

Enumerating DNA polyhedral links

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Received: 13 November 2012 / Accepted: 20 January 2013 / Published online: 7 February 2013
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Abstract With the fast-growing of DNA self-assembly techniques, a large number of DNA catenanes or more specifically, DNA polyhedral links were synthesized in the past decade. As a sequel of a recent paper (J. Math. Chem. 50, p. 1693, 2012) by the present authors on the enumeration problem of polyhedral links, this paper considers the enumeration problem of DNA polyhedral links. In contrast to a general molecular link, a DNA polyhedral link has four notable features: 1. the memory of DNA chain direction; 2. the accurate DNA complementary base pairing; 3. the twist patterns of the double-helical strands; 4. the migration in branched junction. These features put forward particular requests for treating the enumeration problem of DNA polyhedral links. In addition to using the standard Pólya's counting theory, we here introduce the generating function and edge direction retentivity analysis to the enumeration problem, by which we establish explicit expressions of the numbers of DNA polyhedral links for three typical models. These models have been used as strategies or are potential strategies in the synthesis of DNA polyhedral links.

Keywords Catenane · DNA polyhedral link · Enumeration

Research supported by NSFC (No. 10831001).

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1 Introduction

Enumeration of molecules is one of the fundamental problems in bioinformatics, chemoinformatics and has attracted chemists, biologists and mathematicians for more than one century [1,2]. It is also important from a practical viewpoint because it plays an important role in drug discovery, experimental structure elucidation (e.g., by NMR or MS), molecular design [3], virtual libraries constructing, hypotheses testing and experiments optimizing [4].

Motivated by the problem of chemical isomer enumeration, in the 1930s Pólya [2] developed a powerful combinatorial theory for the enumeration of symmetry-mediated equivalence classes of ‘colorings’. This enumeration theory has now become standard fare in combinatorics texts and named after him, i.e., Pólya’s theorem or Redfield-Pólya theorem. Following Pólya there have been further refinements for this chemical problem in a very large number of papers, the earlier of which was nicely reviewed by Read [5] who also gave a translation (made by Aeppli) of the Pólya’s foundational paper [2]. The works on this problem for the past few decades can be found, for example in [6–16] and the references cited therein.

In [17], the present authors considered the enumeration problem of a particular three-dimensional molecular or chemical compound system which has a polyhedral frame where the vertices, edges, and faces correspond to ‘units’ such as atoms, bonds, ligands, polymers, or other objects of chemical interests. This enumeration problem is mathematically modeled as the so called ‘total coloring’ enumeration problem of a polyhedron. Here, the notion ‘total coloring’ means to color all the vertices, edges and faces of the polyhedron by using three or more corresponding color sets. By extending the fundamental version of Pólya’s enumeration theorem, a theoretical approach for the number of total colorings of a polyhedron was established. Applying this approach, the authors gave explicit expressions for the number of certain types of polyhedral links, a particular type of catenanes, which belongs to the family of ‘3-cross-curve and double-twist-line covering’ polyhedral links proposed by Qiu [18] inspired by the recent advances on the study of catenanes, e.g., [19–22].

As a sequel of the above paper, this paper considers the enumeration problem of DNA polyhedral links in which edges are associated to DNA double strands. Since the first topological catenane [23] was synthesized in 1961, a large number of DNA catenanes or more specifically, DNA polyhedral links were synthesized in the past decade with the fast-growing of the DNA self-assembly techniques [19–21,24–26]. In fact, DNA polyhedral links exist not only in the synthesized molecules but also in many existing biomolecules in nature, a typical example of which would be the bacteriophage HK97 capsid [22].

Due to the Watson–Crick principle of the accurate complementary base pairing and the reaction of highly specific enzymes, DNA has been one of the most exciting self-assembly molecules and therefore widely used in synthesizing molecules at the nanometer length scale. The theoretical strategy for synthesizing a DNA polyhedral link of the desired architecture involves using careful DNA sequence selection to direct the self-assembly of the structure. In practice, the widely used synthetic strategies in DNA self-assembly technology are using the pre-prepared building blocks to achieve the desired configuration or in particular, the desired polyhedral link. Two typical types

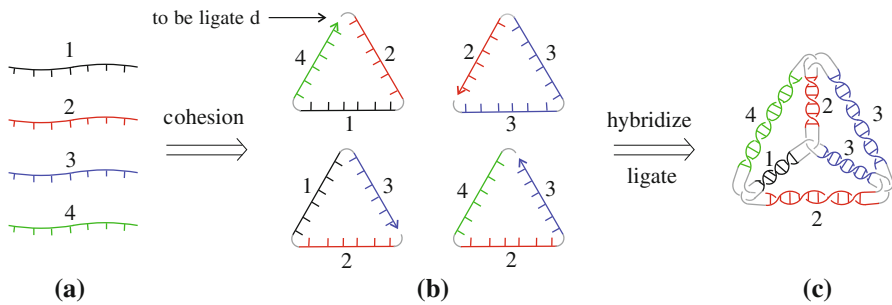


Fig. 1 **a** Four types of pre-prepared DNA strands; **b** four single rings to be hybridized and legated; **c** a tetrahedron link

of building blocks are the DNA single strands [20,21] and branched DNA junctions (for example, the Holliday junction [25,27]).

