A Survey on Knotoids, Braidoids and Their Applications

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Abstract This paper is a survey on the theory of knotoids and braidoids. Knotoids are open ended knot diagrams in surfaces and braidoids are geometric objects analogous to classical braids, forming a counterpart theory to the theory of knotoids in the plane. We survey through the fundamental notions and existing works on these objects as well as their applications in the study of proteins.

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1 Introduction

The theory of knotoids was introduced by Turaev [31] in 2012. A surface knotoid is an oriented curve with two endpoints, in an oriented surface, having finitely many self-intersections that are endowed with under/over data. The endpoints can be in different regions of the diagram. This definition extends the notion of (1, 1)-tangle whose endpoints can assumed to be fixed at the boundary of the disk where the tangle lives. The theory of knotoids in the 2-sphere extends the theory of classical knots and also proposes a new diagrammatic approach to classical knot theory [31]. In [31] basic notions of knotoids were studied comprehensively, including the introduction of several invariants of knotoids in the 2-sphere, such as the complexity (or height) and the Jones/bracket polynomial. Knotoids in S^2 were classified by Bartholomew in [5] and up to 5 crossings by using a generalization of the bracket polynomial for knotoids that was defined by Turaev. There is also a recent classification table for prime knotoids of positive height with up to 5 crossings [23] given by Korablev, May and Tarkaev, obtained by using the correspondence between the knotoids in S^2 and the knots in thickened torus. The first and the second listed authors introduced several new invariants in [12, 14] in analogy with invariants from virtual knot theory. Recently, knotoids have been studied in the field of biochemistry as they suggest new topological models for open linear protein chains. The invariants introduced in [12, 14, 31] have been used for determining the topological entanglement of open protein chains in [10, 11]. Some other recent works on knotoids are on biquandle coloring invariants, by the first listed author and Nelson [18], and on the study of knots that are knotoid equivalent, by Adams, Henrich, Kearney and Scoville [1]. See further [15, 19, 22].

Further, in [12, 16, 17] the theory of braidoids is initiated by the first and the last authors in relation to the theory of planar knotoids. A braidoid diagram extends the notion of classical braid diagram [3, 4] with extra 'free' strands that initiate/terminate at two endpoints located anywhere in the plane of the diagram. The closure operation for braidoids requires special attention due to the presence of the endpoints and their forbidden moves, while a 'braidoiding' algorithm turning any planar knotoid diagram into a braidoid diagram is the proof of an analogue of the classical Alexander theorem [2, 7, 9, 20, 25, 26, 29, 32, 35] for knotoids. With the introduction of L-moves on braidoids, which were originally defined for classical braids by the last author [24–26], a geometric analogue of the classical Markov theorem [6–8, 24–26, 28–30, 33] for braidoids is enabled. In [12, 13, 16] a set of combinatorial elementary blocks for braidoids is also introduced, which are proposed in [16] for an algebraic encoding of the entanglement of open protein chains in 3-dimensional space.

The outline of the paper is as follows. In Sect. 2 we review the basic notions of knotoids and in Sect. 3 we present closure types for knotoids for obtaining knots. In Sect. 3.3 we focus on the spherical knotoids and how they extend the classical knot theory. In Sect. 4 we present geometric interpretations for spherical and planar knotoids. In Sect. 5 we survey through the existing works and results on the invariants of knotoids. In Sect. 6 we review the fundamental notions of braidoids. In Sects. 6.3

and 6.4, we present the key elements for proving an analogue of the Alexander theorem for knotoids/multi-knotoids. In Sect. 6.5 we reprise the definition of the *L*-moves on braidoid diagrams that give rise to an analogue of the Markov theorem for braidoids. Finally, in Sect. 7 we present the applications of knotoids to the study of proteins where we also review the building blocks for braidoid diagrams, which is proposed to be used in encoding open protein chains by algebraic expressions.

2 Knotoids and Knotoid Isotopy

2.1 Knotoid Diagrams

Let Σ be an oriented surface. A *knotoid diagram K* in Σ [31] is an immersion of the unit interval [0, 1] in Σ with a finite number of double points each of which is a transversal self-intersection endowed with over/under data. Such self-intersections of *K* are called *crossings* of *K*. The images of 0 and 1 are two distinct points called the *endpoints* of *K* and are specifically called the *leg* and the *head*, respectively. A knotoid diagram is naturally oriented from its leg to its head. The trivial knotoid diagram is assumed to be an immersed curve without any self-intersections as depicted in Fig. 1a.

The notion of knotoid can be extended to include more components. A *multi-knotoid diagram* in Σ is a union of a knotoid diagram and a finite number of knot diagrams [31].

2.2 Moves on Knotoid Diagrams

Planar isotopy moves generated by the Ω_0-move and the Reidemeister moves Ω_1, Ω_2, Ω_3 (see Fig. 2) that take place in a local disk free of any endpoints are allowed on knotoid diagrams. A special case of planar isotopy moves that involves an endpoint is a *swing move*, whereby an endpoint can be pulled within its region, without crossing any other arc of the diagram, as illustrated in Fig. 2. We refer to all these moves as Ω-moves of knotoids.
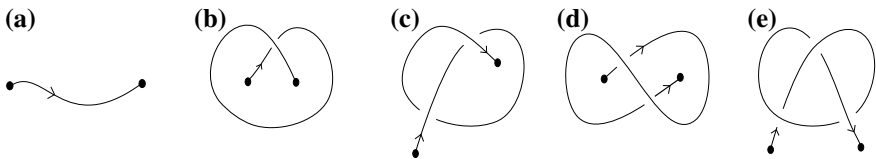

