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Some Invariants of Polyhedral Links

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Abstract

A mathematical method is proposed to describe the complex structure of polyhedral catenanes with two DNA duplexes. In this method, a special oriented tangle diagram T_k is designed to generate a new family of polyhedral links based on the 1-skeleton of polyhedron. We show that the Homfly polynomials of these links can be given by an explicit formula in terms of the Q^d-polynomial of the associated polyhedral graph. As applications, this formula allows us to calculate the span_v of the Homfly polynomial, the braid index and genus of each link we constructed. Our results reveal that the complexity of these polyhedral links depends completely on these building blocks.

1 Introduction

In past decades, the geometry and topology of DNA molecules [1–13] have been realized by using DNA as building material. A variety of DNA polyhedron including DNA tetrahedron [2, 6], DNA cube [3, 7], DNA octahedron [4, 8], DNA dodecahedron [6, 11], DNA icosahedron [9, 12] and DNA bipyramid [13] have been synthesized based on stiffness and flexibility of DNA. These exotic newcomers in biochemistry have attracted considerable attentions due to their graceful structures and potential properties. How to describe and characterize these intriguing DNA nanoarchitecture has became a new challenge in the topological stereochemistry. This paper will be dedicated to exploiting a small fraction of this field.

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A polyhedral link [14–25] is a set of some interlocked and interlinked looped based on 1-skeleton of polyhedron. In fact, it appears as a mathematical model for DNA polyhedron by treating DNA as double strands. In these synthesized DNA polyhedrons, each edge is composed of double-helical DNA [2–5] or two DNA duplexes [6–10], and each vertex a big 'hole' formed by the interaction of the edges. Based on these facts, there are lots of polyhedral links [15–22] constructed by double-helical DNA as two twisted strands. Meanwhile, some related topological indexes, such as the component number, Homfly polynomial, Jones polynomial, genus and index braid, have been discussed in Ref. [17–22]. However, there is very little research on the polyhedral catenane with two DNA duplexes. To this end, this paper introduces a special oriented tangle diagram T_k to construct the new family of polyhedral links. Three important invariants, including the Homfly polynomial, genus and braid index, are all calculated in this paper.

The Homfly polynomial [26, 27] is a very powerful invariant of oriented links, which plays an important role in identifying topological type and chirality [28]. This invariant is closely related to both the genera and braid indexes of oriented links [29–32], which have been used to classify and order molecular catenanes [33, 34]. However, among the three invariants, none of them can be easily calculated in general, particularly for the links with a large number of crossings. In the present paper, the Homfly polynomials of the polyhedral links our constructed have been given by an explicit formula in terms of Q^d-polynomial, a generalized dichromatic polynomial, of the associated polyhedral graph. This formula not only simplifies greatly the calculation of the Homfly polynomial but also leads to obtaining the spans_v of the Homfly polynomials, the genera and braid indexes, of these links. These invariants provide the important mathematical tools for a comprehensive measure of the complexity of polyhedral links, and also give a possible approach to describing and characterizing the structural properties of polyhedral catenanes with two DNA duplexes.

2 The oriented links derived from the plane graphs

In this section, we will begin with some basic terms and definitions.

In graph theory, a planar graph is a graph that can be embedded in the plane. A planar graph already drawn in the plane without edge intersections is called a plane graph. Note that all convex polyhedrons are 3-connected planar graphs [35], and hence each of them has an embedding on the plane. Such an embedding is called a polyhedral graph. In this paper, we will consider all plane graphs, which include the polyhedral graphs as the special case.

A n-twist tangle diagram, denoted by $[n]$, is two parallel strands with n half-twists for any positive integer n. Two 2-tangle diagrams $[\infty]$ and $[0]$ are shown in Fig. 1. The Denominator of a 2-tangle diagram T, denoted by $D_e(T)$, is obtained by joining with simple arcs each pair of the corresponding top and bottom endpoints of T.

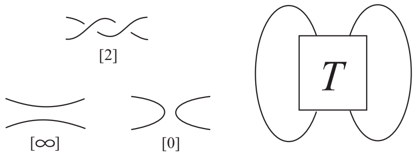

Figure 1. Three 2-tangle diagrams (left) and $D_e(T)$ (right).

A special oriented 2-tangle diagram $T_k = T(2n_1, 2n_1; 2n_2, 2n_2; ...; 2n_k, 2n_k)$ is shown in Fig. 2, where each box $2n_i$ denotes a $2n_i$-twist tangle diagram for $1 \leq i \leq k \geq 1$. Specially, if a box $2n_i$ is replaced by a 2-tangle diagram $[\infty]$ or $[0]$, the resulting link diagram is denoted by the corresponding notation obtained by using 0 or ∞ instead of $2n_i$ in T_k (See Fig. 2).

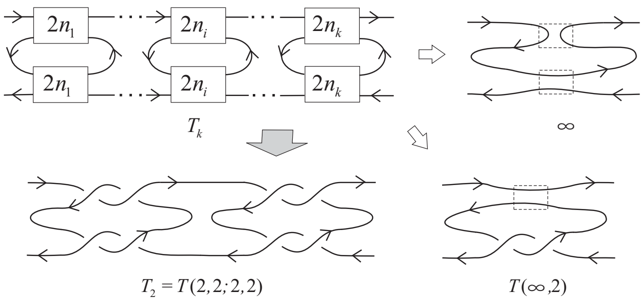

Figure 2. Four oriented tangle diagrams: T_k, T_2, $T(0, \infty)$ and $T(\infty, 2)$.

