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ORIGINAL PAPER

The architecture and the Jones polynomial of polyhedral links

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Abstract In this paper, we first recall some known architectures of polyhedral links (Qiu and Zhai in J Mol Struct (THEOCHEM) 756:163–166, 2005; Yang and Qiu in MATCH Commun Math Comput Chem 58:635–646, 2007; Qiu et al. in Sci China Ser B Chem 51:13–18, 2008; Hu et al. in J Math Chem 46:592–603, 2009; Cheng et al. in MATCH Commun Math Comput Chem 62:115–130, 2009; Cheng et al. in MATCH Commun Math Comput Chem 63:115–130, 2010; Liu et al. in J Math Chem 48:439–456, 2010). Motivated by these architectures we introduce the notions of polyhedral links based on edge covering, vertex covering, and mixed edge and vertex covering, which include all polyhedral links in Qiu and Zhai (J Mol Struct (THEOCHEM) 756:163–166, 2005), Yang and Qiu (MATCH Commun Math Comput Chem 58:635–646, 2007), Qiu et al. (Sci China Ser B Chem 51:13–18, 2008), Hu et al. (J Math Chem 46:592–603, 2009), Cheng et al. (MATCH Commun Math Comput Chem 62:115–130, 2009), Cheng et al. (MATCH Commun Math Comput Chem 63:115–130, 2010), Liu et al. (J Math Chem 48:439–456, 2010) as special cases. The analysis of chirality of polyhedral links is very important in stereochemistry and the Jones polynomial is powerful in differentiating the chirality (Flapan in When topology meets chemistry. Cambridge Univ. Press, Cambridge, 2000). Then we give a detailed account of a result on the computation of the Jones polynomial of polyhedral links based on edge covering developed by Jin, Zhang, Dong and Tay (Electron. J. Comb. 17(1): R94, 2010) and, at the same time, by using this method we obtain some new computational results on polyhedral links of rational type and uniform polyhedral links with small edge covering units. These new computational results are helpful to

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judge the chirality of polyhedral links based on edge covering. Finally, we give some remarks and pose some problems for further study.

Keywords Polyhedral links · Architecture · Jones polynomial · Chirality

1 Introduction

Polyhedral links or catenanes have been synthesized, by using branched DNA molecules, such as DNA cube [1], DNA tetrahedron [2], DNA octahedron [3], DNA truncated octahedron [4], DNA bipyramid [5], DNA dodecahedron [6], DNA dodecahedron and buckyballs [7] etc. In 2000, a topologically linked protein catenane, which consists of 12 pentameric and 60 hexameric rings of covalently joined subunits that loop through each other, was found in the mature empty capsid of the double-stranded DNA bacteriophage [8,9]. Synthetical strategies for some DNA and protein polyhedral links have also been studied by chemists and biologist.

These works motivate Qiu, Zhang and their collaborators to study the architecture of polyhedral links. See [10–16]. It is well known that the analysis of chirality problems is very important in stereochemistry [17,18]. In order to analyze the chirality as well as other topological properties of polyhedral links, many invariants of polyhedral links, such as component number, twist number, genus, the Jones polynomial and its generalization, the Homflypt polynomial are computed by chemists and mathematicians. See [10–16,19,20].

In this paper, we shall study new architectures of polyhedral links. We introduce the notions of polyhedral links based on edge covering, vertex covering, and mixed edge and vertex covering. These new architectures include polyhedral links in [10–16] as special cases. We hope that these new architectures will become the potential synthetical objects of chemists and biologists. Then we review a general method on the computation of the Jones polynomial of polyhedral links based on the edge covering developed by Jin, Zhang, Dong and Tay in [21], at the same time, by using this method to obtain some new computational results on polyhedral links of rational type and uniform polyhedral links with small edge covering units. These new computational results are helpful to judge the chirality of polyhedral links based on edge covering. Finally, we give some remarks and pose some open problems for further study.

There are two motivations for us to concentrate on the Jones polynomial invariant of polyhedral links. First, the Jones polynomial invariant of links is powerful in differentiating the chirality of links. However, computing the Jones polynomial of links is difficult in general [22]. Polyhedral links usually have large numbers of crossings, while the present softwares usually can only deal with links with small number of crossings. Therefore, it is necessary to develop approaches to the computational problem of the Jones polynomial or its main part, the Kauffman bracket polynomial of such polyhedral links with large number of crossings. In this aspect, there have been many works in the field of both mathematics and chemistry, including [21,23–31].

Second, the Jones polynomial is a special case of the partition function of the Potts model in statistical mechanics [32,33]. The study of zeroes in physics originated from two very well-known papers [34,35] on phase transitions by Lee and Yang.

One hopes to gain much information by considering complex variables and studying zeros. Wu and Wang [36], Chang and Shrock [37] initiated the study of zeros of the Jones polynomial. Except the above two, there are also some works in the aspect by Lin [38], Champanerkar and Kofman [39], Jablan et al. [29,30], and the present authors [21,40,41]. In order to study zeros, one usually needs to obtain expressions of Jones polynomials of links firstly.

2 Old and new architectures

2.1 Preliminaries

A link L of n components is a subset of $\mathbb{R}^3$, consisting of n disjoint piecewise linear simple closed curves; a knot is a link with one component. Although links are mathematical objects in $\mathbb{R}^3$, we usually represent them by their 2-dimensional *link diagrams*, that is, the regular projections of links into $\mathbb{R}^2$ with each undercrossing indicated by a gap in an arc. By *a signed graph* we mean a graph with each edge labeled with a sign, $+$ or $-$. We denote by G^s a signed graph. Let e be an edge of the signed graph G^s. We shall denote by $s(e)$ the sign of the edge e. If a signed graph is also a plane graph, we shall call it *a signed plane graph*.

It's well known that there is a one-to-one correspondence between link diagrams and signed plane graphs [42,43]. The correspondence has been known for about one hundred years. Originally it was used to construct a table of link diagrams of all links starting with graphs with a relatively small number of edges and then increasing the number of edges. Indeed, it provides a method of studying links using graphs. Now we give a brief account of the correspondence and firstly we give the definition of the medial graph of a plane graph.

A graph is said to be *trivial* if it is an isolated vertex. The *medial graph $M(G)$* of a connected non-trivial plane graph G is a 4-regular plane graph obtained by inserting a vertex on every edge of G, and joining two new vertices by an edge lying in a face of G if the vertices are on adjacent edges of the face; if G is trivial, its medial graph is a simple closed curve surrounding the vertex (strictly, it is not a graph); if G is not connected, its medial graph $M(G)$ is the disjoint union of the medial graphs of its connected components.

Given a connected link diagram D, shade it as in a checkerboard so that the unbounded face is unshaded. See Fig. 2 for an example. We then associate D with a signed plane graph G^s as follows: For each shaded face F_i, take a vertex V_{F_i}, and for each crossing at which F_i and F_j meet, take an edge $V_{F_i}V_{F_j}$ and give the edge a sign as shown in Fig. 1. The signed plane graph of a non-connected link diagram (viewed as 4-regular graphs) is defined to be the disjoint union of signed plane graphs of its connected components of the link diagram.

Conversely, given a signed plane graph G^s, draw its medial graph $M(G)$ firstly. Then, to turn $M(G)$ into a link diagram $D = D(G^s)$, we turn the vertices of $M(G)$ into crossings by defining a crossing to be positive or negative according to the sign of the edge also as shown in Fig. 1.

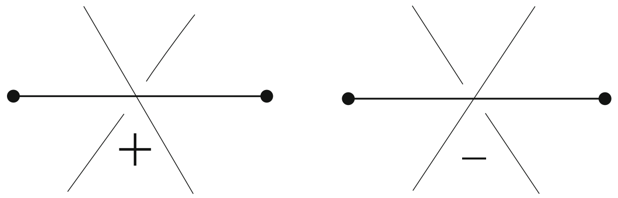


Fig. 1 The correspondence between signed edges of plane graphs and crossings of link diagrams

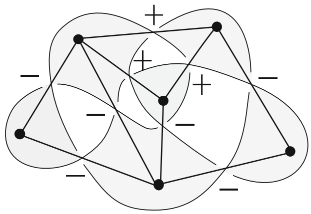


Fig. 2 A knot diagram and its corresponding signed plane graph

An example illustrating the correspondence is given in Fig. 2. It is clear that signed plane graphs with all edges signed "+" or all edges signed "−" correspond to alternating link diagrams. Loops and bridges of signed plane graphs correspond to nugatory, i.e. removable crossings of link diagrams. Block decompositions of plane graphs correspond to the prime decompositions of link diagrams.

