UNIVERSITA' DEGLI STUDI DI CAMERINO

SCUOLA DI SCIENZE E TECNOLOGIE

CORSO DI LAUREA IN MATHEMATICS AND APPLICATIONS (CLASSE LM-40)

Knotoids

Master Thesis in Topology

Relatore

Prof. Riccardo Piergallini

Laureanda

Ilaria Capozucca

Anno Accademico 2020-2021

Alla mia famiglia
presente e futura

Contents

Introduction

The term 'knot' is part of everyday life, like the knot of the shoes, the knot of the tie and many others, but a 'mathematical knot' is different because its ends are joined so that it cannot be untied.
The theory of knots is a branch of geometry, in particular of topology, whose main purpose is to study the topological properties of a closed curve in Euclidean space.
The first to approach such a theory were Vandermonde and Gauss in the second half of the eighteenth century but the most rigorous approach was in 1860, thanks to an idea of the Irish physicist Lord Kelvin, who hypothesized that matter was made up of atoms − vortices (or eddies), i.e. that the elements are knots in the 'ether'. This hypothesis prompted his collaborator, the English physicist Tait, to engage in the classification of knots and in the search for a relationship between the classes of equivalent knots and the types of atoms. Each element of the periodic table had assigned a knot type.
From the point of view of Physics, Kelvin and Tait were on the wrong track, in fact the theories that used an ether (i.e. a substance that fills the space and which is necessary for the propagation of electromagnetic waves) have become obsolete. Instead from the point of view of Mathematics they had discovered a new research topic that is still evolving today. The theory of knots gained new life only in 1900, when its potential was understood as a tool that can also be applied in other scientific fields such as Physics and Biology. In particular, the mathematical knot theory was used to study knots in the protein chains.
In the last twenty-five years numerous studies have revealed that there are proteins whose main chain fold into non-trivial topologies and there is the presence of knots in their conformation.
The precise nature of the structural and functional advantages created by the presence of knots in the protein backbone is a subject of high interest from both experimental and theoretical point of view and to better understand this open problem, several attempts have been made towards the characterization and classification of the protein chains based on their knot type. This

characterization required the accepting that linear chains can be knotted. If we pull the ends of a given strand of string we can decide whether it is knotted or not. Because we hold the ends, the string and our body form a closed circle and there is no danger of untying the knot as it is pulled. In knot theory, any open arc (indipendently of the degree of entanglement) is topologically equivalent to a straight line, since it can be continuously deformed to a straight line.
Proteins in their native folded structure are frequently quite rigid and a continuous deformation from protein chain to a straight line is not allowed. So the analysis of their knottedness is done for their open chains with fixed geometry. Until recently, the characterization of knottedness of proteins required closure of protein chains since available knot invariants could only make sense for closed curves but now we can study the knottedness of protein for open curves, using knotoid invariants.
The theory of knotoids is recent and it was introduced by Vladimir Turaev in 2012.
The purpose of this thesis is to study theory of knotoids that is a generalization of the theory of knots. We will describe the polynomial invariants of knotoids that are currently used to analyze the topology of open protein chains. Namely, the Jones polynomial, the Turaev loop bracket polynomial, the arrow polynomial and the loop arrow polynomia.
Afterwords it will be seen why the planar knotoids provide a more detailed overview of the topology of an open chain compared to knots and to knotoids on the sphere.
Finally, we will describe how the knotoid approach is used to analyse knottedness of entire protein chains and of their all possible subchains.

Chapter 1

Hints of knot theory

1.1 Some definitions

Definition 1.1.1. A *knot* $K \subset \mathbb{R}$ is a closed simple curve in the space $\mathbb{R}^3$, that is, any topological subspace of $\mathbb{R}^3$, topologically equivalent to the circumference S^1.
The circumference, therefore, is also a knot and it is called *trivial knot*. Recall that two topological spaces are said to be topologically equivalent if there is a homeomorphism, that is, a one-to-one function, continuous and with a continuous inverse, which sends one onto the other.

The disjoint union of n knots is called *n-components link* (n-link) or *link*.