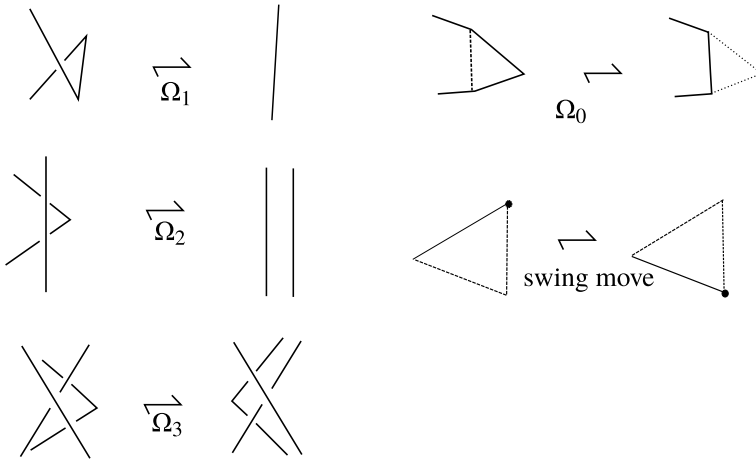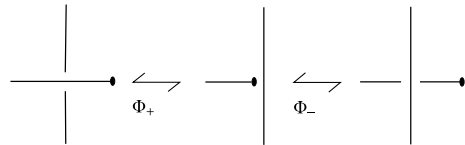**Fig. 1** Examples of knotoid diagrams

Fig. 2 The moves generating isotopy on knotoid diagrams

Fig. 3 Forbidden knotoid moves

The moves consisting of pulling the arc adjacent to an endpoint over or under a transversal arc, as shown in Fig. 3, are the *forbidden knotoid moves* and are denoted by Φ_+ and Φ_-, respectively. Notice that, if both Φ_+ and Φ_--moves were allowed, any knotoid diagram in any surface could be clearly turned into the trivial knotoid diagram.

2.3 Knotoids

The Ω-moves generate an equivalence relation on knotoid diagrams in Σ, called *knotoid isotopy*. Two knotoid diagrams are *isotopic* to each other if there is a finite sequence of Ω-moves that takes one to the other. The isotopy classes of knotoid diagrams in Σ are called *knotoids*. The equivalence relation defined on knotoid diagrams applies also to multi-knotoid diagrams, and the corresponding equivalence classes are called *multi-knotoids*.

Let $\mathcal{K}(\mathbb{R}^2)$ and $\mathcal{K}(S^2)$ denote the set of all knotoids in $\mathbb{R}^2$ and S^2, respectively. We shall call knotoids in $\mathcal{K}(\mathbb{R}^2)$ *planar* and knotoids in $\mathcal{K}(S^2)$ *spherical*.

There is a surjective map [31]

$$\iota : \mathcal{K}(\mathbb{R}^2) \hookrightarrow \mathcal{K}(S^2),$$

induced by the inclusion $\mathbb{R}^2 \hookrightarrow S^2 = \mathbb{R}^2 \cup \{\infty\}$. However, the map ι is not injective. Indeed, there are knotoid diagrams in the plane representing a nontrivial knotoid while they represent the trivial knotoid in S^2. For an example, see Fig. 1b. It is well-known that the knot theory of the plane coincides with the knot theory of the 2-sphere, while the non-injectivity of the map ι implies that the theory of knotoids in $\mathbb{R}^2$ differs from the theory of knotoids in S^2, also yields a more refined theory than the theory of spherical knotoids.

3 Knotoids, Classical Knots and Virtual Knots

3.1 Classical Knots via Knotoids

In [31] the study of knotoid diagrams is suggested as a new diagrammatic approach to the study of knots in three-dimensional space, as any classical knot can be represented by a knotoid diagram in $\mathbb{R}^2$ or in S^2. More precisely, the endpoints of a knotoid diagram can be connected with an arc in S^2 that goes either under each arc it meets or over each arc it meets, as illustrated in Fig. 4. This way we obtain an oriented classical knot diagram in S^2 representing a knot in $\mathbb{R}^3$. The connection types are called the *underpass closure* and the *overpass closure*, respectively. The knot that is represented by a knotoid diagram may differ depending on the type of the closure. For example, the knotoid in Fig. 4 represents a trefoil via the underpass closure and the trivial knot via the overpass closure.

In order to have a well-defined representation of knots via knotoids, we should fix the closure type for knotoid diagrams. When we choose the underpass closure as closure type, we have the following proposition. The statement of the proposition is symmetric for the overpass closure.

Proposition 1 ([31]) *Two knotoid diagrams in S^2 or $\mathbb{R}^2$ represent the same classical knot if and only if they are related to each other by finitely many Ω-moves, swing moves and the forbidden Φ_--moves.*

Given a knot in S^3. We can also consider cutting out an underpassing or an overpassing strand of an oriented diagram of the knot. The resulting diagram is clearly a knotoid

Fig. 4 The overpass and the underpass closures of a knotoid diagram resulting in different knots
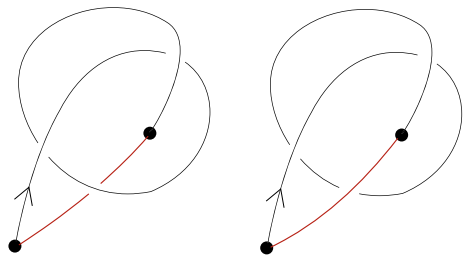
diagram in the plane or the 2-sphere. In fact we can obtain a set of knotoid diagrams by cutting out different strands and the resulting knotoid diagrams all represent the given knot via the underpass or the overpass closure. Knotoid representatives of a knot in S^3 clearly have less number of crossings than any of the diagrams of the knot. For this reason, use of knotoid diagrams to study knots in S^3 provides a considerable amount of simplification for computing knot invariants, such as the knot group [31].

Another interesting question in relation with the knotoid closures has been recently worked in [1]. Two knots K_1, K_2 in S^3 are said to be *knotoid equivalent* if there exists a knotoid κ such that K_1 is the underpass closure of κ and K_2 is the overpass closure of κ. So the question is: *Which pairs of knots are knotoid equivalent?* The authors proved the following theorem.

Theorem 1 ([1, Theorem 2.3]) *Given any two knots K_1, K_2 in S^3, K_1 is knotoid equivalent to K_2.*

3.2   Virtual Knots via Knotoids

The endpoints of a knotoid diagram in S^2 can be tied up also in the virtual way. Namely, the endpoints of a knotoid diagram can be connected with an arc by declaring each intersection of the arc with the diagram as a virtual crossing, as illustrated in Fig. 5. This induces a non-injective (e.g. the knotoids in Fig. 5 are different) and non-surjective mapping from the set of knotoids in S^2 to the set of virtual knots of genus 1, called the *virtual closure map* [15]. Being a well-defined map, the virtual closure map provides a way to extract invariants for knotoids from the virtual knot invariants. In fact, most of the new invariants of knotoids that the first and the second authors have discovered in [14] and we briefly mention in Sect. 3.3, are the result of using the principle that the virtual knot class of the virtual closure of a knotoid is an invariant of the knotoid.