2.2 Some old architectures

In works by chemists and biologists [1–7], many DNA polyhedral links have been synthesized via applying 'branched curves' covering, which is based on the principle of DNA branched junctions (see Seeman et al. [44,45]), and '(twisted) double-lines' covering. In Fig. 3 (left) we provide an example of the planar representations of such polyhedral links—the cubic link obtained by applying 3-branched curves covering and 4-twisted double-lines covering in [1]. Its corresponding signed plane graph is shown in Fig. 3 (right).

In [13], Hu et al. developed a methodology for the construction of polyhedral links on the basis of the Platonic solids by using the n-branched curves and m-twisted double-lines covering. See Fig. 4b, d for the 3-branched curve covering and 4-twisted double-line covering. For an arbitrary polyhedral graph G, Liu et al. introduced the following method to construct polyhedral links in [16]: first make a "chain and sheaf" replacing on edges of G to obtain $\hat{G}$, then apply the operation of X-tangle covering to all edges of $\hat{G}$, where X may be ± 2 horizontal or vertical integer tangle. The chain and sheaf replacing is the same to the construction of the present authors in [26] and the operation of X-tangle covering to all edges of $\hat{G}$ is the same to the construction of Traldi in [46]. Note that in the above two constructions, vertices of degree n of the polyhedral graph are both covered by n-branched curves. The difference between the two lies in the building blocks covering edges of polyhedral graphs.

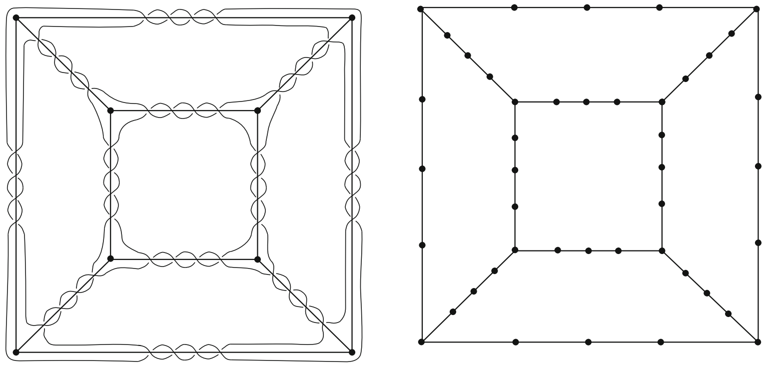


Fig. 3 The planar representation of the cubic link in [1] (*left*). Its corresponding signed plane graph—the signs are all + and hence, omitted (*right*)

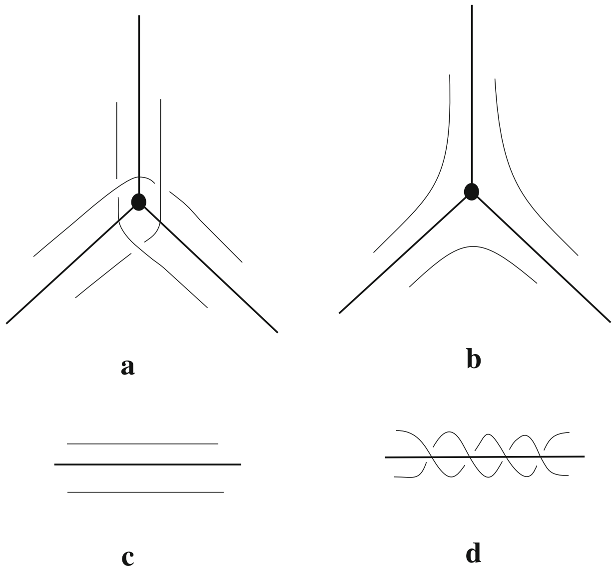


Fig. 4 **a** 3-Cross-curve covering, **b** 3-branched cure covering, **c** double-line covering, and **d** 4-twisted double-line covering

Motivated by the discovery of a topologically linked protein catenane in the mature empty casid of the double-stranded DNA bacteriophage [8,9], Qiu and Zhai developed a method of constructing polyhedral links based on Goldberg polyhedra by means of 'three-cross-curve and double-line covering' in [10]. See Fig. 4a, c for the 3-cross-curve covering and double-line covering. This construction is applied in [11] to carbon nanotubes by Yang and Qiu. To deal with polyhedra having vertices of degrees $n > 3$, in [14,15], '3-cross-curve' covering is generalized to 'n-cross-curve' covering and more generally, to 'branched alternating closed braids' covering. Note that in all these constructions, edges are all covered by double-lines. The difference lies in the building blocks covering the vertices.

In addition, Qiu et al. developed the method of constructing polyhedral links on the basis of Platonic and Archimedean solids by using 'three-cross-curve and twisted double-line covering' in [12].

Note that the surface of a polyhedron is topologically homeomorphic to the sphere S^2. Thus the polyhedral graph consisting of vertices and edges of a polyhedron, i.e the 1-skeleton, is a planar graph via the well-known stereographic projection [47]. Without loss of generality, we can always construct polyhedral links based on connected plane graphs which include polyhedral graphs as special cases. Once the links are constructed, it is not difficult for us to transform them into polyhedral links via spatial deformations.

2.3 New architectures

To generalize the above known constructions of polyhedral links, we first give the definition of the n-tangle. An *n-tangle* is n disjoint properly embedded arcs and perhaps some circles in 3-ball. The $2n$ endpoints of the n arcs are all on the ball's boundary. We can always arrange the $2n$ points on the 3-ball boundary to lie on a great circle and the tangle in general position with respect to the projection onto the flat disc bounded by the great circle. The projection then gives us a tangle diagram, where we make note of overcrossings and undercrossings as with knot diagrams. Usually, one is more interested in 2-tangles.

Polyhedral links based on edge covering are defined to be polyhedral links obtained by using general 2-tangles to cover edges of polyhedral graphs and using n-branched curves to cover vertices of degree n of polyhedral graphs and connecting the two kinds of building blocks. In fact, in [13], the authors use integer tangles to cover edges, while in [16], the authors use even integer tangles (horizontal or vertical) and $\pm 2, \pm 2, \ldots, \pm 2$ tangles (horizontal or vertical) [43] to cover edges of the polyhedral graph. Clearly there are many other 2-tangles. Hence polyhedral links based on edge covering are the real generalization of polyhedral links in [13,16]. In Fig. 5 (left), we give an example of such tetrahedral links. Its corresponding signed plane graph is shown in Fig. 5 (right). Many other constructions are given in Fig. 19 of Sect. 3 in the form of graphs with two attached vertices.

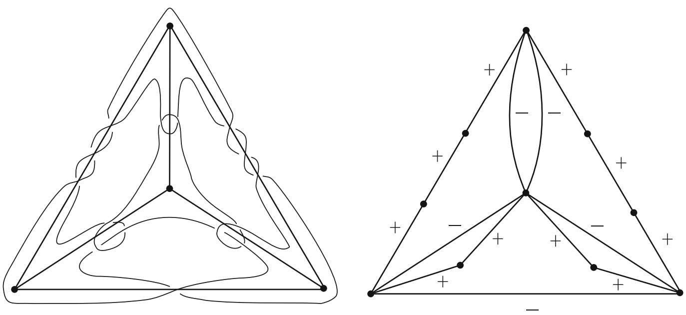


Fig. 5 (*left*) A tetrahedral link based on edge covering and (*right*) its corresponding signed plane graph

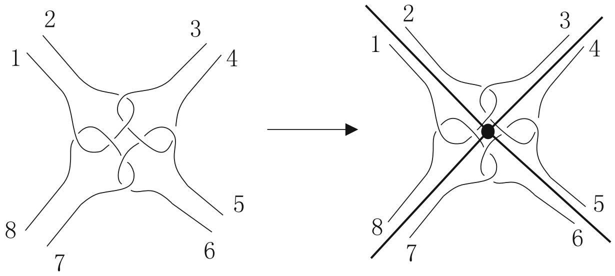


Fig. 6 Diagram of a 4-tangle and its covering of a vertex with degree 4

Note that n-branched curves, n-cross curves and n-branched closed braids are all special cases of n-tangles. We define *Polyhedral links based on vertex covering* to be polyhedral links obtained by using general n-tangles to cover vertices of degree n of polyhedral graphs and using double-lines to cover edges of polyhedral graphs and and connecting the two kinds of building blocks. Clearly, polyhedral links based on vertex covering include polyhedral links in [10,11,14,15] as special cases.

To be precise, given an n-tangle diagram, we number the $2n$-endpoints on the great circle $1, 2, 3, 4, \ldots, 2n-1, 2n$ clockwise. Divide it into the following n pairs: $\{1, 2\}, \{3, 4\}, \ldots, \{2n-1, 2n\}$, which is designed to cover the n edges incident with the vertex of degree n of the polyhedral graph. In Fig. 6 we show the diagram of a 4-tangle and its covering of a vertex of degree 4.