We now associate any plane graph to an oriented link diagram by using a similar method in Ref. [36–38]. Here these special oriented 2-tangle diagrams are used as the building blocks of the oriented links. The constructive process is described as follows:

For any connected plane graph G, its medial graph $M(G)$ is a 4-regular plane graph by inserting a vertex v_e on every edge e of G, and connecting two new vertices by an edge lying in a face of G if the vertices are on adjacent edges of the face. Then, $M(G)$

is shaded as in a checkerboard so that the unbounded face is unshaded, and the boundary of each shaded face is oriented in clockwise direction. At last for each vertex v_e of $M(G)$, the neighborhood $N(v_e)$ is replaced by a special oriented 2-tangle diagram $T_{k_e} = T(2n_1, 2n_1; 2n_2, 2n_2; ...; 2n_{k_e}, 2n_{k_e})$, as shown in Fig. 3(a). The resulting link diagram is denoted by $D(G)$, and T_{k_e} is associated to e. In Fig. 3(b), a link diagram $D(G)$ is obtained from the tetrahedral graph G by using $T(2, 2)$ as the building block.

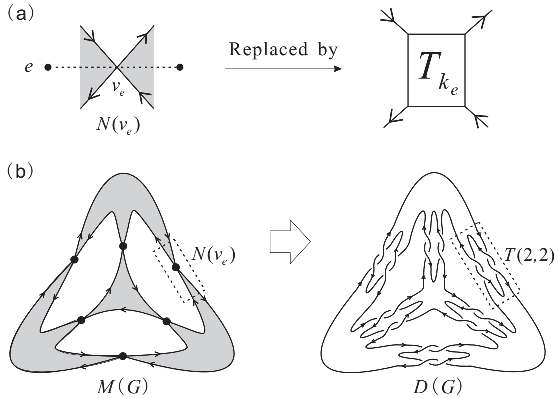

Figure 3. (a)The neighborhood $N(v_e)$ replaced by T_{k_e} (b) The link diagram $D(G)$ derived from the oriented medial graph $M(G)$.

3 Homfly polynomial and Q^d-polynomial

The Homfly polynomial is the invariant of oriented links, which was discovered independently by several authors [26, 27]. This invariant generalizes the Alexander-Conway polynomial and the Jones polynomial. Here we use its definition provided in Ref. [28].

Definition 3.1. *The Homfly polynomial $H(L; v, z) \in \mathbb{Z}[v, z]$ for an oriented link L is defined by the following relationships:*

(1) $H(L; v, z)$ is invariant under ambient isotopy of L.

(2) If L is a trivial knot, then $H(L; v, z) = 1$.

(3) Suppose that three link diagrams L_+, L_- and L_0 are different only on a local region, as shown in Fig. 4. Then $v^{-1}H(L_+; v, z) - vH(L_-; v, z) = zH(L_0; x, y, z)$.

The Homfly polynomial has the following properties:

(1) If L is the connected sum of L_1 and L_2, denoted by $L_1 \sharp L_2$, then

$$H(L) = H(L_1)H(L_2).$$

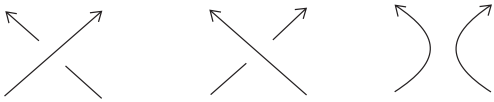

Figure 4. Three link diagrams: L_+, L_-, L_0.

(2) If L is the disjoint union of L_1 and L_2, denoted by $L_1 \cup L_2$, then

$$H(L) = (\frac{v^{-1} - v}{z})H(L_1)H(L_2).$$

A double weighted graph is a graph G together with two functions α and β, where α (β, respectively) maps from $E(G)$ into some commutative ring with unity R_α(R_β, respectively). Let e be any edge of G, and let $\alpha(e)$ and $\beta(e)$ be two weights of e respectively. Hereafter we use $G - e$ and G/e to denote the graphs obtained from graph G by deleting and contracting e respectively.

Definition 3.2. *The Q^d-polynomial $Q^d(G) = Q^d(G; t, z)$ for a double weighted graph G is defined by the following recursive rules:*
1. Let E_n be n isolated vertices. Then $Q^d(E_n) = t^n$.
2. Suppose that $\alpha(e) = \alpha_e$ and $\beta(e) = \beta_e$. Then
(a) when e is a loop,

$$Q^d(G) = (\alpha_e z + \beta_e)Q^d(G - e);$$

(b) when e is a bridge,

$$Q^d(G) = (\alpha_e + \beta_e t)Q^d(G/e);$$

(c)otherwise,

$$Q^d(G) = \alpha_e Q^d(G/e) + \beta_e Q^d(G - e).$$

In fact, Q^d-polynomial is a naturally generalization of the dichromatic polynomial $Q(G; t, z)$ of a weighted graph G [37]. We can recover this dichromatic polynomial from Q^d-polynomial by setting $\alpha_e = 1$. Hence Q^d-polynomial can be defined as follows:

$$Q^d(G) = \sum_{F \subseteq E(G)} \left(\prod_{e \in F} \alpha_e \right) \left(\prod_{e \in E(G) - F} \beta_e \right) t^{k<F>} z^{n<F>}, \qquad (1)$$

where $k < F >$ and $n < F >$ are the number of connected components and the nullity of the spanning subgraph $< F >$, induced by F, of G, respectively.

