MATCH
Communications in Mathematical
and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **76** (2016) 569-594

ISSN 0340 - 6253

A Survey on Several Invariants of Three Types of Polyhedral Links*

Xian'an Jin

School of Mathematical Sciences, Xiamen University,
Xiamen, Fujian 361005, P.R.China
`xajin@xmu.edu.cn`

(Received April 6, 2016)

Abstract

Polyhedral links were introduced as the mathematical model for DNA and protein polyhedra. Various invariants of polyhedral links were computed to understand and quantize DNA and protein polyhedra. In this paper we focus on two types of DNA polyhedral links and one type of protein polyhedral links and four invariants: Jones polynomial, HOMFLY polynomial, braid index and genus, give a survey of results in these aspects. We also raise several questions for further study.

1 Introduction

In 1961, Frisch and Wasserman [1] first synthesized a pair of linked rings, known as the Hopf link in knot theory and as catenanes in chemistry. Twenty eight years later, the first molecular knot in the form of the trefoil knot was synthesized by Dietrich-Buchecker and Sauvage [2]. Many molecules in the form of other knots, links and more general spatial graphs have been synthesized artificially in the laboratory or found in nature by chemists and biologists in the past more than fifty years.

Small molecules are usually rigid and their structures are topologically simple. Macromolecules are relatively flexible and could have more complicated spatial structures, and in this case topological techniques are applied. For example, in 1982, Walba, Richards, and Haltiwanger synthesized the first Möbius ladder with three rungs [3] and in 1986

---

*Dedicated to Professor Fuji Zhang on the occasion of his 80th birthday

Simon [4] proved Walba's conjecture: the Möbius ladder with three or more rungs is topologically chiral in the sense that rungs are transformed to rungs and sides to sides. Another manifest is the description and quantization of the action of cellular enzymes on circular DNA [5,6]. For applications of topology to chemistry as well as molecular biology, we refer the readers to the survey paper [7] and the monograph [8].

Knot theory is a branch of topology which mainly study knots and links, i.e. circles, $\mathbb{S}^1$'s, embedded in the 3-dimensional space $\mathbb{E}^3$, as well as general spatial graphs. Graph theory is a branch of combinatorics which mainly study abstract graphs, as well as planar graphs and graphs embedded in surfaces of higher genuses. The two theories both originated from the Euler's Königsberg's Bridges Problem and are two of three main branches (the third theory is group theory) of mathematics widely used in the study of mathematical chemistry.

As for the interplay between knot theory and graph theory, there is an old 1-1 correspondence between edge-singed plane graphs and link diagrams, the planar representation of links in $\mathbb{E}^3$. The example in Fig. 1 illustrates it clearly. This correspondence was once used to construct a table of link diagrams of all links in the late 19th century [9]. In the late 1980s, the correspondence was used to establish a relation between Jones polynomial [10] in knot theory and Tutte polynomial [11] in graph theory. See [12–14] for details. In 2000s, the relation was generalized to several relations [15–17] between the Jones polynomial of virtual links [18] and the topological Tutte polynomial of ribbon graphs [19,20]. To unify these relations, the classical geometrical duality for cellularly embedded graphs (i.e. ribbon graphs) was generalized to partial duality and further twisted duality in [21] and [22] in recent several years. See the monograph [23] for details.

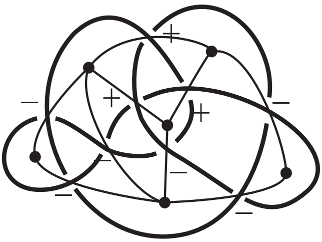


Fig. 1: A link diagram (thick arcs) and its corresponding edge-signed plane graph (thin arcs).

Two graphs are called *homeomorphic* if they both can be obtained from another graph by edge subdivisions. In [24], Read and Whitehead studied a unified way to compute the Tutte polynomial of homeomorphism classes of graphs, reducing it to the chain polynomial of labelled graphs [25]. In [26], Jin and Zhang generalized it from graphs to signed graphs so that it can be used to deal with the Jones polynomial of links formed from a graph by replacing edges by parallel twists. Then they generalized it to two kinds of twists, parallel or perpendicular, in [27]. Finally, the computational method of the general case: replacing edges by 2-tangles, was obtained in [28]. Based on [26], Yang and Zhang further reduced the computation to that of cubic 3-polytopes in [29]. Furthermore, a similar result was also obtained by Jin and Zhang for the HOMFLY polynomial in [30], which extends results in [31] obtained by Jaeger and [32] obtained by Traldi greatly.

To our surprise and delight, our above results on general knots found applications in quantizing many DNA polyhedra synthesized since 1991. The paper is organized as follows. In Section 2, we first recall some DNA and protein polyhedra and their mathematical model. In Section 3, we give a survey of results on invariants of DNA or protein polyhedral links and we shall focus on the following four invariants: Jones polynomial, HOMFLY polynomial, braid index and genus. In the last Section 4, we propose several problems for further study.

2 Polyhedral links

Polyhedral links are mathematical models introduced in recent ten years or so, which were used to describe, understand and quantize DNA and protein polyhedra. Now we recall two types of DNA polyhedra and one type of protein polyhedra, and their corresponding mathematical models.

In 1991, Chen and Seeman gave the first construction of a closed polyhedral object from DNA, the DNA cube [33]. Since then, DNA truncated octahedron [34], DNA octahedron [35], DNA tetrahedron [36,37], DNA bipyramid [38], DNA dodecahedron [39] were synthesized one after another. They are all constructed by means of "d-branched curves and (even) k-twisted double-lines" covering introduced by Hu et al in [40] as shown in Fig. 2.

Let G be a plane graph. We shall denote by $L_k(G)$ such a polyhedral link by covering each vertex of degree d by a d-branched curve and each edge by a k-twisted double-line. When k is even, we call $L_k(G)$ an *even polyhedral link* [41]. This is a special family of

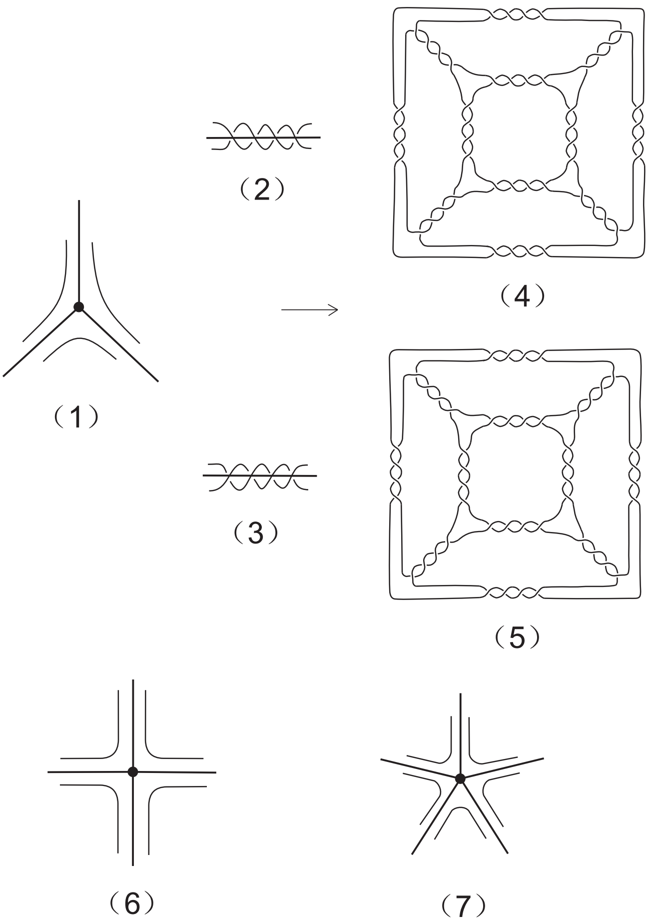


Fig. 2: (1) A 3-branched curve, (2) a -4-twisted double-line, (3) a +4-twisted double-line, (4) the planar representation of the negative DNA cubic link in [33] with $k = -4$, (5) the planar representation of the positive DNA cubic link with $k = +4$, (6) a 4-branched curve and (7) a 5-branched curve.

polyhedral links based on edge covering introduced in [42] by Jin and Zhang.

