

The Homfly polynomial of double crossover links

Xiao-Sheng Cheng · Yujuan Lei · Weiling Yang

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Abstract Motivated by double crossover DNA polyhedra (He et al. in *Nature* 452:198, 2008; Lin et al. in *Biochemistry* 48:1663, 2009; Zhang et al. in *J Am Chem Soc* 131:1413, 2009; Zhang et al. in *Proc Natl Acad Sci USA* 105:10665, 2008; He et al. in *Angew Chem Int Ed* 49:748, 2010), in this paper, we construct a new type of link, called the double crossover link, formed by utilizing the “ n -point star” to cover each vertex of a connected graph G . The double crossover link can be used to characterize the topological properties of double crossover DNA polyhedra. We show that the Homfly polynomial of the double crossover link can be obtained from the chain polynomial of the truncated graph of G with two distinct labels. As an application, by using computer algebra (Maple) techniques, the Homfly polynomial of a double crossover tetrahedral link is obtained. Our result may be used to characterize and analyze the topological structure of DNA polyhedra.

Keywords DNA polyhedron · Polyhedral links · Homfly polynomial · Chain polynomial

1 Introduction

A gigantic challenge in biology is to attain total control of the arrangement of molecular knots and links by the design of building blocks [6–11]. In recent years, biologists

X.-S. Cheng (✉)
Department of Mathematics, Huizhou University, Huizhou 516007, Guangdong,
People’s Republic of China
e-mail: chengxsh@tom.com

X.-S. Cheng · Y. Lei · W. Yang
School of Mathematical Sciences, Xiamen University, Xiamen 361005, Fujian,
People’s Republic of China

have synthesized the DNA tetrahedron, cube, octahedron, dodecahedron, icosahedron and buckyball by “ n -point star” strategy [1–5]. These fancy DNA nanostructures present tremendous potential in a number of areas, including drug encapsulation and release, regulation of the folding and activity of encaged proteins, as host molecules for nanomaterials and as building blocks for 3D-networks for catalysis and biomolecule crystallization [1]. The study of such DNA polyhedra will spur the further progress of theoretical synthesis.

A central question in knot theory is whether two knot diagrams represent the same knot. One tool used to answer the question is a knot polynomial, which is computed from a diagram of the knot and can be shown to be an invariant of the knot, i.e. diagrams representing the same knot have the same polynomial. The converse is not true. The Homfly polynomial [12,13] is one such invariant and a powerful tool to analyze biological properties of DNA polyhedra.

Many of the molecules that are important in nature are chiral, these include proteins (and their constituent amino acids), which control most processes within biological systems, and the nucleic acids DNA and RNA which are responsible for holding the information necessary for proteins to be synthesized. The Homfly polynomial is even better at detecting chirality of these DNA polyhedra.

The Homfly polynomials of some types of DNA polyhedra are calculated. For example, tangled platonic DNA polyhedra [14]. In addition, some mathematical models, called polyhedral links, are built to model and characterize DNA polyhedra. A polyhedral link is a link with the shape of a polyhedron. Homfly polynomials of some type of polyhedral links are also calculated in [15,16]. In [17], the authors established a relation between Homfly polynomial of the associated oriented link $L(G)$ and the dichromatic polynomial of the plane graph G by using arbitrary alternating oriented 2-tangle to cover every edge of the graph G . The oriented links indicate that the above polyhedral links can be understood as special cases. The relation gave a more general method to compute the Homfly polynomial of DNA polyhedra.

For the type of DNA polyhedra synthesized by “ n -point star” strategy was called a double crossover links [1–5]. Now we describe the construction of double crossover links. Given a graph G with $\delta(G) \geq 3$ ($\delta(G)$ denotes the minimum degree of the graph G), to construct a double crossover link, “ n -point star” building blocks are needed. An “ n -point star” (See Fig. 1) is proposed to cover every vertex with degree n of the graph G (See Fig. 2). By connecting these “ n -point stars”, we obtain an alternating link called a double crossover link. An example is shown in Fig. 3. In [18], the authors determined the number of seifert circles, the component number and the crossing number of the double crossover link. In [19], the authors gave the braid index of the double crossover links by utilizing the maximal degree and minimal degree of v of their Homfly polynomial.

The purpose of this paper is to calculate explicit expression of their Homfly polynomials. We provide a general method by establishing a relation between the Homfly polynomials and the chain polynomials. As an example, we obtain that the Homfly polynomial of double crossover tetrahedral link. Our results may provide further insight into the theoretical characterization of the DNA polyhedral links.

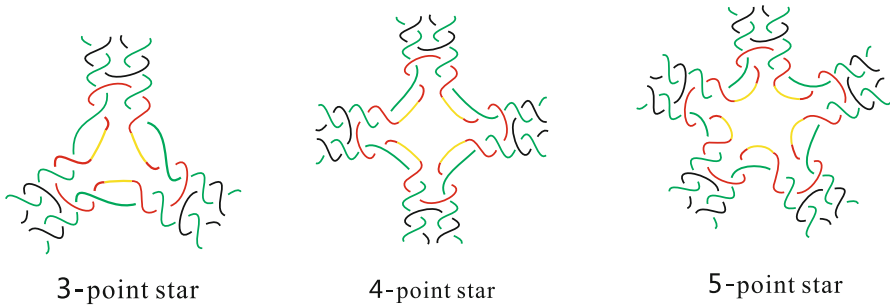


Fig. 1 3-point star, 4-point star and 5-point star

2 The Homfly, dichromatic and chain polynomials

In this section, we will describe, independently, the Homfly, dichromatic and chain polynomials.

2.1 The Homfly polynomial

The Homfly polynomial is an invariant of oriented links, introduced in [12] and [13] independently. Now we recall the definition of the Homfly polynomial. The Homfly polynomial of an oriented link L , denoted by $P_L(v, z)$, can be defined by the three following axioms [20].

- (1) $P_L(v, z)$ is invariant under ambient isotopy of L .
- (2) If L is the trivial knot then $P_L(v, z) = 1$.
- (3) It satisfies the skein relation: $v^{-1}P_{L_+}(v, z) - vP_{L_-}(v, z) = zP_{L_0}(v, z)$, where L_+ , L_- and L_0 are link diagrams which are identical except near one crossing where they are as in Fig. 4 and are called a skein triple.