Fig. 5 The virtual closure of two knotoids
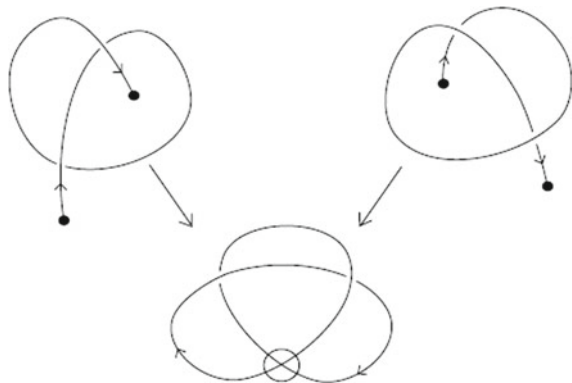
3.3 Spherical Knotoids Extend the Classical Knot Theory

There is a well-defined injective map from the set of oriented classical knots to $\mathcal{K}(S^2)$ [31]. This map is induced by specifying an oriented diagram for a given oriented knot in S^3 and cutting out an open arc from this diagram that does not contain any crossings. The resulting diagram is a knotoid diagram in S^2 with its endpoints lying in the same local region of S^2. Such a knotoid diagram is a *knot-type knotoid diagram* and the isotopy class of the diagram is a *knot-type knotoid*. Figure 1a, b and e are some examples of knot-type knotoid diagrams. It is clear that this map gives a one-to-one correspondence between the set of oriented classical knots and the set of knot-type knotoids in S^2. There are also knotoids that do not lie in the image of this map. They are called *proper knotoids*. The endpoints of any of the representative diagram of a proper knotoid can lie in any but different local regions of the diagram. Figure 1c, d illustrate some examples of proper knotoids.

3.3.1 The Monoid of Knotoids

As Turaev explains in [31], two knotoids K_1, K_2 in S^2 can be concatenated end-to-end in the following way. One can cut out regular disk-neighborhoods of the head of K_1 and the leg of K_2 and identify the remaining surfaces with boundary along their boundaries with an orientation-reversing homeomorphism carrying the unique intersection point of K_1 with the regular neighborhood of the head of K_1 to the unique intersection point of K_2 with the regular neighborhood of the leg of K_2. The resulting diagram is a composite knotoid diagram in S^2, denoted by $K_1 \# K_2$. Equipped with the binary operation #, the set of spherical knotoids, $K(S^2)$, carries a monoid structure [31].

4 Geometric Interpretations of Knotoids

4.1 A Geometric Interpretation of Spherical Knotoids

A Θ-*graph* is a spatial graph with two vertices v_0, v_1, called the *leg* and the *head* respectively, and three edges, e_+, e_0, e_- connecting v_0 to v_1, as exemplified in Fig. 6. The isotopy on Θ-graphs is defined to be the ambient isotopy of the 3-dimensional space preserving the labeling of vertices and the edges, and the set of Θ-graphs consists of the isotopy classes of Θ-graphs.

There is a binary operation on the set of Θ-graphs, called the *vertex multiplication* [34] given as follows. Let Θ_1 and Θ_2 be two Θ-graphs, take out an open 3-disk neighborhood of the head of Θ_1 and an open 3-disk neighborhood of the leg of Θ_2, each intersecting with the graphs along 3-radii (simple parts from e_0, e_+, e_-). Then identify the remaining manifolds with boundary along their boundaries with an orientation-reversing homeomorphism. With the vertex multiplication, the set of
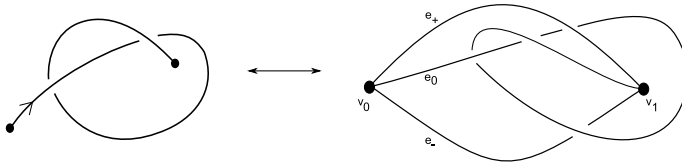
Fig. 6 A knotoid and the corresponding simple Θ-graph

Θ-graphs forms a monoid. A Θ-graph is called *simple Θ-graph* if the union of its edges, e_+ and e_- (the upper and the lower edge, respectively) is the trivial knot. Simple Θ-graphs form a submonoid [31].

Turaev showed the following correspondence between the spherical knotoids and the simple Θ-graphs that gives also rise to a geometric interpretation of spherical knotoids via Θ-curves.

Theorem 2 ([31, Theorem 6.2]) *There is an isomorphism of monoids of spherical knotoids and of simple Θ-graphs.*

### 4.2 A Geometric Interpretation of Planar Knotoids

It is explained in [14] that the theory of planar knotoids is related naturally to open space curves on which an appropriate isotopy is defined. An open curve located in $\mathbb{R}^3$ corresponds to a planar knotoid diagram when projected regularly along the two lines passing through its endpoints and are perpendicular to a chosen projection plane. View Fig. 7. Conversely, an open space curve with two specified parallel lines passing from its endpoints can be viewed as a *lifting* of the related knotoid diagram. A *line isotopy* [14] between two open space curves is an ambient isotopy of $\mathbb{R}^3$ transforming one curve to the other one in the complement of the lines, keeping the endpoints on the lines and fixing the lines. The isotopy classes of planar knotoids (considered in the chosen projection plane) are in one-to-one correspondence with the line isotopy classes of open space curves [14]. Furthermore, in [21] Kodokostas and the third author make the observation that this interpretation of planar knotoids as space curves is related to the knot theory of the handlebody of genus two and they propose the construction of knotoid invariants through this connection. These ideas are further explored in [22].