In 2000, a topologically linked catenane, which consists of 12 pentameric and 60 hexameric rings of covalently joined protein subunits that loop through each other, was observed in the bacteriophage HK97 capsid [43, 44]. Such a protein catenane can be modelled mathematically by a polyhedral link obtained by "3-cross curve and untwisted double-line" covering introduced by Qiu and Zhai in [45] as shown in Fig. 3. The construction was further generalized by Cheng et al in [46] to d-cross curves and branched alternating closed braids, and by Jin and Zhang in [42] to $2d$-tangles to obtain *polyhedral links based on vertex covering.*

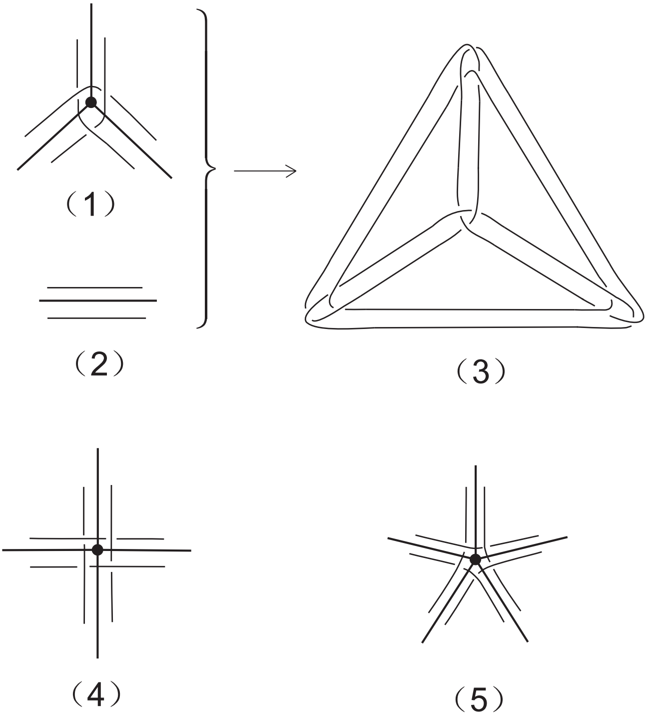


Fig. 3: (1) A 3-cross curve, (2) an untwisted double-line, (3) the planar representation of the protein tetrahedral link, (4) a 4-cross curve and (5) a 5-cross curve.

Let G be a plane graph. We shall denote by $L_v(G)$ such a polyhedral link by covering each vertex of degree d by a d-cross curve and each edge by a untwisted double-line. When G is d-regular, we call $L_v(G)$ a *d-regular polyhedral link* for simplicity.

Since 2008 or so, a type of more complicated DNA polyhedra such as DNA cube (with 4 turns) [47], DNA octahedron [48], DNA icosahedron [49], DNA tetrahedron , dodecahedron and buckyball [50], have been reported. They are all synthesized by covering each vertex of degree n of the polyhedron by "n-point star motif (tiles)" and through sticky-end association between the tiles. The "n-point star motif" has an n-fold rotational symmetry and consists of $2n+1$ single strands: a long repetitive central DNA strand, n identical medium DNA strands and n identical short DNA strands. The part at the center of the motif represents n unpaired DNA single-strands whose lengths can be adjusted to change bending degree of the whole structure. See also [51, 52]. In fact they are called *double crossover DNA polyhedra* in [53].

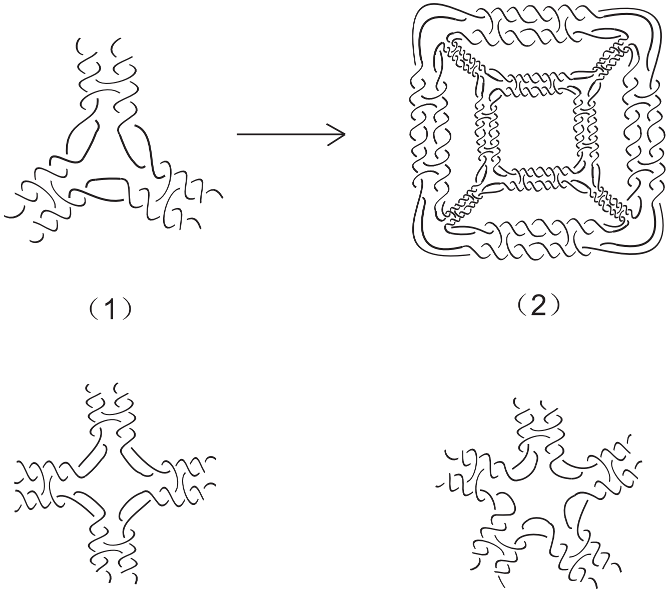
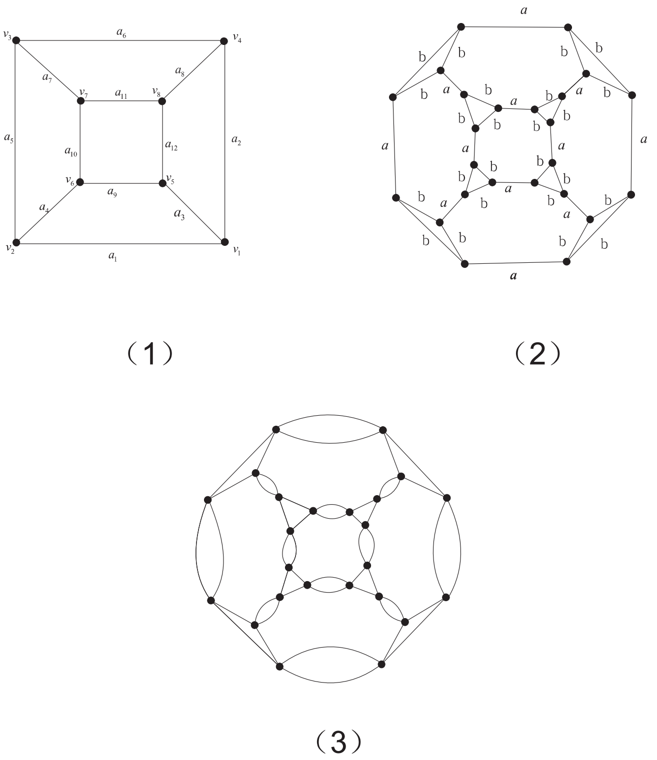

(1) (2) (3) (4)

Fig. 4: (1) A 3-point star motif, (2) the planar diagram of the (negative) double crossover hexahedral link, (3) a 4-point star motif and (4) a 5-point star motif.