4 The Homfly polynomials of links

In this section, we establish the relationship between the Homfly polynomials of the family of links constructed in section 2 and the Q^d-polynomial of the associated plane graph. Let G be any connected plane graph, and $D(G)$ be the link diagram derived from G using the method in section 2. Let $D_{e:T}(G)$ be the same as $D(G)$ only except the 2-tangle diagram associated to e is T. Hereafter, we denote by $V(G)$, $E(G)$ and $F(G)$ the vertex, edge, face set of G respectively.

Lemma 4.1. *Let $T = T(2n, 2n)$ be a special oriented 2-tangle diagram. Then*

$$H(D_e(T); v, z) = v^{4n} \cdot \frac{v^{-1} - v}{z} + vz \cdot \frac{v^{4n} - 1}{v^2 - 1}. \tag{2}$$

Proof: We proceed by induction on the crossing number n, and suppose that $n = 1$ firstly. Repeatedly applying the definition (3) of Homfly polynomial to the crossings of T, we have

$$\begin{aligned} H(D_e(T)) =& v^2 H(D_e(T(\infty, 2))) + vz \\ =& v^2[v^2 H(D_e(T(\infty, \infty))) + vz] + vz \\ =& v^4 \frac{v^{-1} - v}{z} + v^3 z + vz \ . \end{aligned}$$

Now we suppose that $n \geq 2$. Using the definition (3) of Homfly polynomial, then

$$\begin{aligned} H(D_e(T)) =& v^2 H(D_e(T(2n-2, 2n))) + vz \\ =& v^2[v^2 H(D_e(T(2n-2, 2n-2))) + vz] + vz \\ =& v^4 H(D_e(T(2n-2, 2n-2))) + v^3 z + vz \ . \end{aligned}$$

By our induction hypothesis, we have

$$H(D_e(T(2n-2, 2n-2))) = v^{4(n-1)} \cdot \frac{v^{-1} - v}{z} + vz \cdot \frac{v^{4(n-1)} - 1}{v^2 - 1}.$$

Hence we can obtain the following equation:

$$\begin{aligned} H(D_e(T)) =& v^4[v^{4(n-1)} \cdot \frac{v^{-1} - v}{z} + vz \cdot \frac{v^{4(n-1)} - 1}{v^2 - 1}] + v^3 z + vz \\ =& [v^{4n} \cdot \frac{v^{-1} - v}{z} + vz \cdot \frac{v^{4n} - v^4}{v^2 - 1}] + vz \cdot \frac{v^4 - 1}{v^2 - 1}. \end{aligned}$$

□

Lemma 4.2.

$$H(D_{e:T(2n,\infty)}(G)) = H(D_{e:T(\infty,2n)}(G)) = (v^{2n} \cdot \frac{v^{-1}-v}{z} + vz \cdot \frac{v^{2n}-1}{v^2-1})H(D_{e:T(0,\infty)}(G)).$$

Proof: Since $T(\infty, 2n)$ and $T(2n, \infty)$ represent the same tangle type, we have

$$H(D_{e:T(2n,\infty)}(G)) = H(D_{e:T(\infty,2n)}(G)).$$

Hence we only need to show that lemma 4.2 holds for the link diagram $D_{e:T(2n,\infty)}(G)$. We proceed by induction on the crossing number n, and suppose that $n = 1$ firstly. Applying the definition (3) of Homfly polynomial to a crossing of T, we have

$$\begin{aligned} H(D_{e:T(2,\infty)}(G)) =& v^2 H(D_{e:T(\infty,\infty)}(G)) + vzH(D_{e:T(0,\infty)}(G)) \\ =& v^2(\frac{v^{-1}-v}{z})H(D_{e:T(0,\infty)}(G)) + vzH(D_{e:T(0,\infty)}(G)) \\ =& (v^2 \cdot \frac{v^{-1}-v}{z} + vz)H(D_{e:T(0,\infty)}(G)). \end{aligned}$$

Now we suppose that $n \geq 2$. Using the definition (3) of Homfly polynomial, then

$$H(D_{e:T(2n,\infty)}(G)) = v^2 H(D_{e:T(2n-2,\infty)}(G)) + vzH(D_{e:T(0,\infty)}(G)).$$

Apply our induction hypothesis to the link diagram $D_{e:T(2n-2,\infty)}(G)$, we have

$$\begin{aligned} H(D_{e:T(2n,\infty)}(G)) =& v^2[v^{2(n-1)}(\frac{v^{-1}-v}{z}) \\ &+ vz \cdot \frac{v^{2(n-1)}-1}{v^2-1}]H(D_{e:T(0,\infty)}(G)) + vzH(D_{e:T(0,\infty)}(G)) \\ =& [v^{2n}\frac{v^{-1}-v}{z} + vz \cdot \frac{v^{2n}-v^2}{v^2-1} + vz \cdot \frac{v^2-1}{v^2-1}]H(D_{e:T(0,\infty)}(G)). \end{aligned}$$