Definition 1.1.2. Two countinuous applications $f, g : X \to Y$ between topological spaces are *homotopic* if there exists a family of countinuous applications $h_t : X \to Y$ which depend in continuous way of the parameter

$t \in [0,1]$, such that $h_0 = f$ and $h_1 = g$. It is therefore required that the application be continuous $H : X \times [0,1] \to Y$ is defined $H(x,t) = h_t(x)$ for every $(x,t) \in X \times [0;1]$.
H is called *homotopy* between f and g

Definition 1.1.3. Two continuous applications $f, g : S \to S$ of a topological space S are isotopic if there exist a homotopy H between f and $g$such that $h_t : S \to S$ is a topological transformation for every $t \in [0,1]$.
In this case H is called *isotopy* between f and g. Moreover, if f is the identity of S, then we say that $g : S \to S$ is realisible by isotopy.

Definition 1.1.4. Two knots K_1 e K_2 are *equivalent* if there exists a homeomorphism $h : \mathbb{R}^3 \to \mathbb{R}^3$ such that $h(K_1) = K_2$.

Definition 1.1.5. Two knots K_1 e K_2 are *isotopically equivalent* if there exists a homeomorphism of $\mathbb{R}^3 \to \mathbb{R}^3$ isotopic to the identity such that $h(K_1) = K_2$. In this case we write $K_1 \equiv K_2$

Example

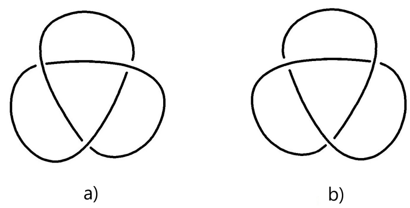
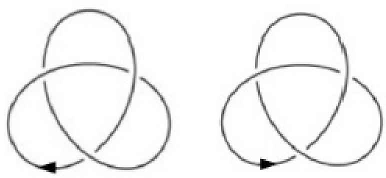


Figure 1.1: The right-handed trefoil knot a) is equivalent to the left-handed trefoil knot b) but it is not isotopically equivalent to it (there not exists a continuous deformation from a) to b)). The equivalence is realized only with a homeomorphism that inverts the orientation.

Definition 1.1.6. An *oriented knot* is a knot with a specified orientation. Similarly, we define an oriented link as a link with a specified orientation on each component.



Definition 1.1.7. A knot K isotopic to its symmetric is called an *achiral* knot, i.e. if $K \equiv \sigma(K)$ where σ is a reflection. Otherwise it is called a *chiral* knot.
For example the trefoil knot is chiral.

Definition 1.1.8. A link $K \subset \mathbb{R}^3$ is called
trivial if it is isotopic to a the disjoint union of copies of S^1, i.e. it is possible to deform the knot so as to obtain a finite number of circumferences in the plane

$$K \equiv S^1 \sqcup ... \sqcup S^1 \subset \mathbb{R}^2;$$

symmetric if it is isotopic to a mirror reflection

$$K \equiv \bar{K} = \sigma(K), \text{ where } \sigma \text{ is a reflection;}$$

invertible if it is isotopic at the same knot with the opposite orientation

$$K \equiv -K.$$

1.2 Knots and their diagrams

Given a knot K, we choose a direction v in space and a plane perpendicular to it on which we draw an orthogonal projection $\pi(K)$ of the knot.
The orthogonal projection in $\mathbb{R}^2$ satisfies the following properties:

- no more than two distinct points are projected in the same point;
- the projections of the two strands in each double point must not be tangent
- the projection is a regular map, i.e there is not vertical tangency;

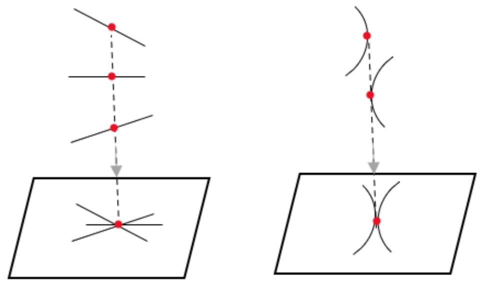


Figure 1.2: Unacceptable situations

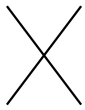
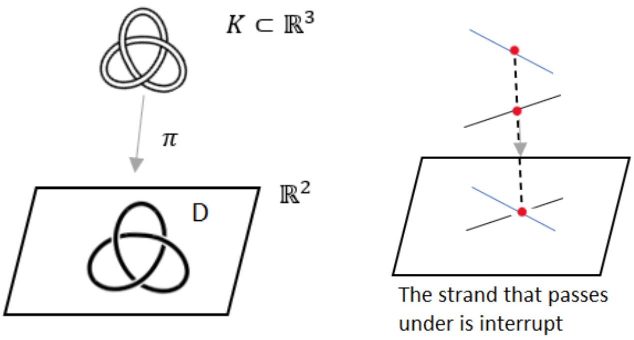


Figure 1.3: Double point

Definition 1.2.1. A diagram $D \in$ of a knot $K \subset \mathbb{R}^3$ is a projection into a plane with the over/under crossing data at each double point.



