are denoted by *O-dual links*.

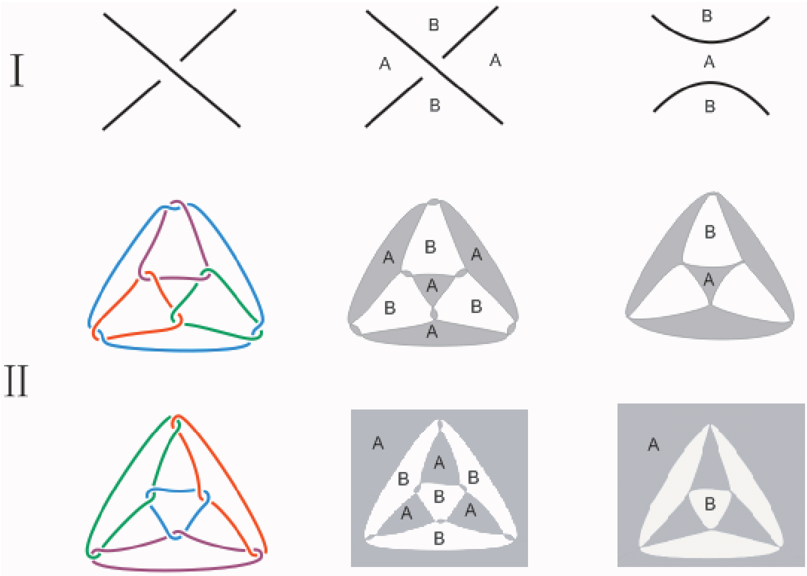

Figure 4. (Ⅰ) The operation of *A-split*; (Ⅱ) The operation of *all-A-split*. From two interlaced links (the leftmost graph), and two *all-A-split* states (the rightmost graph) of them are obtained.

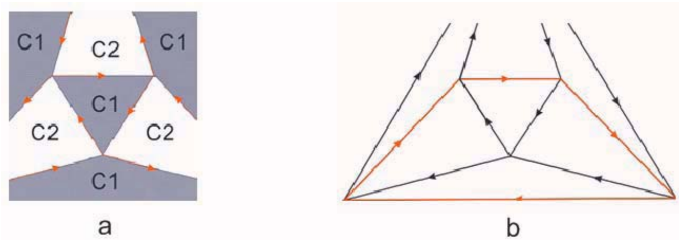

Figure 5. G_e and G_o

It is clear that orientations of *E-dual links* and *O-dual links* are determined by G_e and G_o, respectively. Further, the chirality of oriented link *K'* can be determined by the linking numbers *l(K')*: the link is denoted *D* configurations if *l(K')* > 0 and *L* configurations if *l(K')* < 0 [28]. For an oriented link, $\varepsilon(p)$ is given a sign according to the convention, as shown in Figure 6, the linking numbers *l(K')* can be calculated by the following equations:

$$l(K') = \frac{1}{2} \sum_{p \in \alpha_i \cap \alpha_j} \varepsilon(p)$$

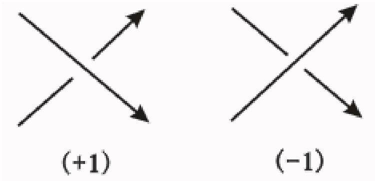

Figure 6. Convention used to assign crossings

Where $\varepsilon(p)$ defined to be ±1 if the overpass slants from top left to bottom right or from bottom left to top right, and $\alpha_i \cap \alpha_j$ is the set of crossings of two different components.

4. Construction of dual links

For our benefit, the plane graph of cubo-octahedron is selected to construct dual links. In geometry, hexahedron and octahedron are dual polyhedra, and when we cut them by planes perpendicular to their diagonals to the midpoints of edges, cubo-octahedron is obtained [5]. Cubo-octahedron owns 12 vertices, 8 trigonal and 6 quadrangular faces, and 4 *CC*. Two types of orientation of cubo-octahedron are given: G_e (Figure 7(a)) and G_o (Figure 9(a)).