Note that if we close the ends $2i-1$ and $2i$ for $i = 1, 2, \ldots, n$, then we obtain a link diagram $\hat{T}$ with period n. Conversely, we can also obtain n-tangle with an n-fold symmetry from links with period n. Since nature prefers symmetry, we provide some symmetrical 3-tangles as shown in Fig. 7.

More generally, we can combine polyhedral links based on edge covering with polyhedral links based on vertex covering to obtain polyhedral links based on mixed edge and vertex coverings, i.e. links obtained from polyhedral graphs by applying n-tangles to cover vertices of degree n and 2-tangles to cover edges and connecting the two kinds of building blocks. It is clear that polyhedral links based on mixed edge and vertex covering are generalizations of polyhedral links based on edge covering and polyhedral links based on vertex covering and include polyhedral links in [12] as a special case. The planar representations of examples of polyhedral links based on vertex covering and mixed edge and vertex covering are shown in Figs. 8 and 9, respectively.

3 The Jones polynomial of polyhedral links based on edge covering

In this section we shall first review a general method developed by the present authors in [21] of computing the Jones polynomial of polyhedral links based on edge covering, i.e. polyhedral links obtained by using 'branched curves and 2-tangles' covering. This method appeared in Section 2 of [21], it is very condensed, here we give a detailed

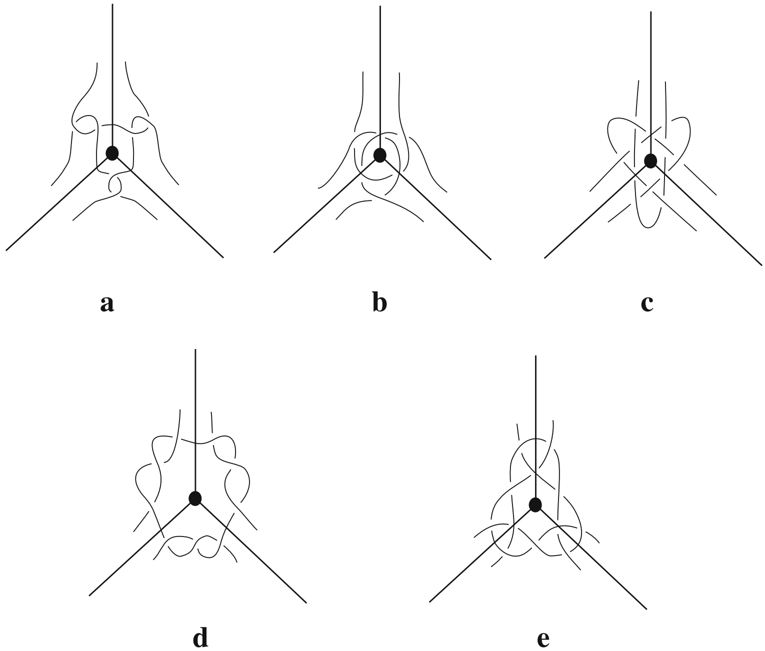


Fig. 7 Some symmetrical 3-tangles: **a** branched 6_1^3; **b** branched Borromean ring 6_2^3, i.e. the branched regular alternating closed braids $(\sigma_1^{-1}\sigma_2)^3$ in [14]; **c** a branched 12-crossing link; **d** branched 9_1; **e** a branched 12-crossing knot

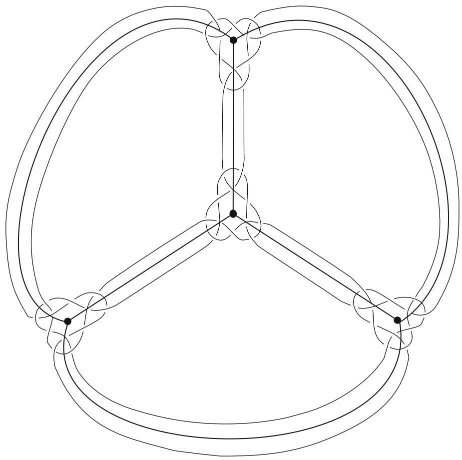


Fig. 8 An example of polyhedral links based on vertex covering obtained from the tetrahedron by applying 3-tangle shown in Fig. 7e covering

account of it and at the same time, we think this method may be not known by chemists. Then we provide new computational results on polyhedral links of rational-type and uniform polyhedral links with small edge covering units.

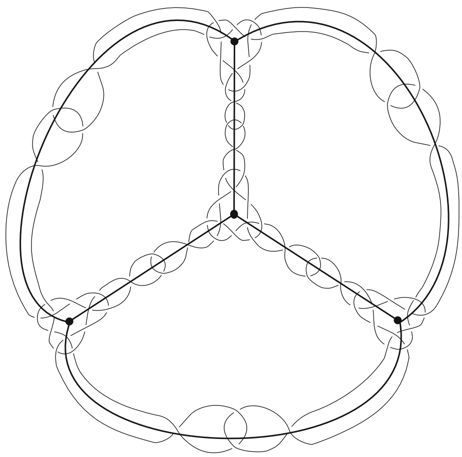


Fig. 9 An example of polyhedral links based on mixed edge and vertex covering obtained from the tetrahedron by applying 3-tangle shown in Fig. 7e and 2-tangle shown in Fig. 20 (down) covering

3.1 A general method

Originally, the Jones polynomial was given in terms of the trace of a matrix representation of the braid group into a Temperley–Lieb algebra (see Jones [48,49]). In 1987, Kauffman constructed a state model for the Jones polynomial using his bracket polynomial [50,51], which provided another way of calculating the Jones polynomial. Let $V_L(t)$ be the Jones polynomial of an oriented link L. Let D be a link diagram of the oriented link L, and $\langle D\rangle$ be the Kauffman bracket polynomial in one variable A of D with orientations neglected. Then

$$V_L(t) = (-A^3)^{-w(D)}\langle D\rangle|_{A=t^{-1/4}}, \tag{1}$$

where $w(D)$ is the writhe of D.

Note that the writhe of an oriented link diagram is easily calculated. Hence the main difficulty in computing the Jones polynomial of an oriented link is to compute the Kauffman bracket polynomial of its corresponding unoriented link diagram.

Note. Let $[D] = [D](A, B, d)$ be the Kauffman square bracket polynomial of the unoriented diagram D in three variables A, B and d. Then it is related to the one-variable Kauffman bracket polynomial $\langle D\rangle = \langle D\rangle(A)$ in the variable A by [50,51]

$$\langle D\rangle(A) = [D](A, A^{-1}, -A^2 - A^{-2}). \tag{2}$$

In this paper, we need not give the original definitions of the Jones polynomials and the (square) Kauffman bracket polynomials. For the definitions, we refer the reader to Jones [48] and Kauffman [50], respectively. It is enough for the readers to know the relation between the Jones polynomial and the Kauffman bracket polynomial, and the relation between the Kauffman bracket polynomial and the Kauffman square bracket polynomial.

Based on the 1–1 correspondence between signed plane graphs and link diagrams, Kauffman converted the Kauffman square bracket polynomial to the Tutte polynomial of signed (not necessarily planar) graphs in [51,52] which is a generalization of the Tutte polynomial [53] of unsigned graphs in graph theory.

Let G^s be a signed graph, We will denote by $Q[G^s] = Q[G^s](A, B, d) \in \mathbb{Z}[A, B, d]$ the Tutte polynomial of G^s and we also call it the Q-polynomial. Note that when G^s is a signed plane graph, we have [51,52]

$$[D(G^s)](A, B, d) = Q[G^s](A, B, d). \tag{3}$$

Therefore, later we shall focus on the Tutte polynomial of signed graphs.

Definition 1 The Tutte polynomial $Q[G^s] = Q[G^s](A, B, d) \in \mathbb{Z}[A, B, d]$ for a signed graph G^s can be redefined by the following recursive rules:

1. The Tutte polynomial of the empty graph E_n which consists of n disjoint vertices and no edges is d^{n-1}, that is,

$$Q[E_n] = d^{n-1}.$$

2. Let e be an edge of a signed graph G^s. We denote by $G^s - e$ and G^s/e the graphs obtained from G^s by deleting and contracting (that is, deleting e and identifying its two end-vertices) the edge e, respectively.