Polyhedral links modelling the double crossover DNA polyhedra are called *double crossover polyhedral links*. See Fig. 4 for an example. Let G be a plane graph. We shall denote by $L_e(G)$ such a polyhedral link by covering each vertex of degree d by a d-point star motif. When G is d-regular, we call $L_e(G)$ a *the double crossover d-regular polyhedral link* for simplicity. The double crossover polyhedral link is in fact a type of polyhedral links based on edge covering. Let P be a polyhedral graph. Let DTP be the plane graph obtained from P by truncating P firstly and then doubling edges originally in P. See Fig. 5. It is not difficult to see that

$$L_e(P) = L_4(DTP). \tag{1}$$



(1)

(2)

(3)

Fig. 5: (1) A cubic graph P, (2) its truncation and (3) doubling edges to obtain DTP.

One can combine the edge covering and the vertex covering to obtain more complicated polyhedral links based on mixed edge and vertex covering [42]. For more information on mathematical models of DNA polyhedra, we also refer the readers to the survey [54].

3 Invariants

As far as we know by now actual DNA and protein polyhedral links are all alternating. We use the orientation of the 2 backbone strands of the dsDNA to orient DNA polyhedral links, thus consider DNA polyhedral links as oriented links with antiparallel orientations. Under these assumptions k must be even (the corresponding plane graph explained in the Section 1 must be bipartite [55]), $L_k(G)$ is right-handed if $k > 0$ and left-handed if $k < 0$. See Fig. 6. We shall view protein polyhedral links as unoriented ones. We point out that four invariants we shall consider in the following are all sensitive to orientations of links. There are unoriented versions of these four invariants which we shall take when we consider protein polyhedral links.

Fig. 6: Right-handed (+) and left-handed crossings (−).

3.1 Jones polynomial

The Jones polynomial [10, 56] was discovered in 1984. It is an invariant of oriented links up to ambient isotopy. Let L be an oriented link, we shall denote by $V_L(t)$ the Jones polynomial of L. It is a Laurent polynomial in the variable $\sqrt{t}$, determined by the following three axioms:

(i) Jones polynomial is an ambient isotopic invariant of oriented links.

(ii)

$$V_O(t) = 1, \tag{2}$$

where O is an unknot.

(iii) (Skein relation)

$$t^{-1}V_{L_+}(t) - tV_{L_-}(t) = (\sqrt{t} - \frac{1}{\sqrt{t}})V_{L_0}(t), \tag{3}$$

where L_+, L_- and L_0 are link diagrams which are identical (outside the dotted circles) except near one crossing where they are as in Fig. 7 and are called a skein triple.

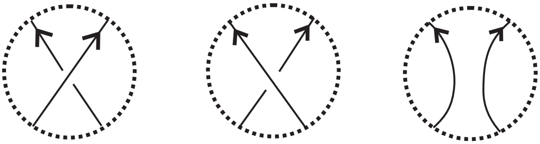


Fig. 7: L_+ (positive), L_- (negative) and L_0 in Eq. (3).

In 1987, L. H. Kauffman constructed a state model for the Jones polynomial using his bracket polynomial [12, 13], which provided another way of calculating the Jones polynomial. Let D be a link diagram of the oriented link L, and $< D >$ be the Kauffman bracket polynomial in one variable A of D with orientations neglected. Then

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

where $w(D)$ is the writhe (i.e. the sum of signs of crossings) of D inheriting the orientation of L.

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. In [57], Jin and Zhang gave a computational formula of the Kauffman bracket polynomial of $L_k(G)$ in terms of the Tutte polynomial $T_G(x, y)$ of G. For the detail of the Tutte polynomial we refer the reader to [11, 58].

Theorem 3.1 *Let G be a connected plane graph, having p vertices and q edges. For any integer k, even or odd, then*

$$< L_k(G) >= A^{-qk} \left[\frac{(-A^4)^k - 1}{-A^2 - A^{-2}}\right]^{q-p+1} T_G((-A^4)^k, \frac{(-A^4)^k + A^4 + 1 + A^{-4}}{(-A^4)^k - 1}).$$

This result is obtained by combining the relation [26] between the Kauffman bracket polynomial and the chain polynomial, and the relation [57] between the chain polynomial and the Tutte polynomial. 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. Jones polynomials of Platonic polyhedral links are thus obtained in [57]. In [27], Jin and Zhang generalized the relation in [26] to deal with Kauffman bracket polynomials of rational links (i.e. 2-bridge links).

Based on the 1-1 correspondence between link diagrams and signed plane graphs, in [14] Kauffman converted the Kauffman bracket polynomial to the Tutte polynomial of signed graphs, which are not necessarily planar. Let G be a signed graph. We shall denote by $Q[G] = Q[G](A, A^{-1}, -A^2 - A^{-2}) \in \mathbb{Z}[A]$ the Tutte polynomial of G.

Let G 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 a connected signed graph H_a with two attached vertices u and w that has only the vertices u and w in common with $\widehat{G - a}$. Let H'_a be the graph obtained from H_a by identifying u and w, the two attached vertices of H_a. Let $d = -A^2 - A^{-2}$. Let

$$\alpha_a = \alpha[H_a] = \frac{1}{d^2 - 1}(dQ[H_a] - Q[H'_a]), \tag{5}$$

$$\beta_a = \beta[H_a] = \frac{1}{d^2 - 1}(dQ[H'_a] - Q[H_a]), \tag{6}$$

$$\gamma_a = \gamma[H_a] = 1 + d\frac{\alpha[H_a]}{\beta[H_a]} \tag{7}$$

In [28], Jin, Zhang, Dong and Tay established a relation between the Tutte polynomial of $\hat{G}$ and the chain polynomial of G as follows. We first recall the definitions of labeled graphs and chain polynomials.

A *labeled graph* is a graph whose edges have been labeled with elements of a commutative ring with unity. The *chain polynomial* of labeled graphs was introduced by Read and Whitehead Jr. in [25] for studying the chromatic polynomials of homeomorphic graphs. The chain polynomial of labeled graphs can also be computed by using the following recursive rules.

1. If G^l is edgeless, then

$$Ch[G^l] = 1. \tag{8}$$

2. Let a be an edge of G^l.

   (a) If a is a loop of G^l, then

$$Ch[G^l] = (a - w)Ch[G^l - a]. \tag{9}$$

   (b) If a is not a loop, then

$$Ch[G^l] = (a - 1)Ch[G^l - a] + Ch[G^l/a]. \tag{10}$$

Theorem 3.2 *Let G 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* $Ch(G)$*, then we have*

$$Q[\hat{G}] = \frac{\prod_{a \in E(G)} \beta_a}{d^{q(G)-p(G)+1}} Ch[G]\,, \tag{11}$$

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

We point out that the Tutte polynomial of $\hat{G}$ was studied by Woodall in [59] and similar results were also obtained by Diao et al in [60,61]. In theory Theorem 3.2 solved the computational problem of Jones polynomials of polyhedral links based on edge covering, although in practice it is still a difficult task to obtain explicit expressions of Jones polynomials of large ones. In [42], Jin and Zhang obtained some such explicit expressions of polyhedral links of rational type and uniform polyhedral links with small edge covering units.

In [62,63], Jablan et al computed the Jones polynomial of 3- and 4-pyramidal knots and 3- and 4-prismatic knots. Cheng et al computed the Jones polynomial of cycle-crossover polyhedral links in [64]. Other related works on computing the Jones polynomial include [29,65–67].

3.2 HOMFLY polynomial

The discovery of the Jones polynomial is a very exciting event in the study of invariants of links which provokes the discovery of the Homfly [68,69] as well as many types of polynomials. The HOMFLY polynomial of an oriented link L, denoted by $P_L(v,z) \in \mathbb{Z}[v^{\pm}, z^{\pm}]$, can be defined by the three following axioms:

(i) $P_L(v,z)$ is invariant under ambient isotopy of L.

