### ORIGINAL PAPER

# The HOMFLY polynomials of odd polyhedral links

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**Abstract** This paper extends the methodology for the construction of odd polyhedral links. Building blocks are odd chain tangles, each of which consists of finitely many 2n + 1-twist tangles for any nonnegative integer n. For any polyhedral graph G, replacing each edge with an odd chain tangle results in an infinite collection of odd polyhedral links. The relationship between the HOMFLY polynomials of these odd links and the  $Q^d$ -polynomial of G is established. It leads to the determination of the span of the HOMFLY polynomial, the bound on the braid index and the genus of each odd link. Our results show that these indices depend not only on the building blocks but also on the graph G.

**Keywords** Polyhedral links · HOMFLY polynomial · Dichromatic polynomial · Braid index · Genus

#### 1 Introduction

Knots and links are significant structural features in DNA [1–6]. They, together with slipknots, are also gradually recognized in some proteins [7–9] and play an important role in the chemical and physical properties of both natural and synthetic compounds [10–14]. To date, a wide variety of molecules with topological characteristics [15–27], such as trefoil knots [15–18], composite knots [17], Hopf links [19,20] and Borromean rings [21,22], have been synthesized in the laboratory. Among these interesting

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topological molecules, Polyhedral catenanes [23–27] assembled based on the remarkable programmability and flexibility of DNA, are the interlocked and interlinked architectures and have received a great deal of attention. In recent reports, the building blocks consisting of DNA star-shaped motifs have led to the highly complex topology of these 3D nanostructure [28–32]. In these newly assembled objects, each edge is composed of two DNA duplexes instead of the originally double-helical DNA, and each face forms a big hole by the intersection of the edges. These facts encourage us to employ some new methods for the construction of polyhedral links with two DNA duplexes, thereby enriching and broadening the original assembly strategy.

Knot theory [33], the study of simple closed curves in Euclidean 3-space ( $R^3$ ), has been proven to be effective in describing knotted and linked molecules [34,35]. In particular, some knot invariants such as linking number, component number, Jones polynomial, the HOMFLY polynomial, genus and braid index have been used to characterize polyhedral links [36–47]. The HOMFLY polynomial [48,49] is a powerful invariant of oriented links, which generalizes the Alexander–Conway polynomial and the Jones polynomial. Furthermore, it is closely related to the genera and braid indices of oriented links [50–53], which play significant roles in classifying and ordering molecular catenanes [54,55]. However, the calculation of the HOMFLY polynomial is believed to be NP-hard [56,57], and the other two invariants are also difficult to obtain in general. Therefore, we need an effective method to simplify their calculation.

Odd polyhedral links are defined initially by using 2n + 1-twist tangle [2n + 1] in Refs. [40,41] (Fig. 1a). Their HOMFLY polynomials are difficult to compute, due to each edge (i.e. a 2n + 1-twist tangle) having an unpredictable orientation. In the present paper, odd chain tangles are used as building blocks, each of which consists of finitely many  $2n_i + 1$ -twist tangles (Fig. 2a). These odd tangles not only increase the complexity of the previous ones but also have a determined orientation. Therefore for any polyhedral graph G, replacing each edge e with an odd chain tangle  $T_{k_e}$  will result in infinitely many oriented odd polyhedral links. We show that the HOMFLY polynomials of these odd links can be obtained by using the  $Q^d$ -polynomial of the polyhedral graph G. Furthermore, the span $_v$  of the HOMFLY polynomial, the upper and lower bounds on the braid index and the genus of each odd link are all determined in this paper. Our results are expected to provide a theoretical rule on the design and synthesis of the complex structure of polyhedral catenanes.

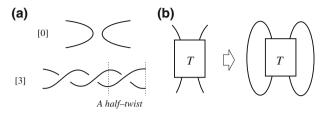
# 2 The construction of odd polyhedral links

In this section, we begin by introducing some notation and basic definitions.

In graph theory, *a planar graph G* is a graph that can be drawn in the plane with no edge crossings. Such a drawing is called *a plane graph* of *G*. In particular, all convex polyhedrons are 3-connected planar graphs [58], and a plane graph of a polyhedron is also called *a polyhedral graph*. Hence in this paper, the graphs we considered are all plane graphs, including polyhedral graphs as special cases.

A *n*-twist tangle, denoted by [n], consists of two parallel strands with n half-twists, where n is any nonnegative integer. Two tangles [0] and [3] are shown in Fig. 1a. The Denominator of a 2-tangle T, denoted by  $\overline{T}$ , is obtained by joining with simple arcs each pair of the corresponding top and bottom endpoints of T, as shown in Fig. 1b.





**Fig. 1** a Two tangles [0] and [3]; b 2-tangle T and its Denominator  $\overline{T}$ 

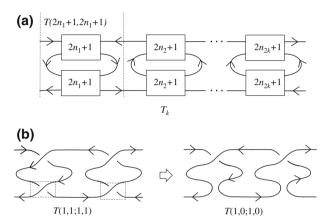


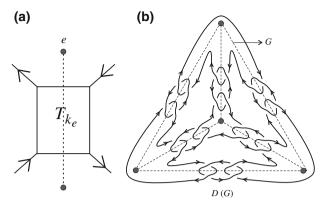
Fig. 2 a A general form of  $T_k$ ; **b** an odd chain tangle T(1, 1; 1, 1) and a 2-tangle T(1, 0; 1, 0) obtained from it

