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Enumerating the total colorings of a polyhedron and application to polyhedral links

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Abstract In this paper we consider the enumeration problem of a particular three-dimensional molecular or chemical compound system which has a polyhedral frame where the vertices, edges and faces represent 'units' such as atoms, bonds, ligands, polymers, or other objects of chemical interests. In this system, chirality is also taken into account. This enumeration problem is mathematically modeled as the 'total coloring' enumeration problem of a polyhedron: i.e., the number of ways to color all the vertices, edges and faces of the polyhedron by using three or more corresponding color sets, in which some colors may be chiral. We establish a general formula for this enumeration problem by extending the fundamental version of Pólya's enumeration theorem. In particular, we apply this technique to the enumeration problem of polyhedral links which have received special attention from biochemists, mathematical chemists and mathematicians over the past two decades.

Keywords Total coloring · Polyhedral link · Catenane · Enumeration

1 Introduction

Motivated by the chemical isomer problem, in the 1930s Pólya [1] developed a powerful combinatorial theory for the enumeration of symmetry-mediated equivalence

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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. Beyond the formal mathematical theory, Pólya also applied his theory to a few chemical problems and, in particular, the classic problem of alkane isomer enumeration which was recently reviewed by Fujita in his survey paper [2]. Following Pólya there have been further refinements for this chemical problem in a large number of papers. Some earlier results can be found, for example in [3–10] and the references cited therein. In particular, the pre-1986 work on this problem was nicely reviewed by Read [11] who also gave a translation (made by D. Aeppli) of the Pólya's foundational paper [1].

Pólya's enumeration theory has now developed to be a universal tool in dealing with the enumeration problems of various systems, in addition to alkane isomers and its original version. In 1992, Fujita [12] considered in detail many theoretical extensions (primarily concerning chirality and symmetry questions, not only for isomers, but also for reaction processes). In his series of articles [13–17], Fujita also considered the alkanes as stereoisomers and therefore, developed the unit-subduced-cycle-index (USCI) approach by means of an algebraic derivation as well as by means of a diagrammatical formulation. Yeh considered the asymmetric dendrimers [18], the acyclic chemical compounds generated by asymmetric building blocks. The earlier works beyond the acyclic compounds are discussed in [9] and after this, a lot of works were also established for various cyclic molecular systems, e.g., the benzenoid hydrocarbons and geometrical non-planar benzenoid hydrocarbons [19–22], conjugated polyene hydrocarbons [23], fluorantenoids and fluorenoids (catacondensed systems) [24], hererofullerenes [25], polyphenacenes [26,27]. In [28], Bytautas and Klein extended this standard combinatorial enumerative techniques to compute average values of certain graph-theoretic invariants.

In this paper we consider 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, in which chirality is taken into account. This enumeration problem is mathematically modeled as the 'total coloring' enumeration problem of a polyhedron. Here, for the notion 'total coloring' we mean to color all the vertices, edges and faces of the polyhedron by using three or more corresponding color sets. For chemical interests, a color may represent an atom, a bond, a ligand, a polymer, or other object and therefore, may be chiral or achiral. Thus, the number of the ways to totally color a polyhedron, in terms of the standard Pólya's theory, could be represented as the number of equivalence classes of the total colorings under the operation of the point group generated by the rotations which leave the polyhedron invariant if chirality is included; or the reflection group generated by the rotations and the mirror reflections which leave the polyhedron invariant if chirality is neglected.

In the second section, we establish a general formula for the 'total coloring' enumeration problem by extending the fundamental version of Pólya's enumeration theorem. This enumeration model is expected to have various applications in counting three dimensional chemical compounds or other three dimensional objects. In particular, we apply this technique to the enumeration problem of polyhedral links which have received special attention from biochemists, mathematical chemists and mathematicians over the past two decades [29–35].

In the third section, by applying the enumeration model obtained in the second section, we give explicit expressions for the number of certain types of polyhedral links belonging to the family of '3-cross-curve and double-twist-line covering' polyhedral links. This concept was proposed by Qiu [32] inspired by the recent advances on the study of catenanes, e.g., [29–31,35].

2 Total colorings of the polyhedrons

For a polyhedron $\mathcal{P}$, we denote by V, E and F its vertex set, edge set and face set, respectively. For convenience, a vertex or edge or face of $\mathcal{P}$ will be generally called an element, if no confusion can occur. Correspondingly, V or E or F is generally called an element set and denoted by W. A total coloring of $\mathcal{P}$ with the vertex color set $\mathscr{C}_v$, edge color set $\mathscr{C}_e$ and face color set $\mathscr{C}_f$ is a mapping from V, E and F to $\mathscr{C}_v, \mathscr{C}_e$ and $\mathscr{C}_f$, i.e., an assignment of each vertex, each edge and each face of $\mathcal{P}$ with a color in $\mathscr{C}_v, \mathscr{C}_e$ and $\mathscr{C}_f$, respectively. We note that a color may be chiral or achiral.