5 Invariants of Knotoids

In [14, 31] several invariants for knotoids are introduced. One of the first invariants introduced by Turaev [31] was the the *bracket* and the *Jones polynomial* for knotoids. The bracket polynomial extends to spherical knotoids in the natural way. More
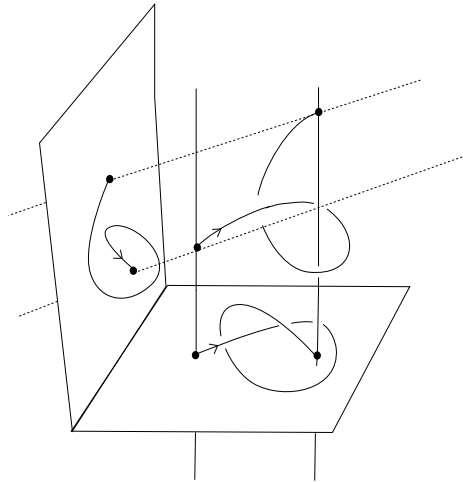
precisely, the bracket expansion is directly applied to knotoid diagrams as shown in
Fig. 8, and in each state we observe a single long segment component with endpoints
and a finite number of circular components. Each circular component contributes to
the polynomial by the value $-A^{-2} - A^2$. The initial conditions given in Fig. 8 are
sufficient for the computation of the bracket polynomial of a knotoid. The closed
formula for the bracket polynomial of knotoids is as follows.

Definition 1 The *bracket polynomial* of a knotoid diagram K is defined as
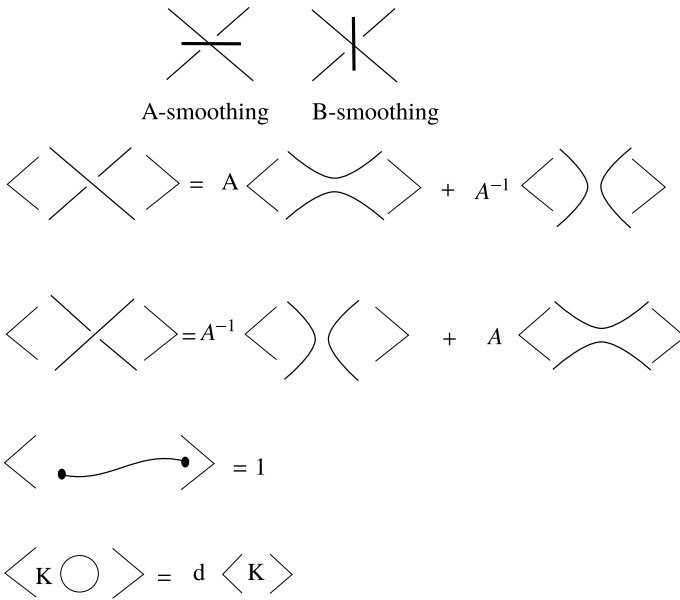
$$< K > = \sum_S A^{\sigma(S)} d^{\|S\|-1},$$

where the sum is taken over all states, $\sigma(S)$ is the sum of the labels of the state S,
$\|S\|$ is the number of components of S, and $d = -A^2 - A^{-2}$.

The bracket polynomial of knotoids in S^2 normalized by the writhe factor,
$(-A^3)^{-\text{wr}(K)}$, generalizes the Jones polynomial with the substitution $A = t^{-1/4}$. Note
that the Jones polynomial of the trivial knotoid is trivial. Furthermore, the following
conjecture [14] extends the long-standing Jones polynomial conjecture.

Conjecture 1 *The Jones polynomial of spherical knotoids detects the trivial knotoid.*

Some other generalizations of the Jones polynomial are: Turaev's *2-variable
bracket polynomial* [31] that is obtained by a use of the intersection number of the
connection arc used in the underpass closure with the rest of the diagram and also
with the state components, and the *arrow polynomial* [14] that keeps track of the
cusp-like structure (see Fig. 11) arising in the oriented bracket expansion (see Fig. 10
for the oriented state expansion) by assigning new variables namely Λ_i's to zig-zag
components. There is a special generalization of the bracket polynomial for planar
knotoids induced by distinguishing the circular state components nested around the
long segment component from the circular state components that do not nest around

A-smoothing   B-smoothing

$$\left\langle \times \right\rangle = A \left\langle)(\right\rangle + A^{-1} \left\langle)(\right\rangle$$

$$\left\langle \times \right\rangle = A^{-1} \left\langle)(\right\rangle + A \left\langle)(\right\rangle$$

$$\left\langle \bullet\!-\!\!-\!\bullet \right\rangle = 1$$

$$\left\langle K \bigcirc \right\rangle = d \left\langle K \right\rangle$$

Fig. 8 State expansion of the bracket polynomial

**Fig. 9** An affine biquandle coloring on knotoid diagrams
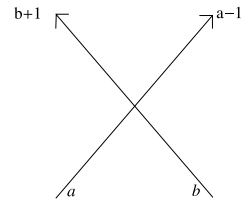
the long segment component. Turaev defined the 3-*variable bracket polynomial* [31] for planar knotoids based on this idea and the *loop bracket polynomial*, which is a specialization of the 3-variable bracket polynomial, was utilized in [11] to classify the knotoid models of protein chains (see Sect. 7). Similarly the first and the second listed authors introduce the *arrow loop polynomial* in [15].

Furthermore, the *affine index polynomial*, given in [14], is induced by a non-trivial biquandle structure on knotoid diagrams (see Fig. 9), and a number of biquandle coloring invariants were studied in [18].

There is also a well-defined parity assigned to crossings of (planar or spherical) knotoid diagrams. The *Gaussian parity* is a mapping that assigns each crossing of a knotoid diagram to either 0 or 1. The importance of an existing parity for knotoids comes from the fact that there is no nontrivial parity for classical knot diagrams. Some parity based invariants for knotoids such as the *odd writhe* and the *parity bracket polynomial* [27] were studied in [14].