(a) If e is a loop, then

$$Q[G^s] = (A + Bd)Q[G^s - e] \text{ when } s(e) = -, \text{ and}$$
$$Q[G^s] = (Ad + B)Q[G^s - e] \text{ when } s(e) = +.$$

(b) If e is not a loop, then

$$Q[G^s] = AQ[G^s - e] + BQ[G^s/e] \text{ when } s(e) = -, \text{ and}$$
$$Q[G^s] = BQ[G^s - e] + AQ[G^s/e] \text{ when } s(e) = +.$$

Observation Under the correspondence between signed plane graphs and link diagrams. Using a 2-tangle to cover an edge is equivalent to using a signed plane graph with two attached vertices to replace the edge.

For example, in Fig. 10 (up) an edge a is covered by a 2-tangle. Under the correspondence between signed plane graphs and link diagrams, it is equivalent to using the signed plane graph H_a to replace a as shown in Fig. 10 (down). The two vertices circled are the attached vertices.

Motivated by the above observation, we give the following definition.

Definition 2 A labeled graph is a graph whose edges have been labeled with elements of a commutative ring with unity. Let G^l be a connected labeled graph. We define $\hat{G}$ to be the signed graph obtained from G by replacing each edge $a = uw$ of G by

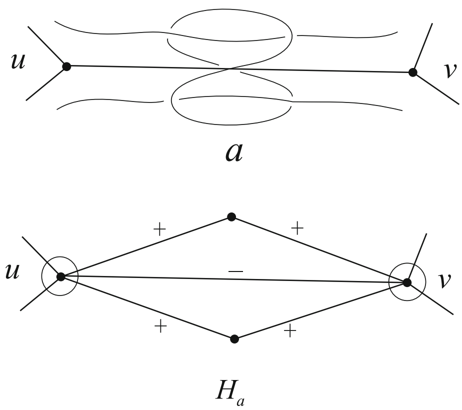


Fig. 10 Relation between an edge replaced by a signed plane graph and the edge covered by a 2-tangle

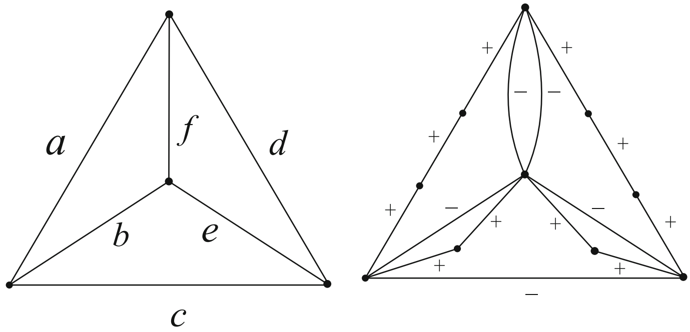


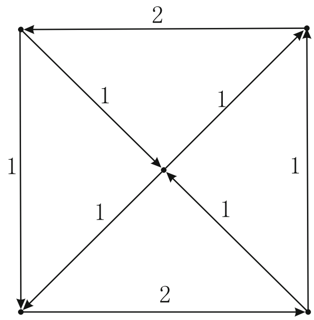
Fig. 11 The labeled tetrahedron T^l (*left*); a signed graph obtained from T^l by edge replacements (right), which is the signed plane graph in Fig. 5 (*right*)

a connected signed graph H_a with two attached vertices u and w that has only the vertices u and w in common with $\widehat{G-a}$.

An example is shown in Fig. 11. Therefore, computing the Kauffman bracket polynomial of polyhedral links based on edge covering is equivalent to computing the Q-polynomial of $\hat{G}$, where G is the polyhedral graph. We need the definition of the chain polynomial of labeled graphs. The chain polynomial of labeled graphs was introduced by Read and Whitehead Jr. in [54] for studying the chromatic polynomials of homeomorphic graphs. To define the chain polynomial, we need firstly recall the definition of the flow polynomial of graphs.

Let G be a graph and let $\overrightarrow{G}$ be an orientation of G obtained by assigning an arbitrary but fixed orientation $\overrightarrow{e}$ to each edge e of G. Let $\overrightarrow{E}$ denote the set of oriented edges of $\overrightarrow{G}$. A map $f : \overrightarrow{E} \longrightarrow \mathbb{Z}_q = \{0, 1, 2, \ldots, q-1\}$ is called a q-flow if, for each vertex $v \in V(\overrightarrow{G})$, the total flow out of v is equal to the total flow into v. A map $f : \overrightarrow{E} \longrightarrow \mathbb{Z}_q$ is called nowhere-zero if, for each $\overrightarrow{e} \in \overrightarrow{E}$, $f(\overrightarrow{e}) \neq 0$. An example of nowhere-zero flows is given in Fig. 12. It is not difficult to see that the number of nowhere-zero q-flows does not depend on the orientation of G, so we are justified in saying the number of nowhere-zero q-flows on G. Let $F[G](q)$ denote the number

Fig. 12 A nowhere-zero q-flow on the 4-wheel for any $q \geq 3$



of nowhere-zero q-flows of G. As we will see in the contraction-deletion formula, $F[G](q)$ is a polynomial in q, and will be called the flow polynomial of G. The flow polynomial can be evaluated by the following contraction-deletion formula.

1. If E_n is an empty graph (that is, a graph without edges) with n vertices, then

$$F[E_n](q) = 1.$$

2. (a) If G has a bridge, then

$$F[G](q) = 0.$$

   (b) If e is a loop of G, then

$$F[G](q) = (q - 1)F[G/e](q).$$

   (c) If e is neither a bridge nor a loop of G, then

$$F[G](q) = F[G/e](q) - F[G - e](q).$$

For more information on the flow polynomial, we refer the reader to Tutte [53], Bollobás [42] and Shahmohamad [55].

Definition 3 The *chain polynomial* $Ch[G^l]$ of a labeled graph G^l is defined as

$$Ch[G^l] = \sum_{Y \subset E} F_{G-Y}(1 - w) \prod_{a \in Y} a$$

where the sum is over all subsets of the edge set E of G, $F_{G-Y}(1 - w)$ denotes the flow polynomial in $q = 1 - w$ of $G - Y$, the graph obtained from G by deleting the edges in Y, and $\prod_{a \in Y} a$ denotes the product of labels in Y.

The chain polynomial of labeled graphs can also be computed by using the following recursive rules [26].

1. If G^l is edgeless, then

$$Ch[G^l] = 1. \tag{4}$$

2. Let a be an edge of G^l.
   (a) If a is a loop of G^l, then

$$Ch[G^l] = (a - w)Ch[G^l - a]. \tag{5}$$

   (b) If a is not a loop, then

$$Ch[G^l] = (a - 1)Ch[G^l - a] + Ch[G^l/a]. \tag{6}$$

Let T be a 2-tangle as shown in Fig. 13a. By joining with simple arcs the two upper and the two lower end-points of the 2-tangle T, we obtain a link called the numerator of T, denoted by $N(T)$, see Fig. 13b. Joining with simple arcs each pair of the corresponding left and right end-points of the tangle T, we obtain a link called the denominator of T, denoted by $D(T)$, see Fig. 13c.

Recall that H_a is the plane graph with two attached vertices corresponding to the 2-tangle T_a covering the edge a. Let H'_a be the graph obtained from H_a by identifying u and w, the two attached vertices of H_a. It is not difficult to see that the graph H_a corresponds to the denominator of the tangle T_a and H'_a corresponds to the numerator of the tangle T_a. See Fig. 14.

In [21], the present authors established a relation between the Q-polynomial of $\hat{G}$ and the chain polynomial of G^l.