2.2 The dichromatic polynomial

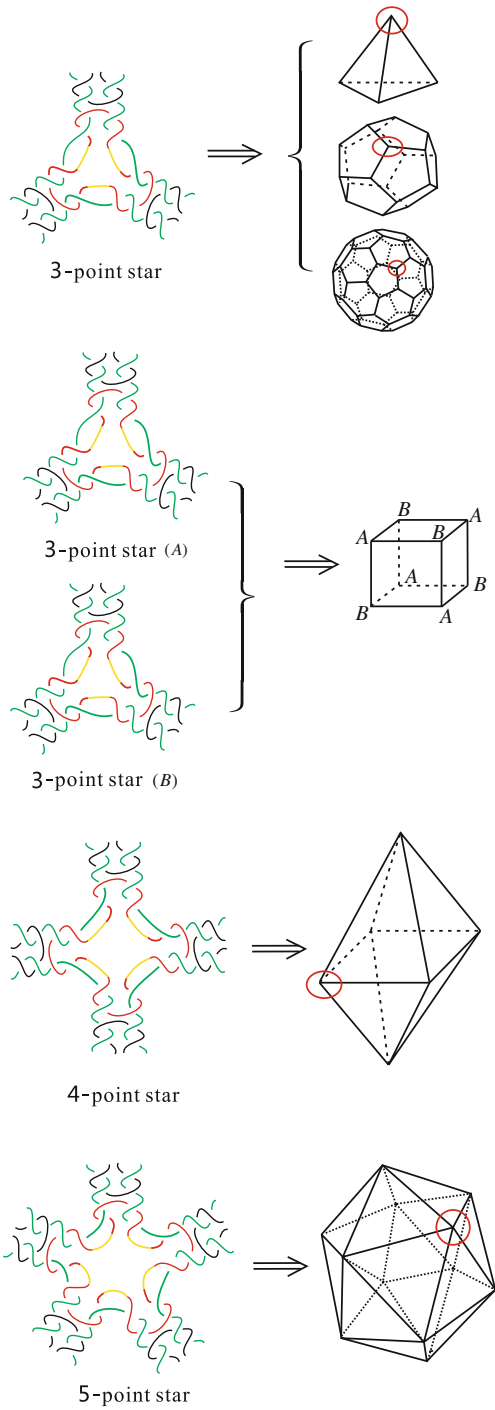
A weighted graph is a graph G together with a function w mapping $E(G)$ into some commutative ring R with unity 1. If e is an edge of the weighted graph G , then $w(e)$ is the weight of the edge e . The dichromatic polynomial for weighted graphs was introduced by Traldi [21], which is a generalization of the Tutte polynomial for signed graphs introduced by Kauffman [22]. We point out there are actually several weighted versions of the Tutte polynomial.

The dichromatic polynomial $Q(t, z)$ of a weighted graph G can be defined as

$$Q(t, z) = \sum_{F \subseteq E(G)} \left(\prod_{f \in F} w(f) \right) t^{k(F)} z^{n(F)}, \tag{1}$$

where the summation is over all edge subsets, F , of G , $k(F)$ and $n(F) = |F| - |V(G)| + k(F)$ are the number of components and the nullity, respectively, of the

Fig. 2 Double crossover links;
Figure 6 of [19]



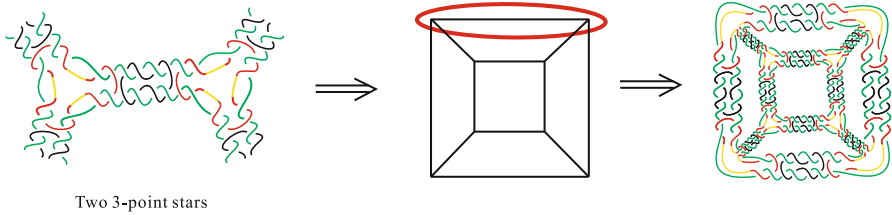
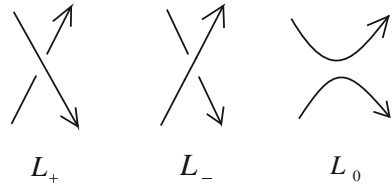


Fig. 3 A cubic double crossover link is constructed by using 8 “3-point stars” to covering each vertex of a cube and connecting their endpoints

Fig. 4 L_+ , L_- and L_0



spanning subgraph $\langle F \rangle$, induced by F , of G . It can also be defined by using the following recursive relations:

- (1) If G is an edgeless graph with $n \geq 1$ vertices, then $Q(G) = t^n$.
- (2) If e is a loop of G , then $Q(G) = (1 + w(e)z)Q(G - e)$.
- (3) If e is not a loop of G , then $Q(G) = Q(G - e) + w(e)Q(G/e)$.

2.3 The chain polynomial

The chain polynomial was proposed by Read and Whitehead [23] for the purpose of studying the chromatic polynomial for homeomorphism class of graphs. Their results are further extended to Tutte polynomial of homeomorphism class of graphs in [24] and signed graphs in [25].

Let G be a labeled graph. We usually identify the edges with their labels for convenience.

Definition 2.1 The chain polynomial $Ch[G]$ of a graph G is defined as

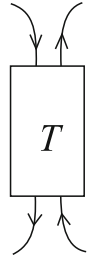
$$Ch[G] = \sum_Y F[E(G) - Y](1 - w)\varepsilon(Y) = \sum_Y F[Y](1 - w)\varepsilon(E(G) - Y),$$

where the summation is over all subsets of $E(G)$; $F(Y)$ (resp. $F[E(G) - Y]$) is the flow polynomial of $\langle Y \rangle$ (resp. $\langle E(G) - Y \rangle$), the spanning subgraph of G only containing all edges in Y (resp. $E(G) - Y$); $\varepsilon(Y)$ (resp. $\varepsilon(E(G) - Y)$) is the product of labels of the edges in Y (resp. $E(G) - Y$).

From the above Definition 2.1, the following proposition can be easily obtained.

Proposition 2.2 [21,23] *Let a be an edge of G , and let $G - a$ and G/a be the graph obtained from G by deleting and contracting the edge a respectively. Then if a is a loop, $Ch[G] = (a - w)Ch[G - a]$, and otherwise, $Ch[G] = (a - 1)Ch[G - a] + Ch[G/a]$.*

Fig. 5 An oriented 2-tangle



According to Definition 2.1 and Proposition 2.2, they have the following theorem.

Theorem 2.3 [26] *Let G be a connected graph, G^w and G^l be the associated weighted graph and labeled graph, respectively. If, in $Ch[G^l]$, we let $w = 1-tz$ and $a = 1 + \frac{t}{w(a)}$ for each edge a , then $Q_{G^w}(t, z) = t^{|V(G)|-|E(G)|} \left(\prod_{a \in E(G)} w(a) \right) Ch[G^l]$.*

3 The Homfly polynomials of double crossover links

In this section, we will calculate the Homfly polynomials of double crossover links.

Let T be an alternating oriented 2-tangle, as shown in Fig. 5. A link diagram $D(G)$ associated with G is defined to be the diagram obtained from a graph G by using each oriented alternating T_e to cover each edge e of the graph G .

Theorem 3.1 [17] *Let G be a plane graph and $D(G)$ be its associated link diagram. Let $\delta = \frac{v^{-1}-v}{z}$. Then*

$$P_{D(G)}(v, z) = \delta^{-1} \left(\prod_{e \in E(G)} \mu(e) \right) Q_G(\delta, \delta),$$

where $\mu(e) = \frac{\delta P_{N_u(T_e)} - P_{D_e(T_e)}}{\delta^2 - 1}$ and the weight $w(e)$ of edge e of G is $w(e) = \frac{\delta P_{D_e(T_e)} - P_{N_u(T_e)}}{\delta P_{N_u(T_e)} - P_{D_e(T_e)}}$.

Here, we must explain the conceptions of $N_u(T)$ and $D_e(T)$.

