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Pyramidal Knots and Links and Their Invariants

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Abstract

We give a survey of different methods for obtaining knots and links in the form of different geometrical polyhedra, that have applications in chemistry. After introducing new graphical notation for decorated polyhedral graphs we derive general formulae for Tutte polynomials of 3- and 4-pyramid decorated graphs. Moreover, we compute different invariants of their corresponding source and generating links.

1. INTRODUCTION

The initial interest in knot theory was stimulated by Kelvin's theory of atomic structure (1867). By the turn of the century, after scientific confirmation of Mendeleev's periodic tables, it was clear that Kelvin's theory was incorrect. Chemists were no longer interested in classifying knots, but topologists continued to study them.

In 1960-ties the focus of chemists turned towards attempts to synthesize molecular knots and links (abbr. KLs). The first pair of linked rings in a form of the Hopf link, a *catenane*, was synthesized by H. Frisch and E. Wasserman in 1961. The first molecular knot, a trefoil made out of 124 atoms was produced by C. Dietrich-Bushecker and J.-P. Sauvage in 1989. They refer to *stereochemical topology*, synthesis, characterization, and analysis of topologically interesting molecular structures [1].

Construction of numerous KLs become possible after the synthesis of first molecular Möbius ladder with three rungs by D. Walba, R. Richards and R.C. Haltiwanger in 1982, and addition of twists to the Möbius ladders managed by Q.Y. Zheng in 1990. In fact, after breaking the rungs, Möbius multi-strand twisted ladders became a molecular closed braid representation of a KL.

In the 1950s F.H.C. Crick and J.D. Watson unraveled the double helix structure of DNA. A molecule of DNA can also take the form of a ring and become knotted. In the process of recombination, a DNA knot is temporarily broken, physically changed, and then reconnected. In the 1970s it was discovered that an enzyme, *topoisomerase*, is responsible for this process. The first electron microscope pictures of knotted DNA were produced in 1985 by S. Wasserman, J. Dungan and N. Cozzarelli [2]. The *linking number* and its splitting into *average writhe* Wr and *twist* Tw is used as a basic tool to analyze the geometry of supercoiled DNA. C. Ernst and D.W. Sumners [3, 4] reconstructed the actions of enzyme (TN3 Resolvase) by solving tangle equations. Distances of rational knots and links were calculated by I.K. Darcy and D.W. Sumners [5, 6].

From the point of view of organic chemistry and molecular biology, the most interesting are complex knotted and linked chemical structures with a high degree of symmetry. However, tabulation of KLs as well as computing of KL invariants is restricted to KLs with relatively small number of crossings.

In some sources the end of the 19^{th} century is called the "dark age of the knot theory", because KLs are recognized "by hand" or some other "non-exact methods". However, first knot tables were created during that period by P.G. Tait, T.P. Kirkman and C.N. Little, after more than five years of a hard work. In knot tabulation, almost nothing important happened for almost a century, until the computer derivation of KL tables by M. Thistlethwaite and his collaborators. Now computations have reached the limit even with the use of supercomputers. The existing knot tables contain alternating knots up to 24 crossings, non-alternating knots up to 16 crossings[1] [7], alternating links up to 18 crossings, and non-alternating up to 12 crossings. For applications in chemistry, KL tables are insufficient, because KLs (mostly links) used in chemistry have higher number of crossings. Also, the majority of tabulated KLs have a low degree of symmetry, unlike knotted natural structures, because nature prefers symmetry and complexity.

[1] Very recently, M. Thistlethwaite tabulated non-alternating knots up to 19 crossings. There are about 250 million non-alternating knots with 19 crossings [8].

The things have changed in the last decade, when chemical scientists and mathematicians started constructing new classes of KLs, derived by different geometrical constructions from regular and Archimedean polyhedra [9], fullerenes and nanotubes [10, 11], Goldberg polyhedra (a kind of multi-symmetric fullerene polyhedra) [12], extended Goldberg polyhedra and their corresponding links with even and odd tangles [13–15], dual polyhedral links [16] *etc.* In addition to new methods for producing KLs, together with mathematicians, chemists developed new methodology for the computation of polynomial and other KL invariants. These invariants include: Jones polynomial [17, 18], Kauffman bracket polynomial [17–19] and HOMFLYPT polynomial [20, 22], and polynomials coming from graph theory: Tutte polynomials, Bolobás-Riordan polynomials, chromatic and dichromatic polynomials, chain and sheaf polynomials [19] that can be applied on KLs with a very large number of crossings and their (signed) graphs. For the first time, chirality of KLs with a high number of crossings obtained as polyhedral links was analyzed [23, 24].

In the series of papers chemists tried to solve a fundamental question in chemistry: to determine whether KLs are new forms of molecular structures [9, 12, 25–27]. Geometrical characteristics and the polyhedral shapes of biological molecules have attracted much attention, and remarkable discoveries were made in the control and syntheses of polyhedral links or catenanes, such as the DNA tetrahedron, DNA cube, DNA truncated octahedron, DNA octahedron, and more recently DNA bipyramids and DNA prisms. Topologically linked protein catenane – a 72-hedral link, is discovered in the context of virology in the mature empty capsid of the double-stranded DNA bacteriophage. This and similar discoveries extended the domain of forms that are possible in the biochemical world. Many questions about chemical structures can be formulated in the language of knot theory and answered by using mathematical-topological and geometrical methods.

One of well known constructions in knot theory, middle edge construction, was extended by F. Jaeger, by replacing single crossings in edge mid-points by bigons collinear with the edge. F. Jaeger proposed this construction in order to compute HOMFLYPT polynomials of these links (called after him Jaeger links) from their Tutte polynomials by substitution of variables [28].

In the paper [27] new methodology for understanding the construction of polyhedral links has been developed on the basis of the Platonic and Archimedean solids by the "three-cross-curve and double-twist-line covering" method introduced by the authors.

The authors analyzed regular and truncated regular knotted polyhedra, providing further insight into the molecular design, and theoretical characterization of the DNA and protein catenanes.

The study of polyhedral links was initiated and defined by Qiu's group in 2005, with several consecutive journal papers published subsequently. Following the same avenue of research, X.-S. Cheng, W.-Y. Qiu and H.-P. Zhang [23] proposed a novel method by replacing three cross curves with branched alternating closed braids to construct a new type of polyhedral links on arbitrary convex polyhedra. They described conditions to determine the chirality of the polyhedral links in terms of generalized Tutte polynomials and Kauffman bracket polynomials.

This paper is based on the results by F. Jaeger, W.-Y. Qiu and his colleagues [9]- [28].

In Section 2 we introduce knot theory basics: Conway notation and families of KLs, flypes, Tait flyping theorem, and the Tutte polynomial. After giving a short overview of basic polyhedra in knot theory in Section 3, in Section 4 we distinguish some classes of basic polyhedra that are real geometrical polyhedra, i.e., 4-valent geometric polyhedra graphs. In order to extend basic polyhedra to twisted polyhedral links, in Section 5 we derive decorated pyramid graphs by using generalized Jaeger construction. We unify methods for the construction of polyhedral links: middle graph construction, Jaeger construction, generalized Jaeger standard and dual construction, cross-curve and double-(twist)-line covering and its dual construction, an introduce new graphical notation for all mentioned constructions and their combinations. From n-pyramid graphs and their corresponding antiprismatic basic polyhedra considered in Section 6, in Section 7 we derive general formulae for the Tutte polynomials of 3- and 4-pyramid decorated graphs. Section 8 is dedicated to the recognition of polyhedral KLs. Section 9 contains the complete survey of knot and link invariants computed for KLs and their families derived from 3- and 4-pyramid decorated graphs, with a concise interpretation of the obtained results, including data about chirality and remarks about the completely open field of problems related to non-alternating polyhedral KLs. At the end of Section 9 we provide "portraits of families", plots of zeros of the Jones polynomials of KL families from which we are able to visually identify KL families and recognize some of their properties.

2. KNOT THEORY BASICS

Knots and links are given in Conway notation [10, 29–31].

A 1-dimensional manifold composed of two arcs and any number of circles, properly embedded in a 3-dimensional ball, is called a *tangle* (or 2-tangle). The same term is used to denote a projection of a tangle into 2-dimensional disk. From the intersections, four arcs emerge pointing in the compass directions NW, NE, SW, SE (Fig. 1a).

Tangle can be closed in two ways (without introducing additional crossings): by joining in pairs NE and NW, and SE and SW ends of a tangle to obtain a *numerator closure*; or by joining in pairs NE and SE, and NW and SW ends we obtain a *denominator closure* (Fig. 1c,d).

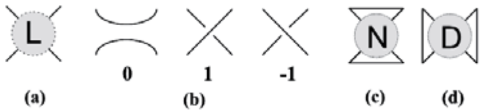

Figure 1: (a) A tangle; (b) the elementary tangles; (c) numerator closure; (d) denominator closure.

The main building blocks in the Conway notation are elementary tangles. We distinguish three elementary tangles, shown in Fig. 1b, denoted by 0, 1 and -1. All other tangles can be obtained by combining elementary tangles, while 0 and 1 are sufficient to obtain alternating KLs. Elementary tangles can be combined by the following operations: *sum*, *product*, and *ramification* (Figs. 2-3). Given tangles a and b, image of a under reflection with mirror line NW-SE is denoted by $-a$, and sum is denoted by $a + b$. Product $a\,b$ is defined as $a\,b = -a + b$, and *ramification* by $(a, b) = -a - b$.

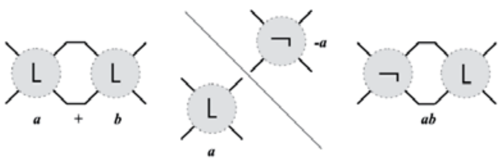

Figure 2: A sum and product of tangles.

A *rational tangle* is any finite product of elementary tangles, and a *rational KL* is a numerator closure of a rational tangle. A tangle is *algebraic* if it can be obtained from

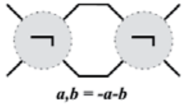

Figure 3: Ramification of tangles.

elementary tangles using the operations of sum and product[2]. KL is *algebraic* if it is a numerator closure of an algebraic tangle.

Basic polyhedron is a 4-regular, 4-edge-connected, at least 2-vertex connected plane graph without bigons [10,29–31]. The basic polyhedron 1^* is the closure of the elementary tangle 1. Basic polyhedron of a given KL can be identified by recursively collapsing all bigons in a KL diagram, until none of them remains (Fig. 4a). Hence, a link L is *algebraic* if there exists at least one diagram of L which can be reduced to the basic polyhedron 1^* by a finite sequence of bigon collapses. Otherwise, it is a *non-algebraic* or *polyhedral link*.

Conway notation for polyhedral KLs contains additional symbol of a basic polyhedron we are working with. The symbol $n^{*m} = n^{*m}1.1.\ldots.1$, where $*m$ is a sequence of m stars, denotes the m-th basic polyhedron in the list of basic polyhedra with n vertices. A KL obtained from a basic polyhedron n^{*m} by substituting tangles t_1, ..., t_k, $k \leqslant n$ instead of vertices, is denoted by $n^{*m}t_1 \ldots t_k$, where the number of dots between two successive tangles shows the number of omitted substituents of value 1. For example, $6^*2:2:2\,0$ means $6^*2.1.2.1.2\,0.1$, and $6^*2\,1.2.3\,2:-2\,2\,0$ means $6^*2\,1.2.3\,2.1.-2\,2\,0.1$ (Fig. 4b).

Definition 0.1. For a link or knot L given in an unreduced[1] Conway notation $C(L)$ denote by S a set of numbers in the Conway symbol excluding numbers denoting basic polyhedron and zeros (determining the position of tangles in the vertices of polyhedron) and let $\tilde{S} = \{a_1, a_2, \ldots, a_k\}$ be a non-empty subset of S. Family $F_{\tilde{S}}(L)$ of knots or links derived from L consists of all knots or links L' whose Conway symbol is obtained by substituting all $a_i \neq \pm 1$, by $sgn(a_i)|a_i + k_{a_i}|$, $|a_i + k_{a_i}| > 1$, $k_{a_i} \in \mathbb{Z}$. [10]

If all k_{a_i} are even integers, the number of components is preserved within the corresponding subfamilies, i.e., adding full-twists preserves the number of components inside the subfamilies.