An odd chain tangle, denoted by  $T_k = T(2n_1 + 1, 2n_1 + 1; 2n_2 + 1, 2n_2 + 1; \ldots; 2n_{2k} + 1, 2n_{2k} + 1)$ , is a special oriented 2-tangle shown in Fig. 2a, where each box  $2n_i + 1$  denotes a  $2n_i + 1$ -twist tangle for  $1 \le i \le 2k \ge 2$ . In particular, if a box  $2n_i + 1$  is replaced by the 0-twist tangle, the resulting link is denoted by the corresponding notation. For example in Fig. 2b, the 2-tangle obtained from T(1, 1; 1, 1) by replacing two 1-twist tangles with two 0-twist tangles is denoted by T(1, 0; 1, 0). In addition for  $1 \le i \le 2k$ , we denote by  $T(2n_i + 1, 2n_i + 1)$  the corresponding 2-tangle in  $T_k$ . In Fig. 2a,  $T(2n_1 + 1; 2n_1 + 1)$  is the 2-tangle bounded by two dotted lines.

Now we will use odd chain tangles as building blocks for the construction of oriented links. This can be described as follows:

For any connected plane graph G, each edge e is replaced by an odd chain tangle  $T_{k_e}$  (Fig. 3a), and then two endpoints of the tangles are connected along the boundary of each face. The resulting link, denoted by D(G), is called *an odd link*. It is also called *an odd polyhedral link* when G is a polyhedral graph. Note that D(G) has a consistent orientation based on the similar methods in Refs. [59–61]. In Fig. 3b, we take a tetrahedral graph G for example. Tetrahedral link D(G) is generated by replacing each edge e with T(1, 1; 1, 1). Hereafter we denote by V(G) its vertex set, by E(G) its edge set, and by v(G), e(G) and f(G) the number of vertices, edges, and faces of G respectively.





**Fig. 3** a An edge e replaced by  $T_{k_a}$ ; **b** an odd tetrahedral link D(G) derived from graph G

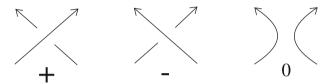


Fig. 4 Three link diagrams  $L_+$ ,  $L_-$  and  $L_0$  differ locally at the site of a single crossing

**Note.** An even chain tangle consists of finitely many 2n-twist tangles. However, it has orientation and other properties which are very different from an odd chain tangle. For example, if we remove any loop in an even or odd chain tangle, this operation will break the whole chain for the latter but the former will change into a 'smaller' even chain tangle. For more details on even chain tangles, please refer to [62].

### 3 The HOMFLY polynomials of odd links

In this section, we establish the relationship between the HOMFLY polynomials of odd links and the  $Q^d$ -polynomial of a plane graph. Let G be any plane graph, and D(G) be an odd polyhedral link obtained from G by using the method in Sect. 2. Let us start with a quick introduction to two polynomial invariants.

**Definition 3.1** [33] 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  $v^{-1}H(L_+; v, z) vH(L_-; v, z) = zH(L_0; v, z)$ .

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

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

(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  $\alpha$  and  $\beta$ , where  $\alpha$  ( $\beta$ , respectively) map E(G) into some commutative ring with unity  $R_{\alpha}(R_{\beta}$ , respectively). Let e be any edge of G, and let  $\alpha(e)$  and  $\beta(e)$  is two weights of e.

**Definition 3.2** [62] 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. Let  $\alpha(e) = \alpha_e$  and  $\beta(e) = \beta_e$ . Then When *e* is a loop,

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

Otherwise,

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

In fact, the  $Q^d$ -polynomial can be directly obtained by generalizing the dichromatic polynomial of a weighted graph [60]. Hence it has an alternative definition as follows:

$$Q^{d}(G) = \sum_{F \subseteq E(G)} \left( \prod_{e \in F} \alpha_{e} \right) \left( \prod_{e \in E(G) - F} \beta_{e} \right) t^{k\langle F \rangle} z^{n\langle F \rangle},$$

where  $k\langle F \rangle$  and  $n\langle F \rangle = e\langle F \rangle - v\langle F \rangle + k\langle F \rangle$  are the number of connected components and the nullity of the spanning subgraph  $\langle F \rangle$ , induced by F, of G, respectively.

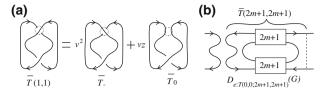
**Lemma 3.3** Let  $T_k$  be an odd chain tangle, and  $T(2n_i + 1, 2n_i + 1)$  be the corresponding 2-tangle in  $T_k$  for  $1 \le i \le 2k$ . Then

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

*Proof* We only need to show that the formula (1) holds for i = 1, 2, and the proof in the case of  $i \ge 3$  is similar. Also,  $T(2n_2 + 1, 2n_2 + 1)$  has a reversed orientation to  $T(2n_1 + 1, 2n_1 + 1)$  on each of its components. Hence we only need to prove that the formula (1) holds for i = 1.

We proceed by induction on the crossing number of  $T = T(2n_1 + 1, 2n_1 + 1)$ , and assume firstly that  $n_1 = 0$ . Since  $\overline{T}$  has only positive crossings, by applying property





**Fig. 5 a** Each diagram in the equation denotes its corresponding HOMFLY polynomial; **b** the link  $D_{e:T(0,0;2m+1,2m+1)}(G)$  and the Denominator of T(2m+1,2m+1) in it

(3) of the definition of the HOMFLY polynomial to a crossing of  $\overline{T}$ , we obtain two links  $\overline{T}_{-}$  and  $\overline{T}_{0}$  as shown in Fig. 5a. Hence we have

$$H(\overline{T}) = v^2 H(\overline{T}_-) + vz H(\overline{T}_0)$$

Note that  $\overline{T}_{-}$  is the disjoint union of two trivial knots and  $\overline{T}_{0}$  is a trivial knot. Hence

$$H(\overline{T}_{-}) = \frac{v^{-1} - v}{z}$$
 and  $H(\overline{T}_{0}) = 1$ .