By joining NW and NE and SW and SE of the 2-tangle T , we obtain a link called the numerator of T , denoted by $N_u(T)$, as seen in Fig. 6 (right). Joining NW and

Fig. 6 $D_e(T)$ and $N_u(T)$

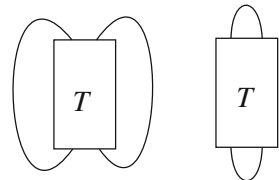


Fig. 7 Double crossover tangle and vertical [4]-tangle

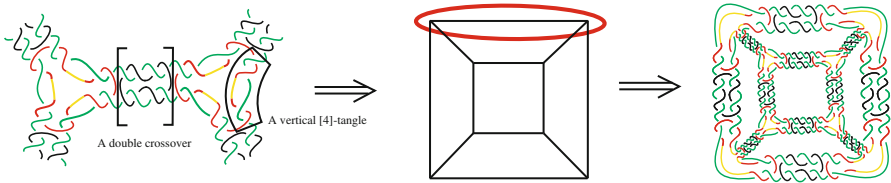
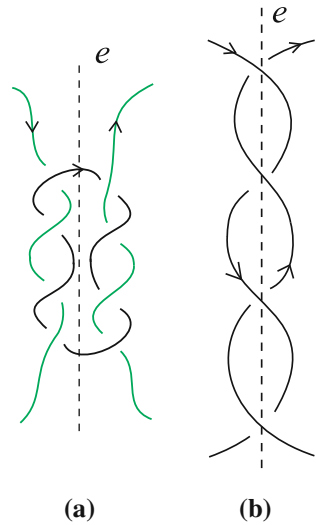


Fig. 8 A double crossover cubic link consists of 12 double crossover and 24 vertical [4]-tangles

SW and NE and SE of the 2-tangle T , we obtain a link called the denominator of T , denoted by $D_e(T)$, as illustrated in Fig. 6 (left).

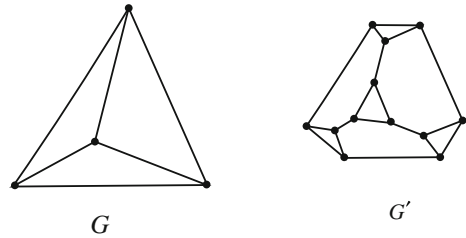
Obviously, a double crossover link can be constructed by two different tangles. One is double crossover tangle as shown in Fig. 7a, the other is vertical [4]-tangle as illustrated in Fig. 7b. For example, A double crossover cubic link consists of 12 double crossover and 24 vertical [4]-tangles, as shown in Fig. 8.

Lemma 3.2 [17] *Let G be a plane graph with edge set $E(G) = e_1, e_2, \dots, e_m$. Let $D_c(G)$ be the associated link diagram obtained from G by replacing the edge e_i by the vertical integer $[2n_i]$ -tangle. If we let the weight of e_i be $\frac{v^{-1}-v}{z} \frac{v^{2n_i}}{1-v^{2n_i}}$, then*

$$P_{D_c(G)}(v, z) = \left(\frac{z}{v^{-1} - v} \right)^{m+1} \left(\prod_{i=1}^m (1 - v^{2n_i}) \right) Q_G(\delta, \delta).$$

To calculate the Homfly polynomial of a double crossover link diagram $D(G)$, we first truncate each vertex of the graph G , then obtain a new truncated graph G' . An example is shown in Fig. 9. According to Theorem 3.1 and Lemma 3.2, we can calculate the Homfly polynomial of a double crossover link. It can be seen as follows.

Fig. 9 A graph G and its truncated graph G'



Theorem 3.3 Let G be a plane graph with $\delta(G) \geq 3$. Let G' be its truncated plane graph and $D(G)$ be a double crossover link diagram. Let x and y denote, respectively, the number of the double crossover tangle and vertical [4]-tangle. Let $w_x(e)$ and $w_y(e)$ denote the weight of edge covered by double crossover tangle and vertical [4]-tangle, respectively. Then

$$P_{D(G)}(v, z) = \frac{z}{v^{-1} - v} ((vz)(1 + v^2))^{2x+y} Q_{G'}(\delta, \delta),$$

$$\text{where } w_x(e) = \frac{2z^2(1+v^2)v^3+v^5-v^7}{z^3(1+v^2)^2}, \quad w_y(e) = \frac{v^3}{z(1+v^2)}.$$

Proof According to the Theorem 3.1, let T_e be a double crossover tangle, we calculate the Homfly polynomial of $N_u(T_e)$, $D_e(T_e)$ as

$$P_{N_u(T_e)} = \left(\frac{z}{v^{-1} - v} \right)^3 (1 - v^4)^2 Q_{G_1}(\delta, \delta),$$

and

$$P_{D_e(T_e)} = \left(\frac{z}{v^{-1} - v} \right)^3 (1 - v^4)^2 Q_{G_2}(\delta, \delta).$$

Where G_1 and G_2 denote, respectively, the plane graph of $N_u(T_e)$ and $D_e(T_e)$. However,

$$\begin{aligned} Q_{G_1}(\delta, \delta) &= (\delta + 2w_y(e) + w_y^2(e)\delta)\delta|_{w_y(e)=\frac{v^3}{z(1+v^2)}} \\ &= \left(\frac{z^2(1+v^4)(1+v^2) + v^6 - v^8}{v(1+v^2)^2z^3} \right) \frac{v^{-1} - v}{z}, \end{aligned}$$

and

$$Q_{G_2}(\delta, \delta) = \delta + 2w_y(e) + w_y^2(e)\delta + (\delta^2 - 1)(2w_y(e) + w_y^2(e)\delta)|_{w_y(e)=\frac{v^3}{z(1+v^2)}}.$$

Then, we have

$$P_{N_u(T_e)} = \left(\frac{z}{v^{-1}-v}\right)^2 (1-v^4)^2 \left(\frac{z^2(1+v^4)(1+v^2)+v^6-v^8}{v(1+v^2)^2z^3}\right),$$

and

$$\begin{aligned} P_{D_e(T_e)} &= \left(\frac{z}{v^{-1}-v}\right)^3 (1-v^4)^2 \left([\delta+2w(e)+w^2(e)\delta]+(\delta^2-1)[2w(e)+w^2(e)\delta]\right) \\ &= \left(\frac{z}{v^{-1}-v}\right)^3 (1-v^4)^2 \times \left(\left(\frac{z^2(1+v^4)(1+v^2)+v^6-v^8}{v(1+v^2)^2z^3}\right)\right. \\ &\quad \left. + \left(\frac{(1-v^2)^2-v^2z^2}{v^2z^2}\right) \left(\frac{2z^2(1+v^2)v^4+v^6-v^8}{v(1+v^2)^2z^3}\right)\right). \end{aligned}$$

Now, we will calculate $\mu_x(e)$ and $w_x(e)$.