(ii)

$$P_O(v,z) = 1, \tag{12}$$

where O is an unknot.

(iii) (Skein relation)

$$v^{-1}P_{L_+} - vP_{L_-} = zP_{L_0}. \tag{13}$$

In [40], Hu et al. first computed HOMFLY polynomial of several specific polyhedral links. Imitating Jaeger's work [31], Jin and Zhang [41] gave a general method to compute the HOMFLY polynomial of even polyhedral links. They obtained:

Theorem 3.3 *Let G be a connected plane graph with p vertices and q edges. Then*

$$P_{L_{2n}(G)}(v,z) = (\frac{z}{v^{-1}-v}(1-v^{2n}))^{q-p+1}v^{2n(p-1)}T_G(v^{-2n}, 1+(\frac{v^{-1}-v}{z})^2\frac{v^{2n}}{1-v^{2n}}).$$

By applying Theorem 3.3 and using computer algebra (Maple) techniques, HOMFLY polynomials of even Platonic polyhedral links are calculated in [41].

Now we give a more general result extending from even twists to the so-called alternatingly oriented 2-tangles. A 2-*tangle* is a part of a link with 4 free ends obtained by cutting two segments of curves of the link. A 2-tangle diagram is the planar representation of a 2-tangle. We usually use a square (with letter T inside) with 4 free ends to denote a general 2-tangle diagram. An oriented 2-tangle diagram is said to be *alternatingly oriented* if the orientation of the diagram induces alternating orientations on the four free ends as shown in Fig. 8.

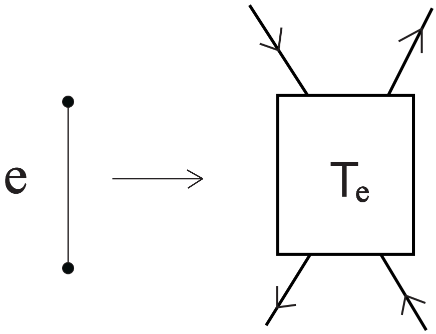


Fig. 8: Alternatingly oriented 2-tangle diagram.

Let T be a 2-tangle. By joining with simple arcs the two upper (i.e. NW and NE) and the two lower end-points (i.e. SW and SE) of the 2-tangle T, we obtain a link called the *numerator* of T, denoted by $Nu(T)$. Joining with simple arcs each pair of the corresponding left end-points (i.e. NW and SW) and right end-points (i.e. NE and SE) of the 2-tangle T, we obtain a link called the *denominator* of T, denoted by $De(T)$, see Fig. 9.

Let $D_T(G)$ be the oriented link diagram obtained from G by covering e with the alternatingly oriented 2-tangle T_e as shown in Fig. 8. Let $\delta = \frac{v^{-1}-v}{z}$,

$$\begin{aligned} w(e) &= \frac{\delta P_{De(T_e)} - P_{Nu(T_e)}}{\delta P_{Nu(T_e)} - P_{De(T_e)}}, \\ \mu(e) &= \frac{\delta P_{De(T_e)} - P_{Nu(T_e)}}{\delta^2 - 1}. \end{aligned}$$

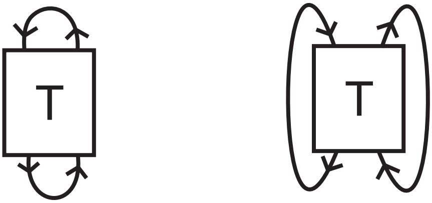


Fig. 9: The numerator (left) and the denominator (right).

Theorem 3.4 *Let G be a connected plane graph, having p vertices and q edges. If we replace w by $1-\delta^2$, and replace a by $1+\frac{\delta}{w(a)}$ for every label a in $Ch(G)$, then*

$$P_{D_T(G)}(v,z) = \delta^{p-q-1}\left(\prod_{e\in E(G)} \mu(e)\right) Ch[G].$$

This result is obtained by combining the relation [30] between the HOMFLY polynomial and the Tutte polynomial of weighted graphs, and the relation [70] between the Tutte polynomial of weighted graphs and the chain polynomial of labelled graphs. In theory Theorem 3.4 solved the computational problem of HOMFLY polynomials of DNA polyhedral links. But in practice it is still difficult to obtain explicit expressions of HOMFLY polynomials of large DNA polyhedral links. For some specific alternatingly oriented 2-tangles, Liu et al did a series of similar works in this aspect, see [71–74].

Now we discuss the double crossover polyhedral links. The double crossover tetrahedral link has 96 crossings, applying Theorem 3.4 its HOMFLY polynomial was obtained by Cheng, Lei and Yang in [75]. However, the double crossover hexahedral link as shown in Fig. 4 (2) has 192 crossings. Applying Theorem 3.4, we cut it into 12 blocks of type 1 and 24 blocks of type 2 as shown in Fig. 10, then we need to compute the chain polynomials of a truncated hexahedral graph with two different labels a and b as shown in Fig. 5 (2), but the truncated hexahedral graph has 36 edges and its chain polynomial is still difficult to be obtained.

In [76], Li, Deng and Jin give a general method to obtain the chain polynomial of a truncated cubic (i.e. 3-regular) graph with two different labels via the chain polynomial of the original cubic graph based on the $Y-\triangle$ transform theorem of chain polynomials and another trivial result of chain polynomials on emerging a path into a single edge [77]. See Fig. 11. As a consequence, for example, by computing the chain polynomial of the labeled hexahedral graph as shown in Fig. 5 (1) they obtain the HOMFLY polynomial of

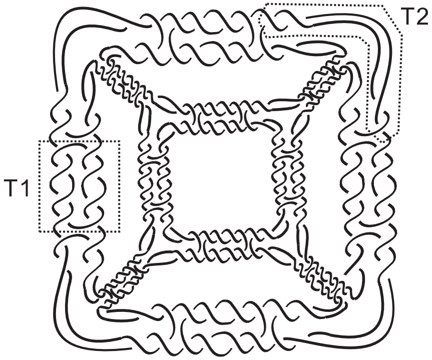


Fig. 10: Two types of building blocks of the double crossover hexahedral link.

the double crossover hexahedral link as shown in Fig. 4 (b).

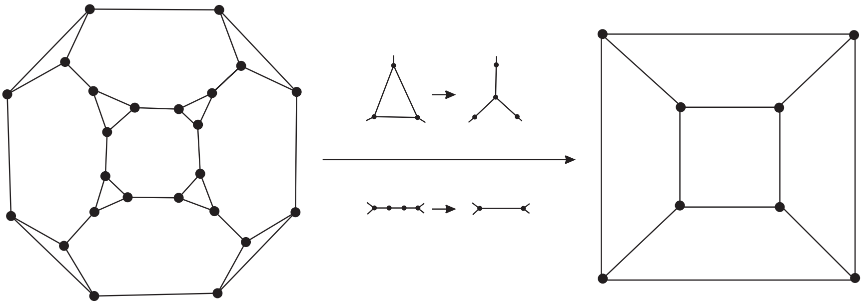


Fig. 11: $\triangle - Y$ transformation and emerging a path of length 3 into a single edge.

3.3 Braid index

Alexander [78], in 1923, showed that every oriented link can be represented as a closed n-string braid. The *braid index* of an oriented link is the minimum number of strings among all closed braid representatives for the given oriented link. Let L be an oriented link. We denote by $b(L)$ the braid index of L.