Hence we obtain

$$H(\overline{T}) = v^2 \frac{v^{-1} - v}{z} + vz.$$

Now assume that  $n_1 \ge 1$ . By applying property (3) of the definition of the HOMFLY polynomial to a crossing of  $\overline{T}$ , we obtain two links  $\overline{T}(2n_1 - 1, 2n_1 + 1)$  and  $\overline{T}'_0$ . Note that  $\overline{T}'_0$  is a trivial knot. Hence we have

$$\begin{split} H(\overline{T}) &= v^2 H(\overline{T}(2n_1 - 1, 2n_1 + 1)) + vz H(\overline{T}'_0) \\ &= v^2 H(\overline{T}(2n_1 - 1, 2n_1 + 1)) + vz. \end{split}$$

Also, $H(\overline{T}(2n_1 - 1, 2n_1 + 1)) = v^2 H(\overline{T}(2n_1 - 1, 2n_1 - 1)) + vz$ . Then we obtain

$$H(\overline{T}) = v^{2}[v^{2}H(\overline{T}(2n_{1} - 1, 2n_{1} - 1)) + vz] + vz$$
  
=  $v^{4}H(\overline{T}(2n_{1} - 1, 2n_{1} - 1)) + v^{3}z + vz$ .

By our inductive hypothesis, we have

$$H(\overline{T}) = v^4 \left[ v^{4n_1 - 2} \frac{v^{-1} - v}{z} + vz \frac{v^{4n_1 - 2} - 1}{v^2 - 1} \right] + v^3 z + vz.$$

The above shows that formula (1) holds for the case of i = 1, and hence for the other cases.



For any nonnegative integer n, hereafter we define

$$d'_n = v^{4n+2} + v^2 z^2 \left(\frac{v^{2n}-1}{v^2-1}\right)^2,$$

$$d''_n = v^{4n+1} z + 2v^{2n+1} z \frac{v^{2n}-1}{v^2-1} \text{ and }$$

$$\Delta_n = v^{4n+2} \frac{v^{-1}-v}{z} + vz \frac{v^{4n+2}-1}{v^2-1}.$$

**Lemma 3.4** Let e be an edge of G, which is replaced by an odd chain tangle T(2n+1, 2n+1; 2m+1, 2m+1) for any nonnegative integers n and m. If e is a loop, then

$$H(D(G)) = \left[ d_n'' d_m'' v^2 \frac{v^{-1} - v}{z} + d_n' \Delta_m + d_n'' d_m' + d_n'' d_m'' vz \right] H(D(G - e)). \tag{2}$$

Otherwise,

$$H(D(G)) = d_n'' d_m'' v^2 H(D(G/e)) + (d_n' \Delta_m + d_n'' d_m' + d_n'' d_m'' vz) H(D(G - e)). \tag{3}$$

*Proof* First, we apply property (3) of the definition of the HOMFLY polynomial to a crossing of the 2n + 1-twist tangle in T(2n + 1, 2n + 1; 2m + 1, 2m + 1), giving

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

Similarly

$$H(D_{e:T(2n-1,2n+1;2m+1,2m+1)}(G))$$

$$= v^2 H(D_{e:T(2n-3,2n+1;2m+1,2m+1)}(G)) + vz H(D_{e:T(0,2n+1;2m+1,2m+1)}(G))$$

Then we obtain

$$H(D(G)) = v^4 H(D_{e:T(2n-3,2n+1;2m+1,2m+1)}(G)) + (v^3 z + vz) H(D_{e:T(0,2n+1;2m+1,2m+1)}(G)).$$

By induction on the crossing number of the 2n + 1-twist tangle, we have

$$\begin{split} H(D(G)) &= v^{2n} H(D_{e:T(1,2n+1;2m+1,2m+1)}(G)) \\ &+ vz \frac{v^{2n}-1}{v^2-1} H(D_{e:T(0,2n+1;2m+1,2m+1)}(G)). \end{split}$$

Similarly for the 2n + 1-twist tangle in T(1, 2n + 1; 2m + 1, 2m + 1), we have

$$\begin{split} H(D_{e:(1,2n+1;2m+1,2m+1))}(G)) &= v^{2n} H(D_{e:T(1,1;2m+1,2m+1)}(G)) \\ &+ vz \frac{v^{2n}-1}{v^2-1} H(D_{e:T(1,0;2m+1,2m+1)}(G)). \end{split}$$



From the above two equations, we obtain

$$\begin{split} H(D(G)) &= v^{4n} H(D_{e:T(1,1;2m+1,2m+1)}(G)) + v^{2n+1} z \frac{v^{2n}-1}{v^2-1} H(D_{e:T(1,0;2m+1,2m+1)}(G)) \\ &+ v z \frac{v^{2n}-1}{v^2-1} H(D_{e:T(0,2n+1;2m+1,2m+1)}(G)). \end{split}$$

Using the definition of the HOMELY polynomial, we have

$$H(D_{e:T(1,1;2m+1,2m+1)}(G)) = v^2 H(D_{e:T(0,0;2m+1,2m+1)}(G)) + vz H(D_{e:T(1,0;2m+1,2m+1)}(G)).$$