Theorem 1 (Redeimester's Theorem)**.** *Two diagrams in $\mathbb{R}^2$ represent isotopically equivalent links if and only if they can be obtained one from the other by a finite sequence of planar isotopies and Reidemeister moves. These moves, or local changes, allow us to vary a small portion of the diagram while leaving the rest unchanged.*

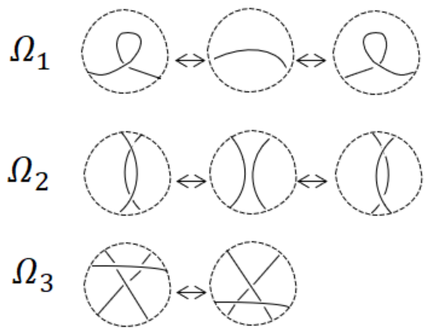


Figure 1.4: Reidemeister moves
Ω_1 adds/removes a curl
Ω_2 overlaps one strand to another
Ω_3 allows the passage of a strand over a crossing

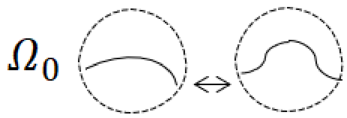
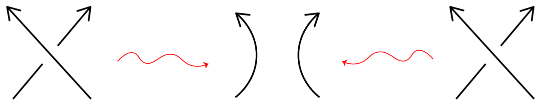


Figure 1.5: Planar isotopy

Definition 1.2.2. The construction of a **Seifert surface** of a knot k^* in S^3 from a knot diagram D of k^*. Every crossing of D admits a unique smoothing compatible with the orientation of k^*.



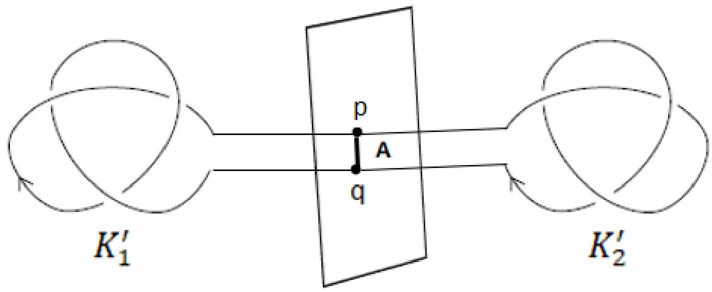
Applying these smoothings to all crossings of D and we obtain a closed oriented 1-manifold $\tilde{D} \subset S^2$. This $\tilde{D}$ consists of disjoint simple closed curves and bounds a system of disjoint disks in S^3 lying above S^2. These disks together with half-twisted strips at the crossings form a compact connected orientable surface S in S^3 bounded by k^*.

The genus of this surface S is equal to $g(S) = \dfrac{c(D) - |\tilde{D}| + 1}{2}$ where $c(D)$ is the number of crossings of D and $|\tilde{D}|$ is the number of components of $\tilde{D}$.
This gives us an estimate from above for the Seifert genus of k^*:
$g(k^*) \leq \dfrac{c(D) - |\tilde{D}| + 1}{2}$

1.3 Connected sum of knots

Definition 1.3.1. Given K_1,$K_2 \subset \mathbb{R}^3$ knots. We produce an other knot K starting from K_1,K_2 doing the **connected sum** of these knots, as follows. We consider $K_i' \equiv K_i$ with K_1' and K_2' separated by a plane except a common arc A=$K_1' \cap K_2'$ in the plane. Then we define:

$$K \equiv K_1 \# K_2 = \mathrm{Cl}(K_1 \cup K_2 - A)$$



The connected sum is **well defined** up to isotopy. In fact, it does not matter K_1' and K_2' are chosen. The arcs on the plane are all equivalent then we can assume A to be a segment.
The connected sum is **commutative and associative**.