$$\begin{aligned} \mu_x(e) &= \frac{\delta P_{N_u(T_e)} - P_{D_e(T_e)}}{\delta^2 - 1} \\ &= (1-v^4)^2 \delta^{-3} \left([\delta+2w_y(e)+w_y^2(e)\delta]-[2w_y(e)+w_y^2(e)\delta]\right) \\ &= (1-v^4)^2 \left(\frac{z}{v^{-1}-v}\right)^3 \\ &\quad \times \left(\left(\frac{z^2(1+v^4)(1+v^2)+v^6-v^8}{v(1+v^2)^2z^3}\right) - \left(\frac{2z^2(1+v^2)v^4+v^6-v^8}{v(1+v^2)^2z^3}\right)\right) \\ &= v^2z^2(1+v^2)^2, \end{aligned}$$

and

$$\begin{aligned} w_x(e) &= \frac{\delta P_{D_e(T_e)} - P_{N_u(T_e)}}{\delta P_{N_u(T_e)} - P_{D_e(T_e)}} \\ &= \frac{\delta[2w_y(e)+w_y^2(e)\delta]}{[\delta+2w_y(e)+w_y^2(e)\delta]-[2w_y(e)+w_y^2(e)\delta]} \\ &= \frac{\frac{2z^2(1+v^2)v^4+v^6-v^8}{v(1+v^2)^2z^3}}{\frac{z^2(1+v^4)(1+v^2)+v^6-v^8}{v(1+v^2)^2z^3} - \frac{2z^2(1+v^2)v^4+v^6-v^8}{v(1+v^2)^2z^3}} \\ &= \frac{2z^2(1+v^2)v^3+v^5-v^7}{z^3(1+v^2)^2}. \end{aligned}$$

In addition, according to Lemma 3.2, we know $\mu_y(e) = vz(1 + v^2)$ and $w_y(e) = \frac{v^3}{z(1+v^2)}$. Hence, the Homfly polynomial of a double crossover is

$$P_{D(G)}(v, z) = \frac{z}{v^{-1} - v} ((vz)(1 + v^2))^{2x+y} Q_{G'}(\delta, \delta).$$

□

According to Theorem 2.3 and 3.3, we have

Theorem 3.4 *Let G be a plane graph with $\delta(G) \geq 3$. Let G' be a truncated plane graph of G and $D(G)$ be a double crossover link diagram. Let G^w and G^l be the associated weighted graph and labeled graph of the graph G' , respectively. Let x and y denote, respectively, the number of the double crossover tangle and vertical [4]-tangle. In $Ch[G^l]$, we let $w = 1 - (\frac{v^{-1}-v}{z})^2$, $a = 1 + \frac{v^{-1}-v}{z} \frac{1}{w(a)}$, and $b = 1 + \frac{v^{-1}-v}{z} \frac{1}{w(b)}$. Then*

$$P_{D(G)}(v, z) = \left(\frac{v^{-1} - v}{z}\right)^{|V(G^l)| - |E(G^l)| - 1} \frac{v^{2x+4y} (2z^2v^3(1+v^2) + v^5 - v^7)^x}{z^x} Ch[G^l].$$

4 An application

For a double crossover tetrahedral link, Note $x = 6, y = 12$. By Theorem 3.4,

$$\begin{aligned} P_{D(G)}(v, z) &= \left(\frac{v^{-1} - v}{z}\right)^{|V(G^l)| - |E(G^l)| - 1} \frac{v^{2x+4y} (2z^2v^3(1+v^2) + v^5 - v^7)^x}{z^x} Ch[G^l]. \\ &= \left(\frac{v^{-1} - v}{z}\right)^{-7} \frac{v^{60} (2z^2v^3(1+v^2) + v^5 - v^7)^6}{z^6} Ch[G^l]. \end{aligned}$$

We know that the graph G' is produced by truncating each vertex of G . Then it can product some new edges, denoted by b . And those no changed edges are denoted by a . An example is shown in Fig. 10. To calculate the chain polynomial, we write a program

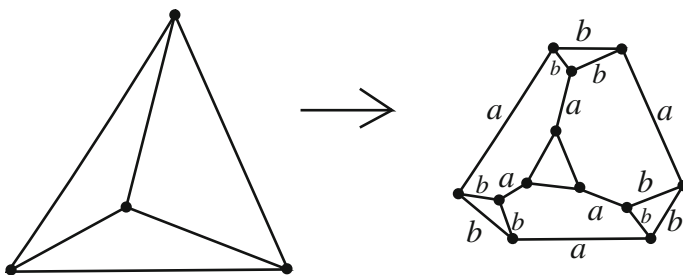


Fig. 10 A graph G and its corresponding labeled graph G^l

in the Maple platform (See “Appendix”). The chain polynomial of the truncated graph G' is shown in the following.

$$\begin{aligned}
 Ch[G'] = & a^6b^{12} - 4a^6b^9w + 6a^6b^6w^2 - 4a^3b^9w - 4a^6b^3w^3 - 12a^3b^8w \\
 & + 12a^3b^7w^2 + 28a^3b^6w^2 - 12a^3b^5w^3 - 3a^2b^8w + a^6w^4 + 20a^3b^6w \\
 & - 24a^3b^4w^3 + 4a^3b^3w^4 - 12a^2b^7w + 12a^2b^6w^2 - 24a^3b^4w^2 - 12a^3b^3w^3 \\
 & + 12a^3b^2w^4 - 6a^2b^6w + 36a^2b^5w^2 - 18a^2b^4w^3 + 54ab^6w^2 - 36ab^5w^3 \\
 & + 6ab^4w^4 - 12a^3b^4w - 8a^3b^3w^2 + 12a^3b^2w^3 + 12a^3bw^4 - 4a^3w^5 \\
 & + 24a^2b^5w - 36a^2b^3w^3 + 12a^2b^2w^4 + 54ab^6w - 150ab^4w^3 + 84ab^3w^4 \\
 & - 12ab^2w^5 + 4a^3b^3w + 24a^3bw^3 - 12a^3w^4 + 15a^2b^4w - 60a^2b^3w^2 \\
 & - 3a^2w^5 + 36ab^5w - 330ab^4w^2 + 204ab^3w^3 + 60ab^2w^4 - 48abw^5 \\
 & + 6aw^6 - 81b^4w^3 + 18a^2b^2w^3 + 12a^2bw^4 + 108b^3w^4 - 54b^2w^5 + 12bw^6 \\
 & - w^7 + 12a^3bw^2 - 12a^3w^3 - 24a^2b^3w + 36a^2bw^3 - 12a^2w^4 + 132ab^3w^2 \\
 & + 324ab^2w^3 - 252abw^4 + 42aw^5 - 243b^4w^2 + 540b^3w^3 - 378b^2w^4 \\
 & + 108bw^5 - 174ab^4w - 11w^6 - 4a^3w^2 - 6a^2b^2w + 36a^2bw^2 - 18a^2w^3 \\
 & + 12ab^3w + 426ab^2w^2 - 480abw^3 + 114aw^4 - 162b^4w + 864b^3w^2 \\
 & - 972b^2w^3 + 384bw^4 - 50w^5 + 12a^2bw - 12a^2w^2 + 174ab^2w - 396abw^2 \\
 & + 150aw^3 + 432b^3w - 1080b^2w^2 + 672bw^3 - 120w^4 - 3a^2w - 120abw \\
 & + 96aw^2 - 432b^2w + 576bw^2 - 160w^3 + 24aw + 192bw - 112w^2 - 32w
 \end{aligned} \tag{2}$$

According to Theorem 3.4, in $Ch[G^I]$, we know

$$\begin{aligned}
 w &= 1 - \left(\frac{v^{-1} - v}{z} \right)^2 \\
 a &= 1 + \frac{v^{-1} - v}{z} \frac{1}{w(a)} = \frac{v^4z^2 + v^6z^2 + v^6 - v^8 + z^2 + v^2z^2}{v^4(2z^2(1 + v^2) + v^2 - v^4)} \\
 b &= 1 + \frac{v^{-1} - v}{z} \frac{1}{w(b)} = \frac{1}{v^4}.
 \end{aligned}$$