Then

$$\begin{split} H(D(G)) &= v^{4n+2} H(D_{e:T(0,0;2m+1,2m+1)}(G)) + vz \frac{v^{2n}-1}{v^2-1} H(D_{e:T(0,2n+1;2m+1,2m+1)}(G)) \\ &+ \left(v^{4n+1}z + v^{2n+1}z \frac{v^{2n}-1}{v^2-1}\right) H(D_{e:T(1,0;2m+1,2m+1)}(G)). \end{split}$$

Repeatedly applying property (3) of the definition of the HOMFLY polynomial, we have

$$\begin{split} &H(D_{e:T(0,2n+1;2m+1,2m+1)}(G)) = v^2 H(D_{e:T(0,2n-1;2m+1,2m+1)}(G)) + vz H(D_{e:T(0,0;2m+1,2m+1)}(G)) \\ &= v^2 [v^2 H(D_{e:T(0,2n-3;2m+1,2m+1)}(G)) + vz H(D_{e:T(0,0;2m+1,2m+1)}(G))] \\ &+ vz H(D_{e:T(0,0;2m+1,2m+1)}(G)) \\ &= v^4 H(D_{e:T(0,2n-3;2m+1,2m+1)}(G)) + (v^3 z + vz) H(D_{e:T(0,0;2m+1,2m+1)}(G)) \\ &\cdots = v^{2n} H(D_{e:T(0,1;2m+1,2m+1)}(G)) + vz \frac{v^{2n} - 1}{v^2 - 1} H(D_{e:T(0,0;2m+1,2m+1)}(G)). \end{split}$$

Hence we have

$$\begin{split} H(D(G)) &= v^{4n+2} H(D_{e:T(0,0;2m+1,2m+1)}(G)) \\ &+ \left( v^{4n+1}z + v^{2n+1}z \frac{v^{2n}-1}{v^2-1} \right) H(D_{e:T(1,0;2m+1,2m+1)}(G)) + vz \frac{v^{2n}-1}{v^2-1} \\ &\cdot \left[ v^{2n} H(D_{e:T(0,1;2m+1,2m+1)}(G)) + vz \frac{v^{2n}-1}{v^2-1} H(D_{e:T(0,0;2m+1,2m+1)}(G)) \right] \\ &= \left[ v^{4n+2} + v^2 z^2 \left( \frac{v^{2n}-1}{v^2-1} \right)^2 \right] H(D_{e:T(0,0;2m+1,2m+1)}(G)) \\ &+ \left( v^{4n+1}z + 2v^{2n+1}z \frac{v^{2n}-1}{v^2-1} \right) H(D_{e:T(1,0;2m+1,2m+1)}(G)). \end{split}$$

Similarly for the two 2m + 1-twist tangles in T(0, 0; 2m + 1, 2m + 1), we obtain

$$H(D_{e:(1,0;2m+1,2m+1)}(G)) = d_m' H(D_{e:T(1,0;0,0)}(G)) + d_m'' H(D_{e:T(1,0;1,0)}(G)).$$



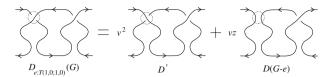


Fig. 6 Each diagram in the equation denotes its corresponding HOMFLY polynomial

Hence we have

$$H(D(G)) = d'_n H(D_{e:T(0,0;2m+1,2m+1)}(G)) + d''_n d'_m H(D_{e:T(1,0;0,0)}(G)) + d''_n d''_m H(D_{e:T(1,0;1,0)}(G)).$$

$$(4)$$

Note that  $D_{e:T(0,0;2m+1,2m+1)}(G)$  can be described in Fig. 5b. Using the property (1) of the HOMFLY polynomial and Lemma 3.3, we have

$$\begin{split} H(D_{e:T(0,0;2m+1,2m+1)}(G)) &= H(\overline{T}(2m+1,2m+1)\sharp D(G-e)) \\ &= H(\overline{T}(2m+1,2m+1))H(D(G-e)) \\ &= \Delta_m H(D(G-e)) \\ &\text{and} \\ H(D_{e:T(1,0;0,0)}(G)) &= H(D(G-e)). \end{split}$$

Hence we obtain

$$H(D(G)) = d'_n \Delta_m H(D(G - e)) + d''_n d'_m H(D(G - e)) + d''_n d''_m H(D_{e:T(1,0;1,0)}(G)).$$

Applying property (3) of the definition of the HOMFLY polynomial to the 2-tangle T(1, 0; 1, 0), we obtain two links D' and D(G - e) as shown in Fig. 6. Hence

$$\begin{split} H(D(G)) &= (d'_n \Delta_m + d''_n d'_m) H(D(G-e)) + d''_n d''_m (v^2 H(D') + vz H(D(G-e))) \\ &= (d'_n \Delta_m + d''_n d'_m + d''_n d''_m vz) H(D(G-e)) + d''_n d''_m v^2 H(D'). \end{split}$$

If e is a loop, then

$$H(D') = \frac{v^{-1} - v}{z} H(D(G - e)).$$

Hence we have

$$H(D(G)) = \left[ d_n'' d_m'' v^2 \left( \frac{v^{-1} - v}{z} \right) + d_n' \Delta_m + d_n'' d_m' + d_n'' d_m'' vz \right] H(D(G - e)).$$

If e is not a loop, then

$$H(D') = H(D(G/e)).$$



Hence we have

$$H(D(G)) = d''_n d''_m v^2 H(D(G/e)) + (d'_n \Delta_m + d''_n d''_m + d''_n d''_m vz) H(D(G - e)).$$

For any two nonnegative integers n and m, we can define

$$E'(n,m) = d''_n d''_m v^2$$
 and  $E''(n,m) = d'_n \Delta_m + d''_n d''_m + d''_n d''_m vz$ .