Fig. 10 Arrow state sum expansion

$$K \bigcirc \quad = \quad (-A^2 - A^{-2})K$$
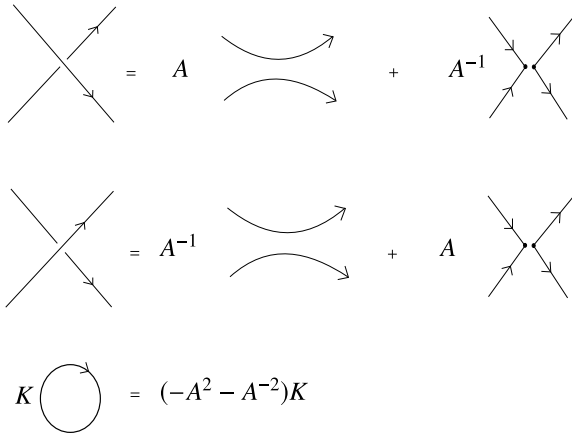
Fig. 11 Cusps
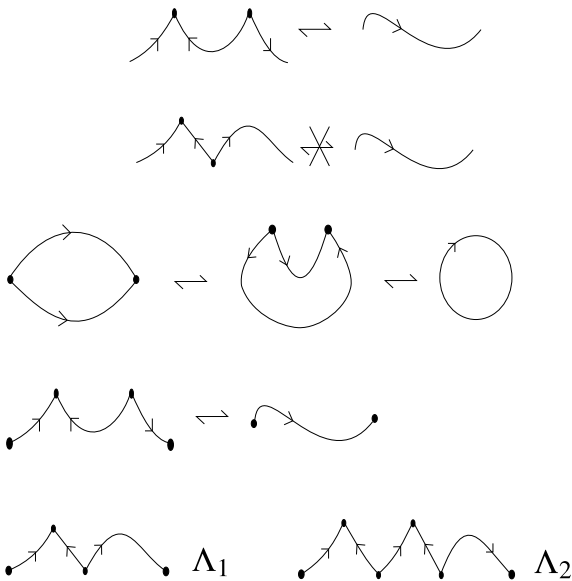
Proper knotoids give rise to interesting questions related to their intrinsic nature, such as the crossing-wise distance between the endpoints, the so-called *height*. More precisely, the *height* of a knotoid diagram in S^2 [31] is the least number of crossings created when the endpoints are joined up by an underpassing strand. The *height* of a knotoid is the minimum of the height of knotoid diagrams in its equivalence class and so forms an invariant for knotoids.

The first and the second listed authors showed that the affine index polynomial and the arrow polynomial establish lower bound estimations for the height of a knotoid. More precisely we have the following lower bound estimations for the height of a knotoid.

Theorem 3 ([14, Theorem 4.12]) *The height of a knotoid is greater than or equal to the maximum degree of its affine index polynomial.*

Theorem 4 ([14, Theorem 5.1]) *The height of a knotoid is greater than or equal to the Λ-degree of its arrow polynomial.*

The interested reader is referred to [15, 19] for ongoing works on knotoids regarding the parity aspect of knotoids and a Khovanov homology construction in analogy with the Khovanov homology for virtual knots/links [19], respectively.

6 The Theory of Braidoids

In this section we reprise the fundamental notions of braidoids introduced by the first and the last listed authors. Braidoids are defined as to form a braided counterpart theory to the theory of planar knotoids.

6.1 Braidoid Diagrams

Let I denote the unit interval $[0, 1] \subset \mathbb{R}$. A *braidoid diagram B* is an immersion of a finite union of arcs into $I \times I \subset \mathbb{R}^2$. The images of arcs are called *strands* of B. There are only finitely many intersection points among the strands of B which are transversal double points endowed with over/under data, the crossings of B. We identify $\mathbb{R}^2$ with the xt-plane with the t-axis directed downward. Following the orientation of I, each strand is naturally oriented downward, with no local maxima or minima, so that it intersects a horizontal line at most once.

A braidoid diagram has two types of strands, the classical strands and the free strands. A *classical strand* is as a braid strand with two ends, one lying in $I \times \{0\}$ and the other lying in $I \times \{1\}$. A *free strand* is a strand that either has one of its ends lying in $I \times \{0\}$ or in $I \times \{1\}$ and the other end lying anywhere in $I \times I$ or it has two of its ends lying anywhere in $I \times I$. There are two such free ends, called the *endpoints* of B and are denoted by a vertex to be distinguished from the fixed ends. For examples see Fig. 12. The two endpoints are called the *leg* and the *head* and are denoted by l and h respectively, in analogy with the endpoints of a knotoid diagram. The head is the endpoint that is terminal for a free strand while the leg is the starting endpoint for a free strand, with respect to the orientation.

The other ends of the strands of B are named *braidoid ends*. Each braidoid end is numbered accordingly to its order from left to right. Braidoid ends lie equidistantly and two braidoid ends having the same order on $\{t = 0\}$ and $\{t = 1\}$ are vertically aligned. Two braidoid ends whose orders coincide are called *corresponding ends*. See the examples in Fig. 12.
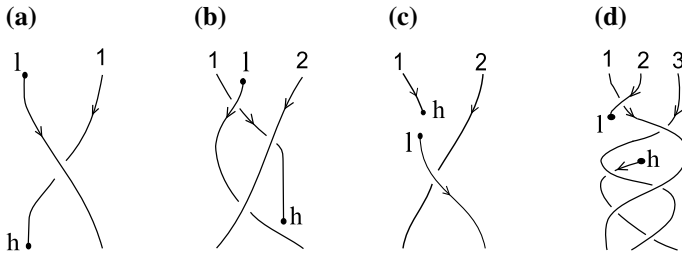
Fig. 12 Some examples of braidoid diagrams

6.2 Isotopy Moves on Braidoid Diagrams

We allow on braidoid diagrams the oriented Reidemeister moves Ω_2 and Ω_3 (recall Fig. 2), which preserve the downward orientation of the arcs in the move patterns. In addition to these moves, the endpoints of a braidoid diagram can be pulled up or down in the vertical direction by a *vertical move*, and right or left in the horizontal direction by a *swing move* in the vertical strip determined by the neighboring corresponding ends, as long as they do not intersect or cross through any strand of the diagram. That is, the pulling of the leg or the head over or under any strand is forbidden. It is clear that allowing both forbidden moves cancels any braiding of the free strands.

The *braidoid isotopy* is induced by keeping the braidoid ends fixed on the top and bottom lines ($t = 0$ and $t = 1$, respectively) but allowing the Reidemeister moves Ω_2 and Ω_3 and planar Δ-moves, as well as the swing and the vertical moves for the endpoints. Two braidoid diagrams are isotopic if one can be obtained from the other by a finite sequence of the above moves. An equivalence class of isotopic braidoid diagrams is a *braidoid*.