□

Similarly, we have

Lemma 4.3.

$$H(D_{e:T(2n,0)}(G)) = H(D_{e:T(0,2n)}(G)) = v^{2n}H(D_{e:T(0,\infty)}(G)) + vz\frac{v^{2n}-1}{v^2-1}H(D(G-e)).$$

For any positive integer n, we define the following notations:

$$\begin{aligned} a_n &= v^{4n} \cdot \frac{v^{-1}-v}{z} + 2vz \cdot v^{2n} \cdot \frac{v^{2n}-1}{v^2-1}, \\ b_n &= (vz \cdot \frac{v^{2n}-1}{v^2-1})^2 \quad \text{and} \\ c_n &= v^{4n} \cdot \frac{v^{-1}-v}{z} + vz \cdot \frac{v^{4n}-1}{v^2-1}. \end{aligned}$$

Lemma 4.4. *Let $T_{k_e} = T(2n_1, 2n_1; 2n_2, 2n_2; ...; 2n_{k_e}, 2n_{k_e})$ be a special oriented 2-tangle diagram associated to an edge e of G. If e is a loop, then*

$$H(D(G); v, z) = [\prod_{i=1}^{k_e} a_{n_i} \frac{v^{-1} - v}{z} + \sum_{j=1}^{n_{k_e}} (\prod_{i=1}^{j-1} a_{n_i} b_{n_j} \prod_{i=j+1}^{k_e} c_{n_i})] H(G - e). \tag{3}$$

Otherwise,

$$H(D(G); v, z) = \prod_{i=1}^{k_e} a_{n_i} H(G/e) + [\sum_{j=1}^{n_{k_e}} (\prod_{i=1}^{j-1} a_{n_i} b_{n_j} \prod_{i=j+1}^{k_e} c_{n_i})] H(G - e). \tag{4}$$

Proof: We proceed by induction on k_e for $1 \leq i \leq k_e$, and have two cases depending on whether e is a loop or not.

(i)We first assume that $k_e = 1$.

Repeatedly applying the definition (3) of Homfly polynomial to the crossings of T_{k_e}, we have

$$\begin{aligned} H(D(G)) =& v^2 H(D_{e:T(2n_1-2,2n_1)}(G)) + vzH(D_{e:T(0,2n_1)}(G)) \\ =& v^2[v^2 H(D_{e:T(2n_1-4,2n_1)}(G)) + vzH(D_{e:T(0,2n_1)}(G))] + vzH(D_{e:T(0,2n_1)}(G)) \\ =& v^4 H(D_{e:T(2n_1-4,2n_1)}(G)) + (v^3 z + vz)H(D_{e:T(0,2n_1)}(G)). \end{aligned}$$

By induction on n_1, we can easily obtain the following formula:

$$H(D(G)) = v^{2n_1} H(D_{e:T(\infty,2n_1)}(G)) + vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1} H(D_{e:T(0,2n_1)}(G)).$$

Using the lemmas 4.2 and 4.3, we have

$$\begin{aligned} H(D(G)) =& v^{2n_1}(v^{2n_1} \cdot \frac{v^{-1} - v}{z} + vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1}) H(D_{e:T(0,\infty)}(G)) \\ &+ vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1}[v^{2n_1} H(D_{e:T(0,\infty)}(G)) + vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1} H(D(G - e))] \\ =& (v^{4n_1} \cdot \frac{v^{-1} - v}{z} + 2vz \cdot v^{2n_1} \cdot \frac{v^{2n_1} - 1}{v^2 - 1}) H(D_{e:T(0,\infty)}(G)) \\ &+ (vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1})^2 H(D(G - e)). \end{aligned}$$

If e is a loop, then

$$H(D_{e:T(0,\infty)}(G)) = (\frac{v^{-1} - v}{z}) H(D(G - e)).$$

And hence we have

$$\begin{aligned} H(D(G)) =& [(v^{4n_1} \cdot \frac{v^{-1} - v}{z} + 2vz \cdot v^{2n_1} \cdot \frac{v^{2n_1} - 1}{v^2 - 1})(\frac{v^{-1} - v}{z}) \\ &+ (vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1})^2] H(D(G - e)). \end{aligned}$$

If e is not loop, then

$$H(D_{e:T(0,\infty)}(G)) = H(D(G/e)).$$

And hence we have

$$\begin{aligned} H(D(G)) =& (v^{4n_1} \cdot \frac{v^{-1} - v}{z} + 2vz \cdot v^{2n_1} \cdot \frac{v^{2n_1} - 1}{v^2 - 1}) H(D(G/e)) \\ &+ (vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1})^2 H(D(G - e)). \end{aligned}$$

