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Ear decomposition of 3-regular polyhedral links with applications

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H I G H L I G H T S

- 3-regular polyhedral links can be used to model bacteriophage HK97 capsid.
- We introduce a notion of ear decomposition of 3-regular polyhedral links.
- We obtain an upper bound for the braid index of 3-regular polyhedral links.
- The results may be used to characterize the structure and complexity of protein polyhedra.

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In this paper, we introduce a notion of ear decomposition of 3-regular polyhedral links based on the ear decomposition of the 3-regular polyhedral graphs. As a result, we obtain an upper bound for the braid index of 3-regular polyhedral links. Our results may be used to characterize and analyze the structure and complexity of protein polyhedra and entanglement in biopolymers.

1. Introduction

One of the exotic newcomers in biochemistry is the polyhedral links, which is molecular catenane via template on polyhedral substrates. In mathematical terms, a polyhedral link is a topological entity entangled with a collection of finitely separate closed curves based on the 1-skeleton of the polyhedron. To date, a type of DNA polyhedra whose edges are DNA double helix have been synthesized one after another, for example, DNA cube (Chen and Seeman, 1991), DNA tetrahedron (Goodman et al., 2004), DNA octahedron (Shih et al., 2004), DNA truncated octahedron (Zhang and Seeman, 1994), DNA bipyramid (Erben et al., 2007), DNA dodecahedron (Zimmermann et al., 2008), DNA buckyballs (Bhatia et al., 2009; Zhang et al., 2008a). And another type of more complex double crossover DNA polyhedral links such as He et al. (2008), Lin et al. (2009), Zhang et al. (2009), Zhang et al. (2008b), and He et al. (2010) have been synthesized. These DNA polyhedra 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 (He et al., 2008). The interest in these species is rapidly increasing because of not only their potential applications, but also their aesthetically pleasing topological architectures. To realize these benefits, their many mathematical properties were characterized. For the first type of DNA polyhedra, polyhedral links were used to model these DNA polyhedra (Qiu et al., 2008; Hu et al., 2009; Qiu et al., 2010a, 2010b), and their many polynomial invariant, such as Homfly, Jones and dichromatic polynomials are computed (Jin and Zhang, 2010, 2011, 2012). In other aspects, their genus and braid index are given (Hu et al., 2010; Cheng et al., 2012). For the second type of DNA polyhedra, their genus, braid index and Homfly polynomials are also calculated (Hu et al., 2010; Cheng and Jin, 2012; Cheng et al., 2014).

Another noteworthy case of polyhedral links is the topologically linked protein discovered in the bacteriophage HK97 capsid in 2000 (Wikoff et al., 2000). This is a 72-hedral catenane interlinked by 12 pentameric and 60 hexameric rings, which are believed to provide additional stability. After, this capsid is further researched (Twarock and Hendrix, 2006). Motivated by this topologically complex polyhedral catenane, W.Y. Qiu and his group developed the method of 'three-cross-curve and double lines covering' to construct polyhedral links

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based on 3-regular polyhedra (Qiu and Zhai, 2005; Yang and Qiu, 2007). We shall call such polyhedral links 3-regular polyhedral links. An example is shown in Fig. 1. For this type of links, recently, S.Y. Liu and H. Zhang computed their genus (Liu and Zhang, 2012). In addition, the 3-regular polyhedral link models were generalized to a more universal polyhedral links (Cheng et al., 2009) by the method of 'branched alternating closed braids and double lines covering'. Due to these advances in the architecture of polyhedral links, it is necessary to seek more suitable molecular descriptors to characterize the topological properties of such polyhedral links.

A closed braid is a simple representation of a knotted or interlinked structure, and the braid index can be employed to describe such configuration. The recent example is that knotted hydrocarbon complexes can be modeled as closed braids to facilitate the study of their properties (Cox et al., 2008). Therefore, understanding this topological descriptor is of both fundamental and practical importance. However, it is extremely difficult to calculate them. Up to now, as far as we know, braid indexes of 3-regular polyhedral links have not been studied yet.

Ear decomposition, first proposed by Whitney in 1932, is used to characterize 2-connected graphs. In this paper we introduce the notion of ear decomposition of 3-regular polyhedral links based on the ear decomposition of the 3-regular polyhedral graphs. As a result, we obtain an upper bound for the braid index of 3-regular polyhedral links. Our result is not only a supplement to the theory of knots and links, and may be also used to characterize and analyze the structure and complexity of protein polyhedra and entanglement in biopolymers.

2. Preliminaries

2.1. Knots and links, Seifert surface and braid index

A link L is a finite collection of disjoint circles embedded in R^3-space, and such a circle is called a component of *L*. *A knot* can be described as a link with one component. *An oriented link* $\overrightarrow{L}$ is a link whose each component is assigned a direction. *A reverse link of* $\overrightarrow{L}$, denoted by $-\overrightarrow{L}$, is obtained by reversing the orientations of its all components.