In contrast to other molecular links, a DNA polyhedral link has four notable features, roughly speaking:

1. the memory of DNA chain direction;
2. the accurate DNA complementary base pairing;
3. the twist of two DNA strands around the helical axis;
4. the branch migration in Holliday junction.

These features put forward specific requests for treating the enumeration problem of DNA polyhedral links. The enumeration problem of DNA polyhedral links constructed by means of branched DNA junctions can be mathematically modeled as the typical vertex coloring problem of polyhedrons. This model can be also regarded as a special case of the total coloring problem which has been studied in our previous paper [17].

Here we focus our attention on the DNA polyhedral links constructed by means of DNA single strands, which involve the first three of the above mentioned features. To this end, in addition to using the standard Pólya's counting theory, we here introduce the generating function and edge direction retentivity analysis to extend the counting techniques introduced in [17], by which we establish explicit expressions of the numbers of DNA polyhedral links for three typical models. These models have been used as strategies or are potential theoretical strategies in the synthesis of DNA polyhedral links. In our study, chirality is taken into account.

2 Models

One of the laboratory methods using the pre-prepared DNA single strands to synthesize a DNA polyhedral link is executed as the following steps [21]: 1. hold single strands together by sticky-end cohesion to form single rings designed to run around faces, each of which has a nick to be ligated; 2. hybridize single rings by the Watson–Crick complementary base pairing to form the double helical edges and then form a polyhedral backbone; 3. close nicks by enzymatic ligation to form a polyhedral link, as depicted in Fig. 1.

Using this strategy, Goodman et al. [21] successfully synthesized a DNA tetrahedron, in which strands on different edges are designed to be different.

In some cases, at each vertex of a polyhedron \mathcal{P} , the corresponding single strands may be interlocked, which has been discussed in our previous work [17]. To simplify our discussion, we will not take this case into account in the following discussion. Thus, if we neglect the intermediate chemical synthesizing process then a polyhedral link is determined mathematically by the following factors: 1. the pre-prepared DNA single strands; 2. the direction of a strand on an edge; 3. the *twisting pattern* (i.e., the *clockwise pattern* and *anti-clockwise pattern*) and the *twisting number* (i.e., the times of a strand circling the axis of the double helix) of the double strand on an edge [17].

Let \mathcal{P} be a polyhedron, and let V and E be the vertex set and edge set of \mathcal{P} , respectively. Following [17], we consider a DNA polyhedral link with frame \mathcal{P} as an edge coloring of \mathcal{P} . An edge coloring C is a mapping from the edge set E of \mathcal{P} to a color set \mathcal{C}_E , i.e., an assignment of each edge of \mathcal{P} with a color in \mathcal{C}_E . It is known that a rotation or a mirror reflection π which leaves \mathcal{P} invariant induces a permutation on V and E , respectively. In the following, we do not distinguish between a rotation (or a mirror reflection) π and its induced permutation, i.e., π represents either the rotation (or a mirror reflection) itself or its induced vertex or edge permutation. From symmetric group theory, all rotations which leave \mathcal{P} invariant form a group. We denote this group by $G_{\mathcal{P}}$. Moreover, $G_{\mathcal{P}} \times \{I, \phi\}$ also forms a permutation group acting on each of V and E [28], where I is the unity permutation and ϕ is an arbitrary mirror reflection that leaves \mathcal{P} invariant. We note that, for any $\pi \in G_{\mathcal{P}}$, $\phi\pi$ is also a mirror reflection of \mathcal{P} [6, 28]. This means that a chiral color will be transferred to be its antipode (i.e., its mirror image) under the operation of $\phi\pi$ for any $\pi \in G_{\mathcal{P}}$ while an achiral color does not change.

For a coloring C and a vertex or an edge x , we denote by $C(x)$ the color of x assigned by C . Two colorings C_1 and C_2 are said to be equivalent under the operation of $G_{\mathcal{P}}$ (resp., $G_{\mathcal{P}} \times \{I, \phi\}$) if there is a permutation $\pi \in G_{\mathcal{P}}$ (resp., $\pi \in G_{\mathcal{P}} \times \{I, \phi\}$) such that $C_1(x) = C_2(\pi(x))$ for each x . A coloring is called chiral if it is not equivalent to its mirror image and called achiral otherwise.

Therefore, the edge coloring enumeration of \mathcal{P} , in terms of the standard Pólya's theory, is equivalent to determining the number of equivalent coloring classes of \mathcal{P} with the edge color set \mathcal{C}_E under the operation of $G_{\mathcal{P}}$ if chirality is included; or under the operation of $G_{\mathcal{P}} \times \{I, \phi\}$ if chirality is neglected (we refer to [17] for details).

Thus, we model the DNA polyhedral links as the following three specific types of edge colorings of \mathcal{P} to meet some specific requirements or synthesis strategies.