Let

$$\begin{aligned}
\alpha_a &= \alpha[H_a] = \frac{1}{d^2-1}(dQ[H_a] - Q[H'_a]),\\
\beta_a &= \beta[H_a] = \frac{1}{d^2-1}(dQ[H'_a] - Q[H_a]),\\
\gamma_a &= \gamma[H_a] = 1 + d\frac{\alpha[H_a]}{\beta[H_a]}
\end{aligned}$$

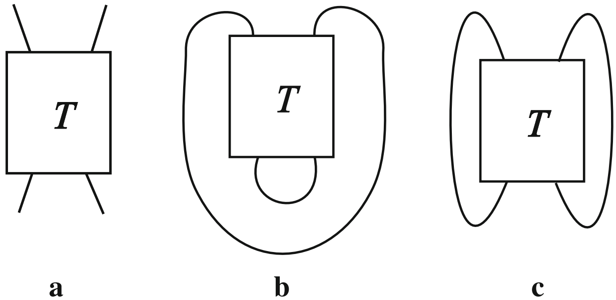


Fig. 13 **a** The general 2-tangle T; **b** the numerator of T; **c** the denominator of T

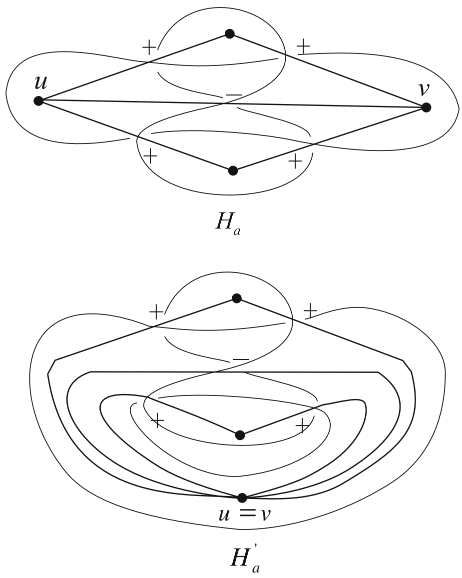


Fig. 14 H_a corresponds to the denominator of the tangle T_a and H'_a corresponds to the numerator of the tangle T_a

Theorem 1 [21] *Let G^l be a connected labeled graph, and $\hat{G}$ be the signed graph obtained from G by replacing the edge* ***a*** *by a connected signed graph H_a for every edge* ***a*** *in G. If we replace w by $1-d^2$, and replace* ***a*** *by γ_a for every label* ***a*** *in $Ch(G^l)$, then we have*

$$Q[\hat{G}] = \frac{\prod_{a \in E(G)} \beta_a}{d^{q(G)-p(G)+1}} Ch[G^l], \tag{7}$$

where $p(G)$ and $q(G)$ are the numbers of vertices and edges of G, respectively.

Note that when G is a connected graph, $q(G) - p(G) + 1$ is called the nullity or cyclomatic number of G. In addition, if G is also a plane graph, then its nullity equals the number of bounded faces of G by the well-known Euler formula [47].

Now we consider a special case, i.e. H_a is uniformly for all edges. By the following lemma, Theorem 1 can be further reduced to computing the Tutte polynomial [53] of the graph G.

Lemma 1 [20] *Let G^u be a uniform labeled graph, i.e. all edges of G are labeled with the same label u. Then the chain polynomial of G^u is related to the Tutte polynomial of G by*

$$Ch[G^u] = (u-1)^{q-p+c} T_G\left(u, \frac{u-w}{u-1}\right). \tag{8}$$

Note that the Maple software has a function called TuttePolynomial in the GraphTheory package, which can be used for us to calculate the Tutte polynomial of small graphs, including many polyhedral graphs.

3.2 New computational results

Now we apply Theorem 1 and Lemma 1 to compute Kauffman bracket polynomials of some families of polyhedral links based on the edge covering. It is sometimes convenient for us to compute the Q-polynomial by using the follow lemma.

Lemma 2 [21,25]

(1) *Let $G_1^s \cup G_2^s$ be the disjoint union of two signed graphs G_1^s and G_2^s. Then*

$$Q[G_1^s \cup G_2^s] = d\,Q[G_1^s]Q[G_2^s]. \tag{9}$$

(2) *Let $G_1^s \cdot G_2^s$ be the union of two signed graphs G_1^s and G_2^s having only one common vertex. Then*

$$Q[G_1^s \cdot G_2^s] = Q[G_1^s]Q[G_2^s]. \tag{10}$$

(3) *If e is a bridge of G^s, then*

$$Q[G^s] = (Ad + B)Q[G^s/e] \text{ if } s(e) = -, \tag{11}$$
$$Q[G^s] = (A + Bd)Q[G^s/e] \text{ if } s(e) = +. \tag{12}$$

3.2.1 *Links of rational-type*

A horizontal (resp. vertical) integer tangle $[m]$ (resp. $\overline{[m]}$) is a twist of two horizontal (resp. vertical) strands $|m|$ times in the positive or negative directions according to the sign of m. The directions are shown in Fig. 15a (resp. Fig. 15b).

A link will be called *rational-type* if it has a diagram which can be obtained from a connected plane graph by 'branched curves and integer tangles' covering. Note that rational links in knot theory (see [43,56]) are typical examples of links of rational-type.

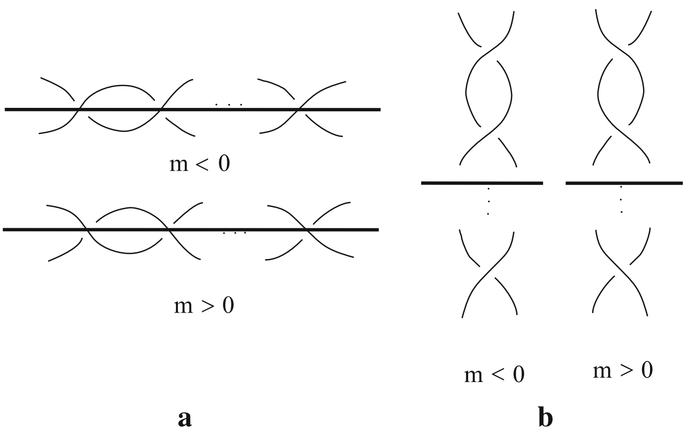


Fig. 15 Horizontal and vertical integer tangles. Note that the *bold lines* are edges to be replaced

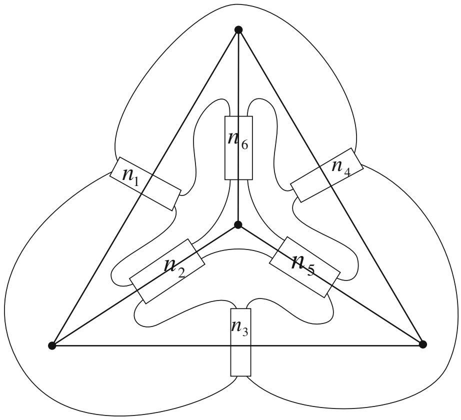


Fig. 16 A rational-type tetrahedral link $D_1(n_1, n_2, n_3, n_4, n_5, n_6)$ obtained from T^l by the following edge covering: the edge a, c, d covered by *vertical* integer tangles $\overline{[n_1]}, \overline{[n_3]}, \overline{[n_4]}$, respectively and b, e, f covered by *horizontal* integer tangles $[n_2], [n_5], [n_6]$, respectively

Note that the denominator of a horizontal integer tangle $[n]$ corresponds to a positive (resp. negative) path P_n^+ (resp. P_n^-) with length n when $n > 0$ (resp. $n < 0$); the denominator of a vertical integer tangle $\overline{[n]}$ corresponds to a positive (resp. negative) multiple edges I_n^+ (resp. I_n^-) with multiplicity n when $n > 0$ (resp. $n < 0$). By Theorem 1, to obtain the Kauffman bracket polynomials of the above family of tetrahedral links, we only need to compute $\beta[P_n^+], \beta[P_n^-], \gamma[P_n^+], \gamma[P_n^-]$ and $\beta[I_n^+], \beta[I_n^-], \gamma[I_n^+], \gamma[I_n^-]$.

When $H_a = P_n^+, H_a' = C_n^+$, the positive cycle with length n; When $H_a = I_n^+$, $H_a' = B_n^+$, the "bouquet of n positive circles", i.e. a signed graph with one vertex and n positive loops. Similarly, when $H_a = P_n^-, H_a' = C_n^-$ and when $H_a = I_n^-, H_a' = B_n^-$. Let $X = A + Bd = -A^{-3}, Y = B + Ad = -A^3$. Recall that $B = A^{-1}, d = -A^2 - A^{-2}$. By Definition 1 and Lemma 2 and after some computations, we obtain the following table:

Example 1 In Fig. 16, we give a family of tetrahedral links of rational-type. Recall that the labeled tetrahedron T^l is illustrated in Fig. 11 (left). Its chain polynomial is computed in [54,57]. That is,

$$\begin{aligned} Ch[T^l] &= abcdef - w(adf + abc + bef + cde) - w(ae + bd + cf) \\ &\quad + (w + w^2)(a + b + c + d + e + f) - w(w + 1)(w + 2). \end{aligned}$$

By Theorem 1 and the data in Table 1, the general formula of the Kauffman bracket polynomial of $D_1(n_1, n_2, n_3, n_4, n_5, n_6)$ can be obtained. However, it is too lengthy and hence omitted.

3.3 Uniform polyhedral links with small edge covering units

Now we consider the so-called *uniform polyhedral links*, that is, the polyhedral links obtained by applying the same 2-tangle to cover each edge of the polyhedral graph. Recall that the 2-tangle corresponds to signed plane graphs with two attached vertices.