In 1950s, Franks, Williams [79] and Morton [80] gave independently a lower bound for the braid index and Ohyama in 1993 [81] provided a upper bound for a non-splittable oriented link L. That is

$$\frac{1}{2}\ span_v P_L(v,z) + 1 \leq b(L) \leq \frac{c(L)}{2} + 1, \tag{14}$$

where $span_v P_L(v,z)$=max $\deg_v P_L(v,z) -$ min $\deg_v P_L(v,z)$, and max $\deg_v P_L(v,z)$ and min $\deg_v P_L(v,z)$ denote, respectively, the maximal degree and minimal degree of v in the polynomial $P_L(v,z)$. In addition, by a result [82] due to Menasco that states that a link with an alternating diagram will be non-splittable if and only if the diagram is connected, we know that polyhedral links considered in this survey are all non-splittable. In some cases the upper and lower bounds coincide and thus we could obtain the braid index.

Using this method, in [83], Cheng et al determined the braid index of even polyhedral links. In [84], Cheng and Jin further determined the braid index of double crossover polyhedral links and cycle-crossover polyhedral links. In fact they consider so-called Jaeger's links (more general Traldi's links) which contain, as special cases, even polyhedral links, double crossover polyhedral links and cycle-crossover polyhedral links.

Let G be a connected plane graph. Let $D_a(G)$ be the oriented link diagram constructed based on G by covering each edge of G with oriented clasp (a) in Fig. 12. Oriented link diagrams $D_b(G), D_c(G)$ and $D_d(G)$ can be defined similarly. Let $D_{a,d}(G)$ be the oriented link diagram constructed based on G by covering some edges of G with oriented clasps (a) and other edges with oriented clasps (d) in Fig. 12. Oriented link diagrams $D_{b,c}(G)$ can be defined similarly. Note that $D_{a,d}(G)$ (resp. $D_{b,c}(G)$) are both alternating and contains Jaeger's link $D_a(G), D_d(G)$ (resp. $D_b(G), D_c(G)$) as special cases. More generally, $D_{a,b,c,d}(G)$ is defined to be the oriented link diagram obtained from G by covering each edge with one of four types of clasps $(a), (b), (c)$ and (d). The corresponding link is called Traldi's link.

Theorem 3.5 *b Let G be a connected bridgeless and loopless plane graph with $q(G)$ edges. Let $L_{a,d}(G)$ (resp. $L_{b,c}(G)$) be the oriented link that $D_{a,d}(G)$ (resp. $D_{b,c}(G)$) represents. Then*

$$b(L_{a,d}(G)) = q(G) + 1,$$
$$b(L_{b,c}(G)) = q(G) + 1.$$

The family of polyhedral links considered in [73] is a special family of Jaeger's links. Theorem 5.4 in [73] coincides with Theorem 3.5. An example of alternating Traldi's links, denoted by L_{Tr}, is shown in Fig. 13 which is constructed from a theta graph by replacing edges e_1, e_2 by oriented clasp (a) and e_3 by clasp (c). On the one hand, by using the

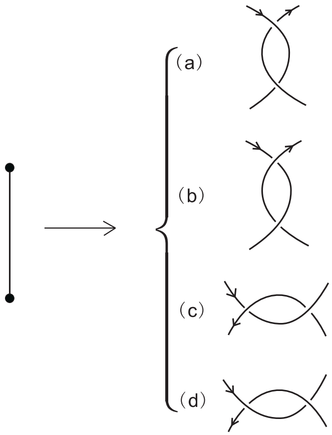


Fig. 12: Replace an edge by four types of oriented clasp.

software KnotGTK, we obtain

$$P_L(v,z) = z^{-1}(-v^5 + v^3) + z(-v^5 + 3v^3) + z^3v^3 \tag{15}$$

and hence, $span_v P_L(v,z) = 2$. On the other hand, we have $c(L) = 4$. Therefore,

$$2 = \frac{span_v P_L(v,z)}{2} + 1 \leq b(L) \leq \frac{c(L)}{2} + 1 = 3. \tag{16}$$

Another such a family of polyhedral links upper and lower bounds of whose braid index are not equal, can be found in Theorem 4.6 of [74].

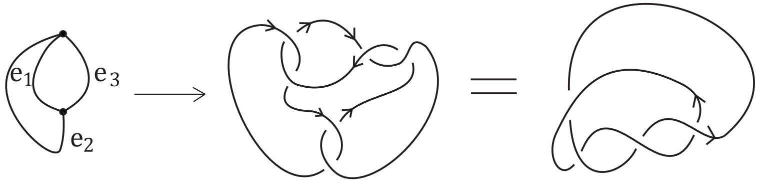


Fig. 13: An alternating Traldi's link upper and lower bounds of whose braid index are not equal.

The braid index of an unoriented link is defined to be the minimum taken over the braid indexes of its all orientations. In 1987, Yamada proved that the braid index of a link equals the minimal number of its Seifert circles [85]. In [86], Cheng, Zhang, Jin and Qiu introduced a notion of ear decomposition of 3-regular polyhedral links based on the ear decomposition of the 3-regular polyhedral graphs. By applying Yamada's result and considering a fixed orientation depending on the ear decomposition, they obtained a upper bound for the braid index of 3-regular polyhedral links. Other works include [87, 88].

3.4 Genus

Let L be an oriented link. An orientable, connected surface that has L as its boundary is called a *Seifert surface* of L. Given a diagram D of L, using Seifert algorithm [89] in 1935, we can obtain a Seifert surface called *projection surface* formed by disks and twisted bands (a kind of ribbon graphs in the Section 1). An example is given as shown in Fig. 14.

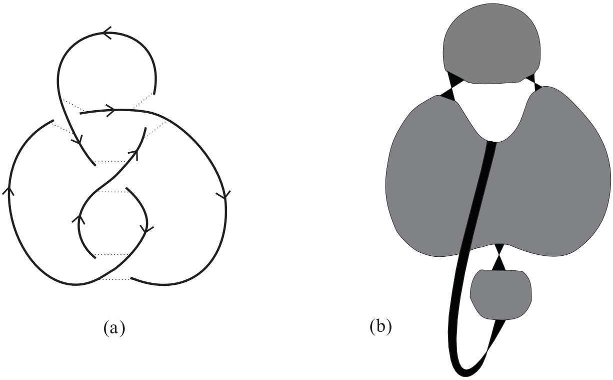


Fig. 14: The Listing knot and its projection surface.

The genus of an oriented link is the minimum genus of all Seifert surfaces of the oriented link. The genus of an unoriented link is the minimum taken over all possible choices of orientation. We denote the genus of an (oriented or unoriented) link L by $g(L)$.

Let D be an alternating link diagram. Let L be the link D represents. Let $\bar{s}_{\max}(D)$ be the maximal number of circles by applying Seifert's algorithm [89] to all orientations of D. According to [90–92], we have:

$$g(L) = \frac{2 - \bar{s}_{\max}(D) + c(D) - \mu(D)}{2}, \tag{17}$$

where $c(D)$ and $\mu(D)$ are the number of crossings and link components of D. In general it is difficult to obtain the genus of an unoriented alternating link with large number of components since we need consider $2^{\mu(L)-1}$ orientations for the link L with $\mu(L)$ components.

Let P_n be the n-pyramid. In [93], Cheng et al proved that

$$g(L_v(P_n)) = \begin{cases} n-2 & if 3|n, \\ n-1 & otherwise. \end{cases}$$

In [94], Liu and Zhang generalized this result from n-pyramid to any 2-connected plane graph G.