[2]These two operations are sufficient, since a ramification $(a, b) = -a - b$ can be represented as the product $a(-b)$.

[1]The Conway notation is called unreduced if in symbols of polyhedral links elementary tangles 1 in single vertices are not omitted.

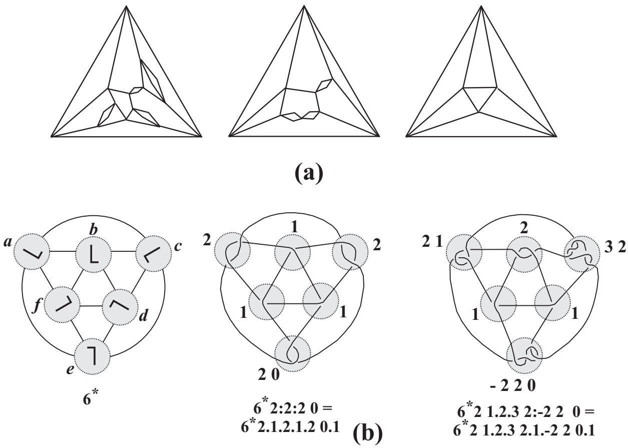

Figure 4: (a) A link shadow collapsing into the basic polyhedron 6^* – an octahedron; (b) basic polyhedron 6^* and the knots $6^*2.1.2.1.2\,0.1$ and $6^*2\,1.2.3\,2 : -2\,2\,0$.

A link given by Conway symbol containing only tangles ± 1 and ± 2 is called a *source link*, and link given by Conway symbol containing only tangles ± 1, ± 2 and ± 3 is called *generating link*.

Suppose an alternating KL diagram contains a tangle T. Let us fix four ends a, b, c, d of T and then rotate it by a 2-fold rotation (half-turn). The twist on the left in Fig. 5 is moved to the right. Such an operation is called a *flype*.

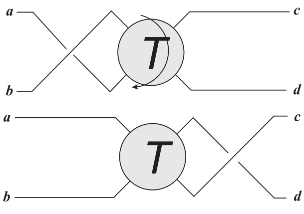

Figure 5: A flype.

The famous Tait's Flyping Conjecture was proved by Menasco and Thistlethwaite in 1993, a century after P.G.Tait formulated it:

Theorem 0.1. *(Tait's Flyping Theorem) Suppose that* L' *and* L'' *are two reduced alternating diagrams of an alternating link* L *on the sphere* S^3. *Then we can change* L' *into*

L'' by performing a finite number of flypes [32, 33].

There is a nice bijective correspondence between KLs and graphs: to obtain a graph from a projection of KL, first color regions of the KL diagram black or white in a checker-board manner, so that the infinite outermost region is black. In the *checker-board coloring* (or *Tait coloring*) of the plane obtained, put a vertex at the center of each white region. Two vertices of a graph are connected by an edge if there was a crossing between corresponding regions in a KL diagram[3]. Graph corresponding to a link diagram D_L will be denoted by $G(D_L)$.

For a graph of KL we can compute its Tutte polynomial, which is a kind of magician hat – many different polynomial invariants of graphs and KLs: chromatic polynomial, dichromatic polynomial, Jones polynomial (Kauffman bracket polynomial), and HOMFLYPT polynomial[4] can be obtained from Tutte polynomial by replacements of variables.

Two operations are essential for understanding the Tutte polynomial definition: *edge deletion* denoted by $G - e$, and *edge contraction* G/e. The latter involves first deleting e, and then merging its endpoints.

Definition 0.2. The *Tutte polynomial* of a graph $G(V, E)$ is a two-variable polynomial $T(G) = T(x, y)$ defined as follows:

$$T(G) = \begin{cases} 1 & E(\emptyset) \\ xT(G/e) & e \in E \text{ and } e \text{ is a bridge} \\ yT(G-e) & e \in E \text{ and } e \text{ is a loop} \\ T(G-e) + T(G/e) & e \in E \text{ and } e \text{ is not a loop or a bridge} \end{cases}$$

The definition of the Tutte polynomial outlines a simple recursive way for computing it, but the order in which rules are applied is not unique.

The Tutte polynomial of the graph $\overline{G}$, dual graph of G, can be obtained from $T(G)$ by replacements $x \to y$, $y \to x$, i.e., $T(\overline{G})(x, y) = T(G)(y, x)$.

According to Thistlethwaite's Theorem, Jones polynomial of an alternating link, up to a factor, can be obtained from Tutte polynomial of its corresponding graph by replacements: $x \to -x$ and $y \to -\frac{1}{x}$ [34–37]. Moreover, from general formulae for Tutte polynomials with negative values of parameters we obtain Tutte polynomials expressed as Laurent polynomials. By the same replacements we obtain, up to a factor, Jones polynomials of non-alternating links.

[3] In addition, to each edge of a graph we can assign the sign of its corresponding vertex of the KL diagram.

[4] For Jaeger links.

Every KL diagram is an embedding of a 4-valent planar graph on a sphere S^2 with denoted overcrosings and undercrossings. In this paper we consider only planar graphs and restrict our attention to alternating KLs obtained from them.

3. BASIC POLYHEDRA IN KNOT THEORY

The first class of graphs we consider are basic polyhedra which are already 4-valent, so need no additional constructions in order to be turned into 4-valent graphs and alternating KLs.

The smallest basic polyhedron is the regular octahedron (i.e., 3-antiprism) corresponding to Borromean rings 6^*. The number of the basic polyhedra with $n \leqslant 20$ crossings is given in the following table

n	6	8	9	10	11	12	13	14	15	16	17	18	19	20
	1	1	1	3	3	12	19	64	155	510	1514	5146	16966	58782

The complete data-base is available in the program *LinKnot* [10].

The list of basic polyhedra includes 2-vertex connected basic polyhedra[5] which are not actual geometrical polyhedra.

If we have any polyhedral graph G, we can obtain its corresponding *middle graph* $M(G)$ determined by mid-edge points of G by connecting mid-edge points belonging to adjacent edges of G. Clearly, the result $M(G)$ is always a 4-valent graph. Every at least 3-vertex connected basic polyhedron can be obtained as the middle graph from some geometrical polyhedron. After turning $M(G)$ into an alternating link diagram D_L, by introducing overcrossings and undercrossings in an alternating manner, the graph G is the graph of the link diagram D_L, i.e., $G(D_L) = G$, so the constructions of a graph of a link diagram $G = G(D_L)$ and a middle graph $D_L = M(G)$ are mutually dual.

4. BASIC POLYHEDRA DERIVED FROM GEOMETRICAL POLYHEDRA

For chemists the most interesting basic polyhedra are the most symmetrical ones, which can be ordered in recognizable recursively defined families of graphs, i.e., basic polyhedra that originate from families of geometrical polyhedra.

[5]The first example of that kind is the basic polyhedron 12E.

Typical examples are $2n$-antiprisms, representing the basic polyhedra $(2n)^*$ $(n \geqslant 3)$, which have two n-gonal, and $2n$ triangular faces. Antiprismatic basic polyhedra $(2n)^*$ are 3-component links for $n = 0 \pmod 3$ and knots otherwise. They are closures of 3-braids $(Ab)^n$ $(n \geqslant 3)$ [38]. The graph of a knot or link $(2n)^*$ is the wheel graph $Wh(n+1)$. The general formula for the Tutte polynomials of wheel graphs is

$$T(G((2n)^*) = T(Wh(n+1)) = \left[\frac{1}{2}\left[(1+x+y)+[(1+x+y)^2-4xy]^{1/2}\right]\right]^n +$$

$$\left[\frac{1}{2}\left[(1+x+y)-[(1+x+y)^2-4xy]^{1/2}\right]\right]^n + xy - x - y - 1.$$

Since graphs $Wh(n+1)$ are self-dual, all their corresponding knots or links $(2n)^*$ are amphicheiral.

Because wheel graphs $Wh(n+1)$ are n-pyramids $(n \geqslant 3)$, all knots and links $(2n)^*$ can be obtained as the middle graphs of n-pyramids. This example illustrates the recursive derivation of basic polyhedra by using middle graphs of a family of polyhedra (e.g., n-pyramids, n-prisms, n-bipyramids, *etc.*)

According to Thistlethwaite's Theorem, the Jones polynomial of an alternating link, up to a factor, can be obtained from the Tutte polynomial by substitutions: $x \to -x$ and $y \to -\frac{1}{x}$ [34–37]. Hence, the Jones polynomials of wheels $(2n)^*$ can be directly obtained from their Tutte polynomials. Moreover, we can plot zeros of the Jones polynomials, i.e., the "portrait of family" of KLs $(2n)^*$ [39].

Signature of all knots and links $(2n)^*$ is 0. BJ-unknotting (unlinking) numbers, which can be used as the measure of the complexity of links are computed in *LinKnot* according to the Bernhard-Jablan conjecture [10]. They are equal to n for $n = 0 \pmod 3$, and $n-1$ otherwise.[6]. All the links of the family $(2n)^*$ $(n = 0 \pmod 3)$ have the Borromean property: their cutting number is 1 and by cutting any component the link brakes in unlinks.

Basic polyhedra 6^* and 8^* belong to the family $(2n)^*$. The next basic polyhedron 9^* is the first member of the family of basic polyhedra 9^*, 12C, ..., with $3n$ crossings, two n-gonal faces, $2n$ triangular, and n 4-gonal faces, derived from n-prisms $(n \geqslant 3)$ as middle graphs. For $n = 1 \pmod 2$ we obtain knots, for $n = 2 \pmod 4$ 2-component links, and

[6] Unlinking numbers are computed for $n \leqslant 10$.

for $n = 0$ (mod 4) 4-component links, defined by braid words $AbA(CbA)^{n-2}CbC$ [38]. The signature of obtained KLs is 2 for $n = 3$, 1 for $n = 4$, and $n - 1$ for $n \geqslant 5$. All 4-component links from this family have cutting number 2, and all obtained KLs are chiral. Since n-prisms and n-bipyramids are mutually dual, the same basic polyhedra (i.e., their mirror image KLs) can be obtained as middle graphs corresponding to n-bipyramids.

All polyhedral alternating KLs can be can be obtained from basic polyhedra by vertex substitutions: we substitute every vertex of a basic polyhedron by an algebraic tangle [29][7].

Unlike algebraic KLs, in order to denote polyhedral KLs we need to use a database of basic polyhedra determined by their 4-valent graphs, ordering of vertices and positions of tangles in each of them. Hence, for the use in chemistry and other natural sciences, more natural is the geometrical approach to knot theory, based on usual geometrical objects: geometrical polyhedra and KLs derived from them by "polyhedral knotting" [9]- [27].

5. DECORATED GRAPHS

For any plane graph G we can construct a 4-valent graph G, representing a KL shadow, i.e., KL diagram without information about overcrossings and undercrossings. After introducing overcrossings or undercrossing in each vertex of G' we obtain a KL diagram. All constructions we describe can be applied to any plane graph, but in order to obtain KLs that could be structurally interesting from the chemistry point of view, we usually start from a polyhedral graph G, desirably with a high degree of symmetry, e.g., from graphs (Schlegel diagrams) of polyhedra forming infinite families (pyramids, prisms, antiprisms, *etc.*), regular polyhedra, uniform (Archimedean) polyhedra, Johnson solids, *etc.* Usually, we work with alternating KLs derived from such graphs, guaranteeing in this way the minimality of the KL diagrams obtained, knowing that every reduced alternating KL diagram, according to Tait theorem on alternating KLs proved by M. Thislethwaite, L. Kauffman, and K. Murasugi in 1987, has the minimal number or crossings and cannot be reduced to a KL with a smaller number of crossings.