Table 1 The parameters for integer tangles

H	P_n^+	P_n^-	I_n^+	I_n^-
$Q[H]$	X^n	Y^n	$\frac{Y^n-B^n}{d}+dB^n$	$\frac{X^n-A^n}{d}+dA^n$
$Q[H']$	$\frac{X^n-A^n}{d}+dA^n$	$\frac{Y^n-B^n}{d}+dB^n$	Y^n	X^n
$\alpha[H]$	$\frac{X^n-A^n}{d}$	$\frac{X^n-A^n}{d}$	B^n	A^n
$\beta[H]$	A^n	B^n	$\frac{Y^n-B^n}{d}$	$\frac{X^n-A^n}{d}$
$\gamma[H]$	$(X/A)^n$	$(Y/B)^n$	$1+\frac{d^2}{(Y/B)^n-1}$	$1+\frac{d^2}{(X/A)^n-1}$

Now we shall firstly list all signed plane graphs with two attached vertices with smaller numbers of edges, i.e. small edge covering units. Then we compute the parameters of such units used in Theorem 1.

Recall that loops correspond to nugatory crossing. We suppose G is a connected non-trivial loopless plane graph. We denote by $p(G)$ and $q(G)$ the numbers of vertices and edges of G, respectively. Since G is connected loopless and non-trivial, we have $2 \leq p(G) \leq q(G)+1$. When $p(G)=2$, G is the multiple edge $I_{q(G)}$; when $p(G)=q(G)+1$, G is a tree with $q(G)$ edges. All trees with $q(G) \leq 11$ edges are listed in [58]. In the following we shall hence only consider the cases: $3 \leq p(G) \leq q(G)$. Recall that the circumference of G is the length of the longest cycle of G. We denote by $c(G)$ the circumference of G.

Lemma 3 *The connected loopless plane (multi-)graphs with edge numbers between 1 and 5 except the trees and multiple edges are shown in Fig. 17.*

Proof It is clear that graphs with edge numbers no more than 5 are all planar. If $q(G)=1$, then $G=I_1$ and if $q(G)=2$, then $G=I_2$ or P_3.

1. $q(G)=3$, we have $p(G)=3$.
   (a) If $c(G)=2$, then G is $3-1$;
   (b) If $c(G)=3$, then G is the $3-2$.
2. $q(G)=4$, we have $3 \leq p(G) \leq 4$.
   (a) If $p(G)=3$, then
      i. If $c(G)=2$, then G is $4-1$ or $4-2$;
      ii. If $c(G)=3$, then G is the $4-3$.
   (b) If $p(G)=4$, then
      i. If $c(G)=2$, then G is $4-4$, $4-5$ or $4-6$;
      ii. If $c(G)=3$, then G is the $4-7$;
      iii. If $c(G)=4$, then G is the $4-8$.
3. $q(G)=5$, we have $3 \leq p(G) \leq 5$.
   (a) If $p(G)=3$, then
      i. If $c(G)=2$, then G is $5-1$ or $5-2$;
      ii. If $c(G)=3$, then G is $5-18$ or $5-19$.
   (b) If $p(G)=4$, then
      i. If $c(G)=2$, then G is $5-3$, $5-4$, $5-5$, $5-6$, $5-7$ or $5-8$;

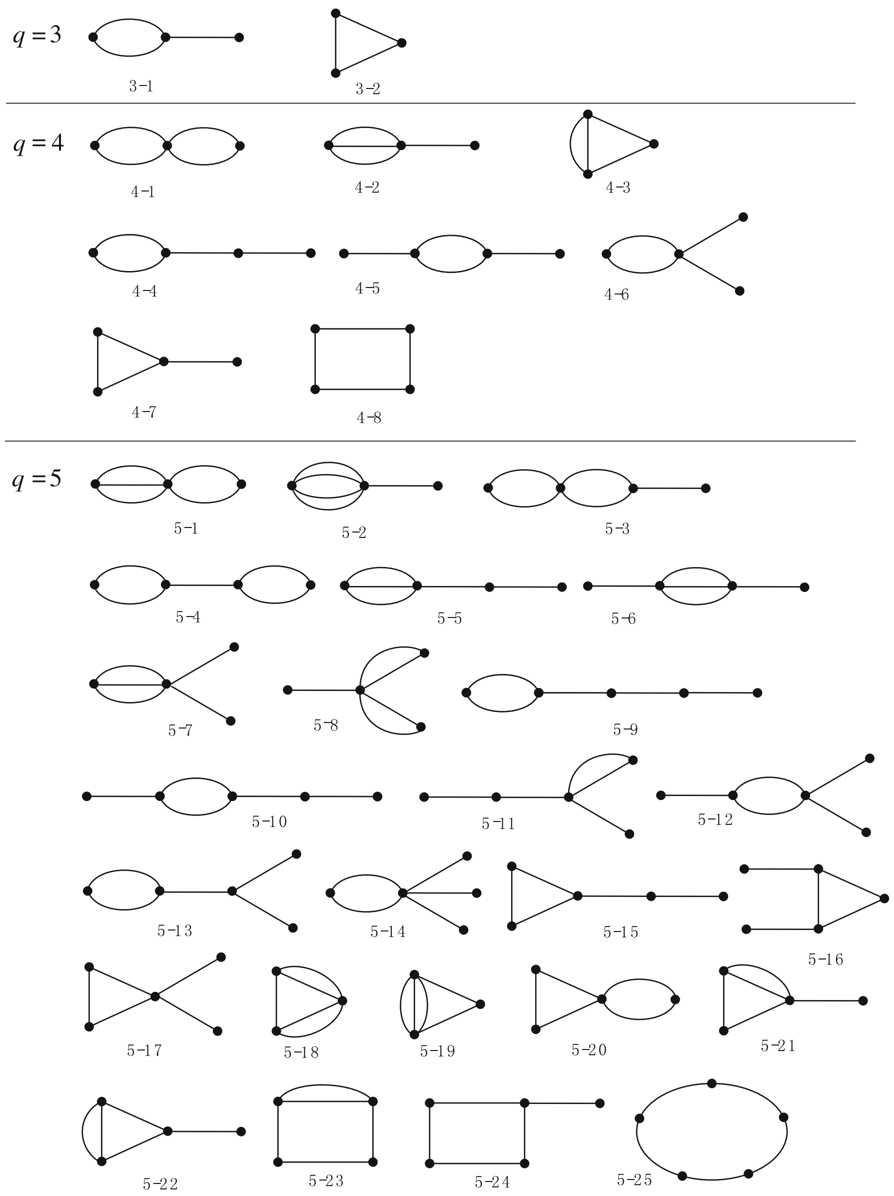


Fig. 17 The connected loopless plane graph with $1 \leq q(G) \leq 5$ except the trees and multiple edges

ii. If $c(G) = 3$, then G is $5 - 20$, $5 - 21$ or $5 - 22$;
iii. If $c(G) = 4$, then G is the $5 - 23$.

(c) If $p(G) = 5$, then
   i. If $c(G) = 2$, then G is $5 - 9$, $5 - 10$, $5 - 11$, $5 - 12$, $5 - 13$ or $5 - 14$;
   ii. If $c(G) = 3$, then G is $5 - 15$, $5 - 16$ or $5 - 17$;

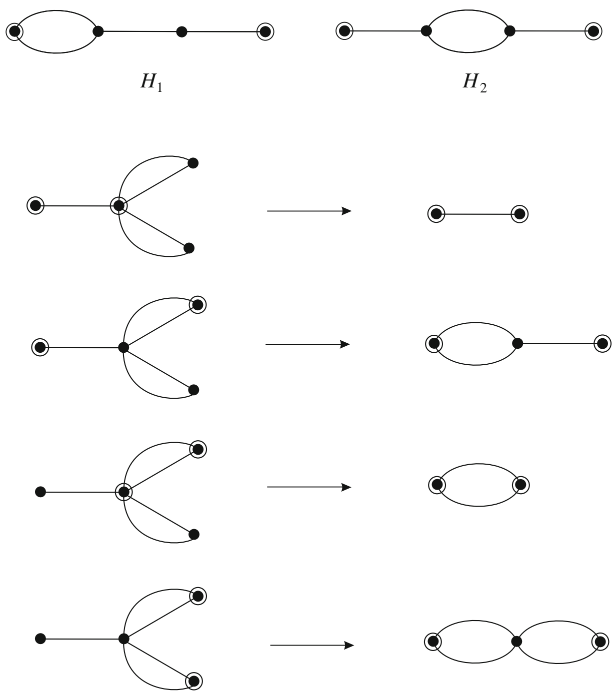


Fig. 18 (*up*) The pair with the same parameters; (*down*) the four 5–8 with two attached vertices are all reduced

iii. If $c(G) = 4$, then G is $5 - 24$;
iv. If $c(G) = 5$, then G is the $5 - 25$.