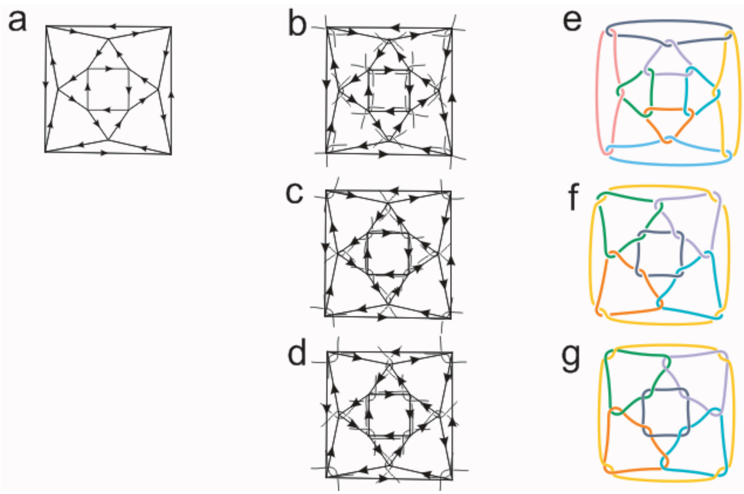

Figure 7. The *E-dual links* of G_e with *E-tangles*. The left is the G_e of cubo-octahedron. In the medial, (b) is G_e which vertices are covered by *2-tangles*; each *2-tangles* of (b) is 90°-rotated and reflected obtain (c) and (d), respectively. In the right, (e), (f) and (g) are the results of tangle composition, (e) and (f) are *L* configurations, and (g) is *D* configurations.

Figure 7 shows the process of constructing *E-dual links* by G_e and *2-tangles*. Firstly, twelve *2-tangles* cover 12 vertices of G_e (Figure 7(b)). Secondly, two new graphs (Figure 7(c) and (d)) are obtained by rotating and reflecting these *2-tangles*, respectively. Finally, undergoing the tangle composition, three links (Figure 7(e), (f) and (g)) are constructed. *l(K')* values of the three links show that Figure 7(e), (f) and (g) belong to *L, L* and *D* configurations, respectively. Moreover, two of them (Figure 7(f) and (g)) with 6 components are mirror images to each other, which are dual to the other one (Figure 7(e)) with 8 components. The results show that *E-dual links* constructed by 90°-rotation of *E-tangles* have the same chirality, and *E-dual links* constructed by reflection of *E-tangles* have opposite chirality. The orientations of 12 tangles are opposite in each oriented links.

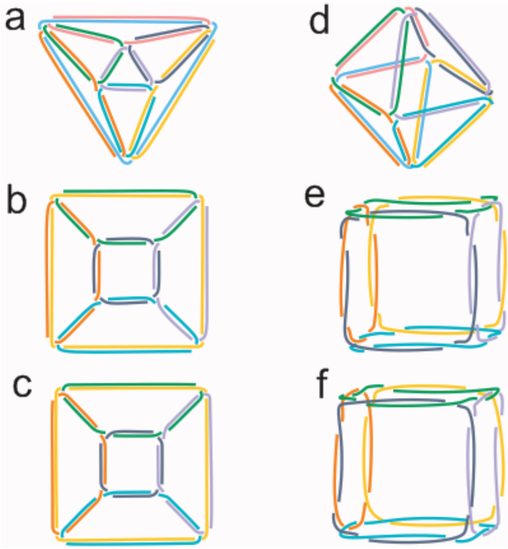

Figure 8. Topological transformation of *E-dual* cubo-octahedron links. The top are octahedral links, and the others are hexahedral links. The left links are in 2-dimensional space, and the right links are in 3-dimensional space