It is well known that a rotation or a mirror reflection π which leaves $\mathcal{P}$ invariant induces a permutation on an element set W: i.e., $\pi|_W : W \to W$ is a bijection. So in the following, we do not distinguish between a rotation or a mirror reflection and its induced permutation. From symmetric group theory, all rotations which leave $\mathcal{P}$ invariant form a group. We denote this group by $G_\mathcal{P}$ here after. Moreover, $G_\mathcal{P} \times \{I, \phi\}$ also forms a permutation group acting on each element set W [36], where I is the unity permutation and ϕ is an arbitrary mirror reflection that leaves $\mathcal{P}$ invariant. We note that, for any $g \in G_\mathcal{P}$, ϕg is also a mirror reflection of $\mathcal{P}$ [12,36]. This means that a chiral color will be transferred to be its antipode [12,36] (i.e., its mirror image) under the operation of ϕg for any $g \in G_\mathcal{P}$ while an achiral color does not change.

For a total coloring C and an element u, we denote by $C(u)$ the color of u assigned by C. Two total 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 $C_1(u) = C_2(\pi(u))$ for all elements u. A total coloring of $\mathcal{P}$ is called chiral if it is not equivalent to its mirror image and called achiral otherwise.

Therefore, the total 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 color sets $\mathscr{C}_v, \mathscr{C}_e$ and $\mathscr{C}_f$ 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 denote this number by $n(\mathcal{P}, \mathscr{C}_v, \mathscr{C}_e, \mathscr{C}_f)$ if chirality is included or $n^*(\mathcal{P}, \mathscr{C}_v, \mathscr{C}_e, \mathscr{C}_f)$ if chirality is neglected.

Before continuing our discussion, let's recall some elementary concepts of the classic Pólya's and Burnside's enumeration theory. For a permutation g of a permutation group G on an m-elements set S, it is well known that g can be split into disjoint cycles in a unique way. If g splits into b_1 disjoint cycles of length 1, b_2 disjoint cycles of length $2, \ldots, b_m$ disjoint cycles of length m ($m = b_1 + 2b_2 + \cdots + mb_m$), then we form the product $x_1^{b_1} x_2^{b_2} \cdots x_m^{b_m}$. The cycle index of G is therefore defined by

$$P_G(x_1, x_2, \ldots, x_m) = \frac{1}{|G|} \sum_{g \in G} x_1^{b_1} x_2^{b_2} \cdots x_m^{b_m}. \quad (1)$$

Consider the number of equivalent coloring classes of S using p colors under the operation of the group G. Burnside's lemma tells us this number is

$$n(S, G) = \frac{1}{|G|} \sum_{g \in G} \Psi(g)$$

or, in terms of Pólya's theorem,

$$n(S, G) = P_G(p, p, \ldots, p),$$

where $\Psi(g)$ is the number of the colorings left fixed by g [37].

We now return to the numbers $n(\mathcal{P}, \mathscr{C}_v, \mathscr{C}_e, \mathscr{C}_f)$ and $n^*(\mathcal{P}, \mathscr{C}_v, \mathscr{C}_e, \mathscr{C}_f)$. By (1), we may write the cycle index of $G_{\mathcal{P}}$ as the form

$$\begin{aligned} &P_{G_{\mathcal{P}}}(x_{11}, \ldots, x_{1|V|}; x_{21}, \ldots, x_{2|E|}; x_{31}, \ldots, x_{3|F|}) \\ &= \frac{1}{|G_{\mathcal{P}}|} \sum_{g \in G_{\mathcal{P}}} \prod_{i=1,2,3} \prod_{j=1,2,\ldots,\sigma_i} x_{ij}^{b_{ij}} \end{aligned}$$

where b_{1j}, b_{2j} and b_{3j} ($j \in \{1, 2, \ldots\}$) are the number of cycles of length j in g restricted to V, E and F, respectively, and $\sigma_1 = |V|, \sigma_2 = |E|, \sigma_3 = |F|$.

For $g \in G_{\mathcal{P}}$, let $\varepsilon_v(g)$ (resp., $\varepsilon_e(g)$ or $\varepsilon_f(g)$) be the number of the cycles in g restricted to V (resp., E or F). Then the number of the colorings left fixed by g is exactly equal to $\Psi(g) = \prod_{i=1,2,3} \prod_{j=1,2,\ldots,\sigma_i} x_{ij}^{b_{ij}}$ by setting $x_{1j} = |\mathscr{C}_v|, x_{2j} = |\mathscr{C}_e|, x_{3j} = |\mathscr{C}_f|$, $j = 1, 2, \ldots$, i.e.,

$$\Psi(g) = |\mathscr{C}_v|^{\varepsilon_v(g)} |\mathscr{C}_e|^{\varepsilon_e(g)} |\mathscr{C}_f|^{\varepsilon_f(g)}.$$

Thus, the following result is immediate.