**Theorem 3.5** Let e be an edge of G, which is replaced by an odd chain tangle  $T_{k_e} = (2n_1 + 1, 2n_1 + 1; \ldots; 2n_{2k_e} + 1, 2n_{2k_e} + 1)$  for any nonnegative integer  $n_i$   $(1 \le i \le 2k_e \ge 2)$ .

If e is a loop, then

$$H(D(G)) = \left[ \sum_{s=1,3,\dots,2k_e-1} \prod_{i=1,3,\dots,s-2} E'(n_i, n_{i+1}) E''(n_s, n_{s+1}) \prod_{i=s+2}^{2k_e} \Delta_{n_i} + \prod_{i=1,3,\dots,2k_e-1} E'(n_i, n_{i+1}) \frac{v^{-1} - v}{z} \right] H(D(G - e)).$$
 (5)

Otherwise,

$$H(D(G)) = \sum_{s=1,3,\dots,2k_e-1} \prod_{i=1,3,\dots,s-2} E'(n_i, n_{i+1}) E''(n_s, n_{s+1}) \prod_{i=s+2}^{2k_e} \Delta_{n_i} H(D(G-e)) + \prod_{i=1,3,\dots,2k_e-1} E'(n_i, n_{i+1}) H(D(G/e)).$$
(6)

*Proof* We proceed by induction on  $k_e$ . Note that the case of  $k_e = 1$  has been shown in Lemma 3.4. Now we suppose that  $k_e \ge 2$ . Using the above formula (4), we have

$$\begin{split} H(D(G)) &= d_{n_1}' H(D_{e:T(0,0;2n_2+1,2n_2+1;\ldots)}(G)) + d_{n_1}'' d_{n_2}' H(D_{e:T(1,0;0,0;2n_3+1,2n_3+1;\ldots)}(G)) \\ &+ d_{n_1}'' d_{n_2}'' H(D_{e:T(1,0;1,0;2n_3+1,2n_3+1;\ldots)}(G)). \end{split}$$

Note that

$$H(D_{e:T(0,0;2n_2+1,2n_2+1;...)}(G)) = H(D(G-e)\sharp \overline{T}(2n_2+1,2n_2+1)\sharp ...\sharp \overline{T}(2n_{2k_e}+1,2n_{2k_e}+1)).$$



Hence using property (1) of the HOMFLY polynomial and Lemma 3.3, we have

$$H(D_{e:T(0,0;2n_2+1,2n_2+1;...)}(G)) = \prod_{i=2}^{2k_e} H(\overline{T}(2n_i+1,2n_i+1))H(D(G-e))$$

$$= \prod_{i=2}^{2k_e} \Delta_{n_i} H(D(G-e))$$

$$= \Delta_{n_2} H(D_{e:T(1,0;0,0;2n_3+1,2n_3+1;...)}(G)).$$

Then

$$\begin{split} H(D(G)) &= d_{n_1}' \prod_{i=2}^{2k_e} \Delta_{n_i} H(D(G-e)) + d_{n_1}'' d_{n_2}' \prod_{i=3}^{2k_e} \Delta_{n_i} H(D(G-e)) \\ &+ d_{n_1}'' d_{n_2}'' H(D_{e:T(1,0;1,0;2n_3+1,2n_3+1;...)}(G)). \end{split}$$

Using property (3) of the definition of the HOMFLY polynomial, we have

$$H(D_{e:T(1,0;1,0;2n_3+1,2n_3+1;...)}(G)) = v^2 H(D_{e:T(2n_3+1,2n_3+1;...)}(G)) + vz H(D_{e:T(0,0;1,0;2n_3+1,2n_3+1;...)}(G)).$$

Hence we obtain

$$\begin{split} H(D(G)) &= \left( d_{n_1}' \prod_{i=2}^{2k_e} \Delta_{n_i} + d_{n_1}'' d_{n_2}' \prod_{i=3}^{2k_e} \Delta_{n_i} \right) H(D(G-e)) \\ &+ d_{n_1}'' d_{n_2}'' (v^2 H(D_{e:T(2n_3+1,2n_3+1;...)}(G)) + vz H(D_{e:T(0,0;1,0;2n_3+1,2n_3+1;...)}(G))). \end{split}$$

Since

$$H(D_{e:T(0,0;1,0;2n_3+1,2n_3+1;...)}(G)) = \prod_{i=3}^{2k_e} \Delta_{n_i} H(D(G-e)),$$

we have

$$\begin{split} H(D(G)) &= d_{n_1}'' d_{n_2}'' v^2 H(D_{e:T(2n_3+1,2n_3+1;...)}(G)) \\ &+ \left( d_{n_1}' \prod_{i=2}^{2k_e} \Delta_{n_i} + d_{n_1}'' d_{n_2}' \prod_{i=3}^{2k_e} \Delta_{n_i} + d_{n_1}'' d_{n_2}'' vz \prod_{i=3}^{2k_e} \Delta_{n_i} \right) H(D(G-e)) \\ &= E'(n_1,n_2) H(D_{e:T(2n_3+1,2n_3+1;...)}(G)) + E''(n_1,n_2) \prod_{i=3}^{2k_e} \Delta_{n_i} H(D(G-e)). \end{split}$$