Cubo-octahedron provides a bridge between hexahedron and octahedron, with the potential emergence in both directions. Similarly, the cubo-octahedron link provides a bridge between hexahedron and octahedron links. Figure 8 shows the results of topological transformation of *E-dual* cubo-octahedron links. Firstly, *N-tangle* is transformed into *n*

-twisted double-edge by the movement of crossings and the polyhedral link is obtained in 2-dimensional space. Then, the polyhedral link in 2-dimensional space is topologically deformed in 3-dimensional structure. An octahedral link (Figure 8(d)) and two hexahedral links (Figure 8(e) and (f)), which are mirror images of each other, are generated in 3-dimensional structure. Chirality of links is kept in topological deformation, and the configurations of Figure 8(d), (e) and (f) are *L, L* and *D*, respectively.

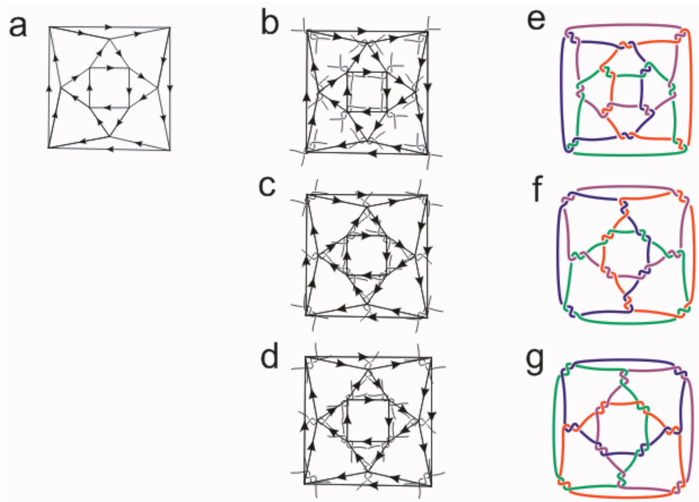

Figure 9. The *O-dual links* of G_o with *O-tangles.* The left is the G_o of cubo-octahedron. In the medial, (b) is G_o which vertices are covered by *3-tangles*; each *3-tangles* of (b) is 90°-rotated and reflected obtain (c) and (d), respectively. In the right, (e), (f) and (g) are the results of tangle composition, (e) and (g) are *L* configurations, and (f) is *D* configurations.

O-dual links which are constructed by G_o and *3-tangles* are shown in Figure 9. Comparing with *E-dual links*, the same manipulations are performed, and different components are needed. Firstly, twelve *3-tangles* substitute into 12 vertices of G_o (Figure 9(b)). Secondly, two new graphs (Figure 9(c) and (d)) are obtained by the manipulation of 90°-rotation and reflection, respectively. Finally, undergoing the tangle composition, three links (Figure 9(e), (f) and (g)) with 4 components are constructed. Different chiral rule with *E-dual links* are found by calculating the *l(K')* values of the three links. In the three links, Figure 9(e) and (g) belong to *L* configurations, and Figure 9(f) belongs to *D* configuration which is the mirror images of Figure 9(g). We have two groups of *O-dual links*: Figure 9(e) and Figure 9(g) have been obtained by reflection with the same chirality, Figure 9(e) and Figure 9(f) have been obtained by 90°-rotation with the opposite chirality. The orientations of 12 tangles show different result with even-dual links. In the 12 tangles, 8 of them have opposite orientation, and the other 4 have the same orientation.

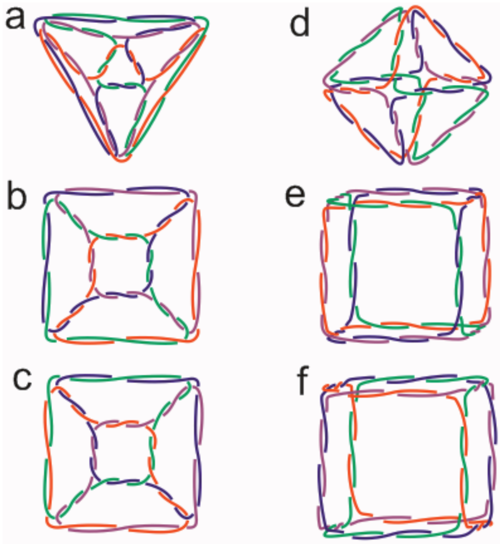

Figure 10. Topological transformation of *O-dual* cubo-octahedron links. The top are octahedral links, and the others are hexahedral links. The left links are in 2-dimensional space, and the right links are in 3-dimensional space