Now we recall the definition of the *medial graph*. Let G be a plane graph. We denote by G_m the medial graph of G. If G is trivial (i.e. an isolated vertex having no edges), G_m is a simple closed curve surrounding the vertex. If G is a connected non-trivial plane graph, G_m 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 two vertices are on adjacent edges of the face. If G is not connected, G_m is defined to be the disjoint union of the medial graphs of its connected components. If G is also an edge-signed, then by turning vertices of G_m into crossings according to signs of G, we shall obtain the link diagram corresponding to the edge-signed plane graph G as shown in Fig. 1. Let G be a plane graph. We shall denote by $D(G)$ the link diagram corresponding to the positive G. It is not difficult to see as shown in Fig. 16 that

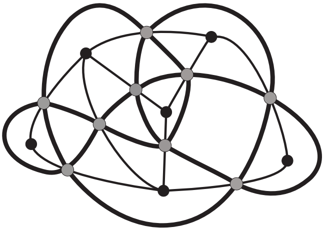


Fig. 15: A plane graph G (colored black) and its medial graph G_m (colored red).

$$L_v(G) = D(G_m). \tag{18}$$

A graph is said to be *even* if each of its vertices has even degree. In particular G_m is even. A connected graph is called *3-edge connected* if it is still connected after removing any its two edges. In [95], Jin et al proved that

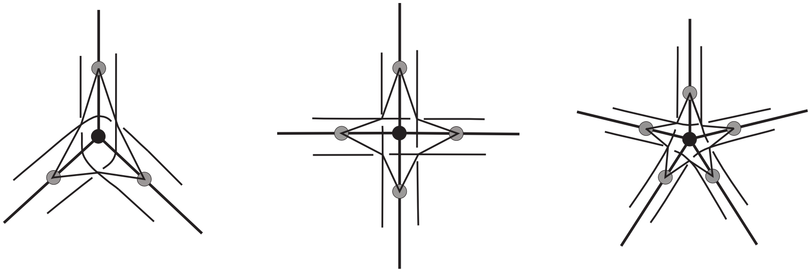


Fig. 16: The interpretation of the equation $L_v(G) = D(G_m)$.

Theorem 3.6 *Let G be a 3-edge connected even plane graph with $p(G)$ vertices. Let $D(G)$ be the alternating link diagram corresponding to the positive G. Let $L(G)$ be the unoriented link $D(G)$ represents. Let $\mu(G)$ be the number of components of $L(G)$. Then*

$$g(L(G)) = \frac{p(G) - \mu(G)}{2}. \tag{19}$$

Theorem 3.6 generalizes Theorem 5.5 in [94] which further contains results of [93] as a special case. As a corollary of Theorem 3.6, we have.

Corollary 3.7 *Let P be a 3-regular polyhedral graph with $p(P)$ vertices. Then*

$$g(L_v(P)) = \frac{p(P)}{2} - 1. \tag{20}$$

Proof. By Eq. (18) and Theorem 3.6, $g(L_v(P)) = g(D(P_m)) = \frac{p(P_m)-f(P)}{2} = \frac{e(P)-f(P)}{2} = \frac{p(P)+2}{2} = \frac{p(P)}{2} - 1$.

□

In addition, by the Euler formula of DNA polyhedral links in [96], it is easy to see that the genuses of the two types of DNA polyhedral links in this paper are both zero. Other related works include [73, 74, 97–99].

4 Questions and discussions

As the research goes on and deepens, some new challenges appeared for us. As for the three kinds of polyhedral links in this survey, there are still some problems unsolved yet. We think that the following two are very fundamental in theory. (1) Efficient ways to compute knot polynomials of (oriented) 3-regular protein polyhedral links have not been found by now. Although 3-regular protein polyhedra has high symmetry, its knot polynomials are difficult to compute. In general, we need to develop computational method for knot polynomials of links obtained from a plane graph by replacing a vertex of degree d by a d-tangle.(2) Theorem 3.4 only dealt with alternatingly oriented 2-tangles, how do we deal with 2-tangles which can not be alternatingly oriented? For example, odd twists. The first step to be solved is how to give an orientation of 2-tangles to form a consistent orientation of the whole link.

There are several concrete problems to be solved technically: (1) The double crossover polyhedral links usually have large number of crossings. Except tetrahedral and cubic links, efficient ways to compute their Jones or HOMFLY polynomial have not been found by now. We have considered double crossover 3-regular polyhedral links. Similar approach may be developed to deal with double crossover 4-regular polyhedral links, and accordingly the HOMFLY polynomial of the double crossover octahedral link may be thus obtained. (2) There are two types of double crossover DNA cube: 4 turns and 4.5 turns. We have only considered the 4-turn DNA cube and it deserves to compute invariants of 4.5-turn DNA cube. (3) Determine the braid index of 3-regular protein polyhedral links.

Usually in chemistry invariants are computed as a complexity indicator of DNA and protein polyhedra. In addition, chirality is very important in stereochemistry, both Jones polynomial and HOMFLY polynomial are sensitive to chirality of links. In [55], the chirality of a type of DNA and protein polyhedral links was studied. More deeply chemical and biological understanding of our computational results deserves further exploring.

Finally, in recent years, more complex DNA surfaces or 3-dimensional structures have been developed by DNA origami [52], sometimes forming complex chemical links. In the other hand, more complex topological links, say, Brunnian cube, have been designed as future possible chemical synthesizing target [100,101]. Topological properties of such links need be studied.

Acknowledgments: This work was supported by Grants from the National Natural Science Foundation of China (No. 11271307) and President's Fund of Xiamen University. We would like to thank Professor Fuji Zhang and Associate Professor Xiaosheng Cheng for some comments.

References

[1] H. Frisch, E. Wasserman, Chemical topology, *J. Am. Chem. Soc.* **83** (1961) 3789–3795.

[2] C. Dietrich–Buchecker, J. P. Sauvage, A synthetic molecular trefoil knot, *Angew. Chem. Int. Ed. Engl.* **28** (1989) 189–192.

[3] D. Walba, R. Richards, R. C. Haltiwanger, Total synthesis of the first molecular Möbius strip, *J. Am. Chem. Soc.* **104** (1982) 3219–3221.

[4] J. Simon, Topological chirality of certain molecules, *Topology* **25** (1986) 229–235.

[5] C. Ernst, D. W. Sumners, A calculus for rational tangles: Applications to DNA recombination, *Math. Proc. Cambridge Philos. Soc.* **108** (1990) 489–515.

[6] D. W. Sumners, Lifting the curtain : using topology to prob the hidden action of enzymes, *Notices Am. Math. Soc.* **42** (1995) 528–537.

[7] E. Flapan, Knots and graphs in chemistry, *Chaos, Solitons Fractals* **9** (1998) 547–560.

[8] E. Flapan, *When Topology Meets Chemistry*, Cambridge Univ. Press, Cambridge, 2000.

[9] K. Murasugi, *Knot Theory and Its Applications*, Birkhauser, 1996.

[10] V. F. R. Jones, A polynomial invariant for knots via von Neumann algebras, *Bull. Amer. Math. Soc.* **12** (1985) 103–112.

[11] W. T. Tutte, A contribution to the theory of chromatic polynomials, *Canad. J. Math.* **6** (1954) 80–91.

[12] L. H. Kauffman, State models and the Jones polynomial, *Topology* **26** (1987) 395–407.