We use two kinds of constructions: the first based on the generalized construction of middle graphs, well known in knot theory, the other based on the truncation and doubling of (twisted) edges [27], called cross-curve and (twisted) double line construction, and the combinations of the mentioned constructions.

[7] This is the method proposed by J. Conway, which results in the Conway notation of polyhedral KLs.

In the classical middle graph construction we introduce crossings (tangles 1 or -1) in the mid-points of a graph G and join the adjacent loose ends so that no additional crossings are created. Instead, we can place place in certain points of an edge of G chains of bigons (positive or negative k-twists) collinear with the edge or perpendicular to it, join adjacent loose ends, and from graph G we again obtain a KL diagram[8] [20, 21]. Another construction resulting in new knotted polyhedra derived from some polyhedron is the "cross-curves and double lines" construction [27]. After introducing bigons, from this construction we obtain "cross-curves and twisted double lines" and "dual cross-curves and twisted double lines" constructions.

In order to simplify the graphical notation of decorated graphs, every k-twist collinear with an edge of G will be denoted by a black circle with the index k, a k-twist perpendicular to an edge by a white circle with the index k (where the indexes 1 can be omitted) belonging to the edge, and every vertex of G of the valence k which is replaced by a k-cross-curve will be surrounded by a circle, while the other vertices of G will be denoted by small black circles. In order to obtain alternating KLs from such decorated graphs we substitute the decorations by appropriate 2-tangles or k-tangles (chains of bigons or k-cross-curves) and join the adjacent loose ends.

Fig. 6a illustrates the meaning of the graphical symbols, and Fig. 6b illustrates the transformation rules: addition and flype, Fig 6c shows the transition from a decorated graph to the corresponding alternating KL, and Fig. 6d the transformation of the decorated graph from Fig. 6c followed by the corresponding ambient isotopy of the links obtained.

In particular, if all edges of G are decorated by black circles of index 2 and there are no other decorations, we obtain Jaeger links [28], and if all vertices of G are surrounded by circles, and there are no other decorations, we obtain polyhedral graphs with cross-curves and double lines without twists [27].

According to Tait flyping theorem, every minimal diagram of a KL can be obtained from some other minimal diagram by a series of flypes. Nice property of our graphical notation is that flypes are represented by a simple graphical transformations: place exchanges of black and white circles belonging to an edge. For black circles holds the simple addition rule: two adjacent black circles of the multiplicity k and l can be replaced by a

[8] After F. Jaeger we can call these two constructions "generalized Jaeger construction" and "generalized dual Jaeger construction".

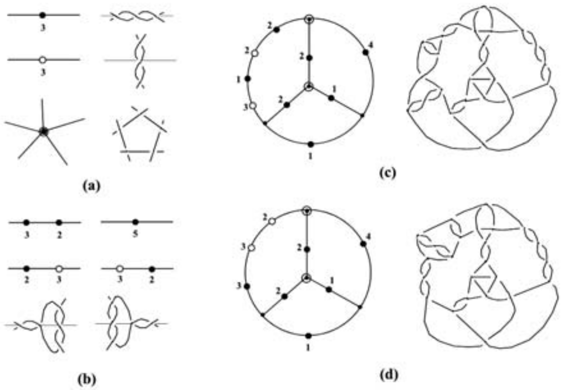

Figure 6: (a) Graphical notation; (b) transformation rules; (c) transition from a decorated graph to the corresponding link; (d) graphical transformations and ambient isotopy.

black circle of the multiplicity $k+l$ (Fig. 6b). Moreover, 2-valent vertices of G have no role and could be deleted. Black or white circles belonging to edges of G, cannot pass over any vertex of G (surrounded by a circle or not). Hence, we can omit 2-valent vertices, and all transformations of KLs can be reduced to the moves of black and white circles belonging to a same edge, i.e., to flypes and additivity of the chains of bigons collinear with the edge.

In order to distinguish the left and right form of an alternating KL we need to consider signs of crossings. For alternating KLs the sign of one crossing determines the rest.

6. ANTIPRISMATIC BASIC POLYHEDRA *(2n)**

First we consider the class of antiprismatic basic polyhedra $(2n)^*$ $(n \geqslant 3)$, which consists of the basic polyhedra 6^*, 8^*, 10^*, $\ldots$ Their corresponding graphs are wheel graphs $Wh(n+1)$, i.e., n-pyramids (Fig. 7), so their Tutte polynomials are given by the general formula [37]:

$$T(G((2n)^*) = T(Wh(n+1)) = \left[\frac{1}{2}\left[(1+x+y)+\left[(1+x+y)^2-4xy\right]^{1/2}\right]\right]^n +$$

$$\left[\frac{1}{2}\left[(1+x+y)-\left[(1+x+y)^2-4xy\right]^{1/2}\right]\right]^n + xy - x - y - 1.$$

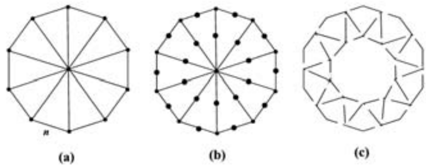

Figure 7: (a) Wheel graph $Wh(n+1)$ $(n = 10)$; (b) the same graph in our graphical notation; (c) its corresponding link.

In order to obtain polyhedral KLs we can use two mutually equivalent constructions: substitutions of vertices by tangles or derivation from decorated graphs.

We can substitute vertices of the basic polyhedron 6^* with arbitrary tangles t_i $(i = 1, \ldots 6)$ or $t_i\,0$, where $t\,0$ is the mirror image of t_i in the diagonal line (see Fig. 2), and obtain KLs given in the Conway notation. For example, by substituting vertices of the basic polyhedron 6^* with integer tangles 2 and $2\,0$ we obtain the link $6^*2\,0.2.2\,0.2.2\,0.2$, or in general $6^*a_1\,0.a_2.a_3\,0.a_4.a_5\,0.a_6$, where a_i $(i = 1, \ldots, 6)$ are integers (Fig. 9).

For further computations of the Tutte polynomials of decorated graphs we use general formulae for the Tutte polynomials of pretzel links [39].

The graph family on Fig. 8 corresponds to the family of pretzel links p, q, r. The general formula for the Tutte polynomial of the graphs $G(p, q, r)$, obtained from Theorem 0.2 [40] is:

$$T(G(p,q,r)) = \frac{x^{p+q+r} + (x^{p+1} + x^{q+1} + x^{r+1})(y-1) - (x^p + x^q + x^r)y}{(x-1)^2} +$$

$$\frac{(xy - x - y)(xy - x - y - 1)}{(x-1)^2}.$$

An *ear* in a graph is a path $v_1 \sim v_2 \sim \ldots \sim v_n \sim v_{n+1}$ where $d(v_1) > 2$, $d(v_{n+1}) > 2$ and $d(v_2) = d(v_3) = \ldots = d(v_n) = 2$. A cycle is viewed as a "special" ear where $v_1 = v_{n+1}$ and the restriction on the degree of this vertex is lifted. If a graph contains an ear or a multi-edge, then all the edges involved can be removed in a single operation. We denote an ear with s edges by E_s and an edge of multiplicity s by e^s. Deletion of an ear $G - E_s$ is defined naturally as meaning the deletion of all the edges of E_s from G. Contraction of a multi-edge G/E_s means to delete all the edges and identify the endvertices, while contraction of an ear means to delete all the edges and identify v_1 and v_{n+1} [40].

Theorem 0.2. *Suppose that G is a biconnected graph that properly contains an ear E_s. Then*

$$T(G) = \frac{x^s - 1}{x - 1} T(G - E_s) + T(G/E_s).$$

Since multiple edges are dual to ears, for multiple edges we immediately obtain the Tutte polynomial of a dual graph.

Notice that n-pretzel links $p_1, p_2, \ldots, p_n$ $(n \geqslant 3)$ are obtained from decorated multi-edge graphs e^n with black circles with indexes p_1, …, p_n on the edges.

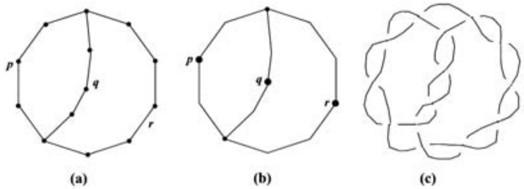

Figure 8: (a) Graph $G(p, q, r)$ $(p = 4,\ q = 4,\ r = 6)$; (b) the same graph in our graphical notation; (c) its corresponding alternating pretzel link.

7. TUTTE POLYNOMIALS OF n-PYRAMID DECORATED GRAPHS

We consider generalized Jaeger and generalized dual Jaeger construction applied to n-pyramids (i.e., wheel graphs $Wh(n+1)$).

Generalized Jaeger links (Fig. 9b) are obtained by introducing chains of bigons a_1, …, a_6 collinear with the edges of 3-pyramid (tetrahedron) graph, i.e., from the decorated 3-pyramid graph $G(a_1, a_2, a_3, a_4, a_5, a_6)$.

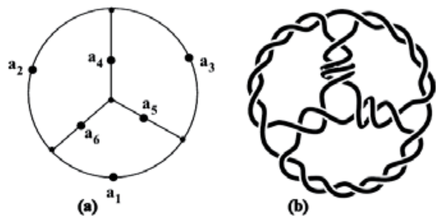

Figure 9: (a) Decorated graph $G_3 = G(a_1, a_2, a_3, a_4, a_5, a_6)$; (b) its corresponding link for $a_1 = 7, a_2 = 6, a_3 = 5, a_4 = 4, a_5 = 3, a_6 = 2$.

Theorem 0.3. *The Tutte polynomial of a decorated 3-pyramid graph* $G_3 = G_3(a_1, a_2, a_3, a_4, a_5, a_6)$ *is given by the general formula:*

$$T(G_3) = C_1(x)T(G(a_2 + a_6, a_4, a_5)) + C_2(x)T(G(a_3 + a_4, a_5, a_6 + 1))+$$

$$C_3(x)T(G(a_4 + 1, a_5 + 1, a_6)) + C_4(x)T(G(a_5 + a_6, 2, 1))+$$

$$C_5(x)T(G(a_6 + 1, 2, 1)) + C_6(x)T(G(2, 2, 1)) + T(Wh(4)),$$

where

$$C_i(x) = \frac{x^{a_i} - x}{x - 1},$$

$G(p, q, r)$ *is the pretzel link graph, and* $Wh(4)$ *is the 3-pyramid graph (4-wheel) with the Tutte polynomial*

$$T(Wh(4)) = 2x + 3x^2 + x^3 + 2y + 4xy + 3y^2 + y^3.$$

The proof of this theorem follows from a series of recursive contractions/deletitions and applications of Theorem 0.2 in the process of the reduction of multiple edges which can be followed on Fig. 10.

Let us notice that the link $L(G_3(a_1, a_2, a_3, a_4, a_5, a_6))$ is the same as the link $6^* a_1\, 0.a_2.a_3\, 0.a_4.a_5\, 0.a_6$ obtained by vertex substitutions. Because wheel graphs are self-dual, generalized dual Jaeger construction produces the same links.

The Jaeger links $L(G_3(2, 2, 2, 2, 2, 2))$ and their HOMFLYPT polynomials [28] are a special case obtained from the Tutte polynomials of graphs $G_3(a_1, a_2, a_3, a_4, a_5, a_6)$ for $a_1 = \ldots = a_6 = 2$. According to Thistlethwaite's Theorem, we obtain the general formula for the Jones polynomials of all the corresponding links $L(G_3)$ for arbitrary integer values of the parameters a_i, including negative values of parameters giving Tutte polynomials of signed graphs and Jones polynomials of the corresponding non-alternating KLs.