Two links are called *equivalent* if one can be transformed into the other via an ambient isotopy deformation.

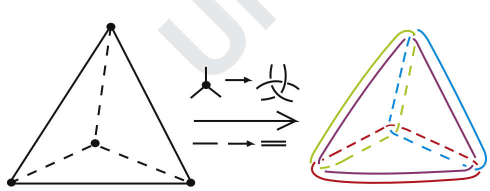

Fig. 1. An example of 3-regular polyhedral links: the tetrahedral link.

A Seifert surface of an oriented link $\overrightarrow{L}$ is a compact, connected and oriented surface S in S^3 that has L as its oriented boundary. In 1934, Seifert (1934) gave an algorithm which, given a diagram of the oriented link $\overrightarrow{L}$, produces such a surface S.

Here, we restate the algorithm. Given a diagram $\overrightarrow{D}$ of an oriented link $\overrightarrow{L}$, first we smooth each crossing of the diagram $\overrightarrow{D}$ by replacing a crossing with two orientation preserving parallel arcs, which results in a set of nonintersecting circles called Seifert circles and the number of such circles is denoted by $s(\overrightarrow{D})$. And then, we connect these circles each other at the position of crossings by half-twisted bands. At last, we can obtain the corresponding Seifert surface of $\overrightarrow{D}$. In Fig. 2, we give the process of the construction for Seifert surfaces of figure-eight knot.

We use $s_{max}(D)$ (or $s_{min}(D)$) to denote the maximum (or minimum) number of Seifert circles taken over all possible choices of orientation of D.

Definition 2.1 (*Cromwell, 2004; Murasugi, 1958; Crowell, 1959; Gabai, 1986*). The genus of an oriented link $\overrightarrow{L}$ is the minimum genus of any Seifert surfaces of $\overrightarrow{L}$. The genus of an unoriented link L is the minimum taken over all possible choices of orientation of L. The genus of a link L is denoted by $g(L)$.

A braid b is a set of n strings in a 3-dimensional cube $I \times I \times I$, where $I = [0, 1]$, all of which are attached to a horizontal bar at the top $\{\frac{1}{2}\} \times I \times \{1\}$ and at the bottom $\{\frac{1}{2}\} \times I \times \{0\}$. A closed braid $\hat{b}$ can be obtained from a braid b by connecting the top ends to the bottom ends of b. An example is illustrated in Fig. 3.

A classical result states that every oriented link can be represented simply by a closed braid (Alexander, 1923).

Definition 2.2 (*Cromwell, 2004*). The braid index of a link is defined by the least number of strings in a braid corresponding to a closed braid representation of the link. The braid index of a link L is denoted by $b(L)$.

It is well-known that the braid index is extremely difficult to calculate.

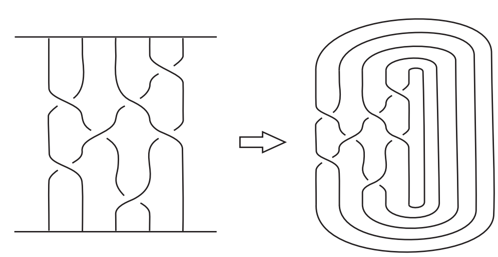

Fig. 3. A braid b and its closed braid $\hat{b}$.

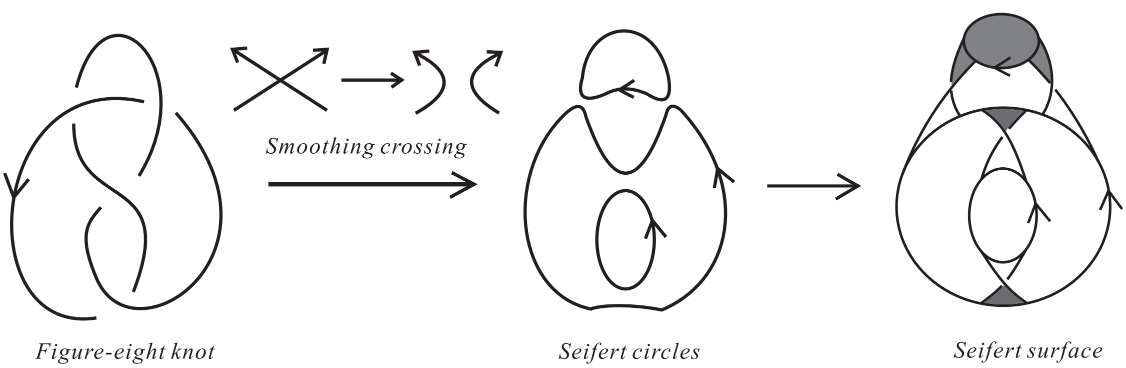

Fig. 2. Seifert circles and surfaces constructed from eight-figure knot by Seifert's algorithm.