[13] L. H. Kauffman, New invariants in the theory of knots, *Amer. Math. Monthly* **95** (1988) 195–242.

[14] L. H. Kauffman, A Tutte polynomial for signed graphs, *Discr. Appl. Math.* **25** (1989) 105–127.

[15] S. Chmutov, I. Pak, The Kauffman bracket of virtual links and the Bollobás–Riordan polynomial, *Moscow Math. J.* **7** (2007) 409–418.

[16] S. Chmutov, J. Voltz, Thistlethwaite's theorem for virtual links, *J. Knot Theory Ramif.* **17** (2008) 1189–1198.

[17] O. Dasbach, D. Futer, E. Kalfagianni, X. S. Lin, N. Stoltzfus, The Jones polynomial and graphs on surfaces, *J. Comb. Theory* **98B** (2008) 384–399.

[18] L. H. Kauffman, Virtual knot theory, *Eur. J. Comb.* **20** (1999) 663–990.

[19] B. Bollobas, O. Riordan, A polynomial of graphs on orentable sufraces, *Proc. London Math. Soc.* **83** (2001) 513–531.

[20] B. Bollobas, O. Riordan, A polynomial of graphs on surfaces, *Math. Ann.* **323** (2002) 81–96.

[21] S. Chmutov, Generalized duality for graphs on surfaces and the signed Bollobás-Riordan polynomial, *J. Comb. Theory* **99B** (2009) 617–638.

[22] J. A. Ellis–Monaghan, I. Moffatt, Twisted duality for embedded graphs, *Trans. Amer. Math. Soc.* **364** (2012) 1529–1569.

[23] J. A. Ellis–Monaghan, I. Moffatt, *Graphs on Surfaces: Dualities, Polynomials, and Knots*, Springer, 2013.

[24] R. C. Read, E. G. Whitehead, The Tutte polynomial for homeomorphism classes of graphs, *Discr. Math.* **243** (2002) 267–272.

[25] R. C. Read, E. G. Whitehead Jr., Chromatic polynomials of homeomorphism classes of graphs, *Discr. Math.* **204** (1999) 337–356.

[26] X. Jin, F. Zhang, The Kauffman brackets for equivalence classes of links, *Adv. Appl. Math.* **34** (2005) 47–64.

[27] X. Jin, F. Zhang, The replacements of signed graphs and Kauffman brackets of link families, *Adv. Appl. Math.* **39** (2007) 155–172.

[28] X. Jin, F. Zhang, F. Dong, E. G. Tay, Zeros of the Jones polynomial are dense in the complex plane, *El. J. Comb.* **17** (2010) #R94.

[29] W. Yang, F. Zhang, Links and cubic 3-polytopes, *Math. Comp.* **77** (2008) 1841–1857.

[30] X. Jin, F. Zhang, The Homfly and dichromatic polynomials, *Proc. Amer. Math. Soc.* **140** (2012) 1459–1472.

[31] F. Jaeger, Tutte polynomials and link polynomials, *Proc. Amer. Math. Soc.* **103** (1988) 647–654.

[32] L. Traldi, A dichromatic polynomial for weighted graphs and link polynomials, *Proc. Amer. Math. Soc.* **106** (1989) 279–286.

[33] J. Chen, N. C. Seeman, Synthesis from DNA of a molecule with the connectivity of a cube, *Nature* **350** (1991) 631–633.

[34] Y. Zhang, N. C. Seeman, The construction of a DNA truncated octahedron, *J. Am. Chem. Soc.* **116** (1994) 1661–1669.

[35] W. M. Shih, J. D. Quispe, G. F. Joyce, A 1.7-kilobase single–stranded DNA that folds into a nanoscale octahedron, *Nature* **427** (2004) 618–621.

[36] R. P. Goodman, R. M. Berry, A. J. Turberfield, The single–step synthesis of a DNA tetrahedron, *Chem. Commun.* **12** (2004) 1372–1373.

[37] R. P. Goodman, I. A. T. Schaap, C. F. Tardin, C. M. Erben, R. M. Berry, C. F. Schmidt, A. J. Turberfield, Rapid chiral assembly of rigid DNA building blocks for molecular nanofabrication, *Science* **310** (2005) 1661–1665.

[38] C. M. Erben, R. P. Goodman, A. J. Turberfield, A self–assembled DNA bipyramid, *J. Am. Chem. Soc.* **129** (2007) 6992–6993.

[39] J. Zimmermann, M. P. J. Cebulla, S. Mönninghoff, G. V. Kiedrowski, Self–assembly of a DNA dodecahedron from 20 trisoligonucleotides, with C_{3h} linkers, *Angew. Chem. Int. Ed.* **47** (2008) 3626–3630.

[40] G. Hu, X. D. Zhai, D. Lu, W. Y. Qiu, The architecture of Platonic polyhedral links, *J. Math. Chem.* **46** (2009) 592–603.

[41] X. Jin, F. Zhang, The Homfly polynomial for even polyhedral links, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 657–677.

[42] X. Jin, F. Zhang, The architecture and the Jones polynomial of polyhedral links, *J. Math. Chem.* **49** (2011) 2063–2088.

[43] W. R. Wikoff,L. Liljas, R. L. Duda, H. Tsuruta, R. W. Hendrix, J. E. Johnson, Topologically linked protein rings in the bacteriophage HK97 capsid, *Science* **289** (2000) 2129–2133.

[44] C. Helgstrand, W. R. Wikoff, R. L. Duda, R. W. Hendrix, J. E. Johnson, L. Liljas, The refined structure of a protein catenane: The HK97 bacteriophage capsid at 3.44 Å resolution, *J. Mol. Biol.* **334** (2003) 885–899.

[45] W. Y. Qiu, X. D. Zhai, Molecular design of Goldberg polyhedral links, *J. Mol. Struct. (Theochem)* **756** (2005) 163–166.

[46] X. S. Cheng, W. Y. Qiu, H. P. Zhang, A novel molecular design of polyhedral links and their chiral analysis, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 115–130.

[47] C. Zhang, S. H. Ko, M. Su, Y. Leng, A. E. Ribbe, W. Jiang, C. Mao, Symmetry controls the face geometry of DNA polyhedra, *J. Am. Chem. Soc.* **131** (2009) 1413–1315.

[48] Y. He, M. Su, P. Fang, C. Zhang, A. E. Ribbe, W. Jiang, C. Mao, On the chirality of self-assembled DNA octahedra, *Angew. Chem. Int. Ed.* **49** (2010) 748–751.

[49] C. Zhang, M. Su, Y. He, X. Zhao, P. Fang, A. E. Ribbe, W. Jiang, C. Mao, Conformational flexibility facilitates self–assembly of complex DNA nanostructures, *Proc. Natl. Acad. Sci. USA* **105** (2008) 10665–10669.

[50] Y. He, T. Ye, M. Su, C. Zhang, A. E. Ribbe, W. Jiang, C. Mao, Hierarchical self–assembly of DNA into symmetric supramolecular polyhedra, *Nature* **452** (2008) 198–202.

[51] C. Lin, Y. Liu, H. Yan, Designer DNA nanoarchitectures, *Biochemistry* **48** (2009) 1663–1674.

[52] A. Kuzuya, M. Komiyama, DNA origami: Fold, stick, and beyond, *Nanoscale* **2** (2010) 310–322.

[53] T. J. Fu, N. C. Seeman, DNA double–crossover molecules, *Biochemistry* **3**2 (1993) 3211–3220.