The same method can be applied to links $8^* a_8\, 0.a_1.a_5\, 0.a_4.a_6\, 0.a_3.a_7\, 0.a_2$ (Fig. 11a) derived from an edge-decorated 4-pyramid graph (i.e., wheel graph $Wh(5)$)) (Fig. 11b). General formulae for the Tutte polynomials of the decorated graphs $G(a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8)$ are obtained by using the preceding theorem, and general formulae for the Tutte

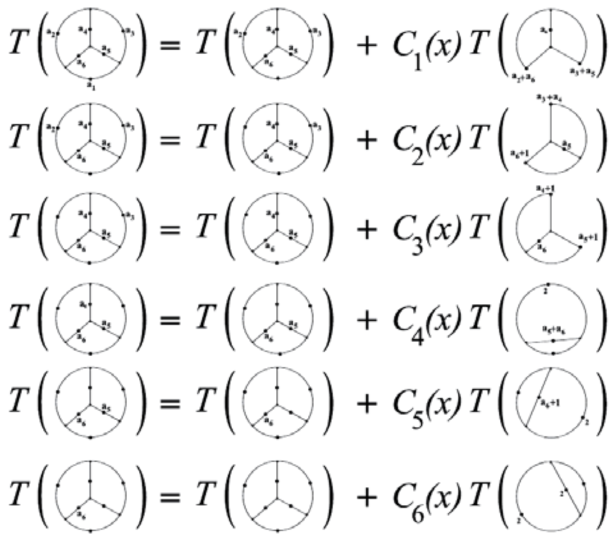

Figure 10: (a) Resolving graph $G_3 = G(a_1, a_2, a_3, a_4, a_5, a_6)$.

polynomials of pretzel link graphs $G(p, q, r)$ and graphs $G((p, q)\, r\,(s, t))$ (Fig. 11c) corresponding to the links $(p, q)\, r\,(s, t))$ [39]. The general formula for the Tutte polynomial of the graphs $G((p, q)\, r\,(s, t))$ is:

$$T(G((p, q)\, r\,(s, t))) = \frac{x^t - 1}{x - 1} T(G(p, q, (r + s))) + T(G(p, q, r)))T(G(s))$$

where $G(s)$ is the graph of the s-cycle E_s with the Tutte polynomial

$$T(G(s)) = \frac{x^s - 1}{x - 1} + y - 1.$$

Theorem 0.4. *Tutte polynomial of the decorated 4-pyramid graph* $G_4 = G_4(a_1,\, a_2, a_3, a_4,$ $a_5, a_6, a_7, a_8)$ *is given by the general formula:*

$$G_4 = G_4(a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8) =$$

$$C_1(x)T(G((a_2 + a_8, +a_7)\, a_3\,(a_6, a_4 + a_5)) + C_2(x)T(G((a_3 + a_7, a_6)\, a_4\,(a_5, a_8 + 1))+$$

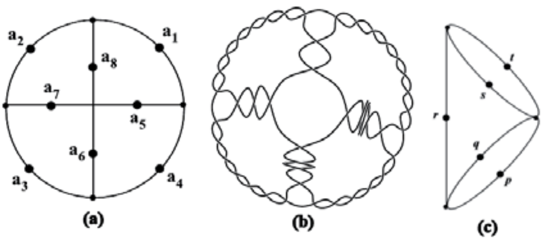

Figure 11: (a) Decorated graph $G(a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8)$; (b) its corresponding link for $a_1 = 9, a_2 = 8, a_3 = 7, a_4 = 6, a_5 = 5, a_6 = 4, a_7 = 3, a_8 = 2$; (c) graph $(p, q)\, r\, (s, t)$.

$$C_3(x)T(G((a_4 + a_6, a_5)\, 1\, (a_8, a_7 + 1)) + C_4(x)T(G((a_5 + 1, a_8)\, 1\, (a_7, a_6 + 1))+$$

$$C_5(x)T(G_3(2, 1, 1, a_7, a_6, a_8)) + C_6(x)T(G_3(2, 1, 1, a_8, a_7, 1))+$$

$$C_7(x)T(G_3(2, 1, 1, 1, a_8, 1)) + C_8(x)T(G_3(2, 1, 1, 1, 1, 1)) + T(Wh(5)),$$

where

$$C_i(x) = \frac{x^{a_i} - x}{x - 1},$$

G_3 is the decorated 3-pyramid graph from Theorem 0.3, $G(p, q, r)$ is the 3-pretzel link graph, $G((p, q)\, r\, (s, t))$ is the graph of the link $(p, q)\, r\, (s, t)$, and $Wh(5)$ is the 4-pyramid graph (5-wheel) with the Tutte polynomial

$$T(Wh(5)) = 3x + 6x^2 + 4x^3 + x^4 + 3y + 9xy + 4x^2y + 6y^2 + 4xy^2 + 4y^3 + y^4.$$

The Tutte polynomials of dual graphs are obtained by substitutions $x \to y$, $y \to x$, and the duality is apparent on the level of decorated graphs (Fig. 12a,b).

8. RECOGNITION OF KLs DERIVED FROM POLYHEDRAL GRAPHS

The most important question is to describe the equivalence relation on decorated graphs and recognize graphs resulting in the same alternating KLs. For all source and generating KLs derived from decorated graphs we compute their minimal Dowker codes

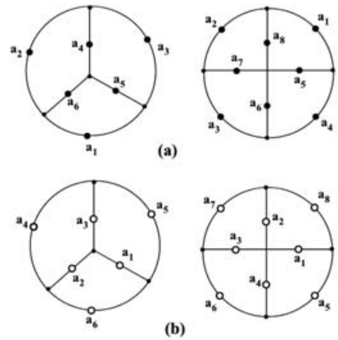

Figure 12: (a) Decorated graphs $G_3(a_1, a_2, a_3, a_4, a_5, a_6)$ and $G_4(a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8)$; (b) their dual graphs.

and select a representative KL (i.e., the decorated graph) for each of different codes. Unlike distinction based on polynomial KL invariants, distinction of different KLs based on minimal Dowker codes is complete, including distinction of mutant KLs that cannot be recognized as different by polynomial invariants. Morover, for large KLs, computation of minimal Dowker codes is much faster then the computation of polynomial invariants.

If all parameters a_i $(i = 1, \ldots, 6)$ are different, using minimal Dowker codes we conclude that among 6!=720 decorated graphs obtained in the class $G_3 = G_3(a_1, a_2, a_3, a_4, a_5, a_6)$ by permutations of parameters, only 30 of them represent different alternating KLs given by the permutations of values of parameters $a_i = i + 1$ $(i = 6, \ldots 1)$, in the following table:

Table 8.1

7,6,5,4,3,2	7,6,4,5,3,2	7,6,3,5,4,2	7,5,6,4,3,2	7,5,4,6,3,2	7,5,3,6,4,2
7,4,6,5,3,2	7,4,5,6,3,2	6,7,5,4,3,2	6,7,4,5,3,2	6,7,3,5,4,2	6,5,7,4,3,2
6,5,4,7,3,2	6,5,3,7,4,2	6,4,7,5,3,2	6,4,5,7,3,2	5,7,6,4,3,2	5,7,4,6,3,2
5,7,3,6,4,2	5,6,7,4,3,2	5,6,4,7,3,2	5,6,3,7,4,2	5,4,7,6,3,2	5,4,6,7,3,2
4,7,6,5,3,2	4,7,5,6,3,2	4,6,7,5,3,2	4,6,5,7,3,2	4,5,7,6,3,2	4,5,6,7,3,2

There are 11 different alternating source links or generating links derived from G_3 (Fig. 13). Their list is given in Table 8.2. The corresponding generating links are obtained by the substitution $1 \rightarrow 3$. Hence, from the decorated pyramid graphs G_3 we obtain 11 different link families that we can analyze by computing their various invariants.

Table 8.2

1	2,2,1,1,1,1	**2**	2,2,1,1,1,2	**3**	2,2,1,2,1,1	**4**	2,1,1,1,1,1
5	2,1,1,2,1,1	**6**	2,2,2,1,1,1	**7**	2,2,2,2,1,1	**8**	2,2,1,2,2,1
9	1,1,1,1,1,1	**10**	2,2,2,2,2,1	**11**	2,2,2,2,2,2		

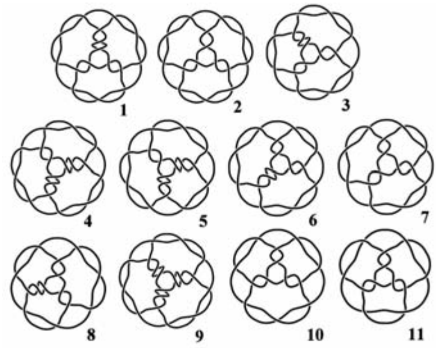

Figure 13: Generating links from Table 8.2.

If all parameters a_i are mutually different, among $8! = 40320$ decorated graphs from the class $G_4(a_1, a_2, a_3,\ a_4, a_5, a_6, a_7, a_8)$ there are 5040 different alternating KLs. This computational result, obtained from minimal Dowker codes, can be confirmed by Polya theorem. The advantage our approach is that we construct links, while Polya's theorem is just a count.

There are 51 different alternating source links or generating links derived from G_4, given in Table 8.3. The corresponding generating links are obtained by the substitution $1 \to 3$. The invariants of the obtained KL families are given in the next section, in Table 9.2.

Table 8.3

1	1,1,1,1,1,1,1,1	**2**	1,1,1,1,2,1,1,1	**3**	2,1,1,1,1,2,1,1	**4**	1,1,1,1,2,1,2,1
5	2,2,1,1,1,1,1,1	**6**	1,1,1,1,2,2,2,1	**7**	2,1,1,1,2,2,1,1	**8**	2,2,1,1,2,1,1,1
9	2,1,1,1,2,1,2,1	**10**	2,2,1,1,1,1,1,2	**11**	2,2,1,1,1,2,1,1	**12**	2,1,1,1,2,2,2,1
13	2,2,1,1,2,2,1,1	**14**	1,1,1,1,2,2,2,2	**15**	2,1,2,1,2,1,2,1	**16**	2,2,2,1,1,1,2,1
17	2,2,2,1,2,1,1,1	**18**	2,2,1,1,1,2,1,2	**19**	2,1,2,1,2,2,1,1	**20**	2,1,1,1,1,1,1,1
21	2,1,1,1,2,1,1,1	**22**	2,1,2,1,2,1,1,1	**23**	2,1,1,1,2,2,1,2	**24**	2,2,1,1,2,1,1,2
25	2,1,1,1,2,2,2,2	**26**	2,2,1,1,2,2,1,2	**27**	2,1,2,1,2,2,2,1	**28**	2,2,2,1,2,1,1,2
29	2,2,2,1,1,1,2,2	**30**	2,2,2,1,1,1,1,1	**31**	2,2,2,2,2,1,1,1	**32**	1,1,1,1,2,2,1,1
33	2,1,1,1,1,2,2,1	**34**	2,2,1,1,2,1,2,1	**35**	2,2,1,1,2,2,2,1	**36**	2,2,2,1,2,1,2,1
37	2,2,2,1,2,2,1,1	**38**	2,1,2,1,1,1,1,1	**39**	2,1,1,1,2,1,1,2	**40**	2,1,2,1,2,1,1,2
41	2,2,1,1,2,1,2,2	**42**	2,2,1,1,2,2,2,2	**43**	2,2,2,1,2,1,2,2	**44**	2,1,2,1,2,2,2,2
45	2,2,2,2,2,2,1,1	**46**	2,2,2,1,2,2,2,1	**47**	2,2,2,2,1,1,1,1	**48**	2,2,2,2,2,1,2,1
49	2,2,2,1,2,2,2,2	**50**	2,2,2,2,2,2,2,1	**51**	2,2,2,2,2,2,2,2		

Because in chemistry we are dealing with KLs with very large number of crossings and with polynomial invariants that hardly can be computed by the standard knot theory programs[9], general formulae for the Tutte polynomials, the Jones polynomials obtained from them, and HOMFLYPT polynomials[10] that can be obtained from Tutte polynomials can be very useful, especially in the case of non-alternating KLs[11]. In order to find the number of different 3- and 4-pyramid KLs with a high number of crossings, we can compute the mentioned polynomial invariants from the general formulae.

All source and generating links from Tables 8.1 and 8.2 are completely recognized as different by the Alexander, Conway[12], Jones, Khovanov, HOMFLYPT, and Kauffman (bracket and 2-variable) polynomials.