6.3 A Closure on Braidoids

One way to define a closure operation on braidoid diagrams in order to obtain planar (multi)-knotoid diagrams is by adding an extra property to braidoid diagrams. More precisely, each pair of the corresponding ends in a braidoid diagram is labeled either *o* or *u*, standing for 'over' or 'under', respectively. We attach the labels next to the braidoid ends lying at the top line and call the diagram a *labeled braidoid diagram*. Two labeled braidoid diagrams are called *isotopic* if their braidoid ends possess the same labeling and they are isotopic as unlabeled diagrams. The corresponding equivalence classes are called *labeled braidoids*.

Let B be a labeled braidoid diagram. The *closure* of B, denoted $\widehat{B}$, is a planar (multi)-knotoid diagram that results from B by the following topological operation: each pair of corresponding braidoid ends of B is joined up with a straight arc (with slightly tilted extremes) that lies on the right of the line of the corresponding braidoid

Fig. 13 The closure of an
abstract labeled braidoid
diagram
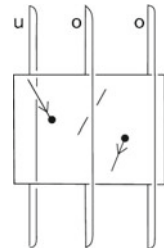
ends in a distance arbitrarily close to this line so that none of the endpoints is located
between the line and the closing arc. The closing arc goes entirely over or entirely
under the rest of the diagram according to the label of the ends. See Fig. 13 for an
abstract illustration of the closure of a labeled braidoid diagram.

Proposition 2 ([16, 17]) *The closure operation induces a well-defined map from
the set of labeled braidoids to the set of planar (multi)-knotoids.*

6.4   How to Turn a Knotoid into a Braidoid?

J.W. Alexander proved in 1923 that any oriented classical knot/link can be represented
by an isotopic knot/link diagram in braided form [2]. See also [9]. The proof of the
Alexander theorem by the last listed author [24–26] utilizes the *L-braiding moves*.
In [16, 17] the first and the last listed authors proved the following analogue of the
Alexander theorem for (multi)-knotoids by utilizing these moves.

Theorem 5 ([16, 17]) *Any (multi)-knotoid diagram in $\mathbb{R}^2$ is isotopic to the closure
of a labeled braidoid diagram.*

Let K be a (multi)-knotoid diagram whose plane is equipped with the top-to-
bottom direction. The basic idea for turning K into a braidoid diagram is to keep the
arcs that are oriented downward, with respect to the top-to-bottom direction, and to
eliminate the ones that are oriented upward (*up-arcs*), producing at the same time
pairs of corresponding braidoid strands, such that the (multi)-knotoid resulting after
closure is isotopic to K. The elimination of the up-arcs is done by the braidoiding
moves.

An *L*-braidoiding move consists in cutting an up-arc at a point and pulling the
resulting two pieces, the upper upward to the line $t = 1$ and the lower downward
to the line $t = 0$, both entirely *over* or *under* the rest of the diagram. The resulting
pieces are pulled so that their ends are kept aligned vertically with the cut-point.
Finally the lower piece is turned into a braidoid strand by Δ-moves. See Fig. 14. For
the purpose of closure, the resulting pair of strands is labeled *o* or *u* depending on our
choice we make for pulling the upper and lower pieces during the braidoiding move.
The reader is referred to Fig. 14 for an illustration of an *L*-braidoiding move where
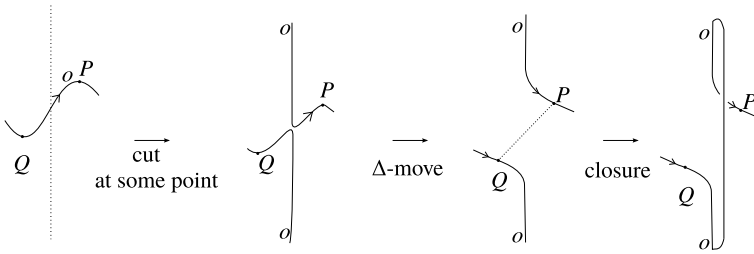
Fig. 14 An *L*-braidoiding move

it can be also verified that the closure of the resulting strands labeled *o* is isotopic to the initial up-arc.

Theorem 5 is proved by applying any one of the braidoiding algorithms. These algorithms are both based on the *L*-braidoiding moves. In Fig. 15 we illustrate the steps of the algorithm that is given in [17]. As for the algorithm in [20] turning any virtual knot/link diagram into a virtual braid diagram, we start by rotating each crossing containing one or two up-arcs by $\frac{\pi}{2}$ or π, respectively, so that we end up with a knotoid diagram whose up-arcs are all free of any crossings. All of these 'free' up-arcs are given an order and a labeling of *o* or *u* each, and are eliminated by the *L*-braidoiding moves one by one. The algorithm terminates in finite steps and results in a labeled braidoid diagram in Fig. 15. The algorithm in [17] which is based on [26], uses braidoiding moves for up-arcs in crossings and is more appropriate for establishing Markov-type theorems for braidoids (see Theorem 6). Yet, an added value of the first algorithm is the following consequence: *Any (multi)-knotoid diagram is isotopic to the uniform closure of a braidoid diagram* [12, 17].

6.5 L-Equivalence

It is clear that due to the choices made in order to prepare a (multi)-knotoid diagram for a braidoiding algorithm (such as subdivision and labeling of the up-arcs) as well as knotoid isotopy moves, we obtain different braidoid diagrams with possibly different numbers of strands and labels. The question that would lead to a Markov-like theorem for braidoids is to ask how these braidoid diagrams are related to each other. Clearly, the braidoid isotopy does not change the number of strands nor the labeling, so braidoid isotopy is not sufficient for determining such relations. The first and the last listed authors showed in [16, 17] that the *L*-moves on braidoid diagrams provide an answer to this question.