Theorem 1 *If chirality is included, i.e., each pair of the chiral total colorings is separately counted, then the number of equivalent total coloring classes of $\mathcal{P}$ with vertex color set $\mathscr{C}_v$, edge color set $\mathscr{C}_e$ and face color set $\mathscr{C}_f$ is given by*

$$\begin{aligned} n(\mathcal{P}; \mathscr{C}_v, \mathscr{C}_e, \mathscr{C}_f) &= \frac{1}{|G_{\mathcal{P}}|} \sum_{g \in G_{\mathcal{P}}} |\mathscr{C}_v|^{\varepsilon_v(g)} |\mathscr{C}_e|^{\varepsilon_e(g)} |\mathscr{C}_f|^{\varepsilon_f(g)} \\ &= P_{G_{\mathcal{P}}}(\underbrace{|\mathscr{C}_v|, \ldots, |\mathscr{C}_v|}_{|V|}; \underbrace{|\mathscr{C}_e|, \ldots, |\mathscr{C}_e|}_{|E|}; \underbrace{|\mathscr{C}_f|, \ldots, |\mathscr{C}_f|}_{|F|}). \end{aligned} \tag{2}$$

□

For a color set $\mathscr{C}_h (h \in \{v, e, f\})$, we denote

$$\mathscr{C}_h^* = \mathscr{C}_h \setminus \{c : c \text{ is chiral and } c \in \mathscr{C}_h, \overline{c} \notin \mathscr{C}_h\},$$

where $\overline{c}$ is the antipode, i.e., the mirror image of c. We call the colors in $\{c : c \text{ is chiral and } c \in \mathscr{C}_h, \overline{c} \notin \mathscr{C}_h\}$ the isolate colors. For a permutation $\pi \in \phi G_{\mathcal{P}}$, let $\delta_v(\pi)$ (resp., $\delta_e(\pi)$ or $\delta_f(\pi)$) be the number of even cycles of π restricted to V (resp., E or F) and let a_v be the number of achiral colors in $\mathscr{C}_v^*$ (resp., $\mathscr{C}_e^*$ or $\mathscr{C}_f^*$). In addition, $\varepsilon_v(\pi)$ (resp., $\varepsilon_e(\pi)$ or $\varepsilon_f(\pi)$) is the number of the cycles in π restricted to V (resp., E or F).

Theorem 2 *If chirality is neglected, i.e., each pair of the chiral total colorings is counted just once, then the number of equivalent total coloring classes of $\mathcal{P}$ with vertex color set $\mathscr{C}_v$, edge color set $\mathscr{C}_e$ and face color set $\mathscr{C}_f$ is given by*

$$n^*(\mathcal{P}; \mathscr{C}_v, \mathscr{C}_e, \mathscr{C}_f) = n(\mathcal{P}; \mathscr{C}_v, \mathscr{C}_e, \mathscr{C}_f) - \frac{1}{2} n\left(\mathcal{P}; \mathscr{C}_v^*, \mathscr{C}_e^*, \mathscr{C}_f^*\right) + \frac{1}{2|G_{\mathcal{P}}|} \sum_{\pi \in \phi G_{\mathcal{P}}} \prod_{h \in \{v,e,f\}} a_h^{\varepsilon_h(\pi) - \delta_h(\pi)} |\mathscr{C}_h^*|^{\delta_h(\pi)} \tag{3}$$

(here we note that $a_h^0 = 1$ for any $a_h \geq 0$).

Proof We first claim that

$$n^*(\mathcal{P}; \mathscr{C}_v, \mathscr{C}_e, \mathscr{C}_f) = n(\mathcal{P}; \mathscr{C}_v, \mathscr{C}_e, \mathscr{C}_f) - n\left(\mathcal{P}; \mathscr{C}_v^*, \mathscr{C}_e^*, \mathscr{C}_f^*\right) + n^*\left(\mathcal{P}; \mathscr{C}_v^*, \mathscr{C}_e^*, \mathscr{C}_f^*\right).$$

In fact, the total colorings C's of $\mathcal{P}$ can be divided into two parts:
Part 1. C does not use any isolate color. The number of such total colorings is clearly equal to $n^*\left(\mathcal{P}; \mathscr{C}_v^*, \mathscr{C}_e^*, \mathscr{C}_f^*\right)$.
Part 2. C uses at least one isolate color. In this case, since the mirror image of an isolate color cannot be used in any coloring, the mirror image of C is not a coloring of $\mathcal{P}$. Thus, the equivalent classes of such colorings are obtained depending only under the operation of the permutation group $G_{\mathcal{P}}$ and therefore, the number of equivalent classes of such colorings is equal to $n(\mathcal{P}; \mathscr{C}_v, \mathscr{C}_e, \mathscr{C}_f) - n\left(\mathcal{P}; \mathscr{C}_v^*, \mathscr{C}_e^*, \mathscr{C}_f^*\right)$. Our claim follows.