So, the Homfly polynomial of the double crossover tetrahedral link is

$$\begin{aligned}
 P_{D(G')}(v, z) = & \frac{v^{13}}{(1 - v^2)^7z^{13}} \left(v^{110} - 24v^{108}z^2 + 276v^{106}z^4 - 2006v^{104}z^6 \right. \\
 & + 10254v^{102}z^8 - 38818v^{100}z^{10} + 111563v^{98}z^{12} - 245348v^{96}z^{14} \\
 & + 410704v^{94}z^{16} - 513958v^{92}z^{18} + 464792v^{90}z^{20} - 286195v^{88}z^{22} \\
 & + 107062v^{86}z^{24} - 18303v^{84}z^{26} - 20v^{108} + 432v^{106}z^2 \\
 & - 4416v^{104}z^4 + 28084v^{102}z^6 - 123048v^{100}z^8 + 388180v^{98}z^{10} \\
 & \left. - 892504v^{96}z^{12} + 1472088v^{94}z^{14} - 1642816v^{92}z^{16} + 1027916v^{90}z^{18} \right)
 \end{aligned}$$

$$\begin{aligned}
& -572390v^{86}z^{22} + 428248v^{84}z^{24} - 109818v^{82}z^{26} + 190v^{106} \\
& -3648v^{104}z^2 + 32568v^{102}z^4 - 176546v^{100}z^6 + 636096v^{98}z^8 \\
& -1555890v^{96}z^{10} + 2472068v^{94}z^{12} - 2028948v^{92}z^{14} - 649500v^{90}z^{16} \\
& + 3800018v^{88}z^{18} - 4260960v^{86}z^{20} + 1975911v^{84}z^{22} - 64676v^{82}z^{24} \\
& -178155v^{80}z^{26} - 1140v^{104} + 19152v^{102}z^2 - 145728v^{100}z^4 \\
& + 646184v^{98}z^6 - 1767864v^{96}z^8 + 2748960v^{94}z^{10} - 1033960v^{92}z^{12} \\
& -5000672v^{90}z^{14} + 10812080v^{88}z^{16} - 8627952v^{86}z^{18} \\
& + 4524212v^{82}z^{22} + 212280v^{78}z^{26} + 4845v^{102} - 69768v^{100}z^2 \\
& + 436356v^{98}z^4 - 1467970v^{96}z^6 + 2451780v^{94}z^8 - 2399944v^{80}z^{24} \\
& + 67134v^{92}z^{10} - 8868946v^{90}z^{12} + 16388196v^{88}z^{14} - 8100944v^{86}z^{16} \\
& + 17245752v^{82}z^{20} - 5425847v^{80}z^{22} - 2210344v^{78}z^{24} \\
& + 977592v^{76}z^{26} - 15504v^{100} + 186048v^{98}z^2 - 900864v^{96}z^4 \\
& -535880v^{86}z^{12} + 33503440v^{80}z^{16} + 1951872v^{88}z^4 + 1915508v^{94}z^6 \\
& + 104136v^{92}z^8 - 9403404v^{90}z^{10} + 17694392v^{88}z^{12} - 3349368v^{86}z^{14} \\
& -11503392v^{84}z^{18} - 28227888v^{84}z^{16} + 31634736v^{82}z^{18} \\
& -15375906v^{78}z^{22} + 4871336v^{76}z^{24} + 38760v^{98} - 372096v^{96}z^2 \\
& + 1238688v^{94}z^4 - 558790v^{92}z^6 - 6725808v^{90}z^8 \\
& + 15536810v^{88}z^{10} + 558144v^{94}z^2 - 1998100v^{80}z^{10} - 365976v^{82}z^4 \\
& -38709312v^{84}z^{14} + 39363896v^{82}z^{16} + 17176916v^{80}z^{18} \\
& -40277492v^{78}z^{20} + 6823451v^{76}z^{22} + 655704v^{74}z^{26} + 8126792v^{74}z^{24} \\
& -1307028v^{72}z^{26} - 77520v^{96} - 2983840v^{90}z^6 + 11324952v^{88}z^8 \\
& -2327960v^{86}z^{10} - 36455960v^{84}z^{12} + 40444152v^{82}z^{14} \\
& -65988568v^{78}z^{18} + 29022808v^{74}z^{22} - 3162280v^{72}z^{24} \\
& -2269200v^{70}z^{26} + 125970v^{94} - 604656v^{92}z^2 - 900864v^{92}z^4 \\
& -365976v^{90}z^4 + 6201668v^{88}z^6 - 5295126v^{86}z^8 + 37703941v^{82}z^{12} \\
& + 33791373v^{80}z^{14} - 80765259v^{78}z^{16} - 9578401v^{76}z^{18} \\
& + 59371212v^{74}z^{20} - 1761039v^{72}z^{22} - 12384064v^{70}z^{24} \\
& -283842v^{68}z^{26} - 167960v^{92} + 403104v^{90}z^2 - 5346840v^{86}z^6 \\
& -23962920v^{84}z^{10} - 9213456v^{84}z^8 + 30112552v^{82}z^{10} \\
& + 17265008v^{80}z^{12} - 78312262v^{78}z^{14} - 7187300v^{76}z^{16} \\
& + 85145370v^{74}z^{18} - 32544886v^{70}z^{22} - 2926744v^{68}z^{24} \\
& + 2012100v^{66}z^{26} + 184756v^{90} - 2683824v^{86}z^4 + 55692v^{84}z^6 \\
& + 17419968v^{82}z^8 - 57830260v^{78}z^{12} + 10109427v^{76}z^{14} \\
& + 90210662v^{74}z^{16} - 8251401v^{72}z^{18} - 56434968v^{70}z^{20} \\
& -5747957v^{68}z^{22} + 8638280v^{66}z^{24} + 1729554v^{64}z^{26} - 167960v^{88} \\
& -403104v^{86}z^2 + 1951872v^{84}z^4 + 5272176v^{82}z^6 - 9916848v^{80}z^8 \\
& -27811680v^{78}z^{10} + 26270192v^{76}z^{12} + 67142868v^{74}z^{14}
\end{aligned}$$