(ii)We now assume that $k_e \geq 2$. By repeatedly applying the definition (3) of Homfly polynomial, we have

$$\begin{aligned} H(D(G)) =& v^2 H(D_{e:T(2n_1-2,2n_1;2n_2,2n_2;...)}(G)) + vzH(D_{e:T(0,2n_1;2n_2,2n_2;..)}(G)) \\ =& v^2[v^2 H(D_{e:T(2n_1-4,2n_1;2n_2,2n_2;...)}(G)) + vzH(D_{e:T(0,2n_1;2n_2,2n_2;..)}(G))] \\ &+ vzH(D_{e:T(0,2n_1;2n_2,2n_2;..)}(G)) \\ =& v^4 H(D_{e:T(2n_1-4,2n_1;2n_2,2n_2;..)}(G)) + (v^3 z + vz) H(D_{e:T(0,2n_1;2n_2,2n_2;..)}(G)) \\ \cdots =& v^{2n_1} H(D_{e:T(\infty,2n_1;2n_2,2n_2;..)}(G)) + vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1} H(D_{e:T(0,2n_1;2n_2,2n_2;...)}(G)). \end{aligned}$$

Using the lemmas 4.2 and 4.3, we have

$$\begin{aligned} H(D(G)) =& v^{2n_1}(v^{2n_1} \cdot \frac{v^{-1} - v}{z} + vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1}) H(D_{e:T(0,\infty;2n_2,2n_2;...)}(G)) \\ &+ vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1}[v^{2n_1} H(D_{e:T(0,\infty;2n_2,2n_2;...)}(G)) + vz \cdot \frac{v^{2n_1} - 1}{v^2 - 1} H(D_{e:T(0,0;2n_2,2n_2;...)}(G))]. \end{aligned}$$

Hence we have

$$H(D(G)) = a_{n_1} H(D_{e:T(0,\infty;2n_2,2n_2;...;2n_{k_e},2n_{k_e})}(G)) + b_{n_1} H(D_{e:T(0,0;2n_2,2n_2;..;2n_{k_e},2n_{k_e})}(G)).$$

Also, $D_{e:T(0,0;2n_2,2n_2;..;2n_{k_e},2n_{k_e})}(G) = D_{e:T(0,0)}(G) \sharp D_e(T(2n_2, 2n_2)) \sharp ... \sharp D_e(T(2n_{k_e}, 2n_{k_e}))$.

By using the property (1) of Homfly polynomial and lemma 4.1, we can obtain the following equation:

$$\begin{aligned} H(D_{e:T(0,0;2n_2,2n_2;..;2n_{k_e},2n_{k_e})}(G)) =& H(D_{e:T(0,0)}(G)) \cdot \prod_{i=2}^{k_e} H(D_e(T(2n_i, 2n_i))) \\ =& H(D(G - e)) \prod_{i=2}^{k_e} c_{n_i}. \end{aligned}$$

Hence we have

$$\begin{aligned} H(D(G)) =& a_{n_1} H(D_{e:T(0,\infty;2n_2,2n_2;..;2n_{k_e},2n_{k_e})}(G)) + b_{n_1} \prod_{i=2}^{k_e} c_{n_i} H(D(G - e)) \\ =& a_{n_1} H(D_{e:T(2n_2,2n_2;..;2n_{k_e},2n_{k_e})}(G)) + b_{n_1} \prod_{i=2}^{k_e} c_{n_i} H(D(G - e)). \end{aligned}$$

If e is a loop, by our induction hypothesis, then

$$H(D_{e:T(2n_2,2n_2;..;2n_{k_e},2n_{k_e})}(G)) = [\prod_{i=2}^{k_e} a_{n_i}\cdot(\frac{v^{-1}-v}{z}) + \sum_{j=2}^{k_e}\prod_{i=2}^{j-1} a_{n_i}\cdot b_{n_j}\cdot \prod_{i=j+1}^{k_e} c_{n_i}]H(D(G-e)).$$

Hence we have

$$\begin{aligned} H(D(G)) =& a_{n_1}[\prod_{i=2}^{k_e} a_{n_i}\cdot(\frac{v^{-1}-v}{z}) \\ &+\sum_{j=2}^{k_e}\prod_{i=2}^{j-1} a_{n_i}\cdot b_{n_j}\cdot \prod_{i=j+1}^{k_e} c_{n_i}]H(D(G-e)) + b_{n_1}\prod_{i=2}^{k_e} c_{n_i}\cdot H(D(G-e)) \\ =&[\prod_{i=1}^{k_e} a_{n_i}\cdot(\frac{v^{-1}-v}{z}) + a_{n_1}\sum_{j=2}^{k_e}\prod_{i=2}^{j-1} a_{n_i}\cdot b_{n_j}\cdot \prod_{i=j+1}^{k_e} c_{n_i} + b_{n_1}\prod_{i=2}^{k_e} c_{n_i}]H(D(G-e)). \end{aligned}$$

Clearly, the formula (3) can be obtained directly from the above equation.