An *L-move* on a braidoid diagram *B* consists in cutting a strand of *B* at an interior point, not vertically aligned with a braidoid end or an endpoint or a crossing, and then pulling the resulting ends away from the cutpoint to the top and bottom of *B* respectively, keeping them aligned with the cutpoint, and so as to create a new pair of
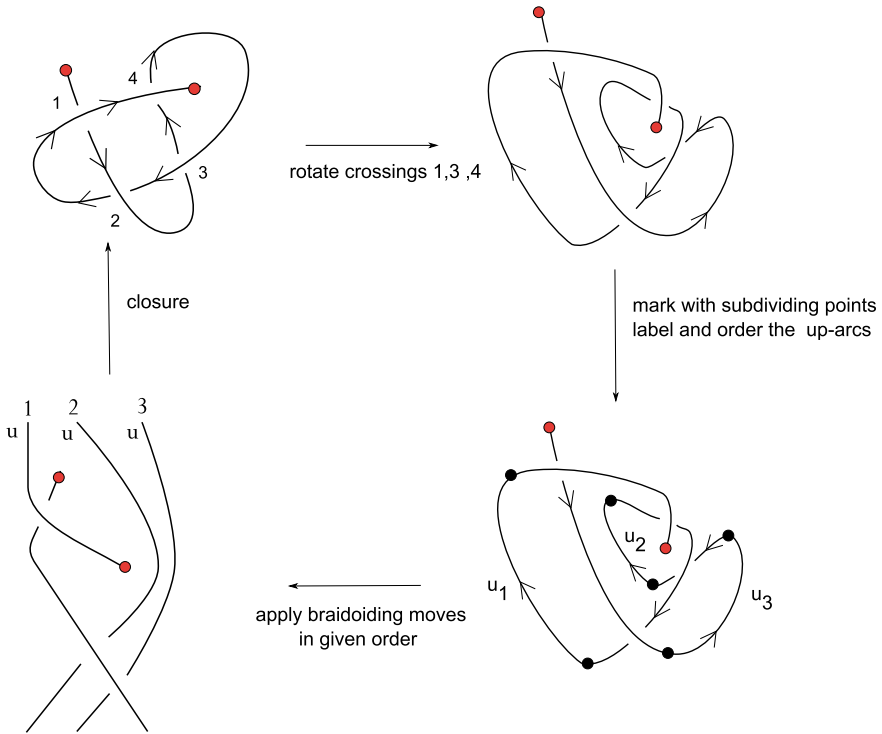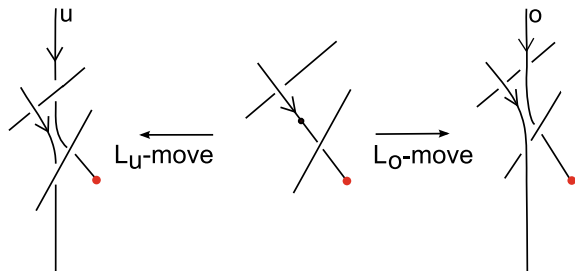
**Fig. 15** An example showing how the algorithm works

Fig. 16 L-moves

corresponding braidoid strands. See Fig. 16 for an illustration of an L-move. There are two types of L-moves, namely L_o and L_u. For an L_o-move the pulling of the resulting new strands is entirely *over* the rest of the diagram. For an L_u-move the pulling of the new strands is entirely *under* the rest of the diagram. The two resulting strands are both labelled according to the type of the L-move. See Fig. 16.

The above definition provides us with the following result, which is an analogue of the classical Markov theorem.

Fig. 17 The configuration of the backbone of the protein 3KZN in 3D and its simplified configuration; image from Dimos Goundaroulis, private communication
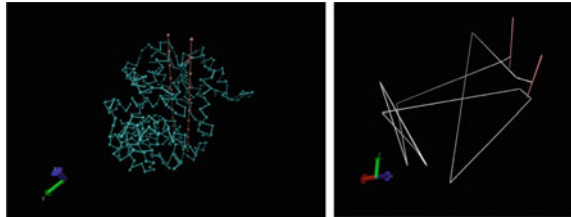

Theorem 6 ([12, Theorem 13]) *The closures of two labeled braidoid diagrams are isotopic (multi)-knotoids in $\mathbb{R}^2$ if and only if the labeled braidoid diagrams are related to each other by a finite sequence of L-moves and braidoid isotopy moves.*