If e is a loop, by our inductive hypothesis, we have

$$\begin{split} H(D_{e:T(2n_3+1,2n_3+1;\dots)}(G)) &= \left(\prod_{i=3,5,\dots,2k_e-1} E'(n_i,n_{i+1}) \cdot \frac{v^{-1}-v}{z} \right. \\ &+ \sum_{s=3,5,\dots,2k_e-1} \prod_{i=3,5,\dots,s-2} E'(n_i,n_{i+1}) \cdot E''(n_s,n_{s+1}) \prod_{i=s+2}^{2k_e} \Delta_{n_i} \right) H(D(G-e)). \end{split}$$

Hence we have

$$\begin{split} H(D(G)) &= E''(n_1, n_2) \prod_{i=3}^{2k_e} \Delta_{n_i} H(D(G-e)) \\ &+ E'(n_1, n_2) \left( \prod_{i=3,5,\dots,2k_e-1} E'(n_i, n_{i+1}) \cdot \frac{v^{-1} - v}{z} \right. \\ &+ \sum_{s=3,5,\dots,2k_e-1} \prod_{i=3,5,\dots,s-2} E'(n_i, n_{i+1}) \cdot E''(n_s, n_{s+1}) \prod_{i=s+2}^{2k_e} \Delta_{n_i} \right) H(D(G-e)). \end{split}$$

The formula (5) can be directly obtained from the above equation. If e is not a loop, by our inductive hypothesis,

$$H(D_{e:T(2n_3+1,2n_3+1;...)}(G))$$

$$= \prod_{i=3,5,...,2k_e-1} E'(n_i, n_{i+1}) H(D(G/e))$$

$$+ \sum_{s=3,5,...,2k_e-1} \prod_{i=3,5,...,s-2} E'(n_i, n_{i+1}) E''(n_s, n_{s+1}) \prod_{i=s+2}^{2k_e} \Delta_{n_i} H(D(G-e)).$$

Hence we have

$$\begin{split} H(D(G)) &= E''(n_1, n_2) \prod_{i=3}^{2k_e} \Delta_{n_i} H(D(G-e)) \\ &+ E'(n_1, n_2) \left[ \prod_{i=3,5,\dots,2k_e-1} E'(n_i, n_{i+1}) H(D(G/e)) \right. \\ &+ \sum_{s=3,5,\dots,2k_e-1} \prod_{i=3,5,\dots,s-2} E'(n_i, n_{i+1}) \cdot E''(n_s, n_{s+1}) \prod_{i=s+2}^{2k_e} \Delta_{n_i} H(D(G-e)) \right]. \end{split}$$

The formula (6) can be directly obtained from the above equation.



In graph G, for each edge e replaced by an odd chain tangle  $T_{k_e}$ , by defining

$$\alpha(e) = \prod_{i=1,3,...,2k_e-1} E'(n_i, n_{i+1})$$
 and

$$\beta(e) = \sum_{s=1,3,\dots,2k_e-1} \prod_{i=1,3,\dots,s-2} E'(n_i, n_{i+1}) E''(n_s, n_{s+1}) \prod_{i=s+2}^{2k_e} \Delta_{n_i},$$

we obtain two functions  $\alpha$  and  $\beta$  from E(G) to the polynomial ring  $\mathbb{Z}[v, z]$ . Now by comparing Theorem 3.5 with the definition of  $Q^d$ -polynomial, we obtain the following theorem.

**Theorem 3.6** Let G be the double weighted graph with two functions  $\alpha$  and  $\beta$  as defined above. Then

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

According to the above theorem and the definition of the  $Q^w$ -polynomial, the HOMFLY polynomials of odd links can be given as a sum over all subsets of E(G) in the following manner.

**Theorem 3.7** *Let G be defined as in Theorem 3.6. Then* 

$$H(D(G)) = \sum_{F \subseteq E(G)} \left( \prod_{e \in F} \alpha_e \right) \left( \prod_{e \in E(G) - F} \beta_e \right) \left( \frac{v^{-1} - v}{z} \right)^{k \langle F \rangle + n \langle F \rangle - 1}.$$

# 4 Applications

In this section, the spans<sub>v</sub> of the HOMFLY polynomials, the bound of the braid indices and the genera of odd polyhedral links are all calculated by using Theorem 3.7.

## 4.1 Span<sub>v</sub> of the HOMFLY polynomial

Let  $\max \deg_v f$  and  $\min \deg_v f$  denote the maximum degree and minimum degree of v in the multi-variable polynomial f taken over terms with non-zero coefficients, respectively. We define  $\operatorname{span}_v f = \operatorname{maxdeg}_v f - \operatorname{mindeg}_v f$ , and begin with some simple lemmas.

**Lemma 4.1** Let  $d'_n$ ,  $d''_n$  and  $\Delta_n$  be defined as in the Sect. 3. Then

- (1)  $\operatorname{maxdeg}_v d'_n = 4n + 2$  and  $\operatorname{mindeg}_v d'_n = 2$ .
- (2)  $\operatorname{maxdeg}_{v} d_{n}^{"} = 4n + 1$  and  $\operatorname{mindeg}_{v} d_{n}^{"} = 2n + 1$ .
- (3)  $\operatorname{maxdeg}_{v} \Delta_{n} = 4n + 3$  and  $\operatorname{mindeg}_{v} \Delta_{n} = 1$ .



The following theorem can be easily obtained from Lemma 4.1.