□

Now we list connected loopless plane graphs with two attached vertices based on Lemma 3. We can apply the following two principles to reduce the numbers of connected loopless plane graphs with two attached vertices.

1. Let H_1 and H_2 are two connected loopless plane graphs with two attached vertices. If $Q[H_1] = Q[H_2]$ and $Q[H_1'] = Q[H_2']$ (hence, the remaining three parameters are also the same), we only choose one of H_1 and H_2 as the representative, usually the one with higher symmetry. For the pair H_1 and H_2 in Fig. 18 (up), according to Lemma 2 (2), $Q[H_1] = Q[H_2]$. Note that $H_1' = H_2'$, hence $Q[H_1'] = Q[H_2']$. We only list H_2 in Fig. 19.
2. Let H be a connected loopless plane graphs with two attached vertices. If H has more than one block, according to Lemma 2 (2), we can reduce H by cutting the blocks containing no attached vertex and some blocks with only one attached vertex. In particular, trees with two attached vertices can be reduced to the path connecting the two attached vertices in the tree. In Fig. 18 (down) we give the example of the reductions of the graph $5 - 8$ in Fig. 17 with different two attached vertices.

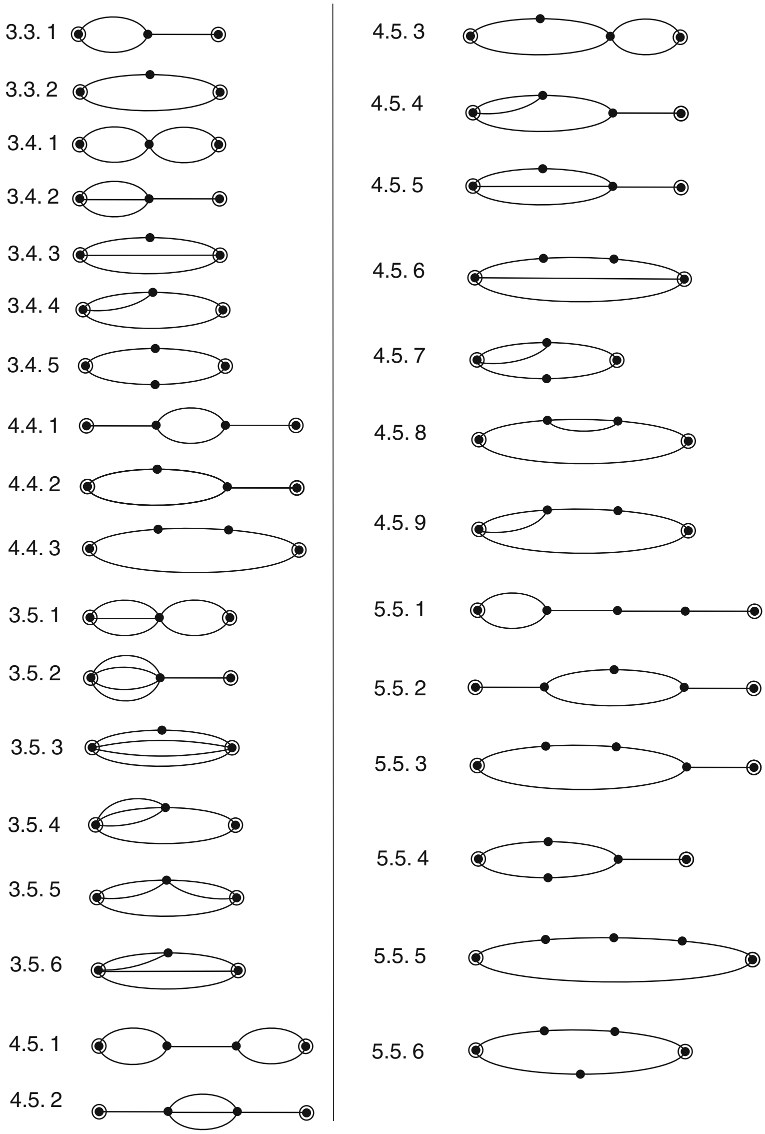


Fig. 19 The connected loopless plane graphs with two attached vertices circled

Finally, we obtain Fig. 19, in which there are 31 connected loopless plane graphs with two attached vertices. In Fig. 19, the notation 4.5.3 means that the corresponding graph is the third one with 4 vertices and 5 edges.

Then we shall suppose the signs on the edges of the 31 graphs are all + (since the polyhedral links synthesized by chemists are all alternating, as far as we know) and compute the parameters used in Theorem 1 of each of them. In Tables 2 and 3, we list the five parameters of units with edge number 3 and 4. In Table 4, we only list

Table 2 The values of $Q[H]$ and $Q[H']$ of units with edge number 3 and 4

The graph H	$Q[H]$	$Q[H']$
3.3.1	$A + A^{-7}$	$A^7 - A^3 - A^{-5}$
3.3.2	$-A^5 - A^{-3} + A^{-7}$	$A^7 + A^{-1}$
3.4.1	$A^8 + 2 + A^{-8}$	$-A^{10} + A^6 - A^2 - A^{-6}$
3.4.2	$-A^4 + 1 + A^{-8}$	$-A^{10} + A^6 - A^2 - A^{-6}$
3.4.3	$A^8 - A^4 + 1 - A^{-4} + A^{-8}$	$-A^{10} - A^2$
3.4.4	$A^8 - A^4 + 1 - A^{-4} + A^{-8}$	$-A^{10} + A^6 + A^{-2}$
3.4.5	$-A^6 - A^{-2} + A^{-6} - A^{-10}$	$A^8 + 2 + A^{-8}$
4.4.1	$-A^{-2} - A^{-10}$	$A^8 - A^4 + 1 - A^{-4} + A^{-8}$
4.4.2	$A^2 + A^{-6} - A^{-10}$	$A^8 - A^4 + 1 - A^{-4} + A^{-8}$
4.4.3	$-A^6 - A^{-2} + A^{-6} - A^{-10}$	$A^8 + 1 - A^{-4}$

Table 3 The values of $\alpha[H]$, $\beta[H]$ and $\gamma[H]$ of units with edge number 3 and 4

The graph H	$\alpha[H]$	$\beta[H]$	$\gamma[H]$
3.3.1	$-A^3 + A^{-1} - A^{-5}$	$-A^5 + A$	$\frac{-1-A^{-8}}{A^4-1}$
3.3.2	$A^{-1} - A^{-5}$	$-A^5 + A - A^{-3}$	$\frac{A^8+1-A^{-4}}{A^8-A^4+1}$
3.4.1	$-2A^2 + A^{-2} - A^{-6}$	$A^8 - 2A^4 + 1$	$\frac{A^8+2+A^{-8}}{A^8-2A^4+1}$
3.4.2	$A^6 - A^2 + A^{-2} - A^{-6}$	$A^8 - A^4 + 1$	$\frac{-A^4+1+A^{-8}}{A^8-A^4+1}$
3.4.3	$A^{-2} - A^{-6}$	$A^8 - A^4 + 2 - A^{-4}$	$\frac{A^{12}-A^8+A^4-1+A^{-4}}{A^{12}-A^8+2A^4-1}$
3.4.4	$-A^2 + A^{-2} - A^{-6}$	$A^8 - 2A^4 + 1 - A^{-4}$	$\frac{A^{12}-A^8+A^4-1+A^{-4}}{A^{12}-2A^8+A^4-1}$
3.4.5	$1 - 2A^{-4} + A^{-8}$	$-A^6 + A^2 - 2A^{-2}$	$\frac{A^8+1-A^{-4}+A^{-8}}{A^8-A^4+2}$
4.4.1	$-A^4 + 2 - A^{-4} + A^{-8}$	$-A^6 + A^2$	$\frac{A^{-4}+A^{-12}}{A^4-1}$
4.4.2	$-A^4 + 1 - 2A^{-4} + A^{-8}$	$-A^6 + A^2 - A^{-2}$	$\frac{-A^4-A^{-4}+A^{-8}}{A^8-A^4+1}$
4.4.3	$1 - A^{-4} + A^{-8}$	$-A^6 + A^2 - A^{-2} + A^{-6}$	$\frac{A^{12}+A^4-1+A^{-4}}{A^{12}-A^8+A^4-1}$

the two parameters of units with edge number 5. We point that, to obtain Tables 2, 3 and 4, we use the Maple program designed for computing Kauffman bracket polynomial of pretzel links in [59]. It is worth noting that the parameters of 4.5.8 and 4.5.9 in Table 4 are the same.

Using results in our tables and Theorem 1 and Lemma 1, we can compute Kauffman bracket polynomials of uniform polyhedral links with small edge (≤ 5) covering unit. Now we give an example.