Model 1 Let t be the number of different types of the pre-prepared DNA single strands. Then the color set used for coloring the edges of a polyhedron \mathcal{P} is defined as

$$\mathcal{C}_E = \{\langle i, j \rangle : i \in \{1, 2, \dots, t\}, j \in \{-1, 1\}\},$$

where i represents the type of the pre-prepared strands and $j \in \{-1, 1\}$ represents one of the two opposite directions of a strand on an edge. In addition, different edges are assigned with different types of strands. \square

Remark for Model 1 In a ‘relaxed’ double-helical DNA segment, the two strands twist around the helical axis once every 10.4–10.5 base pairs of sequence, i.e., the twisting number is proportional to the length of the double strand. For the ‘un-relaxed’ state, a DNA double strand of a given length can have various twisting numbers under different twist strains taken by enzymes. This case can be treated simply by regarding the strands with different twisting numbers as different types of strands. Therefore, Model 1 is still available for modeling this requirement. In addition, to simplify our discussion we do not distinguish the two twisting patterns. \square

In the following models, we will consider the general case in which DNA double strands on edges are not necessarily different. Moreover, the twisting number and the twisting pattern are taken into account.

Model 2 Let t_1 and t_2 be the number of different types of the symmetric and non-symmetric single strands, respectively. Here, for the notion ‘symmetric’ we mean that the base sequence of the DNA strand is symmetric. Let n be the maximum limit of the twisting number on each edge. Then the color set used for coloring the edges of a polyhedron \mathcal{P} is defined as

$$\mathcal{C}_E = \{ \langle i, j, h \rangle : i \in \{1, 2, \dots, t_1 + t_2\}, j \in \{-n, \dots, -1, 0, 1, \dots, n\}, h \in \{-1, 1\} \}$$

where

- (1). i represents a type of the symmetric single strands if $1 \leq i \leq t_1$ or the non-symmetric single strands if $t_1 + 1 \leq i \leq t_1 + t_2$;
- (2). j represents the twisting number in which the positive sign and the negative sign represent the clockwise pattern and anti-clockwise pattern, respectively;
- (3). $h \in \{-1, 1\}$ represents the two directions of a strand on an edge. We note that if $1 \leq i \leq t_1$ then $\langle i, j, -1 \rangle$ and $\langle i, j, 1 \rangle$ represent the same color. \square

Remark for Model 2 The parameter j is generally set to fit with the ‘un-relaxed’ state in which DNA double strands can have various twisting numbers. For ‘relaxed’ state, we may simply set $j = 1$ for clockwise pattern and $j = -1$ for anti-clockwise pattern. Moreover, we note that the two patterns are chiral, i.e., a clockwise pattern is the antipode of an anti-clockwise pattern under the operation of a mirror reflection and vice versa. Since the two single strands on an edge are determined by each other, we only consider one of the two single strands on an edge. Therefore, $\{1, 2, \dots, t_1 + t_2\}$ represents only the types of those single strands in which no two strands are complementary. \square

Model 3 This model is the same as Model 2 with only one additional constraint: the total sum of the twisting numbers on edges is a constant k . \square

Remark for Model 3 This model comes from the fact that, in some cases, the twists on an edge may ‘move’ to another edge through a certain type of the interlocked patterns (e.g., the Holliday junction [25,27] or the T -linkage [26]) at a vertex of the polyhedron. When such movement happens, though the twisting numbers on the relevant edges may change, the sum of twisting numbers of all the edges will keep to be a constant. In particular, the twists of clockwise pattern and anti-clockwise pattern will counteract to each other when twists movement happens.

3 Discussions, results and examples

3.1 Model 1

Since the types of strands on edges are pairwise different and each strand has two possible directions, \mathcal{P} has exactly $2^\varepsilon t(t-1)\cdots(t-\varepsilon+1)$ different edge colorings in total, where ε is the number of edges in \mathcal{P} . Moreover, each coloring is equivalent to exactly $|G_{\mathcal{P}}|$ (the order of $G_{\mathcal{P}}$) colorings of \mathcal{P} under the operation of the group $G_{\mathcal{P}}$. Therefore, the number of equivalent edge coloring classes of \mathcal{P} equals

$$n_{\mathcal{P}}(t) = \frac{2^\varepsilon t(t-1)\cdots(t-\varepsilon+1)}{|G_{\mathcal{P}}|} \quad (1)$$

if chirality is included, i.e., each chiral pair of polyhedral links is separately counted.

Now we consider the case when chirality is neglected, i.e., each chiral pair of polyhedral links is counted just once. Let v be a vertex of \mathcal{P} and let the edges incident to v be assigned with the colors c_1, c_2, \dots, c_d in the clockwise order by an edge coloring C . Then in the mirror image of \mathcal{P} , these colors are mapped to be in the anticlockwise order, i.e., the colors of the edges incident to v in the mirror image are assigned with the colors c_d, \dots, c_2, c_1 . We notice that c_1, c_2, \dots, c_d are pairwise distinct. This means that the coloring C restricted on the edges incident to v cannot be transferred to that of its mirror image. Therefore, C is chiral. Thus, if chirality is neglected then the number of different polyhedral links is exactly the half of $n_{\mathcal{P}}(t)$.