**Lemma 4.2** Let E'(n, m) and E''(n, m) be defined as in the Sect. 3. Then

(1) maxdeg, 
$$E'(n, m) = 4n + 4m + 4$$
 and mindeg,  $E'(n, m) = 2n + 2m + 4$ .

(2) maxdeg, 
$$E''(n, m) = 4n + 4m + 5$$
 and mindeg,  $E''(n, m) = 3$ .

**Theorem 4.3** Let G be any connected plane graph and D(G) be the odd link derived from G using the method in Sect. 2. For each edge e of G, it is replaced by an odd chain diagram  $T_{k_e} = T(2n_1 + 1, 2n_1 + 1; 2n_2 + 1, 2n_2 + 1; \dots; 2n_{2k_e} + 1, 2n_{2k_e} + 1)$  for any nonnegative integer  $n_i$   $(1 \le i \le 2k_e \ge 2)$ . Then

$$\operatorname{maxdeg}_{v} H(D(G)) = \sum_{e \in E(G)} \left[ \sum_{i=1}^{2k_{e}} (4n_{i} + 3) - 1 \right] + v(G) - 1$$
 (7)

and mindeg<sub>v</sub> 
$$H(D(G)) = \sum_{e \in E(G)} (2k_e + 1) - v(G) + 1.$$
 (8)

*Proof* By using Theorem 3.7, we have

$$H(D(G)) = \sum_{F \subseteq E(G)} \left( \prod_{e \in F} \alpha_e \right) \left( \prod_{e \in E(G) - F} \beta_e \right) \left( \frac{v^{-1} - v}{z} \right)^{k \langle F \rangle + n \langle F \rangle - 1}.$$

For any subset F of E(G), by using Lemma 4.2, we have

maxdeg<sub>v</sub> 
$$\alpha_e = \sum_{i=1,3,...,2k_e-1} (4n_i + 4n_{i+1} + 4) = \sum_{i=1}^{2k_e} (4n_i + 2)$$
 and mindeg<sub>v</sub>  $\alpha_e = \sum_{i=1,3,...,2k_e-1} (2n_i + 2n_{i+1} + 4) = \sum_{i=1}^{2k_e} (2n_i + 2).$ 

Similarly, we have

mindeg<sub>v</sub> 
$$\beta_e = \text{mindeg}_v \left\{ E''(n_1, n_2) \prod_{i=3}^{2k_e} \Delta_{n_i} \right\} = 2k_e + 1 \text{ and}$$

$$\text{maxdeg}_v \ \beta_e = \text{maxdeg}_v \left\{ E''(n_1, n_2) \prod_{i=3}^{2k_e} \Delta_{n_i} \right\} = \sum_{i=1}^{2k_e} (4n_i + 3) - 1.$$



Suppose that F is nonempty and |F| is the number of edges in F. Then

$$\begin{aligned} & \max \deg_{v} \left\{ \prod_{e \in F} \alpha_{e} \prod_{e \in E(G) - F} \beta_{e} \cdot \left( \frac{v^{-1} - v}{z} \right)^{k\langle F \rangle + n\langle F \rangle - 1} \right\} \\ &= \sum_{e \in F} \max \deg_{v} \alpha_{e} + \sum_{e \in E(G) - F} \max \deg_{v} \beta_{e} + k\langle F \rangle + n\langle F \rangle - 1 \\ &= \sum_{e \in F} \sum_{i=1}^{2k_{e}} (4n_{i} + 2) + \sum_{e \in E(G) - F} \left[ \sum_{i=1}^{2k_{e}} (4n_{i} + 3) - 1 \right] + 2k\langle F \rangle + |F| - v\langle F \rangle - 1 \\ &= \sum_{e \in E(G)} \left[ \sum_{i=1}^{2k_{e}} (4n_{i} + 3) - 1 \right] - \sum_{e \in F} 2k_{e} + 2k\langle F \rangle + 2|F| - v\langle F \rangle - 1 \\ &= \sum_{e \in E(G)} \left[ \sum_{i=1}^{2k_{e}} (4n_{i} + 3) - 1 \right] - \sum_{e \in F} (2k_{e} - 2) + 2k\langle F \rangle - v\langle F \rangle - 1. \end{aligned}$$

Also, 
$$k\langle F \rangle \leq v\langle F \rangle - 1$$
 and  $\sum_{e \in F} (2k_e - 2) \geq 0$ , we have

$$\begin{aligned} & \operatorname{maxdeg}_v \, \left\{ \prod_{e \in F} \alpha_e \prod_{e \in E(G) - F} \beta_e (\frac{v^{-1} - v}{z})^{k\langle F \rangle + n\langle F \rangle - 1} \right\} \\ & \leq \sum_{e \in E(G)} \left[ \sum_{i=1}^{2k_e} (4n_i + 3) - 1 \right] + 2(v\langle F \rangle - 1) - v\langle F \rangle - 1 \\ & < \sum_{e \in E(G)} \left[ \sum_{i=1}^{2k_e} (4n_i + 3) - 1 \right] + v\langle G \rangle - 1 \\ & = \operatorname{maxdeg}_v \, \left\{ \prod_{e \in E(G)} \beta_e \left( \frac{v^{-1} - v}{z} \right)^{v\langle G \rangle - 1} \right\}. \end{aligned}$$