$$\begin{aligned}
 & -28161252v^{72}z^{16} - 68642568v^{70}z^{18} + 21048972v^{66}z^{22} \\
 & + 5739608v^{64}z^{24} + 59112v^{62}z^{26} + 125970v^{86} + 604656v^{84}z^2 \\
 & - 6206564v^{80}z^6 - 4471272v^{78}z^8 + 25130300v^{76}z^{10} \\
 & + 28196164v^{74}z^{12} - 42790585v^{72}z^{14} - 54853809v^{70}z^{16} \\
 & + 18069396v^{68}z^{18} + 33428240v^{66}z^{20} + 7327137v^{64}z^{22} \\
 & - 1420468v^{62}z^{24} - 797194v^{60}z^{26} - 77520v^{84} - 558144v^{82}z^2 \\
 & - 900864v^{80}z^4 + 3048712v^{78}z^6 + 10989072v^{76}z^8 - 798200v^{74}z^{10} \\
 & - 35251856v^{72}z^{12} - 21096510v^{70}z^{14} + 34727400v^{68}z^{16} \\
 & + 32503776v^{66}z^{18} - 6394698v^{62}z^{22} - 2639656v^{60}z^{24} - 694116v^{58}z^{26} \\
 & + 38760v^{82} + 372096v^{80}z^2 + 1238688v^{78}z^4 + 489940v^{76}z^6 \\
 & - 6970272v^{74}z^8 - 13466700v^{72}z^{10} + 5879824v^{70}z^{12} \\
 & + 31368789v^{68}z^{14} + 13945728v^{66}z^{16} - 12717828v^{64}z^{18} \\
 & - 10729944v^{62}z^{20} - 3260145v^{60}z^{22} - 1167292v^{58}z^{24} - 329970v^{56}z^{26} \\
 & - 15504v^{80} - 186048v^{78}z^2 - 900864v^{76}z^4 - 1882784v^{74}z^6 \\
 & + 542640v^{72}z^8 + 9631984v^{70}z^{10} + 12013520v^{68}z^{12} - 5440704v^{66}z^{14} \\
 & - 16570824v^{64}z^{16} - 7068120v^{62}z^{18} - 125592v^{58}z^{22} - 252712v^{56}z^{24} \\
 & - 33416v^{54}z^{26} + 4845v^{78} + 69768v^{76}z^2 + 436356v^{74}z^4 \\
 & + 1471282v^{72}z^6 + 2196162v^{70}z^8 - 1360690v^{68}z^{10} - 8565019v^{66}z^{12} \\
 & - 7361490v^{64}z^{14} + 1645368v^{62}z^{16} + 3646191v^{60}z^{18} + 861744v^{58}z^{20} \\
 & + 125430v^{56}z^{22} + 197630v^{54}z^{24} + 109245v^{52}z^{26} - 1140v^{76} \\
 & - 19152v^{74}z^2 - 145728v^{72}z^4 - 663068v^{70}z^6 - 1751496v^{68}z^8 \\
 & - 1924860v^{66}z^{10} + 1327880v^{64}z^{12} + 4452012v^{62}z^{14} + 2333160v^{60}z^{16} \\
 & - 224262v^{58}z^{18} + 376452v^{54}z^{22} + 277280v^{52}z^{24} + 126774v^{50}z^{26} \\
 & + 190v^{74} + 3648v^{72}z^2 + 32568v^{70}z^4 + 189686v^{68}z^6 + 714240v^{66}z^8 \\
 & + 1474470v^{64}z^{10} + 1029404v^{62}z^{12} - 822982v^{60}z^{14} - 1112392v^{58}z^{16} \\
 & + 17875v^{56}z^{18} + 347516v^{54}z^{20} + 223726v^{52}z^{22} + 175316v^{50}z^{24} \\
 & + 91837v^{48}z^{26} - 20v^{72} - 432v^{70}z^2 - 4416v^{68}z^4 - 33880v^{66}z^6 \\
 & - 182808v^{64}z^8 - 571392v^{62}z^{10} - 778888v^{60}z^{12} - 118152v^{58}z^{14} \\
 & + 439960v^{56}z^{16} + 188512v^{54}z^{18} + 71000v^{50}z^{22} + 80816v^{48}z^{24} \\
 & + 49848v^{46}z^{26} + v^{70} + 24v^{68}z^2 + 276v^{66}z^4 + 3590v^{64}z^6 \\
 & + 33252v^{62}z^8 + 164838v^{60}z^{10} + 353582v^{58}z^{12} + 201570v^{56}z^{14} \\
 & - 132186v^{54}z^{16} - 120416v^{52}z^{18} + 12060v^{50}z^{20} + 22092v^{48}z^{22} \\
 & + 14444v^{46}z^{24} + 21912v^{44}z^{26} - 252v^{62}z^6 - 5208v^{60}z^8 - 42620v^{58}z^{10} \\
 & - 142248v^{56}z^{12} - 148036v^{54}z^{14} + 5392v^{52}z^{16} + 52320v^{50}z^{18} \\
 & - 26816v^{46}z^{22} - 3136v^{44}z^{24} + 7768v^{42}z^{26} + 18v^{60}z^6 + 720v^{58}z^8 \\
 & + 9410v^{56}z^{10} + 49848v^{54}z^{12} + 81018v^{52}z^{14} + 19328v^{50}z^{16} \\
 & - 25788v^{48}z^{18} - 27780v^{46}z^{20} - 12004v^{44}z^{22} + 368v^{42}z^{24} - 648v^{40}z^{26}
 \end{aligned}$$

$$\begin{aligned}
& -72v^5z^8 - 1560v^5z^{10} - 14904v^5z^{12} - 38808v^5z^{14} - 20880v^5z^{16} \\
& -744v^4z^{18} + 2808v^4z^{22} - 2752v^4z^{24} - 5640v^3z^{26} + 6v^5z^8 \\
& + 156v^5z^{10} + 3627v^5z^{12} + 16185v^4z^{14} + 12541v^4z^{16} \\
& -395v^4z^{18} + 2732v^4z^{20} - 1151v^4z^{22} - 6910v^3z^{24} - 7219v^3z^{26} \\
& -672v^4z^{12} - 6078v^4z^{14} - 7588v^4z^{16} + 1534v^4z^{18} - 5110v^3z^{22} \\
& -6520v^3z^{24} - 6570v^3z^{26} + 84v^4z^{12} + 2007v^4z^{14} + 4686v^4z^{16} \\
& -107v^4z^{18} - 3072v^3z^{20} - 2925v^3z^{22} - 4192v^3z^{24} - 5139v^3z^{26} \\
& -524v^4z^{14} - 2500v^4z^{16} - 1320v^3z^{18} - 740v^3z^{22} - 2536v^3z^{24} \\
& -3720v^3z^{26} + 99v^4z^{14} + 1051v^3z^{16} + 876v^3z^{18} + 72v^3z^{20} \\
& -427v^3z^{22} - 1516v^3z^{24} - 2610v^2z^{26} - 6v^3z^{14} - 360v^3z^{16} \\
& -432v^3z^{18} - 114v^3z^{22} - 1096v^2z^{24} - 1764v^2z^{26} + v^3z^{14} \\
& + 120v^3z^{16} + 300v^3z^{18} + 16v^3z^{20} - 165v^2z^{22} - 892v^2z^{24} \\
& -1034v^2z^{26} - 24v^3z^{16} - 168v^3z^{18} - 216v^2z^{22} - 520v^2z^{24} \\
& -408v^2z^{26} + 6v^3z^{16} + 99v^2z^{18} - 69v^2z^{22} - 124v^2z^{24} + 66v^2z^{26} \\
& -30v^2z^{18} + 78v^2z^{22} + 152v^2z^{24} + 356v^1z^{26} + 15v^2z^{18} \\
& + 60v^2z^{20} + 93v^2z^{22} + 296v^1z^{24} + 462v^1z^{26} + 108v^1z^{22} \\
& + 296v^1z^{24} + 432v^1z^{26} + 20v^1z^{20} + 69v^1z^{22} + 220v^1z^{24} \\
& + 332v^1z^{26} + 30v^1z^{22} + 136v^1z^{24} + 216v^1z^{26} + 15v^1z^{22} \\
& + 64v^1z^{24} + 120v^1z^{26} + 24v^1z^{24} + 56v^1z^{26} + 6v^1z^{24} + 21v^1z^{26} \\
& + 6v^2z^{26} + z^{26}.
\end{aligned}$$

Remark For a double crossover tetrahedral link, we can also compute its Homfly polynomial by Theorem 4.2. But, if we compare formula (2) with (3), then we can immediately find that it is very easy to calculate the Homfly polynomials of double crossover links by using Theorem 3.4. The reason can be elaborated in the following.