Example 1 Consider the DNA tetrahedral link synthesized by Goodman et al. [21] in which six types of DNA strands are pre-prepared, i.e., $t = 6$. Then, by (1) we have $n_{\mathcal{P}}(6) = 3840$ if chirality is included.

3.2 Model 2

Let π be a permutation on the edge set induced by a rotation or a mirror reflection of the polyhedron \mathcal{P} . Let $O = e_1 e_2, \dots, e_l$ be a cycle of π and let u_i, v_i be the two end vertices of the edge $e_i, i = 1, 2, \dots, l$. With no loss of generality, we assume that $\pi(u_i) = u_{i+1}, \pi(v_i) = v_{i+1}$ for $i = 1, 2, \dots, l-1$. We say that e_1 is *direction-preserved* by π if $\pi(u_1) = u_1$ and $\pi(v_1) = v_1$. Otherwise, i.e., $\pi(u_1) = v_1$ and $\pi(v_1) = u_1$, e_1 is said to be *direction-reversed*. We note that, by the symmetry of O , if e_1 is direction-preserved (resp., direction-reversed) then each edge on O is direction-preserved (resp., direction-reversed) and therefore, O is called direction-preserved (resp., direction-reversed). Let C be an edge coloring of \mathcal{P} left fixed by π . It can be seen that if O is direction-reversed then the colors of each edges on O assigned by C must be symmetric. Conversely, if O is direction-preserved then the color of edges assigned by C can be either symmetric or asymmetric.

Property 1 Let $O = e_1 e_2, \dots, e_l$ be a cycle of the permutation on edges induced by a rotation $\pi \in G_{\mathcal{P}}$. Then O is direction-reversed if and only if $\pi \neq I$ and $l = 1$.

Proof If $\pi = I$, then e_1 is clearly direction-preserved by the definition of the unity permutation. We now assume that $\pi \neq I$.

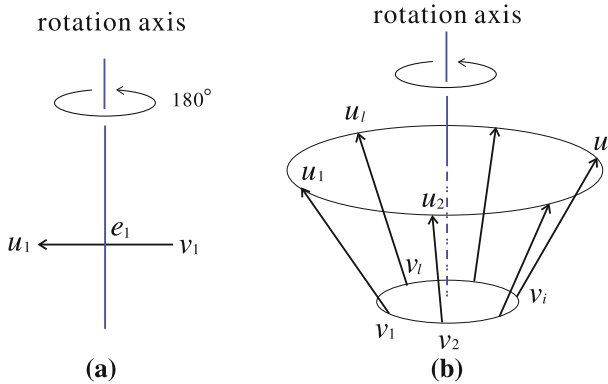


Fig. 2 Edge(s) under the operation of a rotation

If $l = 1$, i.e., $\pi(e_1) = e_1$, then we have $\pi(u_1) = u_1$ and $\pi(v_1) = v_1$ or $\pi(u_1) = v_1$ and $\pi(v_1) = u_1$. If $\pi(u_1) = u_1$ and $\pi(v_1) = v_1$, i.e., π fixes two points of the polyhedron \mathcal{P} , then π is the unity permutation since \mathcal{P} is rigid in the three dimensional space, which contradicts the assumption that $\pi \neq I$. Thus, $\pi(u_1) = v_1, \pi(v_1) = u_1$, i.e., e_1 is direction-reversed, see Fig. 2a.

Now suppose that $l > 1$. Note that π is a rotation which leaves the polyhedron \mathcal{P} invariant. Therefore, e_1, e_2, \dots, e_l , lie in the three dimensional space symmetrically around the rotation axis. Thus, the two end vertices of each edge belong to two different cycles of π , respectively, see Fig. 2b. This implies that $\pi(u_i) = u_i$ and $\pi(v_i) = v_i$, i.e., e_i is direction-preserved. This completes the proof. \square

For a permutation π on the edge set of a polyhedron \mathcal{P} and $i \in \{1, 2, \dots, \varepsilon\}$, let $b_i(\pi)$ ($\varepsilon = b_1(\pi) + 2b_2(\pi) + \dots + \varepsilon b_\varepsilon(\pi)$) be the number of cycles of length i in the disjoint cycle decomposition of π . The cycle index of π is defined by

$$\pi(x_1, x_2, \dots, x_\varepsilon) = x_1^{b_1(\pi)} x_2^{b_2(\pi)} \dots x_\varepsilon^{b_\varepsilon(\pi)}.$$

Theorem 1 *If chirality is included, then the number of the DNA polyhedral links of Model 2 is given by*

$$\begin{aligned} n(\mathcal{P}, t_1, t_2, n) &= \frac{1}{|G_{\mathcal{P}}|} \left(\beta^\varepsilon + \sum_{\pi \in G_{\mathcal{P}} \setminus I} \alpha^{b_1(\pi)} \prod_{i=2}^{\varepsilon} \beta^{b_i(\pi)} \right) \\ &= \frac{1}{|G_{\mathcal{P}}|} \left(\beta^\varepsilon + \sum_{\pi \in G_{\mathcal{P}} \setminus I} \pi(\alpha, \beta, \dots, \beta) \right), \end{aligned}$$

where $\alpha = t_1(2n + 1)$ and $\beta = (t_1 + t_2)(2n + 1)$.