9. INVARIANTS OF ANTIPRISMATIC KLs DERIVED FROM 3- AND 4-PYRAMID DECORATED GRAPHS

In this section we compute different invariants of obtained KL families, believing that used together they provide more complete insight into the complexity of the obtained polyhedral KLs.

9.1. NUMBER OF COMPONENTS

The first and simplest invariant of a KL is the number of components. For KLs obtained from the graphs $G_3 = G_3(a_1, a_2, a_3,\ a_4, a_5, a_6)$ we obtain 4-component links *iff* all a_i are even, 3-component links if one a_i is even and all others are odd or if all of them are odd, and 2-component links if two or five of them are odd, and the others are even. If tree of parameters are odd and three even, we obtain 2-component links *iff* $a_1 = a_2 = a_3 = 0 \pmod 2$, $a_1 = a_5 = a_6 = 0 \pmod 2$, $a_2 = a_4 = a_6 = 0 \pmod 2$, or $a_3 = a_4 = a_5 = 0 \pmod 2$, and knots otherwise. If two parameters are even, and the remaining four even, 2-component links will be obtained *iff* $a_1 = a_4 = 0 \pmod 2$, $a_2 = a_5 = 0 \pmod 2$ or $a_3 = a_6 = 0 \pmod 2$, and knots otherwise.

From graphs $G_4(a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8)$ we obtain 5-component links *iff* all parameters are even, and 4-component links *iff* one of them is odd, and the others are even.

[9] The existing computer programs can work with KLs with at most $n = 50$ crossings.

[10] HOMFLYPT polynomials can be obtained from Tutte polynomials only for Jeager links.

[11] Alternating KLs can be distinguished by using the program *LinKnot* [10] and computing minimal Dowker codes, without fixed limit on the number of crossings.

[12] Alexander and Conway polynomials cannot distinguish the left and right form of the same KL.

If two parameters are odd, and the others even, we obtain 3-component links, and if all parameters are odd we obtain knots. If three parameters are odd, and the others even we obtain 3-component links if $a_3 = a_4 = a_6 = 0$ (mod 1), $a_2 = a_3 = a_7 = 0$ (mod 1), $a_1 = a_4 = a_5 = 0$ (mod 1), or $a_1 = a_2 = a_8 = 0$ (mod 1), and 2-component links otherwise. If four parameters are odd, and four even we obtain 3-component links if $a_1 = a_2 = a_3 = a_4 = 0$ (mod 2), $a_1 = a_3 = a_5 = a_8 = 0$ (mod 2), $a_1 = a_3 = a_6 = a_7 = 0$ (mod 2), $a_2 = a_4 = a_5 = a_6 = 0$ (mod 2), or $a_2 = a_4 = a_7 = a_8 = 0$ (mod 2), 2-component links for the following sets of even parameters:

1,2,5,7	1,2,5,8	1,2,7,8	1,4,5,6	1,4,5,8	1,4,6,8	1,5,6,8	1,5,7,8	2,3,6,7	2,3,6,8
2,3,7,8	2,5,7,8	2,6,7,8	3,4,5,6	3,4,5,7	3,4,6,7	3,5,6,7	3,6,7,8	4,5,6,7	4,5,6,8

and knots otherwise. If three parameters are even, we obtain 3-component links for the following triples of even parameters:

1,5,8	2,7,8	3,6,7	4,5,6

2-component links for

1,2,3	1,2,4	1,3,4	1,3,5	1,3,6	1,3,7	1,3,8	1,6,7
2,3,4	2,4,5	2,4,6	2,4,7	2,4,8	2,5,6	3,5,8	4,7,8

and knots otherwise. If two parameters are even, we obtain 3-component links for $a_1 = a_3$ (mod 2) or $a_2 = a_4$ (mod 0), 2-component links for the following pairs:

1,5	1,8	2,7	2,8	3,6	3,7	4,5	4,6	5,6	5,8	6,7	7,8

and knots otherwise. Finally, if only one parameter is even, we obtain 2-component links if it occupies one of the first four positions, and knots otherwise.

The links obtained from decorated graphs G_3 can be divided into 11 families in Table 8.2. The fist three families **1-3** are knots, **4-8** are 2-component links, **9-10** are 3-component links, and **11** is the family of 4-component links.

The source links obtained from decorated graphs G_4 define 51 families from Table 8.3. The fist 19 families **1-19** are knots, **20-37** are 2-component links, **38-48** are 3-component links, **49-50** are 4-component links, and **51** is the family of 5-component links.

9.2. CUTTING NUMBER

Next invariant we look at is the cutting number: the number of components of a link L that need to be cut in order to obtain split link. It is an invariant of link families: all members of a KL family have the same cutting number. Certainly, for every 2-component link the cutting number is 1. However, cutting number is not necessarily equal to $c-1$, where c is number of components. For example, for Borromean rings the cutting number is 1. All 4-component links obtained from the graph $G_3(a_1,a_2,a_3,a_4,a_5,a_6)$ have cutting number 3, and all 3-component links with one odd parameter have cutting number 2. For 3-component links with all odd parameters we obtain more interesting results. If all parameters are equal to 1, we have Borromean rings with the cutting number 1, but this is not the only link obtained from $G_3(a_1,a_2,a_3,a_4,a_5,a_6)$ with this property: among 3-component links there are 36 possible sets of parameters giving families of links with cutting number 1, and one single link – the Borromean rings. The symbols corresponding to the links with cutting number 1 must have at least two parameters equal to 1, $a_3=a_6=1$, $a_2=a_5=1$ or $a_1=a_4=1$, and the other parameters can be arbitrary odd numbers. Borromean rings are only link among them with the Borromean property: cutting of any component results in a trivial link.

Among links derived from graphs $G_4(a_1,a_2,a_3,a_4,a_5,a_6,a_7,a_8)$ the following sets of parameters yield families of links which have cutting number $c-2$, where c is the number of components:

- 4-component links which have all parameters even;
- 3-component links that have an odd parameter at any of the first four positions, and all the other parameters even;
- 3-component links $a_2=a_4=1 \pmod 2$ or $a_1=a_3=1 \pmod 2$, and with other parameters even.

There are also some other 3-component links with cutting number 1, but some of their parameters must be equal 1. Such links are:

- links with $a_1=a_3=0 \pmod 2$, the remaining parameters are odd, and $a_6=a_7=1$ or $a_5=a_8=1$;

- links with $a_1 = a_3 = 0 \pmod 2$, the remaining parameters are odd, and $a_6 = a_7 = 1$ or $a_5 = a_8 = 1$;
- links with $a_1 = a_3 = 0 \pmod 2$, the remaining parameters are odd, and $a_6 = a_7 = 1$ or $a_5 = a_8 = 1$;
- links with $a_2 = a_4 = 0 \pmod 2$, the remaining parameters are odd, and $a_3 = 1$;
- links with $a_1 = a_3 = 0 \pmod 2$, the remaining parameters are odd, and $a_5 = a_6 = 1$ or $a_7 = a_8 = 1$;
- links with $a_2 = a_7 = a_8 = 0 \pmod 2$, the remaining parameters are odd, and $a_4 = 1$;
- links with $a_3 = a_6 = a_7 = 0 \pmod 2$, the remaining parameters are odd, and $a_1 = 1$;
- links with $a_4 = a_5 = a_6 = 0 \pmod 2$, the remaining parameters are odd, and $a_2 = 1$.

The above sets of parameters can result in equal (ambient isotopic) links.

Since cutting numbers are invariants of families, cutting numbers of all 3- and 4-pyramidal links we obtain from their source and generating links given in Tables 8.2 and 8.3.

9.3. UNKNOTTING NUMBER

Next we compute BJ-unknotting (unlinking) numbers for the mentioned families of KLs by using BJ-unknotting numbers of the corresponding source links and distances of KLs.

Definition 0.3. For a given crossing v of a diagram D representing link L, let D_v denote the link diagram obtained from D by the crossing change in v (Fig. 14).

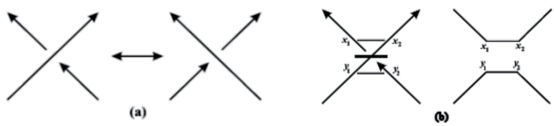

Figure 14: (a) crossing change; (b) ∞-operation.

a) The *unlinking number* $u(D)$ of a link diagram D is the minimal number of crossing changes on the diagram required to obtain an unlink.

b) The *classical unlinking number* of a link L, denoted by $u(L)$ can be defined by $u(L) = \min_D u(D)$ where the minimum is taken over all minimal diagrams D representing L.

c) The *BJ-unlinking number* $u_{BJ}(D)$ of a diagram D is defined recursively in the following manner:

1. $u_{BJ}(D) = 0$ iff D represents an unlink.
2. $u_{BJ}(D) = 1 + \min_{D_v} u_{BJ}(D_v)$ where the minimum is taken over all minimal diagrams of a link represented by D_v for which the value is already defined.

d) $u_M(L) = \min_D u(D)$ where the minimum is taken over all minimal diagrams D representing L.

e) The *BJ-unlinking number* $u_{BJ}(L)$ of a link L $u_{BJ}(L) = \min_D u_{BJ}(D)$ where the minimum is taken over all minimal diagrams D representing L.

J.A. Bernhard in 1994 and independently S. Jablan in 1995 conjectured:

Conjecture 0.1. *(Bernhard-Jablan Conjecture) For every link L we have that $u(L) = u_{BJ}(L)$.*

In other words, we consider all minimal projections of a KL[13], make a crossing change in every crossing, and then minimize all the projections obtained. The same algorithm is applied to the first, second, ... k^{th} generation of the KLs obtained. The BJ-unlinking number is the minimal number of steps k in this recursive unlinking process. If the BJ-conjecture does not hold, BJ-unlinking numbers are still the best upper bound for unlinking numbers.

Definition 0.4. A *distance of a link projection* L'_1 *from a link projection* L'_2 is the minimal number of crossing changes in L'_1 required to obtain L'_2.

A *distance of links* L_1 and L_2 (or Gordian distance), denoted by $d(L_1, L_2)$, is the minimal number of crossing changes in L_1 required to obtain L_2, the minimum taken over all projections of L_1 and L_2.

BJ-unlinking number of a pyramidal knot or link L is obtained from BJ-unlinking number of its source link L_0 as $u_{BJ}(L_0) + d(L, L_0)$[14].

[13] For alternating KLs, one minimal diagram is sufficient.

[14] For computation of KL distances of pyramidal links we used only one minimal diagram for each link.

Example: let us compute BJ-unknotting number of the 3-pyramidal knot K given by the parameters $(a_1, a_2, a_3, a_4, a_5, a_6) = (4, 4, 3, 4, 3, 3)$ belonging to the family **3**. Its distance from the source link K'=**3** given by parameters $(a'_1, a'_2, a'_3, a'_4,\ a'_5, a'_6) = (2, 2, 1, 2, 1, 1)$ is $\sum_{i=1}^{6} \frac{a_1 - a'_1}{2} = 4$, and because the unknotting number of the source link K' is 2, BJ-unknotting number of the knot K is 6.

We restrict our computations to KL families from Tables 8.2 and 8.3, and summarize results in Tables 9.1 and 9.2.

9.4. ∞-UNKNOTTING NUMBER

The ∞-unknotting operation is defined by S. Jablan in 1998. Every crossing of an oriented knot can be resolved by *smoothing* that preserves number of components, introducing a "two-sided mirror" as in Fig. 14. Similar to Definition 0.3 of BJ-unknotting number, we define the ∞-unknotting number $u_\infty(K)$ restricted to minimal projections.

Every ∞-change (i.e., smoothing) transforms an alternating knot to an alternating knot, so the set of all alternating knots is closed with regard to ∞-changes. According to Tait's Flyping Theorem (Theorem 0.1), all minimal projections of an alternating knot have the same ∞-unknotting number, so for every alternating knot it is sufficient to use only one minimal projection. We compute u_∞ numbers of knots, using their minimal diagrams. For links, u_∞ is the minimal number of steps necessary to obtain a link without self crossings, i.e., without crossings that belong to a single component. The u_∞ number is an invariant of a family, so the lists of ∞-unknotting numbers $u_\infty(L)$ computed for source and generating links L are sufficient.