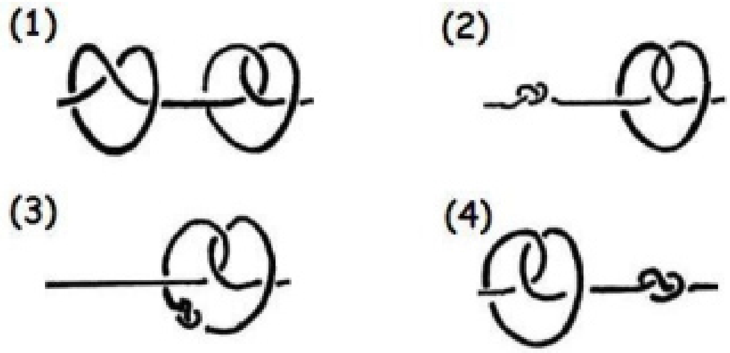
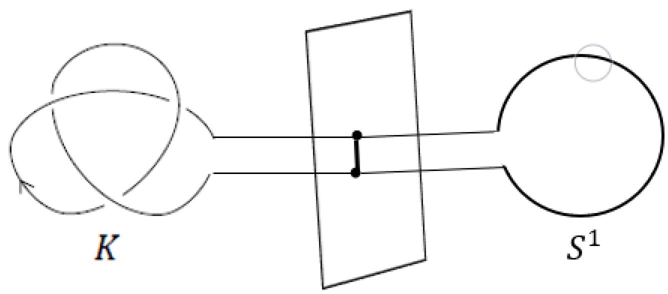


Figure 1.6: Commutative property

$K_1 \# K_2$ has as neutral element the circumference S^1

$$K \# S^1 \equiv K$$

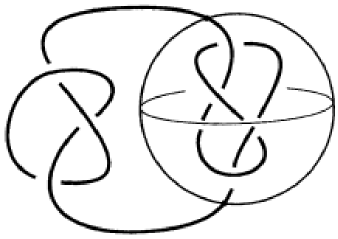


We can contract the circunference at an arc and we obtain K.

In other words the connect sum of two knots is given by: $K \equiv K_1 \# K_2$ if and only if there exists a sphere $S \subset \mathbb{R}^3$ such that $K \cap S = \{p, q\}$

$$K_1 \equiv (K \cap I(S)) \cup A$$
$$K_2 \equiv (K \cap E(S)) \cup A$$

where $A \subset S$ is an arc between p and q, $I(S)$ is the interior of S and $E(S)$ is the exterior of S.



Definition 1.3.2. $K \subset \mathbb{R}^3$ knot is **prime** if any time that we write K as connected sum $K \equiv K_1 \# K_2$, K_1 or K_2 is trivial. Otherwise K is **composite**.

1.4 Hints of virtual knot

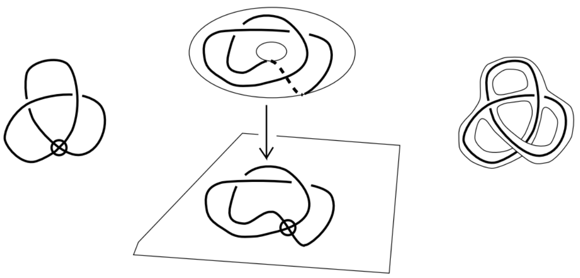


Figure 1.7: Virtual knot representations

Definition 1.4.1. A **virtual knot** in a thickened surface of some genus can be represented by a virtual knot diagram in S^2 or in $\mathbb{R}^2$ that contains a finite number of classical crossings and virtual corssings.
A **virtual crossing** is neither an over-crossing nor an under-crossing and it is indicated by a small circle placed around a crossing point as shown in Figure 1.8. The arcs containing a virtual crossing correspond to arcs of the virtual knot one of which lies at the front of a handle and the other lies at the back of the same handle of the thickened surface. The moves on virtual knot diagrams are generated by the Reidemeister moves (Figure **??**) plus the **detour move**. The detour move allows a segment with consecutive sequence of virtual crossings to be excised and replaced any other such a segment with a consecutive virtual crossings as shown in Figure 1.10. Two virtual knot diagrams are virtually equivalent if they can be related to each other by a finite sequence of the Reidemeister and detour moves. A virtual knot is a virtual equivalence class of virtual knot diagrams.