Proof By Burnside's lemma,

$$n(\mathcal{P}, t_1, t_2, n) = \frac{1}{|G\mathcal{P}|} \sum_{\pi \in G\mathcal{P}} \Psi(\pi),$$

where $\Psi(\pi)$ is the number of the edge colorings C left fixed by π [29].

We now determine the number $\Psi(\pi)$. Let $O = e_1e_2, \dots, e_l$ be a cycle of π . Then by the Pólya's counting theory [29], the colors of all the edges of O assigned by C are the same with $C(e_1)$ and is therefore called the color of the cycle O assigned by C .

First assume that $\pi = I$, i.e., each cycle is formed by one edge. Then by Property 1, each cycle is direction-preserved. Therefore, the color of each cycle, i.e., each edge, assigned by C can be either symmetric or asymmetric. This means that the number of colorings left fixed by π is exactly $|\mathcal{C}_E|^\varepsilon = [(t_1 + 2t_2)(2n + 1)]^\varepsilon$ since the number of cycles of π , i.e., the number of edges, is ε .

Now we assume that $\pi \neq I$. Let $O = e_1e_2, \dots, e_l$ be a cycle of π . If $l = 1$ then, by Property 1, O is direction-reversed. Thus, if a coloring C is left fixed by π then only symmetric colors can be used for the edges on O . The number of such colors is exactly $t_1(2n + 1)$.

If $l > 1$ then, again by Property 1, O is direction-preserved. That is, any colors can be used for O . The number of such colors is clearly $(t_1 + 2t_2)(2n + 1)$.

From the above argument we can conclude that

$$\Psi(\pi) = [(t_1 + 2t_2)(2n + 1)]^\varepsilon$$

if $\pi = I$; or

$$\Psi(\pi) = [t_1(2n + 1)]^{b_1(\pi)} \prod_{i=2}^{\varepsilon} [(t_1 + 2t_2)(2n + 1)]^{b_i(\pi)}$$

if $\pi \neq I$. This completes our proof. \square

Let $\pi \in \phi G$, where ϕ is an arbitrary mirror reflection of \mathcal{P} . For $i \in \{1, 2, \dots, \varepsilon\}$, let

- (1). $\alpha_i = t_1(2n + 1)$ if i is even and $\alpha_i = t_1$ otherwise;
- (2). $\beta_i = (t_1 + 2t_2)(2n + 1)$ if i is even and $\beta_i = t_1 + 2t_2$ otherwise;
- (3). $r_i(\pi)$ and $p_i(\pi)$ be the numbers of direction-reversed and direction-preserved cycles of length i in π , respectively.

Theorem 2 *If chirality is neglected, then the number of the DNA polyhedral links of Model 2 is given by*

$$n^*(\mathcal{P}, t_1, t_2, n) = \frac{1}{2}n(\mathcal{P}, t_1, t_2, n) + \frac{1}{2|G\mathcal{P}|} \sum_{\pi \in \phi G\mathcal{P}} \prod_{i=1}^{\varepsilon} \alpha_i^{r_i(\pi)} \beta_i^{p_i(\pi)}.$$

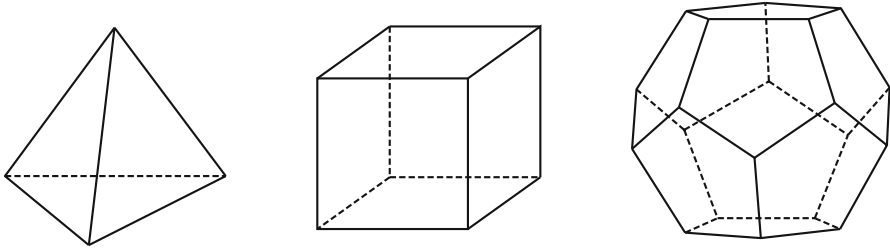


Fig. 3 The tetrahedron \mathcal{P}_4 (left), cube \mathcal{P}_6 (middle) and dodecahedron \mathcal{P}_{12} (right)

Proof Again by Burnside’s lemma,

$$\begin{aligned} n^*(\mathcal{P}, t_1, t_2, N) &= \frac{1}{|\{I, \phi\} \times G_{\mathcal{P}}|} \sum_{\pi \in \{I, \phi\} \times G_{\mathcal{P}}} \Psi(\pi) \\ &= \frac{1}{2|G_{\mathcal{P}}|} \sum_{\pi \in G_{\mathcal{P}}} \Psi(\pi) + \frac{1}{2|G_{\mathcal{P}}|} \sum_{\pi \in \phi G_{\mathcal{P}}} \Psi(\pi) \\ &= \frac{1}{2}n(\mathcal{P}, t_1, t_2, n) + \frac{1}{2|G_{\mathcal{P}}|} \sum_{\pi \in \phi G_{\mathcal{P}}} \Psi(\pi). \end{aligned}$$