From the above argument, we need only to prove that $n^*\left(\mathcal{P}; \mathscr{C}_v^*, \mathscr{C}_e^*, \mathscr{C}_f^*\right)$ equals

$$\frac{1}{2} n\left(\mathcal{P}; \mathscr{C}_v^*, \mathscr{C}_e^*, \mathscr{C}_f^*\right) + \frac{1}{2|G_{\mathcal{P}}|} \sum_{\pi \in \phi G_{\mathcal{P}}} \prod_{h \in \{v,e,f\}} a_h^{\varepsilon_h(\pi) - \delta_h(\pi)} |\mathscr{C}_h^*|^{\delta_h(\pi)}.$$

By Burnside's lemma [37],

$$\begin{aligned} n^*\left(\mathcal{P}; \mathscr{C}_v^*, \mathscr{C}_e^*, \mathscr{C}_f^*\right) &= \frac{1}{2|G_{\mathcal{P}}|} \sum_{\pi \in G_{\mathcal{P}} \times \{I, \phi\}} \Psi(\pi) \\ &= \frac{1}{2|G_{\mathcal{P}}|} \sum_{\pi \in G_{\mathcal{P}}} \Psi(\pi) + \frac{1}{2|G_{\mathcal{P}}|} \sum_{\pi \in \phi G_{\mathcal{P}}} \Psi(\pi). \end{aligned}$$

Let $\pi \in G_{\mathcal{P}} \times \{I, \phi\}$. Consider the number $\Psi(\pi)$ of the total colorings left fixed by π.

Case 1. $\pi \in G_{\mathcal{P}}$.

In this case the number of the colorings left fixed by π is exactly equal to $\Psi(\pi) = |\mathscr{C}_v^*|^{\varepsilon_v(\pi)}|\mathscr{C}_e^*|^{\varepsilon_e(\pi)}|\mathscr{C}_f^*|^{\varepsilon_f(\pi)}$ and therefore,

$$\frac{1}{2|G_{\mathcal{P}}|}\sum_{\pi \in G_{\mathcal{P}}} \Psi(\pi) = \frac{1}{2}n\left(\mathcal{P}; \mathscr{C}_v^*, \mathscr{C}_e^*, \mathscr{C}_f^*\right)$$

by the same argument as that for Theorem 1.

Case 2. $\pi \in \phi G_{\mathcal{P}}$.

Let $\mathscr{C}_v^a$ denote the set of the a_v achiral colors in $\mathscr{C}_v^*$. Let C be a total coloring left fixed by π and let $v_1 \in V$. Then there is a cycle of π, say $v_1 v_2 \cdots v_l$, which contains v_1 and moreover, $v_1, v_2, \ldots, v_l \in V$.

First assume that l is odd. If $C(v_1)$ is chiral then $C(v_1) = \overline{C(v_2)} = C(v_3) = \overline{C(v_4)} = \cdots = C(v_l) = \overline{C(v_1)}$, which is a contradiction since $C(v_1) \neq \overline{C(v_1)}$, where $\overline{C(v_i)}$ represents the mirror image of $C(v_i)$. This implies that $C(v_1)$ is achiral and therefore, $C(v_1) = C(v_2) = \cdots = C(v_l) \in \mathscr{C}_v^a$. In other words, there are exactly $|\mathscr{C}_v^a| = a_v$ colors that can be chosen for the cycle $v_1 v_2 \cdots v_l$.

Now assume that l is even. In this case, each color in $\mathscr{C}_v^*$ can be used for the cycle $v_1 v_2 \cdots v_l$, i.e., there are $|\mathscr{C}_v^*|$ colors that can be chosen for $v_1 v_2 \cdots v_l$.

From the above discussion we can conclude that:

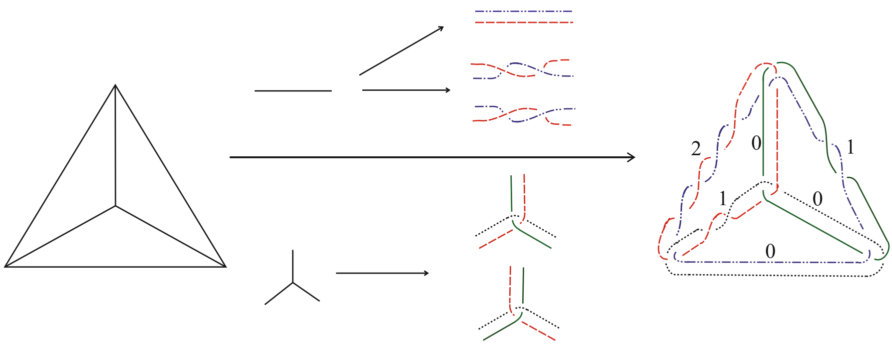
1. If $\delta_v(\pi) = \varepsilon_v(\pi)$, then all the cycles of π restricted to V have even length and, therefore, any color in $\mathscr{C}_v^*$ can be used. Thus the number of the colorings left fixed by π for V is $|\mathscr{C}_v^*|^{\varepsilon_v(\pi)}$. On the other hand, we notice that $\delta_v(\pi) = \varepsilon_v(\pi)$ also implies that $a_v^{\varepsilon_v(\pi)-\delta_v(\pi)}|\mathscr{C}_v^*|^{\delta_v(\pi)} = |\mathscr{C}_v^*|^{\varepsilon_v(\pi)}$ since $a_v^{\varepsilon_v(\pi)-\delta_v(\pi)} = a_v^0 = 1$ for any $a_v \geq 0$, as desired.
2. If $\delta_v(\pi) < \varepsilon_v(\pi)$, then π has an odd cycle in V. So if $a_v = 0$ then no color can be used for this odd cycle. This implies that no coloring is left fixed by π, i.e., $\Psi(\pi) = 0$. On the other hand, $a_v = 0$ and $\varepsilon_v(\pi) - \delta_v(\pi) \neq 0$ imply that $a_v^{\varepsilon_v(\pi)-\delta_v(\pi)}|\mathscr{C}_v^*|^{\delta_v(\pi)} = 0$, again as desired. Now if $a_v > 0$, then it is obvious that the number of the colorings left fixed by π for V is $a_v^{\varepsilon_v(\pi)-\delta_v(\pi)}|\mathscr{C}_v^*|^{\delta_v(\pi)}$.

The discussion for the edge set and face set are analogous, which completes our proof. □

Note 1. From Theorem 2, if π has an odd cycle in V (resp., E or F) and $\mathscr{C}_v^*$ (resp., $\mathscr{C}_e^*$ or $\mathscr{C}_f^*$) contains no achiral color, i.e., $a_v = 0$ (resp., $a_e = 0$ or $a_f = 0$), then there is no coloring left fixed by π. This can greatly simplify the calculation for the last term in (3).

3 Application to polyhedral links

A polyhedral link is mathematically modeled as a topological link based on a polyhedral skeleton in a certain 'linking-locking' pattern. In this section, we focus on



(a) **(b)** **(c)**

Fig. 1 **a** The tetrahedron. **b** Un-twisting pattern and two twisting patterns on an edge (*top*); two locking patterns at a vertex (*bottom*). **c** A 3-cross double-twist tetrahedral link, in which the number on each edge represents the number of twistings

the '3-cross-curve and double-twist-line covering' [32] pattern, which is based on a 3-vertex-regular polyhedron $\mathcal{P}$ (i.e., each vertex has degree 3):

1. at each vertex of $\mathcal{P}$, the three corresponding single rings are interlocked, as illustrated in Fig. 1b;
2. each edge of $\mathcal{P}$ corresponds to parts of two single rings that may be twisted or not, as illustrated in Fig. 1b. Only full twists (full means 360°) are allowed. For convenience, in the following we call the section of a single ring situated on an edge a 'single string';
3. the boundary of each face of $\mathcal{P}$ is associated to a single ring.

We call such polyhedral links the 3-cross double-twist polyhedral links. See Fig. 1c for an example, where the number on each edge represents the number of twistings (here, a 'twisting' means twisting the double line 360°).

From the geometric point of view, at each vertex the three corresponding rings can be locked in two patterns, i.e., the right-hand locking pattern and the left-hand locking pattern, see Fig. 1b. Moreover, these two patterns are chiral and are the antipodes of each other. Similarly, the two corresponding rings on an edge can be twisted in two chiral patterns, i.e., the clockwise pattern and anti-clockwise pattern, both of which are antipodes of each other, see Fig. 1b.

A polyhedral link can be formed in various ways to meet some specific requirements or synthesis strategies, e.g., formed by using the single strings which are given in advance, or formed by using the single rings which are given in advance. Different requirements may lead to different vertex (resp., edge or face) color sets and therefore, lead to different enumeration results by Theorem 1 and Theorem 2. In the following, we give two models of the 3-cross double-twist polyhedral links, for concrete example.

Model 1 Rings which are independent from each other are given; that is, any two (resp., three) rings are allowed to meet at an edge (resp., at a vertex) without any constraints. Furthermore, all the sections of a ring are treated as the same.