If e is not a loop, by our induction hypothesis, then

$$H(D_{e:(2n_2,2n_2;..;2n_{k_e},2n_{k_e})}(G)) = \prod_{i=2}^{k_e} a_{n_i} H(D(G/e)) + \sum_{j=2}^{k_e}\prod_{i=2}^{j-1} a_{n_i}\cdot b_{n_j}\cdot \prod_{i=j+1}^{k_e} c_{n_i} H(D(G-e)).$$

Hence, we have

$$\begin{aligned} H(D(G)) =& a_{n_1}[\prod_{i=2}^{k_e} a_{n_i} H(D(G/e)) \\ &+\sum_{j=2}^{k_e}\prod_{i=2}^{j-1} a_{n_i}\cdot b_{n_j}\cdot \prod_{i=j+1}^{k_e} c_{n_i} H(D(G-e))] + b_{n_1}\prod_{i=2}^{k_e} c_{n_i}\cdot H(D(G-e)) \\ =&\prod_{i=1}^{k_e} a_{n_i} H(D(G/e)) + [a_{n_1}\sum_{j=2}^{k_e}\prod_{i=2}^{j-1} a_{n_i}\cdot b_{n_j}\cdot \prod_{i=j+1}^{k_e} c_{n_i} + b_{n_1}\prod_{i=2}^{k_e} c_{n_i}]H(D(G-e)). \end{aligned}$$

Clearly, the formula (4) can be obtained directly from the above equation. □

Let e be any edge of G, and T_{k_e} be the 2-tangle associated to e. We define

$$\alpha_e = \prod_{i=1}^{k_e} a_{n_i} \quad and \quad \beta_e = \sum_{j=1}^{n_{k_e}}(\prod_{i=1}^{j-1} a_{n_i} b_{n_j} \prod_{i=j+1}^{k_e} c_{n_i}).$$

Hence we obtain two functions α and β from $E(G)$ to $\mathbb{Z}(v,z)$ by defining $\alpha(e)=\alpha_e$ and $\beta(e)=\beta_e$ respectively. Then G is a double weighted graph with α and β. Therefore, the following Theorem can be obtained by comparing Theorem 4.4 with the definition of Q^d-polynomial.

Theorem 4.5. *Let G be a double weighted graph together with two functions α and β as defined above. Then*

$$H(D(G), v, z) = \frac{z}{v^{-1} - v} Q^d(G; \frac{v^{-1} - v}{z}, \frac{v^{-1} - v}{z}).$$

By using the definition of Q^d-polynomial, we can easily obtain

Theorem 4.6. $H(D(G)) = \sum_{F \subseteq E(G)} (\prod_{e \in F} \alpha_e)(\prod_{e \in E(G)-F} \beta_e)(\frac{v^{-1}-v}{z})^{k<F>+n<F>-1}$.

5 Span, braid index and genus

In this section, the spans$_v$ of Homfly polynomials, the braid indexes and genera of the oriented links we constructed are all calculated. Let maxdeg$_v f$ and mindeg$_v f$ denote the maximum degree and minimum degree in variable v of multi-variable polynomial f taken over terms with non-zero coefficients, respectively. Define span$_v f$= maxdeg$_v f$−mindeg$_v f$, and we denote by $v(G)$, $e(G)$, and $f(G)$ the number of vertices, edges, and faces of the plane graph G respectively.

5.1 The span of Homfly polynomial

Lemma 5.1. *Let a_n, b_n and c_n be three polynomials as defined in the section 4. Then*

$$\text{maxdeg}_v\ a_n = 4n + 1 \quad \text{and} \quad \text{mindeg}_v\ a_n = 2n + 1; \tag{5}$$

$$\text{maxdeg}_v\ b_n = 4n - 2 \quad \text{and} \quad \text{mindeg}_v\ b_n = 2; \tag{6}$$

$$\text{maxdeg}_v\ c_n = 4n + 1 \quad \text{and} \quad \text{mindeg}_v\ c_n = 1. \tag{7}$$

Theorem 5.2. *Let G be any connected plane graph, and $D(G)$ be the link diagram obtained by using the method in the section 2. For each edge e of G, it is associated to a special oriented 2-tangle diagram T_{k_e}. Then*

$$\text{mindeg}_v\ H(D(G)) = \sum_{e \in E(G)} \sum_{i=1}^{k_e} (4n_i + 1) + f(G) - 1; \tag{8}$$

$$\text{maxdeg}_v\ H(D(G)) = \sum_{e \in E(G)} (k_e + 1) - v(G) + 1. \tag{9}$$

Proof: By using theorem 4.6, we have

$$H(D(G)) = \sum_{F \subseteq E(G)} (\prod_{e \in F} \alpha_e)(\prod_{e \in E(G)-F} \beta_e)(\frac{v^{-1} - v}{z})^{k<F>+n<F>-1},$$

where $\alpha_e = \prod_{i=1}^{k_e} a_{n_i}$ and $\beta_e = \sum_{j=1}^{n_{k_e}} (\prod_{i=1}^{j-1} a_{n_i} b_{n_j} \prod_{i=j+1}^{k_e} c_{n_i})$.