Just like the topological deformation of *E-dual* cubo-octahedron links, *O-dual* cubo-octahedron links can topologically deform into hexahedral and octahedral links with odd crossings. Figure 10 shows the process and the construction of an octahedral link (Figure 10(d)) and two hexahedral links (Figure 10(e) and (f)) which are mirror images of each other. The chirality of Figure 10(d), (e) and (f) are *L, D* and *L* configuration, respectively.

5. Topological comparing *E-dual links* with *O-dual links*

The two types of dual cubo-octahedron links which have been constructed represent the topological property of *E-dual links* and *O-dual links*. The topological differences of *E-dual* *links* and *O-dual links* are represented as follows:

1. The component rule of dual links is different. In *E-dual links*, each component rounds a face of graph, so a pair of dual links has different components. Whereas, in *O-dual links*, each component is a central circuit *CC*, and the number of central circuit *CC* of a 4- plant graph is invariable, so a pair of dual links has the same components. *E-dual links* have different components, which are equal to the number of C_1 and C_2, respectively. *O-dual links* have the same components, which are equal to the number of *CC*.

2. The chiral rule of dual links is different. The linking numbers *l(K')* determines configuration descriptors class (*D* and *L*) of links . In the manipulation of reflection, *E-dual links* have the same chirality, and the chirality of *O-dual links* are opposite; on the contrary, *O-dual links* have the same chirality in the manipulation of 90°- rotation, and the chirality of *E-dual links* are opposite.

3. The oriented rule of tangles in links is different. In the method, the orientation of each component of oriented link is directed. *E-tangles* have opposite orientations in oriented link, however, the orientation of *O-tangles* is multiform. In oriented links with odd crossing, *O-tangles* can be divided into two types. Some of them are of opposite orientations, and the others are the same orientations.

6. Conclusion

In graph theory, any 4-valent plane graph can construct a pair of dual graphs by inversing medial graph, and set up relationship of graphs. Our work associates medial graph with tangle, which brings forward a method of constructing dual links. Given a 4-valent plane graph, a set of dual links can be constructed and divided into two types: *E-dual links* and *O-dual links*. The definition and construction of dual links may provide a new insight and methodology for the research and classification of links. The component rule, chiral rule and oriented rule of *E-* and *O-dual links* are different. The study of these rules not only provide further insight into theoretical characterization of the DNA polyhedral catenane, but also bring forward a project to design dual chiral molecule by using the same material.

In our paper, another innovation of the method is the chiral rule. The chirality of dual links which is obtained by reflection of G_e with *E*-tangles and 90°- rotation of G_o with *O-tangles* are opposite. Contrarily, the chirality of dual links which is obtained by 90°-rotation of G_e with *E-tangles* and by reflection of G_o with *O-tangles* are the same. Using the method of "inverse medial graph", any 4-valent plant graph can generate a pair of dual plant graph *G* and *G**. According to the chirality, *G* and *G** can correspond to four pairs of dual links: left *G* and left *G** links, left *G* and right *G** links, right *G* and right *G** links, right *G* and left *G** links, respectively. The same components undergoing the different manipulation can get two chiral results, which is a very interesting question in knot theory. Moreover, given a special 4-valent plant graph, two topological deformations can deform dual links to polyhedral links. This study puts forward the definition of dual links which is a new definition in knot theory, and can also help to set up relationship of links. If two things are dual, they have the same characters, and they can complement each other during research. The method opens a new door for the research and classification of links.

Acknowledgements

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