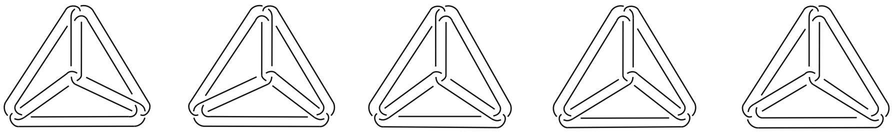


Fig. 2 The tetrahedron links without twisting and with only one type of single ring

We may set the vertex color set as $\mathscr{C}_v = \mathscr{C}_v^* = \{-1, 1\}$ in which -1 and 1 are chiral pairs, i.e., mirror images of each other, representing the right-hand locking pattern and left-hand locking pattern. Let s be the maximum limit of the twisting number at an edge. Since the two single strings on an edge are determined by the two rings they belong to, the color of an edge only represents the twisting pattern and the twisting number of the two corresponding single strings. Thus, we set the edge color set as $\mathscr{C}_e = \mathscr{C}_e^* = \{-s, -s+1, \ldots, -1, 0, 1, 2, \ldots, s\}$ in which i $(0 < i \leq s)$ and $-i$ are chiral pairs representing the clockwise pattern and anti-clockwise pattern with twisting number i, respectively, while 0 is achiral representing the un-twisting pattern. Finally, we set the face color set as $\mathscr{C}_f = \mathscr{C}_f^* = \{1, 2, \ldots, t\}$ in which each color is achiral representing a type of single ring and t is the maximal number of different types of single rings.

Consequently, we have $a_v = 0$, $|\mathscr{C}_v| = |\mathscr{C}_v^*| = 2$, $a_e = 1$, $|\mathscr{C}_e| = |\mathscr{C}_e^*| = 2s + 1$ and $a_f = |\mathscr{C}_f| = |\mathscr{C}_f^*| = t$. In particular, if we set $s = 0$ and $t = 1$, then there are exactly five tetrahedral links of this model, as depicted in Fig. 2, in which 1, 1* and 2, 2* are two chiral pairs. □

Model 2 Strings are given instead of rings. The single ring in a face of the polyhedron is then formed by connecting the corresponding single strings on its boundary. The two strings on an edge are determined by each other. This type models, for an example, a certain type of DNA polyhedral link [35] in which the two strings on an edge represent two DNA single strands and therefore, are determined by each other by the Watson-Crick principle of complementary base pairing.

In general, a DNA strand may have an orientation. To simplify our discussion, in this model we neglect the orientations. Furthermore, since the two strings on an edge are determined uniquely by each other, they are treated as one unit and therefore are assigned with one color. We call such a pair of single strings a double string. Let s be the maximum limit of the twisting number at each edge and let t be the number of different types of double strings (where type may refer, for example, to DNA sequence, but not to twisting number). As an example of isolate colors, we here assume that all types of un-twisted double strings are achiral while all types of twisted double strings are chiral and that all twistings are clockwise, which implies that all colors used for twisted edges are isolate.

From the above requirements, we may set the vertex color set as in Model 1, i.e., $\mathscr{C}_v = \mathscr{C}_v^* = \{-1, 1\}$. The edge color set is set as

$$\mathscr{C}_e = \{\langle i, j\rangle : i \in \{0, 1, \ldots, s\}, j \in \{1, 2, \ldots, t\}\}$$

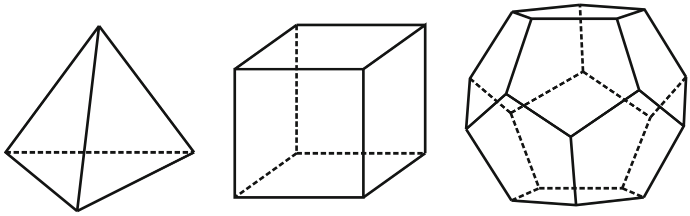


Fig. 3 The tetrahedron $\mathcal{P}_4$ (*left*), the cube $\mathcal{P}_6$ (*middle*) and the dodecahedron $\mathcal{P}_{12}$ (*right*)

and $\mathscr{C}_e^* = \{\langle 0, j\rangle : j \in \{1, 2, \ldots, t\}\}$ in which $\langle i, j\rangle$ with $i \neq 0$ is isolate and $\langle 0, j\rangle$ is achiral, where i and j represent the twisting number and the type of the double string, respectively. Finally, since each face is determined by the corresponding double strings on its boundary, the number of colors for faces is treated as 1. That is, the face color set consists of one achiral color and is set as $\mathscr{C}_f = \mathscr{C}_f^* = \{1\}$.

As a result, we have $a_v = 0$, $|\mathscr{C}_v| = |\mathscr{C}_v^*| = 2$, $a_e = |\mathscr{C}_e^*| = t$, $|\mathscr{C}_e| = (s+1)t$ and $a_f = |\mathscr{C}_f| = |\mathscr{C}_f^*| = 1$. □

As an application of Theorems 2 and 3, in the following we deduce the explicit enumerating expressions of Model 1 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 dodecahedral $\mathcal{P}_{12}$ [36], as shown in Fig. 3.