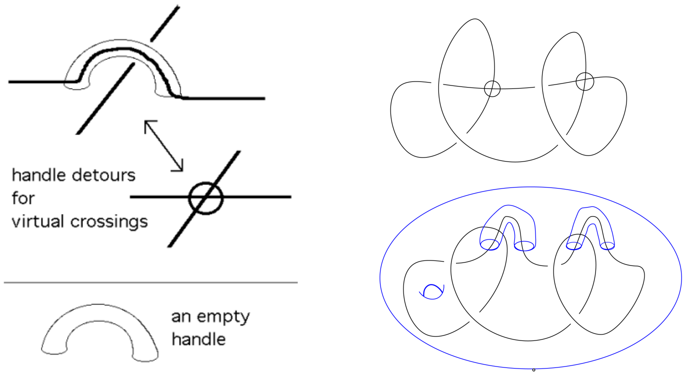


Figure 1.8: Handle detours for virtual crossings

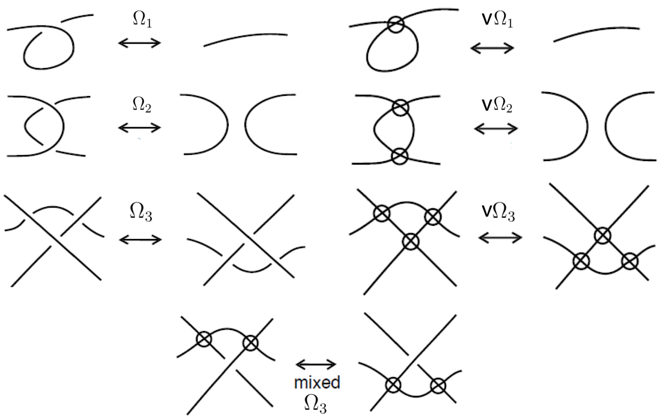


Figure 1.9: Reidemeister moves

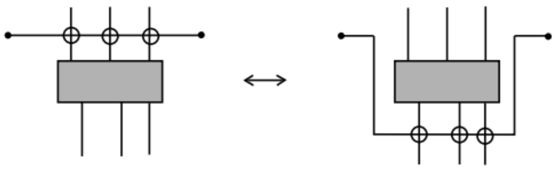


Figure 1.10: Detour move

Chapter 2

Knotoids

Knotoids were first introduced by Vladimir Turaev in 2021 as a generalisation of knots in S^3.
The main purpose of knotoids is to deal with the problem of defining and classifying knottiness for open curves.

2.1 Preliminary definitions

Definition 2.1.1. A **knotoid diagram** K in a surface $\Sigma = \mathbb{R}^2$ *or* S^2 is a generic immersion of the interval $[0, 1]$ in Σ with finitely many transverse double points endowed with over/undercrossing data.
A double point of the diagram is called *classical crossing.*
The images of the points 0 and 1 are called *tail* and *head* respectively, and denoted by v_0 and v_1, moreover they are the *endpoints* of the diagram.
These two points are distinct from each other and from each other point.
Knotoid diagrams are oriented from the tail to the head.

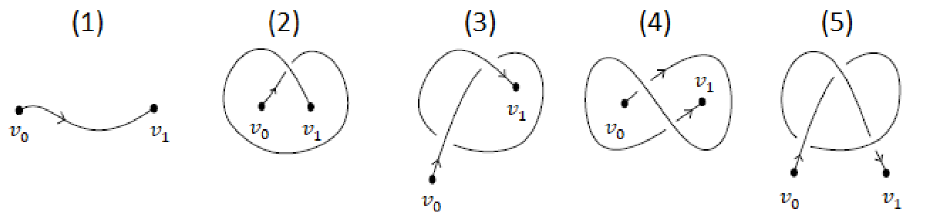


Figure 2.1: Examples of knotoids diagrams

The *trivial knotoid* diagram is an embedding of the unit interval into S^2 or $\mathbb{R}^2$. It is depicted by an arc without any crossings as shown in Figure (1).

Definition 2.1.2. A **multi-knotoid diagram** in an oriented surface Σ is a generic immersion of a single oriented segment and a number of oriented circles in Σ endowed with under/over-crossing data.