By the formula (5) of lemma 5.1, we have

$$\text{maxdeg}_v\ \alpha_e = \sum_{i=1}^{k_e} \text{maxdeg}_v\ a_{n_i} = \sum_{i=1}^{k_e}(4n_i+1)$$

$$\text{and}\ \ \text{mindeg}_v\ \alpha_e = \sum_{i=1}^{k_e} \text{mindeg}_v\ a_{n_i} = \sum_{i=1}^{k_e}(2n_i+1).$$

And using lemma 5.1 again, we have

$$\text{maxdeg}_v\ \beta_e = \text{maxdeg}_v\ \{b_{n_1}\prod_{i=2}^{k_e} c_{n_i}\} = 4n_1 - 2 + \sum_{i=2}^{k_e}(4n_i+1) = \sum_{i=1}^{k_e}(4n_i+1) - 3$$

$$\text{and}\ \ \text{mindeg}_v\ \beta_e = \text{mindeg}_v\ \{b_{n_1}\prod_{i=2}^{k_e} c_{n_i}\} = 2 + \sum_{i=2}^{k_e} 1 = k_e + 1.$$

Let F be any subset of $E(G)$, and $|F|$ be the number of edges of F. If $|F| < e(G)$, then we have

$$\begin{aligned}
&\text{maxdeg}_v\ \{(\prod_{e\in F}\alpha_e)(\prod_{e\in E(G)-F}\beta_e)(\frac{v^{-1}-v}{z})^{k<F>+n<F>-1}\} \\
&= \sum_{e\in F}\text{maxdeg}_v\ \alpha_e + \sum_{e\in E(G)-F}\text{maxdeg}_v\ \beta_e + k<F> + n<F> - 1 \\
&= \sum_{e\in F}\sum_{i=1}^{k_e}(4n_i+1) + \sum_{e\in E(G)-F}[\sum_{i=1}^{k_e}(4n_i+1) - 3] + k<F> + n<F> - 1 \\
&= \sum_{e\in E(G)}\sum_{i=1}^{k_e}(4n_i+1) - 3(e(G)-|F|) + k<F> + n<F> - 1.
\end{aligned}$$

Also, $k<F> \leq e(G)-|F|+1$ and $n<F> = |F| - v<F> + k<F>$, then

$$\begin{aligned}
&\text{maxdeg}_v\ \{(\prod_{e\in F}\alpha_e)(\prod_{e\in E(G)-F}\beta_e)(\frac{v^{-1}-v}{z})^{k<F>+n<F>-1}\} \\
&\leq \sum_{e\in E(G)}\sum_{i=1}^{k_e}(4n_i+1) - 3(e(G)-|F|) + 2(e(G)-|F|+1) + |F| - v<F> - 1 \\
&\leq \sum_{e\in E(G)}\sum_{i=1}^{k_e}(4n_i+1) - (e(G)-|F|) + |F| - v<F> + 1.
\end{aligned}$$

By $v<F>=v(G)=e(G)-f(G)+2$ and $e(G)-|F|>0$, we have

$$\begin{aligned}
&\text{maxdeg}_v\ \{(\prod_{e\in F}\alpha_e)(\prod_{e\in E(G)-F}\beta_e)(\frac{v^{-1}-v}{z})^{k<F>+n<F>-1}\}\\
&=\sum_{e\in E(G)}\sum_{i=1}^{k_e}(4n_i+1)-(e(G)-|F|)+|F|-(e(G)-f(G)+2)+1\\
&\le\sum_{e\in E(G)}\sum_{i=1}^{k_e}(4n_i+1)-2(e(G)-|F|)+f(G)-1\\
&<\sum_{e\in E(G)}\sum_{i=1}^{k_e}(4n_i+1)+f(G)-1.
\end{aligned}$$

Hence we have

$$\text{maxdeg}_v\ H(D(G))=\text{maxdeg}_v\ \{(\prod_{e\in E(G)}\alpha_e)(\frac{v^{-1}-v}{z})^{f(G)-1}\}=\sum_{e\in E(G)}\sum_{i=1}^{k_e}(4n_i+1)+f(G)-1.$$

On the other hand, if $|F|>0$, then we can obtain

$$\begin{aligned}
&\text{mindeg}_v\ \{(\prod_{e\in F}\alpha_e)(\prod_{e\in E(G)-F}\beta_e)(\frac{v^{-1}-v}{z})^{k<F>+n<F>-1}\}\\
&=\sum_{e\in F}\text{mindeg}_v\ \alpha_e+\sum_{e\in E(G)-F}\text{mindeg}_v\ \beta_e-k<F>-n<F>+1\\
&=\sum_{e\in F}\sum_{i=1}^{k_e}(2n_i+1)+\sum_{e\in E(G)-F}(k_e+1)-k<F>-n<F>+1.
\end{aligned}$$

Since $\sum_{i=1}^{k_e}n_i\ge 1$, $k<F>\le v<F>-1$ and $n<F>=|F|-v<F>+k<F>$, we have

$$\begin{aligned}
&\text{mindeg}_v\ \{(\prod_{e\in F}\alpha_e)(\prod_{e\in E(G)-F}\beta_e)(\frac{v^{-1}-v}{z})^{k<F>+n<F>-1}\}\\
&\ge\sum_{e\in F}(k_e+2)+\sum_{e\in E(G)-F}(k_e+1)-2(v<F>-1)-|F|+v<F>+1\\
&=\sum_{e\in E(G)}(k_e+1)-v<F>+3=\sum_{e\in E(G)}(k_e+1)-v<G>+3\\
&>\sum_{e\in E(G)}(k_e+1)-v(G)+1.
\end{aligned}$$

Hence we have

$$\text{mindeg}_v\ H(D(G))=\text{mindeg}_v\ \{\prod_{e\in E(G)}\beta_e(\frac{v^{-1}-v}{z})^{v(G)-1}\}=\sum_{e\in E(G)}(k_e+1)-v(G)+1.$$