In Model 1, we have shown that $a_v = 0$, $|\mathscr{C}_v| = |\mathscr{C}_v^*| = 2$, $a_e = 1$, $|\mathscr{C}_e| = |\mathscr{C}_e^*| = 2s + 1$ and $a_f = |\mathscr{C}_f| = |\mathscr{C}_f^*| = t$. So by (2), (3) and Note 1, the number of different polyhedral links based on a polyhedron $\mathcal{P}$ is given by

$$n(\mathcal{P}) = P_{G_{\mathcal{P}}}(\underbrace{2, \ldots, 2}_{|V|}; \underbrace{2s+1, \ldots, 2s+1}_{|E|}; \underbrace{t, \ldots, t}_{|F|}) \tag{4}$$

if chirality is included, or

$$n^*(\mathcal{P}) = \frac{1}{2}n(\mathcal{P}) + \frac{1}{2|G_{\mathcal{P}}|}\sum_{\pi\in\phi G_{\mathcal{P}},\delta_v=\varepsilon_v} 2^{\varepsilon_v}(2s+1)^{\delta_e}t^{\varepsilon_f} \tag{5}$$

if chirality is neglected, where and here after, for $h \in \{v, e, f\}$, $\varepsilon_h = \varepsilon_h(\pi)$ and $\delta_h = \delta_h(\pi)$ for simplicity.

Tetrahedron links. Let the vertices and edges and faces of $\mathcal{P}_4$ be numbered by 1,2,3,4 and 1,2,3,4,5,6 and 1,2,3,4, respectively, as illustrated in Fig. 4. Let ϕ be chosen as the mirror reflection with respect to the plane P, as illustrated in Fig. 4. For $\pi \in G_{\mathcal{P}_4} \times \{I, \phi\}$, we write π as the form $[\pi_V][\pi_E][\pi_F]$, where $[\pi_V]$, $[\pi_E]$ and $[\pi_F]$ represent the permutations of π restricted to V, E and F, respectively. In this way, the rotation group of the tetrahedron [36] is represented by

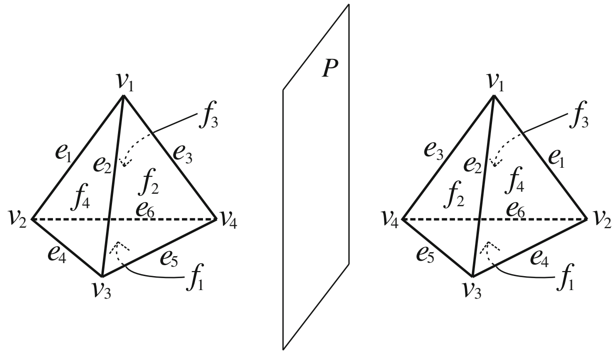


Fig. 4 The tetrahedron (*left*) and its mirror image (*right*) with respect to the plane P (*middle*): v_i, e_i and $f_i (i = 1, 2, \ldots)$ represent the vertex i, edge i and face i, respectively

$$
\begin{aligned}
G_{\mathcal{P}_4} = \{&I, [(234)][(123)(456)][(234)], [(243)][(132)(465)][(243)],\\
&[(134)][(146)(253)][(134)], [(143)][(164)(235)][(143)],\\
&[(124)][(163)(245)][(124)], [(142)][(136)(254)][(142)],\\
&[(123)][(142)(365)][(123)]), [(132)][(124)(356)][(132)],\\
&[(12)(34)][(34)(26)][(12)(34)], [(13)(24)][(15)(34)][(13)(24)],\\
&[(14)(23)][(15)(26)][(14)(23)]\}
\end{aligned}
$$

The cycle index of $G_{\mathcal{P}_4}$ is therefore

$$
\begin{aligned}
&P_{G_{\mathcal{P}_4}}(x_{11}, \ldots, x_{1|V|}; x_{21}, \ldots, x_{2|E|}; x_{31}, \ldots, x_{3|F|})\\
&\quad = \frac{1}{12}\left(x_{11}^4 x_{21}^6 x_{31}^4 + 3x_{12}^2 x_{21}^2 x_{22}^2 x_{32}^2 + 8x_{11}x_{13}x_{23}^2 x_{31}x_{33}\right).
\end{aligned}
$$

Thus, by setting $x_{1j} = 2, x_{2j} = 2s + 1, x_{3j} = t, j = 1, 2, \ldots$, we have

$$
n(\mathcal{P}_4) = \frac{1}{3}\left[4(2s+1)^6 t^4 + 3(2s+1)^4 t^2 + 8(2s+1)^2 t^2\right]. \tag{6}
$$

On the other hand, there are 6 permutations in $\phi G_{\mathcal{P}_4}$ satisfying $\delta_v = \varepsilon_v$:

$$
\begin{aligned}
&[(1324)][(15)(2463)][(1324)], [(1243)][(1652)(34)][(1243)],\\
&[(1342)][(1256)(34)][(1342)], [(1423)][(15)(2364)][(1423)],\\
&[(1234)][(1453)(26)][(1234)], [(1432)][(1354)(26)][(1432)].
\end{aligned}
$$