[54] G. Hu, Z. Wang, W. Y. Qiu, A survey on mathematical models for DNA polyhedra, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 725–742.

[55] X. Jin, X. S. Cheng, Topological chirality of a type of DNA and protein polyhedral links, *J. Math. Chem.* **53** (2015) 1791–1807.

[56] V. F. R. Jones, Hecke algebra representations of braid groups and link polynomials, *Ann. Math.* **126** (1987) 335–388.

[57] X. Jin, F. Zhang, The Jones polynomial for polyhedral links, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 501–520.

[58] B. Bollobás, *Modern Graph Theory*, Springer, Berlin, 1998.

[59] D. R. Woodall, Tutte polynomial expansions for 2-separable graphs, *Discr. Math.* **247** (2002) 201–213.

[60] Y. Diao, G. Hetyei, K. Hinson, Tutte polynomials of tensor products of signed graphs and their applications in knot theory, *J. Knot Theory Ramif.* **18** (2009) 561–590.

[61] Y. Diao, C. Ernst, U. Ziegler, Jones polynomial of knots formed by repeated tangle replacement operations, *Topol. Appl.* **156** (2009) 2226–2239.

[62] S. Jablan, L. Radović, R. Sazdanović, Pyramidal knots and links and their invariants, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 541–580.

[63] S. Jablan, L. Radović, R. Sazdanović, Knots and links derived from prismatic graphs, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 65–92.

[64] X. S. Cheng, H. P. Zhang, G. Hu, W. Y. Qiu, The architecture and Jones polynomials of cycle–crossover polyhedral links, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 637–635.

[65] X. Jin, F. Zhang, On computing Kauffman bracket polynomial of Montesinos links, *J. Knot Theory Ramif.* **19** (2010) 1001–1023.

[66] S. Jablan, L. Radović, R. Sazdanović, Tutte and Jones polynomial of link families, *Filomat* **24** (2010) 19–33.

[67] S. Jablan, L. Radović, R. Sazdanović, Tutte and Jones polynomials of links, polyominoes and graphical recombination patterns, *J. Math. Chem.* **49** (2011) 79–94.

[68] P. Freyd, D. Yetter, J. Hoste, W. B. R. Lickorish, K. Millett, A. Ocneanu, A new polynomial invariant of knots and links, *Bull. Amer. Math. Soc.* **12** (1985) 239–246.

[69] J. H. Przytycki, P. Traczyk, Invariants of links of Conway type, *Kobe J. Math.* **4** (1987) 115–139.

[70] X. Jin, F. Zhang, On the location of zeros of the Homfly polynomial, *J. Stat. Mech.* (2011) #P07011.

[71] S. Y. Liu, X. S. Cheng, H. P. Zhang, W. Y. Qiu, The architecture of polyhedral links and their Homfly polynomials, *J. Math. Chem.* **48** (2010) 439–457.

[72] S. Y. Liu, H. P. Zhang, W. Y. Qiu, The HOMFLY polynomial for a family of polyhedral links, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 65–90.

[73] S. Y. Liu, H. P. Zhang, Some invariants of polyhedral links, *MATCH Commun. Math. Comput. Chem.* **7**0 (2013) 383–400.

[74] S. Y. Liu, H. P. Zhang, The Homfly polynomials of odd polyhedral links, *J. Math. Chem.* **51** (2013) 1310–1328.

[75] X. S. Cheng, Y. Lei, W. Yang, The Homfly polynomial of double crossover links, *J. Math. Chem.* **52** (2014) 23–41.

[76] M. L. Li, Q. Y. Deng, X. Jin, A general method for computing the Homfly polynomial of DNA double crossover 3-regular links, *PLoS One* **10** (2015) #e0125184.

[77] R. C. Read, Chain polynomials of graphs, *Discr. Math.* **265** (2003) 213–235.

[78] J. W. Alexander, A lemma on systems of knotted curves, *Proc. Natl. Acad. Sci. USA* **9** (1923) 93–95.

[79] J. Franks, R. F. Williams, Braids and the Jones polynomial, *Trans. Amer. Math. Soc.* **303** (1987) 97–108.

[80] H. R. Morton, Seifert circles and knot polynomials, *Math. Proc. Cambridge Phil. Soc.* **99** (1986) 107–109.

[81] Y. Ohyama, On the minimal crossing number and the braid index of links, *Canad. J. Math.* **45** (1993) 117–131.

[82] W. Menasco, Closed incompressible surfaces in alternating knot and link complements, *Topology* **23** (1984) 37–44.

[83] X. S. Cheng, X. Jiang, H. Dai, The braid index of polyhedral links, *J. Math. Chem.* **50** (2012) 1386–1397.

[84] X. S. Cheng, X. Jin, The braid index of complicated DNA polyhedral links, *PLoS One* **7** (2012) #e48968.

[85] S. Yamada, The minimal number of Seifert circles equals the braid index of a link, *Invent. Math.* **89** (1987) 347–356.

[86] X. S. Cheng, H. P. Zhang, X. Jin, W. Y. Qiu, Ear decomposition of 3-regular polyhedral links with applications, *J. Theor. Biol.* **359** (2014) 146–154.

[87] G. Hu, W. Y. Qiu, X. S. Cheng, S. Y. Liu, The complexity of Platonic and Archimedean polyhedral links, *J. Math. Chem.* **48** (2010) 401–412.

[88] G. Hu, Z. Wang, W. Y. Qiu, Topological analysis of enzymatic actions on DNA polyhedral links, *B. Math. Biol.* **73** (2011) 3030–3046.

[89] H. Seifert, Über das Geschlecht von Knoten, *Math. Ann.* **110** (1935) 571–592.

[90] K. Murasugi, On the genus of the alternating knot, I, II, *J. Math. Soc. Jpn.* **10** (1958) 94–105, 235–248.

[91] R. H. Crowell, Genus of alternating link types, *Ann. Math.* **69** (1959) 258–275.

[92] D. Gabai, Genera of the alternating links, *Duke Math. J.* **53** (1986) 677–681.

[93] X. S. Cheng, S. Y. Liu, H. P. Zhang, W. Y. Qiu, Fabrication of a family of pyramidal links and their genus, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 623–636.

[94] S. Y. Liu, H. P. Zhang, Genera of the links derived from 2-connected plane graphs, *J. Knot Theory Ramif.* **21** (2012) #1250129.

[95] X. Jin, G. Jun, X. S. Cheng, Y. Lin, The number of circles of a maximum state of a plane graph with applications, *Acta Math. Appl. Sinica*, acceptted.

[96] G. Hu, W. Y. Qiu, A. Ceulemans, A new Euler's formula for DNA polyhedra, *PLoS One* **6** (2011) #e26308.

[97] J. W. Duan, G. Hu, W. Y. Qiu, Topological aspect of DNA cages: genus, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 475–488.

[98] E. Lijnen, A. Ceulemans, Topology-aided molecular design: the platonic molecules of genera 0 to 3, *J. Chem. Inf. Model.* **45** (2005) 1719–1726.

[99] J. W. Duan, W. Li, G. Hu, W. Y. Qiu, Molecular design of DNA polyhedra based on genus, *J. Math. Chem.* **52** (2014) 2380–2394.

[100] N. A. Baas, N. C. Seeman, On the chemical synthesis of new topological structures, *J. Math. Chem.* **50** (2012) 220–232.

[101] N. A. Baas, N. C. Seeman, A. Stacey, Synthesising topological links, *J. Math. Chem.* **53** (2015) 183–199.