Similarly, we have

$$\begin{aligned} & \operatorname{mindeg}_v \ \left\{ \prod_{e \in F} \alpha_e \prod_{e \in E(G) - F} \beta_e \left( \frac{v^{-1} - v}{z} \right)^{k\langle F \rangle + n\langle F \rangle - 1} \right\} \\ &= \sum_{e \in F} \operatorname{mindeg}_v \alpha_e + \sum_{e \in E(G) - F} \operatorname{mindeg}_v \beta_e - k\langle F \rangle - n\langle F \rangle + 1 \\ &= \sum_{e \in F} \sum_{i=1}^{2k_e} (2n_i + 2) + \sum_{e \in E(G) - F} (2k_e + 1) - 2k\langle F \rangle - |F| + v\langle F \rangle + 1 \end{aligned}$$



$$\geq \sum_{e \in F} \sum_{i=1}^{2k_e} (2n_i + 2) + \sum_{e \in E(G) - F} (2k_e + 1) - 2(v\langle F \rangle - 1) - |F| + v\langle F \rangle + 1.$$

Also,  $\sum_{i=1}^{2k_e} (2n_i + 1) \ge 2$ , hence we obtain

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

The following Theorem can be proven by using Theorem 4.3 and Euler's formula.

**Theorem 4.4** 
$$span_v H(D(G)) = \sum_{e \in E(G)} \sum_{i=1}^{2k_e} (4n_i + 2) - 2(f-1).$$

### 4.2 Braid index

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. In the following Theorem 4.5, the lower bound of b(L), known as the MFW inequality, was shown independently by Franks and Williams [50] and Morton [51], and the upper bound was given by Ohyama [52] in 1993.

## Theorem 4.5

$$\frac{1}{2}span_v H(L) + 1 \le b(L) \le \frac{1}{2}c(L) + 1,\tag{9}$$

where c(L) is the crossing number of a link L.

**Theorem 4.6** Let G and D(G) be defined as in Theorem 4.3. Then

$$\sum_{e \in E(G)} \sum_{i=1}^{2k_e} (2n_i + 1) - (f - 2) \le b(D(G)) \le \sum_{e \in E(G)} \sum_{i=1}^{2k_e} (2n_i + 1) + 1. \quad (10)$$



*Proof* Let  $c(T_{k_e})$  and c(D(G)) be the crossing number of  $T_{k_e}$  and D(G), respectively. Note that each  $T_{k_e}$  is an alternating tangle, hence D(G) is an alternating link by the construction method in Sect. 2. Thus

$$c(T_{k_e}) = \sum_{i=1}^{2k_e} (4n_i + 2)$$
 and  $c(D(G)) = \sum_{e \in E(G)} \sum_{i=1}^{2k_e} (4n_i + 2).$ 

Formula (10) can be obtained by using the Theorems 4.4 and 4.5.

## 4.3 Genus

The genus of an oriented link L is the minimum genus of any connected orientable surface having L as its boundary. The following theorem follows directly from Corollary 4.1 and Remark in Ref. [53].

**Theorem 4.7** Let L be a alternating link having a positive diagram, then

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

**Theorem 4.8** Let G be any connected plane graph and D(G) be an odd link obtained from G using the method in Sect. 2. Then

$$g(D(G)) = f(G) - 1.$$

*Proof* Let e be any edge of G, which is replaced by an odd chain tangle  $T_{k_e}$ . Let  $\mu_e$  be the number of the loops in  $T_{k_e}$ ,  $\mu_{D(G)}$  be the component number of D(G). Clearly, each vertex v of G corresponds to a component of D(G). Hence we have the following equations:

$$\mu_e = 2k_e - 1$$
 and  $\mu_e(D(G)) = \sum_{e \in E(G)} \mu_e + v(G) = \sum_{e \in E(G)} (2k_e - 1) + v(G)$ .

Note that each  $T_{k_e}$  only has positive crossings, hence D(G) itself is a positive alternating link diagram. By Theorem 4.7 we have

$$\begin{split} 2g(D(G)) &= \sum_{e \in E(G)} (2k_e + 1) - v(G) + 1 - \left[ \sum_{e \in E(G)} (2k_e - 1) + v(G) \right] + 1 \\ &= 2e(G) - 2v(G) + 2 \\ &= 2f(G) - 2. \end{split}$$



Example 1 Let G be a tetrahedral link as shown in Fig. 3b. Since f(G) = 4 and  $T_{k_e} = T(1, 1; 1, 1)$ , we have

$$span_v H(D(G)) = 6(2+2) - 2(4-1) = 18,$$
  
 $10 \le b(D(G)) \le 6 \cdot (1+1) + 1 = 13$  and  
 $g(D(G)) = 4 - 1 = 3.$ 

#### 5 Conclusion

In this paper, odd chain tangles have been designed to generate odd polyhedral links with two DNA duplexes. Each of them consists of finitely many 2n + 1-twist tangles, with each strand oriented antiparallel to each other. This orientation coincides with the natural direction of DNA strands. Also, we note that removing any loop of an odd chain tangle will break the whole chain, which is essentially different from even chain tangles [62].

Furthermore, the HOMFLY polynomials of odd links have been given by an explicit formula in terms of the  $Q^d$ -polynomial of the associated polyhedral graph G. This formula enables us to obtain the spans $_v$  of the HOMFLY polynomials, the upper and lower bounds on the braid indices and the genera of these odd links. Our results show that the three indices are not only related closely to the odd chain tangles used but also to the face number of G. Also, we observe that these odd links are embedded on the surface with genus n > 0. These facts imply that odd polyhedral links have more complex topological structure than even polyhedral links [38–40,62]. Our work provides novel insights into the synthesis and control of the molecules with remarkably complex topology.

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