Therefore,

$$
\sum_{\pi \in \phi G_{\mathcal{P}_\triangle}, \delta_v = \varepsilon_v} 2^{\varepsilon_v}(2s+1)^{\delta_e} t^{\varepsilon_f} = 6 \times 2 \times (2s+1)^2 \times t = 12(2s+1)^2 t.
$$

Thus, by (5) and (6) we have

$$n^*(\mathcal{P}_4) = \frac{1}{6}\Big[4(2s+1)^6t^4 + 3(2s+1)^4t^2 + 8(2s+1)^2t^2 + 3(2s+1)^2t\Big].$$

Cube links.

$$\begin{aligned}&P_{G_{\mathcal{P}_6}}(x_{11},\ldots,x_{1|V|};x_{21},\ldots,x_{2|E|};x_{31},\ldots,x_{3|F|})\\ &= \frac{1}{24}\Big(x_{11}^8x_{21}^{12}x_{31}^6 + 8x_{11}^2x_{13}^2x_{23}^4x_{33}^2 + 6x_{14}^2x_{24}^3x_{31}^2x_{34} + 3x_{12}^4x_{22}^6x_{31}^2x_{32}^2\\ &\quad +6x_{12}^4x_{21}^2x_{22}^5x_{32}^3\Big).\end{aligned}$$

In addition,

$$\sum_{\pi\in\phi G_{\mathcal{P}_6},\delta_v=\varepsilon_v} 2^{\varepsilon_v}(2s+1)^{\delta_e}t^{\varepsilon_f} = 48(2s+1)^4t^5 + 16(2s+1)^6t^3 + 24(2s+1)^3t^2 +32(2s+1)^2t.$$

Therefore,

$$\begin{aligned}n(\mathcal{P}_6) &= \frac{1}{3}\Big[32(2s+1)^{12}t^6 + 6(2s+1)^6t^4 + 12(2s+1)^7t^3 + 3(2s+1)^3t^3\\ &\quad +16(2s+1)^4t^2\Big].\\ n^*(\mathcal{P}_6) &= \frac{1}{6}\Big[32(2s+1)^{12}t^6 + 6(2s+1)^4t^5 + 6(2s+1)^6t^4 + 12(2s+1)^7t^3\\ &\quad +2(2s+1)^6t^3 + 3(2s+1)^3t^3 + 16(2s+1)^4t^2 + 3(2s+1)^3t^2\\ &\quad +4(2s+1)^2t\Big].\end{aligned}$$

Dodecahedral links.

$$\begin{aligned}&P_{G_{\mathcal{P}_{12}}}(x_{11},\ldots,x_{1|V|};x_{21},\ldots,x_{2|E|};x_{31},\ldots,x_{3|F|})\\ &= \frac{1}{60}\Big(x_{11}^{20}x_{21}^{30}x_{31}^{12} + 20x_{11}^2x_{13}^6x_{23}^{10}x_{33}^4 + 24x_{15}^4x_{25}^6x_{31}^2x_{35}^2 + 15x_{12}^{10}x_{21}^2x_{22}^{14}x_{32}^6\Big).\end{aligned}$$

In addition,

$$\sum_{\pi\in\phi G_{\mathcal{P}_{12}},\delta_v=\varepsilon_v} 2^{\varepsilon_v}(2s+1)^{\delta_e}t^{\varepsilon_f} = 1024(2s+1)^{15}t^6 + 320(2s+1)^5t^2 +96(2s+1)^3t^2.$$

Therefore,

$$n(\mathcal{P}_{12}) = \frac{1}{15}\Big[262144(2s+1)^{30}t^{12} + 3840(2s+1)^{16}t^6 + 1280(2s+1)^{10}t^4 + 96(2s+1)^6t^4\Big].$$

$$n^*(\mathcal{P}_{12}) = \frac{1}{15}\Big[131072(2s+1)^{30}t^{12} + 1920(2s+1)^{16}t^6 + 128(2s+1)^{15}t^6 + 640(2s+1)^{10}t^4 + 48(2s+1)^6t^4 + 40(2s+1)^5t^2 + 12(2s+1)^3t^2\Big].$$

Remark There is a degenerate form of the 3-cross-curve and double-twist-line covering, called the 'three cross-curve and double-line covering' [33] pattern in which no twisting happens on edges, which can be dealt with simply by setting $s = 0$ in (4) and (5). In [34], an analogous pattern, called the '3-branched curves and m-twisted double-lines covering' pattern, was also introduced in which the three single rings at a vertex are not locked. This pattern can be dealt with by replacing the vertex color set in Model 1 by $\mathscr{C}_v = \mathscr{C}_v^* = \{0\}$, in which 0 is achiral.

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