7 Applications

7.1 Applications to the Study of Proteins

The correspondence of line isotopy classes of open space curves and isotopy classes of planar knotoids suggests that a topological analysis of linear physical structures lying in 3-dimensional space can be done by simulating them by open space curves and by taking their orthogonal projections. Through this idea, knotoids, both in S^2 and $\mathbb{R}^2$, have found important applications in the study of open protein chains [10] (see Fig. 17 for an example), as well as of open protein chains with chemical bonds via introducing the notion of *bonded knotoids* [11]. In these papers, open protein chains are studied via their projections into planes. The corresponding knotoid classes are considered in the 2-sphere and in the plane, and they are classified by using the (normalized) bracket polynomial and the Turaev's loop bracket polynomial [11, 31], respectively. In Fig. 18 we see three atlases that contain colored regions. Each of these colored regions corresponds to one topological class of the protein 3KZN when it is closed to some knot, and when it is projected to a knotoid, a spherical knotoid and a planar knotoid, respectively. As seen from Fig. 18, the number of colors increases as we go from the knot representation to the planar knotoid representation. By this data, the authors concluded that planar knotoids yield a more refined analysis for understanding the topological structure of open protein chains than knots or spherical knotoids [11]. This is due to the facts that more knotoids close to the same knot and that the classification of knotoids in the plane is more refined than the classification of spherical knotoids. For example a trivial knotoid in S^2 may happen to be a non-trivial knotoid when considered in $\mathbb{R}^2$ as we discussed in Sect. 2.3.
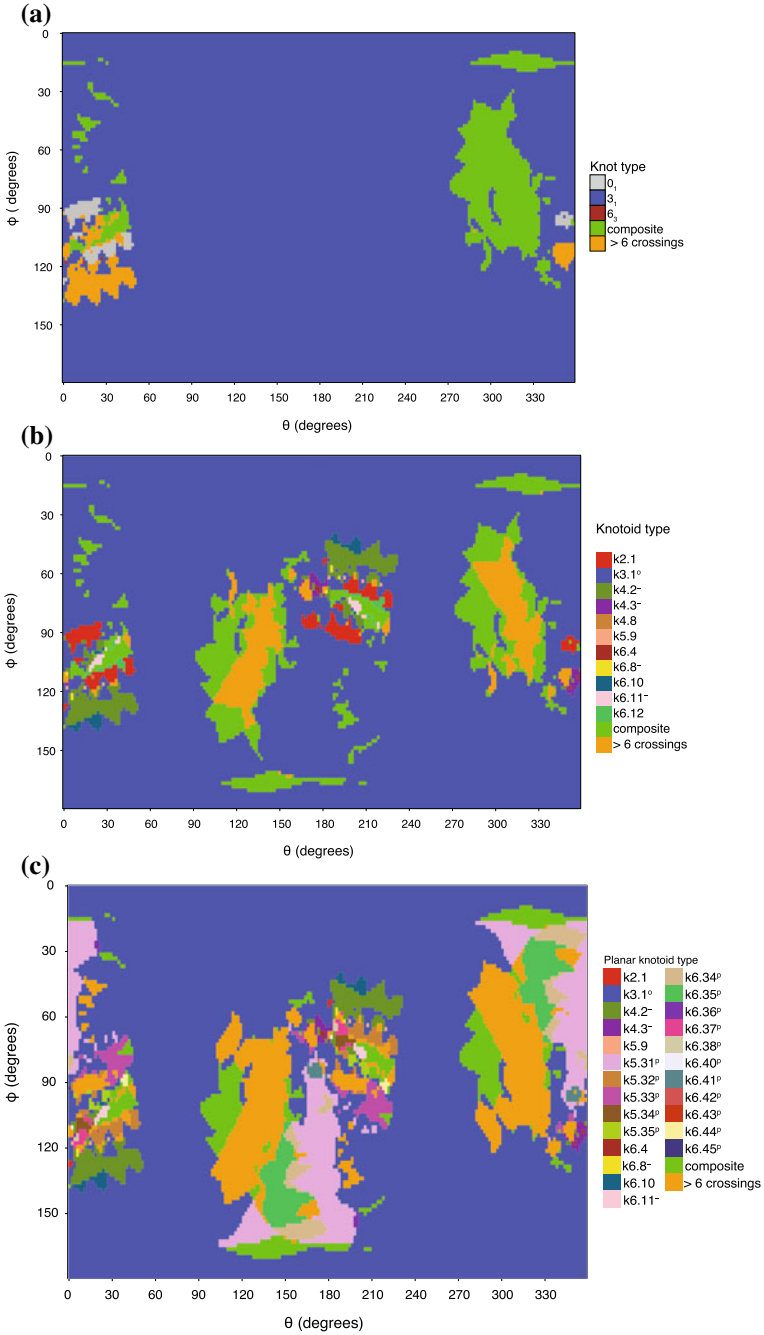
Fig. 18 Atlases showing the topological analysis of 3KZN via knots, spherical knotoids and planar knotoids, image from [11]
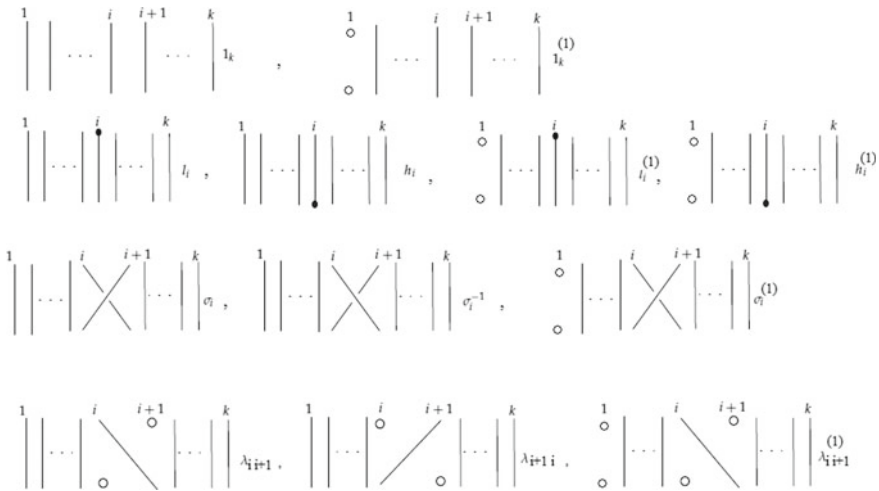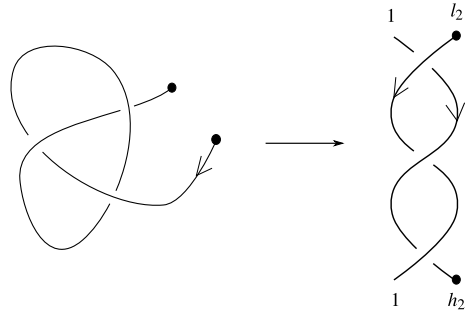
Fig. 19 Elementary k-blocks

7.2 Elementary Blocks and a Proposed Application of Braidoids

As demonstrated in [13, 16], any braidoid diagram can be divided into a finite number of horizontal stripes, each containing one of the blocks that are depicted in Fig. 19. The blocks consist of the classical braid generators, the identity elements containing one endpoint, along with their extensions by the *implicit points*, which are empty nodes put along the vertical direction of the endpoints, and along with the *shifting blocks*, which result from the change of positioning of strands before or after the appearance of an endpoint. A product on the set of elementary n-blocks and relations with respect to this product, induced by the isotopy moves of the braidoid diagrams, is further explored in [13]. Then, any braidoid diagram on n strands can be read, from top to bottom, as a word that corresponds to a combination of finitely many elementary n- or $(n + 1)$-blocks.

Any planar knotoid diagram can be turned into a (labeled) braidoid diagram by Theorem 5, so it can be represented by an expression in terms of elementary blocks. This suggests an algebraic encoding for open protein chains or, in general, for linear polymer chains: they can be projected to planes and the resulting knotoid diagrams can be turned into braidoid diagrams that have algebraic expressions. An example is illustrated in Fig. 20, where the knotoid corresponding to protein 3KZN is turned into a braidoid diagram, which is represented by the word $l_2\sigma_1^3 h_2$ in elementary blocks.

Fig. 20 The knotoid of the protein 3KZN and a corresponding braidoid diagram with algebraic expression $l_2\sigma_1^3 h_2$

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