The following table contains ∞-unlinking numbers for all families of KLs obtained from the graphs $G_3(a_1, a_2, a_3, a_4, a_5, a_6)$, with families given by the lists of parameters corresponding to their source and generating links. In certain cases the $u_\infty(L)$ numbers for a subfamily derived from some source link and for a family derived from the corresponding generating link could be different. In such cases we list both results for a subfamily (derived from a source link) and complete family (obtained from the generating link).

2,2,2,2,2,2	0	2,2,2,2,2,3	1	2,2,2,2,3,2	1	2,2,2,2,3,3	2	2,2,2,3,2,2	1	2,2,2,3,2,3	2
2,2,2,3,3,2	2	2,2,2,3,3,3	3	2,2,3,2,2,2	1	2,2,1,2,2,1	1	2,2,3,2,2,3	2	2,2,3,2,3,2	2
2,2,3,2,3,3	3	2,2,3,3,2,2	2	2,2,3,3,2,3	3	2,2,3,3,3,2	3	2,2,3,3,3,3	3	2,3,2,2,2,2	1
2,3,2,2,2,3	2	2,1,2,2,1,2	1	2,3,2,2,3,2	2	2,3,2,2,3,3	3	2,3,2,3,2,2	2	2,3,2,3,2,3	3
2,3,2,3,3,2	3	2,1,2,1,1,1	3	2,3,2,3,3,3	4	2,3,3,2,2,2	2	2,3,3,2,2,3	4	2,1,1,2,1,2	2
2,3,3,2,3,2	3	2,3,3,2,3,3	3	2,3,3,3,2,2	3	2,3,3,3,2,3	3	2,1,1,1,1,2	3	2,3,3,3,3,2	4
2,3,3,3,3,3	2	3,2,2,2,2,2	1	3,2,2,2,2,3	2	3,2,2,2,3,2	2	3,2,2,2,3,3	3	1,2,2,1,2,2	1
3,2,2,3,2,2	2	3,2,2,3,2,3	3	3,2,2,3,3,2	3	3,2,2,3,3,3	3	3,2,3,2,2,2	2	1,2,1,2,2,1	4
3,2,3,2,2,3	3	3,2,3,2,3,2	3	1,2,1,2,1,1	1	3,2,3,2,3,3	3	3,2,3,3,2,2	4	3,2,3,3,2,3	3
1,2,1,1,1,2	2	3,2,3,3,3,2	4	3,2,3,3,3,3	2	3,3,2,2,2,2	2	3,3,2,2,2,3	3	1,1,2,2,1,2	4
3,3,2,2,3,2	3	1,1,2,2,1,1	1	3,3,2,2,3,3	4	3,3,2,3,2,2	4	3,3,2,3,2,3	3	3,3,2,3,3,2	3
3,3,2,3,3,3	2	3,3,3,2,2,2	3	1,1,1,2,2,1	2	3,3,3,2,2,3	3	1,1,1,2,1,2	1	3,3,3,2,3,2	3
1,1,1,2,1,1	1	3,3,3,2,3,3	2	3,3,3,3,2,2	3	3,3,3,3,2,3	2	3,3,3,3,3,2	2	3,3,3,3,3,3	0

The computations of u_∞ numbers for the families of different source and generating links from Tables 8.2 and 8.3 are given in the Tables 9.1 and 9.2 at the end of this section.

9.5. ADEQUACY NUMBER

Let D be a diagram of an unoriented, framed link $L \in R^3$. A Kauffman state of a diagram D is a function from the set of crossings of D to the set of signs $\{+1, -1\}$. Graphical interpretation is given by smoothing each crossing of D by introducing markers according to the convention illustrated in Fig. 15. A *state diagram* D_s of a diagram D and Kauffman state s, is a system of circles obtained by smoothing all crossings of D [41]. The set of circles in D_s, called *state circles*, is denoted by $C(D)$. Points of state circles which belonged to the same crossing before smoothing are called *self-touch points*. The number of self-touch points belonging to a state circle $c \in C(D)$ is called the *length* of c.

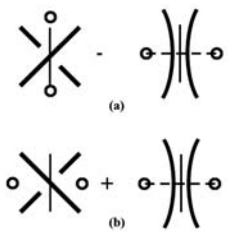

Figure 15: (a) $-$marker; (b) $+$marker. The broken lines represent the edges of the associated graph G_s connecting state circles (represented by dots).

Kauffman states s_+ and s_- with all $+$ or all $-$ signs are called *special states*, and their corresponding state diagrams D_{s_+} and D_{s_-} are called *special diagrams*. All other Kauffman states with both $+$ or $-$ signs are called *mixed states*, and their diagrams are called *mixed state diagrams*.

Definition 0.5. A diagram D is s-adequate if two arcs at every touch-point of D_s belong to different state circles. In particular, a diagram D is $+$adequate or $-$adequate if it is s_+ or s_- adequate, respectively. If a diagram is neither $+$adequate nor $-$adequate it is called *inadequate*. If a diagram is both $+$adequate and $-$adequate, it is called *adequate*, and if it is only $+$adequate or $-$adequate, it is called *semi-adequate* [42, 43].

The definition of adequacy can be extended to an arbitrary mixed state of a link diagram D containing both positive and negative markers.

According to Definition 0.5, a state s of the diagram D is *adequate state* if two segments of D_s obtained by smoothing the same crossing belong to different state circles.

The minimal number of adequate states taken over all diagrams of a link L is called the *adequacy number* of link L and denoted by $a(L)$. All minimal diagrams of an alternating link have the same number of adequate states. The number of adequate states $a(L)$ is the invariant of a family of alternating links L and it is realized on every minimal diagram belonging to a link family [44].

The adequacy numbers of different KL families from Tables 8.2 and 8.3 are given in Tables 9.1 and 9.2. It is interesting to notice that all alternating pyramidal KLs obtained from graphs G_3 and G_4 with all parameters different from 1 have the same adequacy numbers: 15 for all KLs derived from $G_3 = G_3(a_1, a_2, a_3, a_4, a_5, a_6)$ and 43 for all KLs derived from $G_4 = G_4(a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8)$.

9.6. SPLITTING NUMBER

The next invariant defined for links, is the *splitting number*:

Definition 0.6. A *splitting number* $sp(L)$ is the minimum number of crossing changes over all projections of a link L required to obtain a split link, i.e., a link with split components, not necessarily unknotted [45].

Comparing splitting number and unlinking number, C. Adams [45] gave the example of 2-component link $112^*.2\,0 :: -1.-1.-1.-1.-1$ with splitting number 1, and unlinking number 2. A single crossing change turns it into a split link, changing at the same time one of its unknotted components into a trefoil, so its unlinking number is greater then splitting number. In the book [10] we proposed a simpler example of the link with the splitting number 1, and unlinking number 2: the link .2 (or 7^2_6 in the classical notation), that splits by one crossing change which turns one of its unknotted components into a trefoil knot.

From the results given in Tables 9.1 and 9.2 we conclude that for several source links obtained from 3- and 4-pyramid decorated graphs their splitting number is smaller than BJ-unlinking number.

9.7. AMPHICHEIRALITY

Chirality is a geometrical-topological property of many physical systems, and a fundamentally important aspect of chemistry. A KL is *amphicheiral* (or achiral) if it is ambient isotopic to its mirror image. Otherwise, it is *chiral.* There are different knot theory techniques for checking amphicheirality, mostly based on the properties of polynomial KL invariants. One of the most powerful criteria for detection of chirality of alternating links given by their minimal diagrams is based on the Tutte polynomials: a link L is chiral if the Tutte polynomial of its graph is not self-dual, i.e, $T(G_L) \neq T(\overline{G}_L)$. In other words, the Tutte polynomial of its graph does not remain the same after the exchange of variables $x \to y$, $y \to x$.

From general formulae of the Tutte polynomials for n-pyramid graphs ($n = 3, 4$) from Theorems 0.3 and 0.4 it follows that only alternating amphicheiral KLs derived from n-pyramid graphs are the basic polyhedra $(2n)^*$. In general case, amphicheirality of the alternating KLs corresponding to basic polyhedra follows from their minimal braid words $(aB)^n$ and their ambient isotopy with the closed braids $(Ab)^n$ corresponding to the mirror images of KLs in question [10, 38]. Chirality of all remaining alternating KLs derived from n-pyramid graphs can be proved by using methods developed by X.-S. Cheng, W.-Y. Qiu and H.-P. Zhang [23].

9.8. NON-ALTERNATING KLs DERIVED FROM n-PYRAMID GRAPHS

Recognition of non-alternating links is one of the most difficult problems in knot theory. For every polynomial invariant P there exists an infinite number of different KLs that cannot be recognized as different by P. For example, the amount of all KLs with $n \leqslant 12$ crossings that cannot be recognized as different by polynomial invariants (Alexander, Jones, Khovanov, HOMFLYPT, and 2-variable Kauffman polynomial) is between 69% (for the Alexander polynomial) and 9% (for the Kauffman 2-variable polynomial)[15].

Non-alternating knots up to 16 crossings are completely tabulated, and thanks to the recent results of M. Thistlethwaite [8] very soon we expect to have complete tables of non-alternating knots up to 19 crossings. Moreover, the heuristic program *Knotfind*, the part of *Knotscape* [7], successfully recognizes knots up to 50 crossings. From the source

[15] In this amount are included mutant KLs, which cannot be distinguished by any mentioned polynomial invariant.

and generating links from Tables 8.1 and 8.2, by changing signs of positive parameters a_i, $a_i \neq 1$, (i.e., chains of bigons in the corresponding KLs), after making all possible changes, we obtained all non-alternating source and generating links. For the final selection of different KLs from that list we used the program *Knotfind*.

An algebraic tangle t ($t \neq 1$), given in Conway notation, is called *positive* if it contains only positive numbers, and negative if it contains only negative numbers.

Conjecture 0.2. *Replacing a tangle t ($t \neq \pm 1$) in Conway symbol of a minimal diagram of link L by an arbitrary algebraic tangle t' ($t' \neq \pm 1$) of the same sign as t preserves the minimality of the diagram.*

In particular, every replacement of a positive parameter a_i ($a_i \neq 1$) in $G_3 = G_3(a_1, a_2, a_3, a_4, a_5, a_6)$ and $G_4 = G_4(a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8)$ by $-a_i$ preserves the minimality of the corresponding KL diagram. Computations for all non-alternating knots obtained from Tables 8.1 and 8.2 support the conjecture.

From knot families **1-3** in Table 8.1, by crossing changes, we obtain 157 non-alternating source knots giving 10 different families, and from generating knots we obtain 186 non-alternating generating knots giving 47 different families. They are given in Tables 9.8.1 and 9.8.2, respectively.