Let C be a coloring left fixed by $\pi \in \phi G_{\mathcal{P}}$ and let $O = e_1e_2, \dots, e_l$ be a cycle of π . Recall that if O is direction-reversed by π then the color of O assigned by C must be symmetric and if O is direction-preserved then the color of O can be either symmetric or asymmetric. This implies that if O is direction-reversed then the possible colors $c = \langle i, j, k \rangle$ that can be used for O must satisfy $1 \leq i \leq t_1$ and if O is direction-preserved then i can be any integer with $1 \leq i \leq t_1 + t_2$.

On the other hand, noticing that $\pi \in \phi G_{\mathcal{P}}$ is a mirror reflection, we have

$$C(e_1) = \overline{C(e_2)} = C(e_3) = \overline{C(e_4)} = \dots,$$

where $\overline{C(e_i)}$ represents the mirror image of $C(e_i)$ under the operation of π . Thus, if l is odd and $C(e_1)$ is chiral, i.e., $C(e_1) \neq \overline{C(e_1)}$, then $C(e_1) = \overline{C(e_2)} = C(e_3) = \overline{C(e_4)} = \dots = C(e_l) = \overline{C(e_1)}$, which is a contradiction. In other words, no chiral color can be used for an odd cycle of π . Since the clockwise pattern and anti-clockwise pattern with the same twisting number are chiral pair (i.e., mirror images of each other), only those colors $c = \langle i, j, k \rangle$ with twisting number $j = 0$ can be possibly used for an odd cycle.

From the above discussion, we can now conclude that:

- (1). If O is direction-reversed and l is even (resp., l is odd) then the number of colors can be used for O is $t_1(2n + 1)$ (resp., t_1);
- (2). If O is direction-preserved and l is even (resp., l is odd) then the number of colors can be used for O is $(t_1 + 2t_2)(2n + 1)$ (resp., $t_1 + 2t_2$).

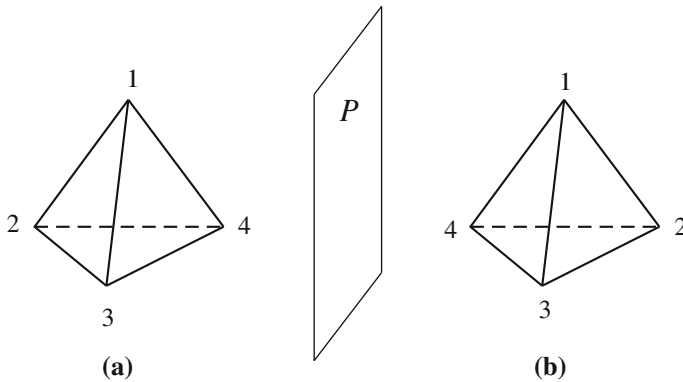


Fig. 4 The tetrahedron (*left*) and its mirror image (*right*) with respect to the plane P

Therefore,

$$\Psi(\pi) = \prod_{i=1}^{\varepsilon} \alpha_i^{r_i(\pi)} \beta_i^{p_i(\pi)},$$

which completes our proof. \square

As an application of Theorems 1 and 2, in the following we deduce the explicit enumerating expressions of Model 2 for the 3-vertex-regular Platonic polyhedra (Plato's solids): i.e., each vertex has degree 3 and all the faces are equal regular polygons. From geometric theory, there are only three such polyhedrons, i.e., the tetrahedron \mathcal{P}_4 , the cube \mathcal{P}_6 and the dodecahedron \mathcal{P}_{12} [28], as shown in Fig. 3.

Example 2 The tetrahedron \mathcal{P}_4 .

Let the vertices of \mathcal{P}_4 be numbered by 1,2,3 and 4, as depicted in Fig. 4a. Then the 12 edge permutations induced by all the 12 rotations of \mathcal{P}_4 , in form of cycle decomposition of edges, are

$$\begin{aligned} & I, & & ([12][13][14])([23][34][42]), \\ & ([12][14][13])([23][42][34]), & & ([12][23][31])([41][42][43]), \\ & ([12][31][23])([41][43][42]), & & ([13][34][41])([21][23][24]), \\ & ([13][41][34])([21][24][23]), & & ([12][24][41])([31][32][34]), \\ & ([12][41][24])([31][34][32]), & & ([12])([34])([14][23])([13][24]), \\ & ([14])([23])([13][24])([12][34]), & & ([13])([24])([14][23])([12][34]), \end{aligned}$$

where $[ij]$ represents the edge ij . Then by Theorem 1, we have

$$\begin{aligned} n(\mathcal{P}_4, t_1, t_2, n) &= \frac{1}{12} (\beta^6 + 3\alpha^2\beta^2 + 8\beta^2) \\ &= \frac{1}{12} \left((t_1+2t_2)^6 (2n+1)^6 + 3t_1^2 (t_1+2t_2)^2 (2n+1)^4 + 8(t_1+2t_2)^2 (2n+1)^2 \right). \end{aligned}$$

For the number $n^*(\mathcal{P}_4, t_1, t_2, n)$, we choose ϕ as the mirror reflection with respect to the plane P , as illustrated in Fig. 4. Therefore, in form of cycle decomposition of vertices, we have $\phi = (24)$. On the other hand, all the 12 permutations of the mirror image of \mathcal{P}_4 (see Fig. 4b) on vertices are $I, (234), (243), (134), (143), (124), (142), (123), (132), (12)(34), (14)(23), (13)(24)$.