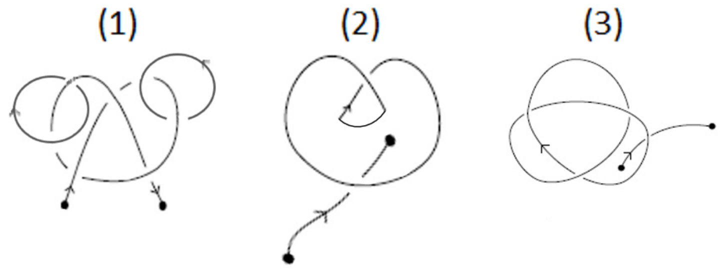


Figure 2.2: Examples of multi-knotoids diagrams

Definition 2.1.3. Two knotoid (or multi-knotoid) diagrams are *(isotopically) equivalent* if they may be obtained from each other by a finite sequence of isotopies and the Reidemeister moves. See Figure 1.2

Definition 2.1.4. There are two **forbidden moves** Ω_- and Ω_+ that pull the strand adjacent to an endpoit (tail or head) under or over a trasversal strands.

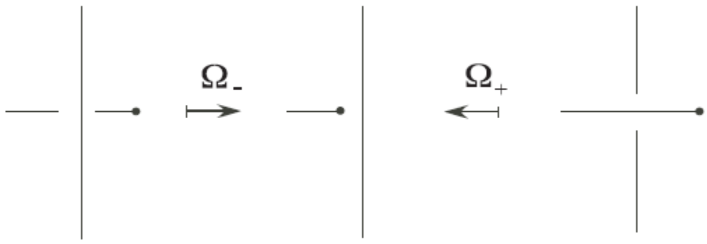
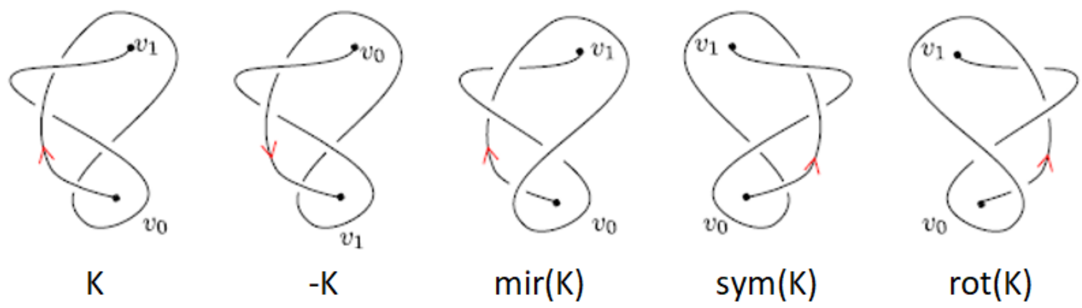


Figure 2.3: Forbidden moves

Notice that if the moves Ω_- and Ω_+ are allowed, any knotoid diagram in Σ can be turned into the trivial knotoid diagram.

Definition 2.1.5. A **knotoid** (or **multi-knotoid**) is an equivalence class of knotoid (multi-knotoids) diagrams determined by the isotopically equivalence relation.
The set of knotoids in Σ is denoted $\mathcal{K}(\Sigma)$.

Definition 2.1.6. The knotoids admit **involutive operations**:

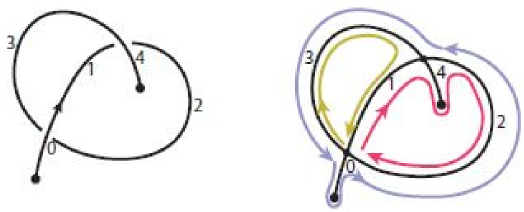


Given a knotoid diagram K:
$-K$ is its **reversion** which consists in changing the orientation of the knotoid diagram (or changing the tail with the head);
mir(K) is its **mirror reflection** that transforms a knotoid into a knotoid represented by the same diagram but with all the crossings changed;
sym(K) is its **symmetric** that reflects a knotoid diagram with respect to the line in $\mathbb{R}^2$ passing through the endpoints;
rot(K) is its **rotation** that is defined as the composition of symmetry and mirror reflection. $\text{rot}(K) = \text{mir}(\text{sym}(K))$