Table 9.8.1

1	$-2,-2,1,1,1,1$	**2**	$-2,2,1,1,1,1$	**3**	$-2,-2,1,1,1,2$	**4**	$-2,-2,1,1,1,-2$
5	$-2,2,1,1,1,2$	**6**	$-2,-2,1,-2,1,1$	**7**	$-2,-2,1,2,1,1$	**8**	$-2,2,1,-2,1,1$
9	$-2,2,1,2,1,1$	**10**	$2,-2,1,2,1,1$				

Table 9.8.2

1	$-2,-2,-3,2,3,-3$	**2**	$-2,-2,3,2,-3,-3$	**3**	$-2,-2,-3,-2,3,3$	**4**	$-2,-2,-3,3,3,-2$
5	$-2,-2,3,-2,-3,3$	**6**	$-2,-2,3,2,3,3$	**7**	$-2,2,-3,-2,-3,3$	**8**	$-2,-2,3,-2,3,3$
9	$-2,2,3,-2,-3,3$	**10**	$-2,-2,3,3,3,2$	**11**	$-2,2,3,-2,3,3$	**12**	$-2,2,-3,-2,3,3$
13	$-2,-2,3,-3,-3,2$	**14**	$-2,-2,3,-3,3,2$	**15**	$-2,-2,-3,2,-3,3$	**16**	$-2,-2,3,2,-3,3$
17	$-2,2,-3,-2,3,-3$	**18**	$-2,-2,-3,-3,3,2$	**19**	$-2,-2,3,2,3,-3$	**20**	$-2,-2,-3,-2,-3,3$
21	$-2,-2,-3,-2,3,-3$	**22**	$-2,-2,-3,-3,3,-2$	**23**	$-2,-2,-3,2,-3,-3$	**24**	$-2,-2,-3,3,3,2$
25	$-2,2,-3,-2,-3,-3$	**26**	$-2,-2,-3,2,3,3$	**27**	$-2,-2,-3,-3,-3,2$	**28**	$-2,-2,3,3,3,-2$
29	$-2,-2,-3,3,3,-3$	**30**	$-2,-2,3,-3,3,-3$	**31**	$-2,-2,3,3,3,3$	**32**	$-2,-2,3,-3,3,3$
33	$-2,-2,3,-3,-3,3$	**34**	$-2,2,-3,-3,3,-3$	**35**	$-2,2,-3,-3,3,3$	**36**	$-2,2,-3,3,3,3$
37	$-2,2,-3,3,3,-3$	**38**	$-2,-2,-3,-3,3,3$	**39**	$-2,2,-3,-3,-3,3$	**40**	$-2,2,-3,3,-3,-3$
41	$-2,-2,3,-3,-3,-3$	**42**	$-2,2,-3,-3,-3,-3$	**43**	$-2,-2,-3,3,3,3$	**44**	$-2,-2,-3,-3,3,-3$
45	$-2,2,-3,3,-3,3$	**46**	$-2,-2,-3,-3,-3,3$	**47**	$-2,-2,3,3,3,-3$		

From knot families **1-19** in Table 8.2, by crossing changes, we obtain 3950 non-alternating source knots giving 81 different families, and from generating knots we obtain 4826 non-alternating generating knots giving 1679 different families.

The Jones polynomial distinguishes all knots in Table 8.1 and source knots in Table 8.2, but fails to distinguish all different generating knots in Table 8.2, distinguishing only 1621 from 1679 different families of generating knots, while two-variable Kauffman polynomial distinguishes all of them.

The non-alternating knots we completely distinguish by using *Knotscape*, but for non-alternating links there is no similar tool. For distinguishing non-alternating links we can use only polynomial invariants, giving just the lower bound of the number of different families.

We used for distinction the Kauffman two-variable polynomial that gives much better lower bound than the Jones polynomial. For 2-component links derived from Table 8.1 this lower bound is 45 for source links and 68 for generating links, for 3-component links it is 19 for source and 28 for generating links, and for 4-component links it is 9 for source and 9 for generating links.

For 2-component links derived from Table 8.2 the lower bound obtained using 2-variable Kauffman polynomial is 221 for source links and 1828 for generating links, for 3-component links it is 264 for source and 888 for generating links, for 4-component links it is 158 for source and 170 for generating links, and for 5-component links it is 42 for source and 42 for generating links.

Another problem important for chemistry is the recognition of amphicheiral KLs. A chiral link L is called *chiral undetectable* by the polynomial invariant P if $P(L) = P(\overline{L})$, where $\overline{L}$ is the mirror image of L. As the first filter we can use the Jones polynomial that is easily computable from the general formulae for the Tutte polynomials (Theorems 0.3 and 0.4), and then make final check by hardly computable colored Jones polynomials, which are probably able to completely recognize chiral KLs undetectable by the other polynomials [10]. Programs *SnapPea* [46] and *SnapPy* [47] provide the complete recognition of chiral KLs.

We provide a few examples of source and generating KLs and their chirality. By using the Jones polynomial as the first filter, the first candidate for an aphicheiral source knot is $G_3(a_1, a_2, a_3, a_4, a_5, a_6) = (-2, 2, 1, 1, 1, 2)$, i.e., $6^* - 2\,0.2 : .2$, but it turns out to be a chiral knot which is chiral-undetectable by all polynomial invariants except the colored Jones polynomial. The first amphicheiral family of non-alternating 2-component links is obtained from G_3. Links $(-2, -3, 3, 2, -3, 3)$ give the family of non-alternating 3-pyramidal 2-component links. From G_4 we obtain 18 amphicheiral generating knots and each of them gives the family of amphicheiral non-alternating knots. For, example, the first of them, knot $8^*-2\,0.-3.-2\,0.3.2\,0.3.2\,0.-3$, gives the family of amphicheiral non-alternating 4-pyramid knots $8^*-(2p)\,0.-(2q+1).-(2r)\,0.(2s+1).(2p)\,0.(2q+1).(2r)\,0.-(2s+1)$ $(p,q,r,s\in\mathbb{N})$.

More detailed discussion of non-alternating pyramidal links will be given in forthcoming paper.

9.9. DIFFERENT INVARIANTS AND PROPERTIES OF ALTERNATING LINKS DERIVED FROM 3- AND 4-PYRAMID DECORATED GRAPHS

For links corresponding to the pyramidal decorated graphs $G_3 = G_3(a_1,a_2,a_3,a_4,$ $a_5,a_6)$ and $G_4 = G_4(a_1,a_2,a_3,a_4,\ a_5,a_6,a_7,a_8)$ we compute all invariants previously mentioned, that can be used as the criteria for valuating KL complexity: cutting number, u_∞-number, adequacy number, splitting number (only for links), and BJ-unknotting (unlinking) number. Except BJ-unlinking number, all of them are invariants of KL families.

In order to present the results for decorated graphs in concise form, we restrict computations to the representatives of different families, and compute invariants of KLs and their families only for generating links. For source and generating links from Tables 8.2 and 8.3 we also compute few well known KL invariants: linking number, signature, hyperbolic volume, genus (only for knots), and data about some KL properties: amphicheirality, period and the order of the symmetry group of the corresponding polyhedron.

Results for KLs derived from 3- and 4-pyramid decorated graphs G_3 and G_4 are given in Tables 9.1. and 9.2. For every invariant or property we provide comparative data for source links SL and generating links GL. If the results for source links and generating links coincide (e.g., for the number of components), or if the results for generating links are not relevant for the future computations (in the case of BJ-unlinking numbers), results are given in one column only. Number of components is denoted by c, BJ-unlinking number by u_{BJ}, ∞-unlinking number by u_∞, adequacy number by a, splitting number by sp, signature by s, hyperbolic volume by hv, linking number by l, cutting number by cu, genus by g, periods by p, amphicheirality by A (1 for amphicheiral KLs and 0 for chiral), order of the symmetry group of the corresponding polyhedron by sym, genus (computed only for knots) by g, linking number by l, and cutting number by cn.

Table 9.1

		SL	SL	GL	SL	GL	SL	GL	SL	GL	SL	GL	SL	GL	SL	GL	SL	GL	SL	GL	SL	GL	SL	GL
	c	u_{BJ}	u_∞	u_∞	a	a	sp	sp	s	s	hv	hv	p	p	A	A	sym	sym	g	g	l	l	cn	cn
1	1	2	3	3	8	15			2	4	10.579	19.8959	2	2	0	0	2	2	3	4				
2	1	2	3	3	9	15			0	6	12.0989	19.0457	3	3	0	0	6	6	2	5				
3	1	2	3	3	10	15			2	8	12.2059	19.0525	2	2	0	0	2	2	3	6				
4	2	2	2	2	7	15	1	5	1	5	8.99735	20.7477	2	0	0	0	4	4			0	0	1	1
5	2	3	3	3	9	15	2	6	1	9	10.667	19.899	2,4	2,4	0	0	8	8			2	6	1	1
6	2	4	3	3	9	15	3	3	3	3	12.0461	19.065	2,3	3	0	0	6	6			3	3	1	1
7	2	2	2	2	11	15	2	3	3	7	13.6313	18.2222	2	2	0	0	2	2			1	1	1	1
8	2	3	1	2	12	15	3	4	3	7	13.844	18.2154	2	2	0	0	8	8			0	0	1	1
9	3	2	0	0	6	15	2	8	0	6	7.32772	21.6051	2,3	3	1	0	48	24			0	0	1	2
10	3	4	1	1	13	15	4	5	4	6	15.1567	17.3998	2	2	0	0	4	4			1	1	2	2
11	4	6	0	0	15	15	6	6	5	5	16.5913	16.5913	2,4	2,4	0	0	48	24			6	6	3	3

Here is a brief comment of the results in Table 9.1:

- links from the family **11** belong to the class of so-called hard links [10], i.e., links with the $u_{BJ} = \frac{n}{2}$, where n is the number of crossings. This is also the only family of 3-pyramid links with 4 components;

- after families are stabilized, i.e., for all 3-pyramid KLs with all parameters greater than 1 adequacy number is 15;

- the lower bound of hyperbolic volume $hv(L)$ of all 3-pyramid KLs is the hyperbolic volume of Borromean rings (source link **9**) $V_m = hv(6^*) = 7.32772$, and the upper bound is the hyperbolic volume of completely augmented link $\overline{L} = 6^*(2,-2)\,0.(2,-2).(2,-2)\,0.(2,-2)(2,-2)\,0.(2,-2)$ with $V_M = hv(\overline{L}) = 5V_m$ [48]. All source and generating links from our list can be distinguished by hyperbolic volume;

- Borromean rings have the highest symmetry among 3-pyramid KLs, and it is the only amphicheiral KL among all 3-pyramid KLs. In general, the same holds for all n-pyramid KLs, where the antiprismatic basic polyhedra $(2n)^*$ are the only amphicheiral links in their classes and possess the highest symmetry. Since 3-antiprism is the regular octahedron with the symmetry group $\mathbf{O}_h$ of order 48, Borromean rings obtained from it have the pyritohedral symmetry group $\mathbf{T}_h$ of order 24, and all the other alternating KLs obtained from antiprysms $(2n)^*$ with the symmetry group $\mathbf{D}_{nd}$ of order $4n$ have dihedral symmetry group $\mathbf{D}_n$ of order $2n$;

- the source and generating links from the families **4**, **8**, and **9** with the linking number 0 can be easily extended to the infinite families of links with the linking number 0 of the form $(2p, 2q-1, 2r-1, 2s-1, 2q-1, 2r-1)$, $(2p, 2p, 2q-1, 2r, 2r, 2s-1)$, and $(2p-1, 2p-1, 2p-1, 2p-1, 2p-1, 2p-1)$ $(p, q, r \in \mathbb{N})$, and the linking number of

4-component links from the family **11** is $d = \sum_{i=1}^{6} \frac{a_i}{2}$ for arbitrary even parameters a_i;

- as we already mentioned, Borromean rings, the only 3-pyramid source link with the cutting number 1, can be extended into subfamilies of 3-pyramid links with the cutting number 1.