If $\rho = I$ then the edge cycle decomposition of $\pi = \phi\rho$ is

$$([12][14])([13])([23][43])([24]).$$

Moreover, by the definitions of direction-reversed and direction-preserved cycle we can check that the cycle $([24])$ is direction-reversed since $\pi(2) = 4$ and $\pi(4) = 2$, while all the other three cycles are direction-preserved. Thus,

$$\prod_{i=1}^{\varepsilon} \alpha_i^{r_i(\pi)} \beta_i^{p_i(\pi)} = \alpha_1 \beta_1 \beta_2^2 = t_1(t_1 + 2t_2)^3(2n + 1)^2.$$

Similarly, if $\rho = (14)(23)$ then the edge cycle decomposition of $\pi = \phi\rho$ is

$$([12][41][34][23])([24][13]),$$

in which the cycle $([24][13])$ is direction-reversed while the other is direction-preserved. Therefore,

$$\prod_{i=1}^{\varepsilon} \alpha_i^{r_i(\pi)} \beta_i^{p_i(\pi)} = \alpha_2 \beta_4 = t_1(t_1 + 2t_2)(2n + 1)^2.$$

In this way, we can calculate

$$\begin{aligned} \sum_{\pi \in \phi G_{\mathcal{P}_4}} \prod_{i=1}^{\varepsilon} \alpha_i^{r_i(\pi)} \beta_i^{p_i(\pi)} &= 6\alpha_1 \beta_1 \beta_2^2 + 6\alpha_2 \beta_4 \\ &= 6t_1(t_1 + 2t_2)^3(2n + 1)^2 + 6t_1(t_1 + 2t_2)(2n + 1)^2. \end{aligned}$$

Then by Theorem 2 we have

$$\begin{aligned} n^*(\mathcal{P}_4, t_1, t_2, n) &= \frac{1}{24} \left[(\beta^6 + 3\alpha^2\beta^2 + 8\beta^2) + (6\alpha_1\beta_1\beta_2^2 + 6\alpha_2\beta_4) \right] \\ &= \frac{1}{24} \left[(t_1 + 2t_2)^6(2n + 1)^6 + 3t_1^2(t_1 + 2t_2)^2(2n + 1)^4 + 8(t_1 + 2t_2)^2(2n + 1)^2 \right. \\ &\quad \left. + 6t_1(t_1 + 2t_2)^3(2n + 1)^2 + 6t_1(t_1 + 2t_2)(2n + 1)^2 \right]. \end{aligned}$$

When $t_1 = 0, t_2 = 1$ and $n = 0$ we have

$$n(\mathcal{P}_4, 0, 1, 0) = 8, n^*(\mathcal{P}_4, 0, 1, 0) = 4.$$

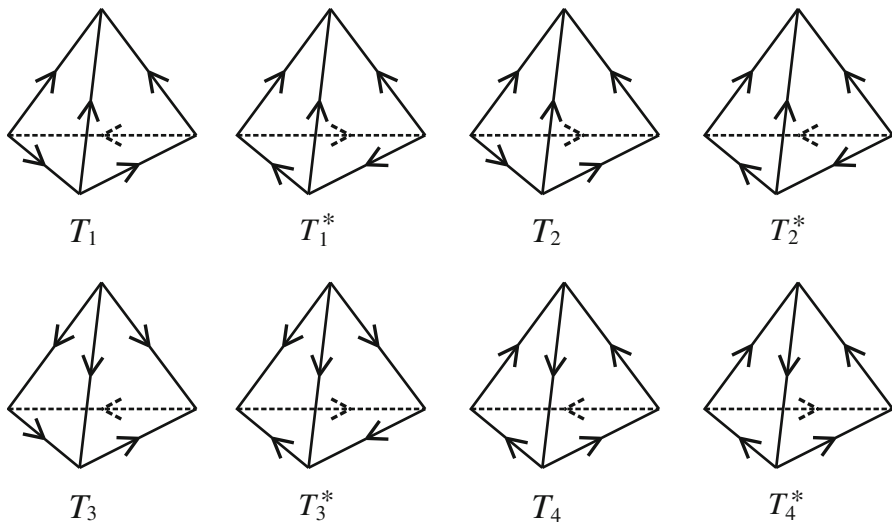


Fig. 5 The 8 tetrahedron links in which T_i and T_i^* are chiral pair, $i = 1, 2, 3, 4$

The corresponding 8 tetrahedral links are depicted as in Fig. 5, all of which are chiral.