□

Corollary 5.3. $\text{span}_v\ H(D(G))=\sum_{e\in E(G)}\sum_{i=1}^{k_e}4n_i.$

5.2 The braid indexes of links

The braid index $b(L)$ of a link L is the minimal number n such that L can be represented as a closed n-string braid. It is well known that Franks and Williams [29] and Morton [30] gave independently a lower bound for the braid index $b(L)$ of a link L in terms of the span_v of the Homfly polynomial as follows:

$$b(L) \geq \frac{1}{2}\mathrm{span}_v H(L) + 1. \tag{10}$$

This inequality (10) is known as MFW inequality, which have been studied extensively for many classes of knots and links [39] such as torus links [29], alternating links [40] and so on. On the other hand, in 1993, Ohyama [31] gave a upper bound for the braid index of a link L in terms of the crossing number of L as follows:

$$b(L) \leq \frac{1}{2}c(L) + 1. \tag{11}$$

where $c(L)$ be the minimal crossing number of L.

In the following theorem, we show $D(G)$ is sharp for MFW inequality, also for the inequality (11).

Theorem 5.4. *Let G be any connected plane graph, and $D(G)$ be the link diagram obtained by using the method in the section 2. For each edge e of G, it is associated to a special oriented 2-tangle diagram T_{k_e}. Then*

$$b(D(G)) = \sum_{e\in E(G)} \sum_{i=1}^{k_e} 2n_i + 1.$$

Proof: Let $c(T_{k_e})$ be the crossing number of T_{k_e}, and $c(D(G))$ be the the crossing number of $D(G)$.

Clearly, T_{k_e} is an alternating tangle diagram for each edge e. Hence $D(G)$ is an alternating link diagram by the constructive process, and also we have

$$c(D(G)) = \sum_{e\in E(G)} c(T_{k_e}) = \sum_{e\in E(G)} \sum_{i=1}^{k_e} 4n_i.$$

Hence $\mathrm{span}_v H(D(G)) = c(D(G)) = \sum_{e\in E(G)} \sum_{i=1}^{k_e} 4n_i$.

By the inequalities (10) and (11), we have

$$b(D(G)) = \frac{1}{2}\mathrm{span}_v D(G) + 1 = \sum_{e\in E(G)} \sum_{i=1}^{k_e} 2n_i + 1.$$

□

5.3 The genera of links

The genus $g(L)$ of an oriented link L is the minimum genus of any connected orientable surface having L as its boundary. The following theorem can be obtained directly by the Corollary 4.1 and the Remark in Ref. [32].

Lemma 5.5. *Let L be an alternating link having a positive diagram, then*

$$g(L) = \frac{1}{2}(\mathrm{mindeg}_v\ H(L) - \mu(L) + 1).$$

Note that each link diagram $D(G)$ we constructed is a positive link diagram, and hence we have the following theorem.

Theorem 5.6. *Let G be any connected plane graph, and $D(G)$ be the link diagram obtained by using the method in the section 2. Let $L_{D(G)}$ be the link corresponding to $D(G)$. Then $g(L_{D(G)}) = 0$.*

Proof: Let e be any edge of G, and T_{k_e} be a special oriented 2-tangle diagram associated to e. Let μ_e and μ_f be the component number associated to the edge e and the face f of G, respectively. According to the tangle diagram T_{k_e}, we have $\mu_e = k_e$ *and* $\mu_f = 1$. Then

$$\mu_{D(G)} = \sum_{e \in E(G)} k_e + f(G).$$

Since $D(G)$ is a positive link diagram, $L_{D(G)}$ is a positive link. By using Theorem 5.5, hence we have

$$\begin{aligned} g(L_{D(G)}) =& \frac{1}{2}[\mathrm{mindeg}_v\ H(D(G)) - \mu(D(G)) + 1] \\ =& \frac{1}{2}\left[\sum_{e \in E(G)} (k_e + 1) - v(G) + 1 - \sum_{e \in E(G)} k_e - f(G) + 1\right] \\ =& \frac{1}{2}[e(G) - v(G) - f(G) + 2] = 0\ . \end{aligned}$$

□

6 Conclusion

In this paper, the new family of polyhedral links is constructed by using a special oriented 2-tangle diagram T_k. These links provide the mathematical models for recently synthetic polyhedral catenanes with double-helical DNA. In T_k, any two twisted components are oriented antiparallel to each other, which coincides with the natural direction of

DNA strands. Notably, the T_k contains some loops, not merely two twisted arcs. Hence our constructed links have the more complex tangled structures than the previous links constructed by using n-twist tangle diagrams [17–23]. Furthermore, we established the relationship between the Homfly polynomial of these links and the Q^d-polynomial, a generalized Dichromatic polynomial, of the origin graph. Using this relationship, we obtained the spans$_v$ of the Homfly polynomials, the braid indexes and genera of these links. Our results show that the former two indexes are directly determined by the corresponding building blocks. And the third index shows that these links all can be embedded on the spherical surface. This work provides a profound understanding and theoretical description of the recently synthesized DNA polyhedrons.

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