Table 9.2

			SL	GL	SL	GL	SL	GL	SL	GL	SL	GL		SL	GL	SL	GL	SL	GL	SL	GL	SL	GL
	c	u_{BJ}	u_∞	u_∞	a	a	sp	sp	s	s	hv	hv	p	A	A	sym	sym	g	g	l	l	cn	cn
1	1	2	1	4	11	43			0	8	12.3509	33.0332	2,4	1	0	16	8	3	7				
2	1	1	3	5	13	43			0	8	14.3446	31.9412	2	0	0	2	2	3	7				
3	1	1	2	5	15	43			0	4	15.9387	31.1777	0	0	0	1	1	3	5				
4	1	3	4	5	16	43			4	4	16.2714	30.856	2	0	0	4	4	2	2				
5	1	2	3	4	13	43			2	6	15.4239	31.4851	2	0	0	2	2	4	6				
6	1	2	4	5	20	43			2	6	18.3111	29.8134	2	0	0	2	2	4	6				
7	1	2	4	4	18	43			2	6	17.8936	30.1129	0	0	0	1	1	4	6				
8	1	1	4	4	16	43			0	4	17.3442	30.4002	0	0	0	1	1	3	5				
9	1	2	4	4	18	43			0	4	17.779	30.0954	0	0	0	1	1	3	5				
10	1	2	4	4	15	43			2	6	17.2512	30.3955	2	0	0	2	2	4	6				
11	1	3	5	5	17	43			4	4	17.4305	30.3928	2	0	0	2	2	2	2				
12	1	2	4	4	24	43			2	10	19.8553	29.0561	0	0	0	1	1	4	8				
13	1	2	4	4	22	43			2	10	19.4053	29.3371	0	0	0	1	1	4	8				
14	1	2	4	4	25	43			0	8	20.3233	28.7694	2,4	0	0	8	8	3	7				
15	1	2	4	4	21	43			4	12	19.3062	29.3465	2	0	0	2	2	4	8				
16	1	2	4	5	18	43			4	12	18.7481	29.6339	0	0	0	1	1	4	8				
17	1	3	4	4	19	43			4	12	18.8383	29.633	0	0	0	1	1	4	8				
18	1	2	4	4	20	43			0	8	19.192	29.312	2	0	0	2	2	3	7				
19	1	2	4	4	21	43			4	12	19.4687	29.3615	2	0	0	2	2	4	8				
20	2	2	1	3	12	43	2	7	1	7	13.9484	32.2681	2	0	0	2	2			1	1	1	1
21	2	1	3	3	14	43	1	6	1	7	15.8513	31.1782	0	0	0	1	1			1	1	1	1
22	2	2	3	3	17	43	2	7	1	3	17.4607	30.4274	0	0	0	1	1			1	5	1	1
23	2	3	3	4	22	43	2	3	3	5	19.7214	29.0666	0	0	0	1	1			1	1	1	1
24	2	2	3	4	19	43	2	3	1	3	19.1768	29.3481	0	0	0	1	1			1	1	1	1
25	2	2	3	3	29	43	2	3	3	9	21.7589	28.0261	2	0	0	2	2			1	1	1	1
26	2	2	3	3	26	43	2	3	3	9	21.1751	28.2886	0	0	0	1	1			1	1	1	1
27	2	3	3	3	27	43	3	3	5	11	21.3007	28.3202	0	0	0	1	1			1	1	1	1
28	2	3	3	3	24	43	3	3	5	11	20.6932	28.5882	0	0	0	1	1			1	1	1	1
29	2	4	3	3	22	43	3	3	5	11	20.6332	28.5823	2	0	0	2	2			3	3	1	1
30	2	3	2	3	15	43	2	7	3	13	16.8987	30.7205	2	0	0	2	2			0	4	1	1
31	2	3	3	3	21	43	3	4	5	11	20.1267	28.8618	2	0	0	2	2			0	0	1	1
32	2	2	1	2	16	43	2	6	1	7	16.3527	30.8763	2	0	0	2	2			0	0	1	1
33	2	2	2	2	20	43	2	6	1	11	17.9481	30.1188	2	0	0	2	2			0	4	1	1
34	2	3	1	2	20	43	3	4	1	3	19.2102	29.3243	2	0	0	2	2			0	0	1	1
35	2	3	1	2	28	43	3	4	3	9	21.3418	28.2848	2	0	0	2	2			0	0	1	1
36	2	3	1	2	23	43	3	4	1	7	20.6254	28.5567	0	0	0	1	1			2	2	1	1
37	2	3	2	2	25	43	3	5	3	9	20.8747	28.573	2	0	0	2	2			1	1	1	1
38	3	3	0	0	14	43	3	9	0	4	15.5509	31.5166	2	0	0	4	4			1	7	1	2
39	3	3	1	3	17	43	3	7	2	6	17.7365	30.1292	2	0	0	2	2			1	1	1	2
40	3	5	2	2	22	43	5	9	2	2	19.3535	29.3832	2	0	0	2	2			5	9	2	2
41	3	6	3	3	24	43	5	5	2	2	21.0441	28.305	2	0	0	2	2			5	5	2	2
42	3	4	2	2	33	43	4	5	4	8	23.1191	27.2653	2	0	0	2	2			1	1	2	2
43	3	4	2	2	29	43	4	5	2	6	22.5113	27.5415	0	0	0	1	1			3	3	2	2
44	3	4	2	2	34	43	4	6	6	10	23.2408	27.2931	2	0	0	4	4			2	2	1	1
45	3	5	2	2	27	43	5	6	4	8	22.0399	27.8145	2	0	0	2	2			4	4	2	2
46	3	4	1	2	31	43	4	6	4	8	22.6715	27.5328	0	0	0	1	1			2	2	2	2
47	3	6	0	0	17	43	6	10	4	12	18.2467	29.9481	2	0	0	8	8			6	10	2	2
48	3	4	1	2	26	43	4	6	2	6	21.9428	27.7875	0	0	0	4	4			2	2	2	2
49	4	6	1	1	38	43	6	7	5	7	24.4976	26.5184	2	0	0	2	2			3	3	2	2
50	4	6	1	1	34	43	6	7	5	7	23.886	26.7736	2	0	0	2	2			5	5	3	3
51	5	8	0	0	43	43	8	8	6	6	25.7619	25.7619	2	0	0	8	8			8	8	3	3

From the results given in Table 9.2 we conclude:

- links from the family **51** belong to the class of hard links [10], i.e., links with the $u_{BJ} = \frac{n}{2}$, where n is the number of crossings. This is the only family of 4-pyramid links with 5 components;

- for all 4-pyramid KLs with all parameters greater than 1 adequacy number is 43;

- the lower bound for the hyperbolic volume $hv(L)$ of all 4-pyramid KLs is the hyperbolic volume of the knot 8^* (source link **1**) $V_m = hv(8^*) = 12.3509$, and the upper bound is the hyperbolic volume of completely augmented link $\overline{L} = 8^*(2,-2)\,0.(2,-2).(2,-2)\,0.(2,-2).(2,-2)\,0.(2,-2).\ (2,-2)\,0.(2,\ -2)$ with $V_M = hv(\overline{L}) = 53.4031$ [48]. All source and generating links from our list can be distinguished by hyperbolic volume;

- the knot 8^* (source link **1** corresponding to the basic polyhedron with dihedral symmetry group $\mathbf{D}_4$ of order 8), derived by alternating from the 4-antiprism with the symmetry group $\mathbf{D}_{4d}$ of order 16, has the highest symmetry among 4-pyramid KLs, and it is the only amphicheiral KL among all 4-pyramid KLs;

- the source and generating links from the families **31**, **32**, **34**, and **35** with the linking number 0 extend to the infinite families of links with the linking number 0, and the linking number of 5-component links from the family **51** is $d = \sum_{i=1}^{6} \frac{a_i}{2}$ for arbitrary even parameters a_i;

- all links from the family **44** have the cutting number 1. Source links from the family **38** give the family of links $(2p, 1, 2, 1, 1, 1, 1, 1)$, and source links from the family **39** give the family of links $(2p, 1, 1, 1, 2, 1, 1, 2)$ $(p \in \mathbb{N})$ with the cutting number 1. All 5-component links from the family **51** have the cutting number 3.

Values of invariants given in Tables 9.1 and 9.2 are initial conditions for computing invariants for other members of the corresponding families. General formulae for complete families, expressed by parameters a_i, can be obtained as linear recursions, in the same way as we obtained general formula for u_{BJ} of the family **3**.

For example, for the same family derived from the generating link $2, 2, 3, 2, 3, 3$ with signature $s = 8$ and genus $g = 6$, the general formula for signature is $s(a_1, a_2, a_3, a_4, a_5, a_6) = 8 + a_2 + a_3 + a_5 + a_6$, and for the genus is $g(a_1, a_2, a_3, a_4, a_5,\ a_6) = 6 + \frac{a_2-2}{2} + \frac{a_3-3}{2} + \frac{a_5-3}{2} + \frac{a_6-3}{2}$.

9.10. ZEROES OF JONES POLYNOMIAL AND PORTRAITS OF KL-FAMILIES

Plots of all zeroes of the Jones polynomial [37, 49, 53] for KL family, referred to as the characteristic "portrait of family". We interpret these plots in the light of results

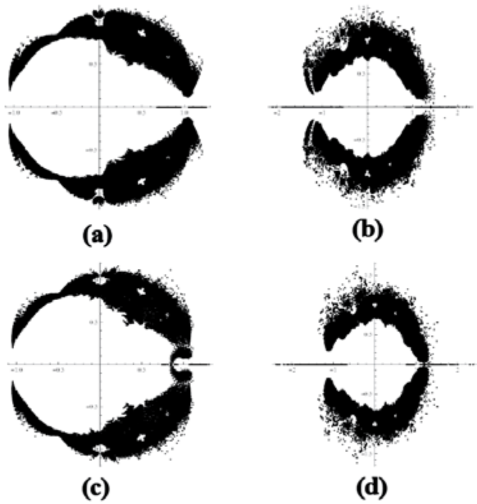

Figure 16: Portraits of the families (a) $6^*(2a_1)\,0.(2a_2).(2a_3+1)\,0.(2a_4+1).(2a_5+1)\,0.(2a_6+1)$ (b) $6^*-(2a_1)\,0.(2a_2).(2a_3+1)\,0.(2a_4+1).(2a_5+1)\,0.(2a_6+1)$ (c) $6^*(2a_1)\,0.(2a_2).(2a_3+1)\,0.(2a_4+1).(2a_5+1)\,0.(2a_6)$ (d) $6^*(2a_1)\,0.(2a_2).-(2a_3+1)\,0.(2a_4+1).(2a_5+1)\,0.(2a_6)$.

in [37, 49–53].

Portraits of the alternating 3-pyramid knot family $6^*(2a_1)\,0.(2a_2).(2a_3+1)\,0.\,(2a_4+1).(2a_5+1)\,0.(2a_6+1)$ and non-alternating knot family $6^*-(2a_1)\,0.(2a_2).(2a_3+1)\,0.(2a_4+1).(2a_5+1)\,0.(2a_6+1)$ are shown in Fig. 16a,b, and portraits of the alternating 3-pyramid knot family $6^*(2a_1)\,0.(2a_2).(2a_3+1)\,0.(2a_4+1).(2a_5+1)\,0.(2a_6)$ and non-alternating knot family $6^*(2a_1)\,0.(2a_2).-(2a_3+1)\,0.(2a_4+1).(2a_5+1)\,0.(2a_6)$ are shown in Fig. 16c,d ($1 \leqslant a_i \leqslant 5$, $i = 1, \ldots, 6$).

Figure 16 suggests that almost all of the roots of the Jones polynomials approach the unit circle under twisting[16], they are dense in the unit circle [53], and critical points are the third [37, 49] and sixth roots of unity. The plots on Fig. 16b,d correspond to non-alternating KL families, because some of the zeros are real and negative [54].

10. CONCLUSION

In this paper we proposed the universal model for analyzing different knotted polyhedral structures relevant for chemistry. It is illustrated on KLs obtained from 3- and

[16] Adding a twist changes the corresponding parameter in a Conway symbol by ± 1.

4-pyramid decorated graphs, based on construction of polyhedral decorated graphs, their graphical notation, and derivation of general formulae for their Tutte polynomials. Moreover, the Jones polynomials of their corresponding alternating and non-alternating KLs are obtained by change of variables in the Tutte polynomials. Invariants for families of polyhedral KLs are obtained recursively from the computations for source and generating links. "Portraits of families", visualized distributions of zeros of the Jones polynomials enable visual recognition of KL families and some of their important properties.

Some constructions discussed in this paper (in particular, constructions based on three-cross curves) are already effectively used for producing examples of three-dimensional DNA structures that include cubes, truncated octahedra and tetrahedra [55]. Hence, we expect that general construction and knot-theory based analysis methods proposed in this paper will find their practical applications in the design of basic DNA building blocks in such a way that basic units will assemble into larger three-dimensional knotted and linked DNA structures.

In the series of the forthcoming papers we will use this model to analyze more complicated decorated polyhedral graphs and their corresponding KLs, beginning from prismatic and bipyramid decorated graphs.

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