By the same discussion as for the tetrahedron, we can get the numbers for \mathcal{P}_6 and \mathcal{P}_{12} as the following two examples.

Example 3 The cube \mathcal{P}_6 .

$$n(\mathcal{P}_6, t_1, t_2, n) = \frac{1}{24} (\beta^{12} + 8\beta^4 + 6\beta^3 + 3\beta^6 + 6\alpha^2\beta^5),$$

$$n^*(\mathcal{P}_6, t_1, t_2, n) = \frac{1}{48} \left[(\beta^{12} + 8\beta^4 + 6\beta^3 + 3\beta^6 + 6\alpha^2\beta^5) \right. \\ \left. + (3\alpha_1^4\beta_2^4 + 6\beta_1^2\beta_2^5 + \beta_2^6 + 6\beta_4^3 + 8\beta_6^2) \right].$$

Example 4 The dodecahedron \mathcal{P}_{12} .

$$n(\mathcal{P}_{12}, t_1, t_2, n) = \frac{1}{60} (\beta^{30} + 20\beta^{10} + 24\beta^6 + 15\alpha^2\beta^{14}),$$

$$n^*(\mathcal{P}_{12}, t_1, t_2, n) = \frac{1}{120} \left[(\beta^{30} + 20\beta^{10} + 24\beta^6 + 15\alpha^2\beta^{14}) \right. \\ \left. + (\beta_2^{15} + 24\beta_{10}^3 + 20\beta_6^5 + 15\alpha_1^2\beta_{14}^2) \right].$$

3.3 Model 3

Let $n_k(\mathcal{P}, t_1, t_2, n)$ and $n_k^*(\mathcal{P}, t_1, t_2, n)$ denote the numbers of DNA polyhedral links in Model 3 in which chirality is included and neglected, respectively. Let $f(x)$ and

$f^*(x)$ be the generating functions of $n_k(\mathcal{P}, t_1, t_2, n)$ and $n_k^*(\mathcal{P}, t_1, t_2, n)$, respectively:

$$f(x) = \sum_{k=1}^{\infty} n_k(\mathcal{P}, t_1, t_2, n)x^k \text{ and } f^*(x) = \sum_{k=1}^{\infty} n_k^*(\mathcal{P}, t_1, t_2, n)x^k.$$

Theorem 3

$$f(x) = \frac{1}{|G\mathcal{P}|} \left[\beta_1(x)^\varepsilon + \sum_{\pi \in G\mathcal{P} \setminus I} \alpha(x)^{b_1(\pi)} \prod_{i=2}^{\varepsilon} \beta_i(x)^{b_i(\pi)} \right],$$

where $\beta_i(x) = (t_1 + 2t_2) \sum_{j=-n}^n x^{ij}$, $i = 1, 2, \dots, \varepsilon$, $\alpha(x) = t_1 \sum_{j=-n}^n x^j$.

Proof Assume firstly that $\pi = I$. Let $k_1 + k_2 + \dots + k_\varepsilon = k$ with $-n \leq k_i \leq n$. Then the number of colorings left fixed by π with twisting number k_i on the i th edge is $(t_1 + 2t_2)^\varepsilon$. Thus, the number of colorings left fixed by π with the total twisting number k (the sum of all the twisting numbers on edges) is exactly

$$\sum_{k_1+k_2+\dots+k_\varepsilon=k} (t_1 + 2t_2)^\varepsilon = P(k)(t_1 + 2t_2)^\varepsilon,$$

where $P(k)$ is the number of integer solutions of the equation

$$x_1 + x_2 + \dots + x_\varepsilon = k$$

with $-n \leq x_i \leq n$. Notice that $P(k)$ is exactly the coefficient of x^k in

$$\left(x^{-n} + \dots + x^{-1} + 1 + x + \dots + x^n \right)^\varepsilon.$$

We now assume that $\pi \neq I$. Let $O = e_1e_2, \dots, e_l$ be a cycle of length l . Since the twisting numbers of the edges on O must be the same, say i , the total number of twistings of O is il . The remaining discussion is analogous to that for the case $\pi = I$ and is omitted here. This completes the proof. □

Theorem 4

$$f^*(x) = \frac{1}{2} f(x) + \frac{1}{2|G\mathcal{P}|} \sum_{\pi \in \phi G\mathcal{P}} \prod_{i=1}^{\varepsilon} \alpha_i(x)^{r_i(\pi)} \beta_i(x)^{p_i(\pi)},$$

where $\alpha_i(x) = t_1 \sum_{j=-n}^n x^{ij}$ if i is even and $\alpha_i(x) = t_1$ otherwise; $\beta_i(x) = (t_1 + 2t_2) \sum_{j=-n}^n x^{ij}$ if i is even and $\beta_i(x) = (t_1 + 2t_2)$ otherwise; $r_i(\pi)$, $p_i(\pi)$ are defined as for Theorem 2.

Proof The proof is the same as that for Theorems 2 and 3 by replacing α and β by $\alpha_i(x)$ and $\beta_i(x)$, respectively. □

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