Definition 4.1 [27] The Tutte polynomial of a graph $G = (V, E)$ is a two-variable polynomial defined as follows:

- (1) if $E(G) = \emptyset$, then $T(G; x, y) = 1$.
- (2) if e is a bridge, then $T(G; x, y) = xT(G/e, x, y)$.
- (3) if e is a loop, then $T(G; x, y) = yT(G - e, x, y)$.
- (4) if e is neither a loop nor a bridge, then $T(G; x, y) = T(G - e, x, y) + T(G/e, x, y)$.

The relation of the Tutte polynomial of a plane graph G and the Homfly polynomial of the graph G corresponding Jaeger link diagram $D(G)$ (See Fig. 11) can be indicated in the following Theorem 4.2.

Theorem 4.2 [28] Let G be a connected plane graph, $D(G)$ a Jaeger link diagram, then

$$P_{D(G)}(v, z) = v^{|E(G)|+|V(G)|-1} z^{|E(G)|-|V(G)|+1} T\left(v^{-2}, 1 + \frac{1-v^2}{z^2}\right).$$

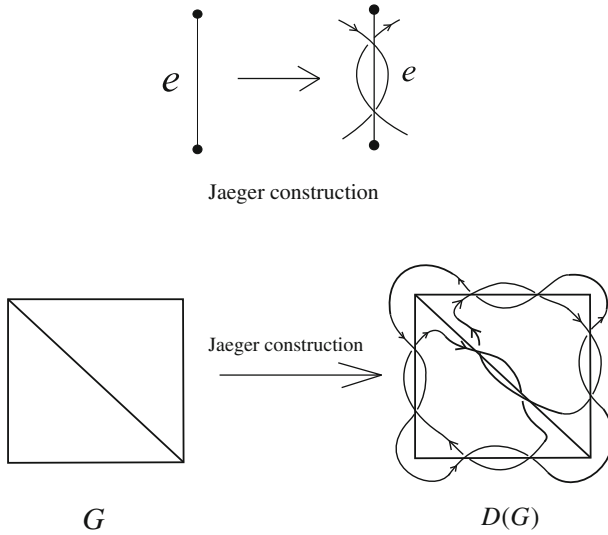


Fig. 11 A graph G and it corresponding Jaeger link diagram $D(G)$

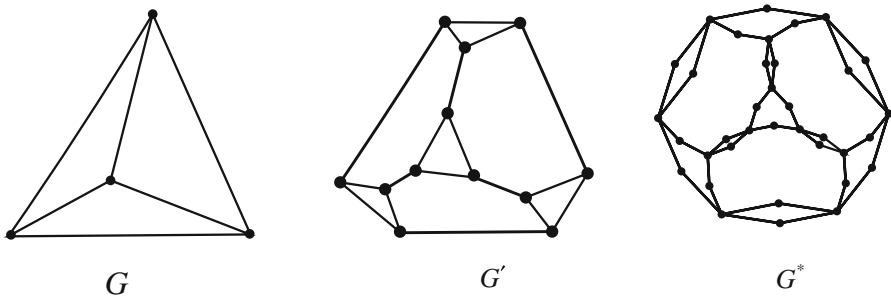


Fig. 12 G , G' and G^*

Hence, in order to calculate the Homfly polynomial of a double crossover tetrahedral link, we first calculate the Tutte polynomial of a graph G^* (See Fig. 12). Computation of this polynomial employed the Maple software.

The Tutte polynomial of the graph G^* is shown in the following.

$$\begin{aligned}
 T(G^*, x, y) = & 32x + 32y + 11y^{12} + 623908x^{24} + 24746968yx^9 + 16894404yx^8 \\
 & + 348796x^{25} + 5165029x^{19} + 3530005x^8 + 66y^{11} + 1051477x^{23} \\
 & + 280y^2 + 944yx + 696x^2 + 6377y^2x + 11937yx^2 + 21206y^3x \\
 & + 65439y^2x^2 + 88932yx^3 + 42556y^4x + 185137y^3x^2 \\
 & + 404610y^2x^3 + 445608yx^4 + 56410y^5x + 318777y^4x^2 \\
 & + 972528y^3x^3 + 1698327y^2x^4 + 1615734yx^5 + 1099y^3 + 7075x^3 \\
 & + 2554y^4 + 44761x^4 + 3914y^5 + 198205x^5 + 4183y^6
 \end{aligned}$$