Example 2 A tetrahedral link, obtained from the tetrahedron by 'branched curve and the tangle $1, 2, 1$' covering, as shown in Fig. 20 (upper). We denote the tetrahedral link by D_2. The $1, 2, 1$ tangle corresponds to the plane graph 4.4.1 in Fig. 19.

Table 4 The values of $\beta[H]$ and $\gamma[H]$ of units with edge number 5

The graph H	$\beta[H]$	$\gamma[H]$
3.5.1	$-A^{11}+2A^7-2A^3+A^{-1}$	$\frac{A^{12}-A^8+A^4-2-A^{-8}}{A^{12}-2A^8+2A^4-1}$
3.5.2	$-A^{11}+A^7-A^3+A^{-1}$	$\frac{-A^8+A^4-1-A^{-8}}{A^{12}-A^8+A^4-1}$
3.5.3	$-A^{11}+A^7-2A^3+2A^{-1}-A^{-5}$	$\frac{A^{16}-A^{12}+2A^8-A^4+1-A^{-4}}{A^{16}-A^{12}+2A^8-2A^4+1}$
3.5.4	$-A^{11}+2A^7-2A^3+A^{-1}-A^{-5}$	$\frac{A^{16}-A^{12}+2A^8-A^4+1-A^{-4}}{A^{16}-2A^{12}+2A^8-A^4+1}$
3.5.5	$-A^{11}+2A^7-3A^3+A^{-1}-A^{-5}$	$\frac{A^{16}-2A^{12}+A^8-2A^4+1-A^{-4}}{A^{16}-2A^{12}+3A^8-A^4+1}$
3.5.6	$-A^{11}+2A^7-2A^3+2A^{-1}-A^{-5}$	$\frac{A^{16}-2A^{12}+A^8-2A^4+1-A^{-4}}{A^{16}-2A^{12}+2A^8-2A^4+1}$
4.5.1	A^9-2A^5+A	$\frac{-A^4-2A^{-4}-A^{-12}}{A^8-2A^4+1}$
4.5.2	A^9-A^5+A	$\frac{1-A^{-4}-A^{-12}}{A^8-A^4+1}$
4.5.3	$A^9-2A^5+2A-A^{-3}$	$\frac{A^{12}+2A^4-1+A^{-4}-A^{-8}}{A^{12}-2A^8+2A^4-1}$
4.5.4	$A^9-2A^5+A-A^{-3}$	$\frac{-A^8+A^4-1+A^{-4}-A^{-8}}{A^{12}-2A^8+A^4-1}$
4.5.5	$A^9-A^5+2A-A^{-3}$	$\frac{-A^8+A^4-1+A^{-4}-A^{-8}}{A^{12}-A^8+2A^4-1}$
4.5.6	$A^9-A^5+2A-2A^{-3}+A^{-7}$	$\frac{A^{16}-A^{12}+A^8-2A^4+1-A^{-4}}{A^{16}-A^{12}+2A^8-2A^4+1}$
4.5.7	$A^9-2A^5+2A-2A^{-3}$	$\frac{A^{12}-A^8+A^4-2+A^{-4}-A^{-8}}{A^{12}-2A^8+2A^4-2}$
4.5.8	$A^9-2A^5+2A-A^{-3}+A^{-7}$	$\frac{A^{16}-A^{12}+A^8-2A^4+1-A^{-4}}{A^{16}-2A^{12}+2A^8-A^4+1}$
4.5.9	$A^9-2A^5+2A-A^{-3}+A^{-7}$	$\frac{A^{16}-A^{12}+A^8-2A^4+1-A^{-4}}{A^{16}-2A^{12}+2A^8-A^4+1}$
5.5.1	$-A^7+A^3$	$\frac{-A^{-8}-A^{-16}}{A^4-1}$
5.5.2	$-A^7+A^3-A^{-1}$	$\frac{1+A^{-8}-A^{-12}}{A^8-A^4+1}$
5.5.3	$-A^7+A^3-A^{-1}+A^{-5}$	$\frac{-A^8-1+A^{-4}-A^{-8}}{A^{12}-A^8+A^4-1}$
5.5.4	$-A^7+A^3-2A^{-1}$	$\frac{-A^4-A^{-4}+A^{-8}-A^{-12}}{A^8-A^4+2}$
5.5.5	$-A^7+A^3-A^{-1}+A^{-5}-A^{-9}$	$\frac{A^{16}+A^8-A^4+1-A^{-4}}{A^{16}-A^{12}+A^8-A^4+1}$
5.5.6	$-A^7+A^3-2A^{-1}+A^{-5}$	$\frac{A^{12}+A^4-1+A^{-4}-A^{-8}}{A^{12}-A^8+2A^4-1}$

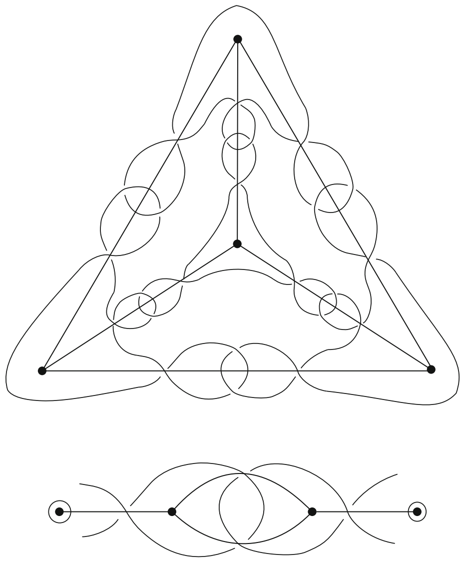


Fig. 20 A uniform tetrahedral link D_2 obtained by applying 1, 2, 1 tangle coverings (*upper*); The 1, 2, 1 tangle and its corresponding signed plane graph 4.4.1 (*down*)

By the data in Table 2, applying Theorem 1 and Lemma 1, and using the Maple program, we obtain

$$\begin{aligned}\langle D_2\rangle = &-A^{42}+9A^{38}-41A^{34}+123A^{30}-278A^{26}+516A^{22}-824A^{18}+1161A^{14}\\ &-1473A^{10}+1704A^{6}-1809A^{2}+1774A^{-2}-1614A^{-6}+1369A^{-10}\\ &-1088A^{-14}+811A^{-18}-569A^{-22}+372A^{-26}-228A^{-30}+126A^{-34}\\ &-66A^{-38}+28A^{-42}-12A^{-46}+3A^{-50}-A^{-54},\end{aligned}$$

which implies D_2 is topologically chiral.

4 Concluding remarks

Firstly, we give some remarks on chain polynomials. The chain polynomial of many graphs or graph families, including the theta graph, wheels, complete graphs, the triangular prisms, laders and Möbius ladders etc, are computed in [57]. As far as the computation of chain polynomials is concerned, in [31] Yang and Zhang shrank all plane graphs to the 3-polytope (i.e. 3-connected 3-regular planar graphs) and two other small graphs. They also calculated chain polynomials of some polyhedra. In [60] L. Traldi proved that the chain polynomial is actually a kind of Tutte polynomials of weighted graphs.

Secondly, there are some results on the Homflypt polynomial of polyhedral links, say [16,19], and polyhedral links in [16] include those in [19] as special cases. Note that the integer tangles used to construct polyhedral links of rational-type can be either even or odd and either horizontal or vertical, they include polyhedral links in [19] and have a very small intersection with polyhedral links in [16]. Note that only 3.4.1 and

3.4.5 in Fig. 19 correspond to horizontal or vertical 2, 2 tangles, therefore, among uniform polyhedral links with small edge $\leq$ 5 covering units, only two polyhedral links belong to polyhedral links in [16]. Hence, the Jones polynomial of only a very small part of two kinds of polyhedral links we considered can be derived from results on Homflypt polynomial in [16]. Here we also point out that our paper [61] generalizes results in [16].

Finally, we posed the notion of polyhedral links based on edge, vertex and mixed edge and vertex covering and constructed a very large family of polyhedral links, but there exists polyhedral links which do not belong to polyhedral links we constructed. See [62,63] for examples. We have given a formula of the Kauffman bracket polynomial of polyhedral links based on edge covering in terms of the chain polynomial of the polyhedral graphs. The Kauffman bracket polynomials (hence, the Jones polynomial) of polyhedral links in [1–7] thus can be obtained. A natural problem is whether we can compute the Kauffman bracket polynomial of polyhedral links based on vertex covering and more general polyhedral links based on mixed edge and vertex covering in terms of some polynomial of the polyhedral graphs. If the answer is "yes", then we shall obtain the Jones polynomial of the linked protein catenane in [8,9].

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