$$\begin{aligned}
&+655836x^6 + y^{13} + 2554599x^{21} + 3449226y^3x^4 + 5170011y^2x^5 \\
&+4446574yx^6 + 1693798x^7 + 8797388y^3x^5 + 11926338y^2x^6 \\
&+9625272yx^7 + 359232yx^{24} + 90060y^4x^{17} + 182383x^{26} \\
&+9068444yx^{18} + 6108253x^9 + 9009515x^{10} + 6085844yx^{19} \\
&+11611086x^{11} + 164430yx^{25} + 33609y^4x^{18} + 1679545x^{22} \\
&+3231y^7 + 14039021x^{13} + 13373865x^{12} + 27079994y^2x^{13} \\
&+16556y^8x + 154479y^7x^2 + 872032y^6x^3 + 1705546y^6x^4 \\
&+2193912y^6x^5 + 6729222y^5x^6 + 16315758y^4x^7 + 26412537y^3x^{10} \\
&+20965708y^3x^{11} + 15376888y^3x^{12} + 12322586y^4x^9 \\
&+15431796y^4x^8 + 27679236yx^{14} + 32038868yx^{13} + 34226y^7x \\
&+281183y^6x^2 + 1355720y^5x^3 + 3318982y^5x^4 + 5593524y^5x^5 \\
&+13784076y^4x^6 + 25023808y^3x^7 + 41074835y^2x^{10} + 38863422y^2x^{11} \\
&+33632422y^2x^{12} + 30088534y^3x^9 + 29963203y^3x^8 + 51898y^6x \\
&+361167y^5x^2 + 1422738y^4x^3 + 4230640y^4x^4 + 8898582y^4x^5 \\
&+16832554y^3x^6 + 21578688y^2x^7 + 31125653yx^{10} + 34545828yx^{11} \\
&+34658048yx^{12} + 38741713y^2x^9 + 31612128y^2x^8 + 6884717x^{18} \\
&+721548yx^{23} + 1288920y^3x^{17} + 143124y^5x^{13} + 264y^{11}x \\
&+3000y^{10}x^2 + 21808y^9x^3 + 11808y^9x^4 + 1236y^9x^5 + 13954y^8x^6 \\
&+108347y^6x^{10} + 39476y^6x^{11} + 12054y^6x^{12} + 11106y^7x^9 \\
&+18488y^5x^{15} + 726y^8x^8 + 218593y^4x^{16} + 1244964y^2x^{20} \\
&+54816y^5x^{14} + 4514y^8x^7 + 630828y^2x^{21} + 650016y^3x^{18} \\
&+303876y^3x^{19} + 294906y^2x^{22} + 12886734yx^{17} + 8786554x^{17} \\
&+17470771yx^{16} + 268y^{10} + 10713947x^{16} + 10553044y^3x^{13} \\
&+5916y^9x + 60582y^8x^2 + 384600y^7x^3 + 570934y^7x^4 \\
&+512124y^7x^5 + 1906398y^6x^6 + 6020424y^5x^7 + 8741264y^4x^{10} \\
&+5670297y^4x^{11} + 3408813y^4x^{12} + 2621860y^5x^9 + 4277022y^5x^8 \\
&+20511066y^2x^{14} + 22566964yx^{15} + 809y^9 + 12432961x^{15} \\
&+1855y^8 + 13645953x^{14} + 6465153y^2x^{17} + 1913625y^4x^{13} \\
&+1530y^{10}x + 16692y^9x^2 + 115058y^8x^3 + 117244y^8x^4 + 59364y^8x^5 \\
&+278106y^7x^6 + 1453055y^5x^{10} + 731592y^5x^{11} + 339876y^5x^{12} \\
&+273455y^6x^9 + 487035y^4x^{15} + 39603y^7x^8 + 2388946y^3x^{16} \\
&+3887574yx^{20} + 1001019y^4x^{14} + 105200y^7x^7 + 2355448yx^{21} \\
&+3959146y^2x^{18} + 2290478y^2x^{19} + 1346664yx^{22} + 4158292y^3x^{15} \\
&+596134y^6x^8 + 10006993y^2x^{16} + 3712397x^{20} + 91x^{33} \\
&+6820936y^3x^{14} + 1182060y^6x^7 + 14705630y^2x^{15} + 3294y^6x^{13} \\
&+2060y^{10}x^3 + 384y^9x^6 + 3039y^7x^{10} + 5503y^5x^{16} + x^{35} + 24y^{12}x \\
&+276y^{11}x^2 + 54y^{10}x^4 + 18y^{10}x^5 + 504y^7x^{11} + 84y^7x^{12}
\end{aligned}$$

$$\begin{aligned}
 &+156y^8x^9 + 112y^6x^{15} + 6y^9x^8 + 672y^6x^{14} + 24y^9x^7 + 4494y^2x^{26} \\
 &+ 3201y^4x^{20} + 4940y^3x^{23} + 759y^4x^{21} + 1160y^3x^{24} + 1014y^2x^{27} \\
 &+ 472yx^{30} + 2202yx^{29} + 1386y^5x^{17} + 300y^5x^{18} + 88411x^{27} \\
 &+ 1742x^{31} + 39299x^{28} + 68280yx^{26} + 130152y^3x^{20} + 125538y^2x^{23} \\
 &+ 50204y^3x^{21} + 47835y^2x^{24} + 13x^{34} + 25276yx^{27} + 8142yx^{28} \\
 &+ 15945y^2x^{25} + 17060y^3x^{22} + 449x^{32} + 5638x^{30} + 11181y^4x^{19} \\
 &+ 7x^{16}y^6 + 165x^{28}y^2 + 135x^{22}y^4 + 200x^{25}y^3 + 72x^{31}y + 48x^{19}y^5 \\
 &+ 15797x^{29} + x^{17}y^6 + 15x^{29}y^2 + 15x^{23}y^4 + 20x^{26}y^3 + 6x^{32}y \\
 &+ 6x^{20}y^5
 \end{aligned}$$

5 Conclusions

In this paper, we present a general approach to compute double crossover DNA polyhedra [1–5] synthesized by Chengde Mao et al. The mathematics in this paper is not difficult. The key step of the approach is to convert the computation of the Homfly polynomial of the DNA polyhedral links to that of the chain polynomial with two distinct labels of the truncated polyhedron, which can be obtained by our given Maple program in “Appendix”. This method can simplify the computation of the HOMFLY polynomial for the DNA polyhedral links, and thus facilitating the subsequent identification of the topological link type. It may be promising that our result may be used to work out a relationship between the polynomials associated with the substrate molecule and the product molecules.

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Appendix

Let GG be a graph, MM the labeled edge matrix of GG , ww algebraic number, so the program of the labled graph GG is written as follows, and the content in “[]” explains the program.

```

ChainPolynomial := proc (GG::GRAPHLN, MM::Matrix, ww::algebraic) [make
a function in order transfer the datas]
local G, chp, AAM, m;
global w;
G := ‘ if ‘ (op(2, GG) = ‘unweighted’, MakeWeighted(GG), GG); [if GG is an
unweighted graph, then can let GG be weighted graph denoted by G]
AAM := MM;
w := ww;
m := nops(op(3, G)); [m equals the vertex number of the graph G]

```

```

chp := proc (G, AAM) [make a function in order to compute the chain poly-
nomial of G]
local i, j, k, ii, jj, e, ee, E, LL, CCM, DDM, n, x, y, z, GDel, GCon, chpp,
GGC, GGD;
option remember;[record the program]
GGC := G;
GGD := G;
E := Edges(G, weights); [E is a list of the weighted edges]
if nops(E) = 0 then return 1 end if;[if G is a null graph, return 1]
e:=E[1]; [e denotes the first edge of E]
ee:=e[1]; [ee are related vertices of e]
ii:=op(1, sort(ee)); [ii is the first vertex of e]
jj:=op(2, sort(ee)); [jj is the first vertex of e]
[the following is the recursive of chain polynomial, where parallel edges are deleted
and contracted at a time]
LL:=AAM[ii, jj];
n:=nops(LL);
x:=1;
for i to n do
x:=x * (LL[i] - 1)
end do;
y:=0;
for k to n do z:=1;
for i to k - 1 do
z:=z * (LL[i] - w)
end do;
for i from k + 1 to n do
z:=z * (LL[i] - 1)
end do;
y:=y + z end do;
GCon := Contract(GGC, ee, multi = true);
GDel := DeleteEdge(GGD, ee);
DDM := matrix(m, m);
CCM:= matrix(m, m);
for i to m do for j to m do
if i = ii and j = jj then
DDM[i, j]:=[]
elif i = jj and j = ii
then DDM[j, i]:=[]
else DDM[i, j]:=AAM[i, j]
end if
end do
end do;
for i to m do
for j to m do
if i ≠ ii and i ≠ jj and j ≠ ii and j ≠ jj

```

```

then CCM[i, j]:=AAM[i, j]
elif i = ii and j ≠ ii and j ≠ jj
then CCM[i, j]:=[op(AAM[ii, j]), op(AAM[jj, j])]
elif j = ii and i ≠ ii and j ≠ jj
then CCM[i, j]:=[op(AAM[i, ii]), op(AAM[i, jj])]
else CCM[i, j]:=[ ]
end if
end do
end do;
chpp := x*procname(GDel, DDM)+y*procname(GCon, CCM);
simplify(chpp)
end proc;
chp(G, AAM)
end proc

```

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