Definition 2.1.7. Local regions of diagrams
If we ignore the over/undercrossing information of a knotoid diagram K, we obtain a *planar graph* with $n + 2$ vertices (n corresponds to the number of crossings of K and 2 correspond at endpoints) and the edges correspond to the arcs of K. This graph G of the knotoid diagram K divides S^2 into $n + 1$ regions.
We label the arcs of the local regions of a diagram in this way:
- we consider G;
- we start from the tail and we lebel it with 0;
- we move along the graph and each time that we meet a crossing, the following arc increases the label by one.
To determinate the local regions of diagram is necessary to do the following:
- we choose a vertex that corresponds to a crossing and we choose an arc that is connected to that vertex;
- we move in a clockwise way and we follow the closed path on the graph that loops back to the chosen arc.
Note that each arc is adjacent to two local regions, except the two arcs that

are directly connected to an endpoint.
For example, the following diagram has $n = 2$ crossings than we have $2 + 1$ local regions, in fact:

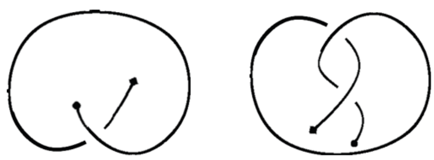
$$r_1 : \ 0, 2, 3$$
$$r_2 : \ 1, 4, 2$$
$$r_3 : \ 3, 1$$



2.2 Differences between planar and spherical knotoids

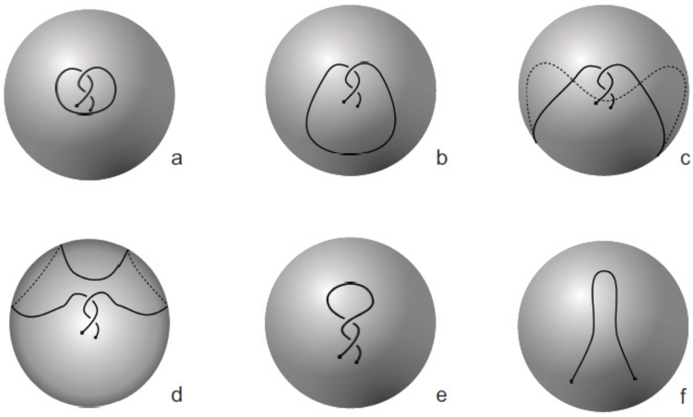
We mostly focus on the case $\Sigma = S^2$ or $\mathbb{R}^2$.
The set of all knotoids in S^2 is denoted $\mathcal{K}(S^2)$ and we shall call these knotoids **spherical**, while the knotoids **planar** are in $\mathbb{R}^2$ and the their set is $\mathcal{K}(\mathbb{R}^2)$.

The planar knotoids provide a more refined way to classify knotoids beacause there are examples of knotoids that are *non-trivial on the plane* but *become trivial* when they are considered *in* S^2.



(A) (B)

If we consider the nontrivial planar knotoids given in the figure, we can deform the knotoid but we will never have the freedom to move arcs in a way that will unknot the curve withouth violating the forbidden moves.
If we consider the same knotoid in the sphere, it's trivial!



We can take an arc of the knotoid diagram in S^2, push it towards a pole of the sphere, across it and all the way around the surface of S^2, with the application of the Reidemeister move Ω_1 for two times, we obtain the trivial knotoid. (The dotted lines indicate parts of the diagram that are on the back side of the sphere.)

There is an application between the two sets of knotoids
$\iota : \mathcal{K}(\mathbb{R}^2) \to \mathcal{K}(S^2)$ that is induced by the inclusion $\mathbb{R}^2 \hookrightarrow S^2 \equiv \mathbb{R}^2 \cup \infty$.
The map ι is surjective but not injective. Indeed, for example, the knotoids (A) and (B) are equivalent in S^2 but not in $\mathbb{R}^2$.

2.2.1 Knotoids and knot theory

Definition 2.2.1. Given a knotoid diagram K, one way to obtain a knot diagram is to connect the endpoints of K by an arc which goes under (or over) each strand of the diagram that it meets. This arc is called a shortcut of K.
The knot diagram obtained by connecting the endpoints of K with a shortcut is called an underpass closure (or overpass closure) of K. These operations induce well defined maps:

$$\omega_{\pm} : \{Knotoids\} \to \{Knots\}$$

ω_- is the *underpass closure map* while ω_+ is the *overpass closure map*
We can indicate the knot diagram obteined by overpass(or underpass) closure by K_+ and K_-, respectively.

Remark 2.2.1. The overpass closure and the underpass closure of a knotoid diagram may give rise to non-isotopic knots.

For example:

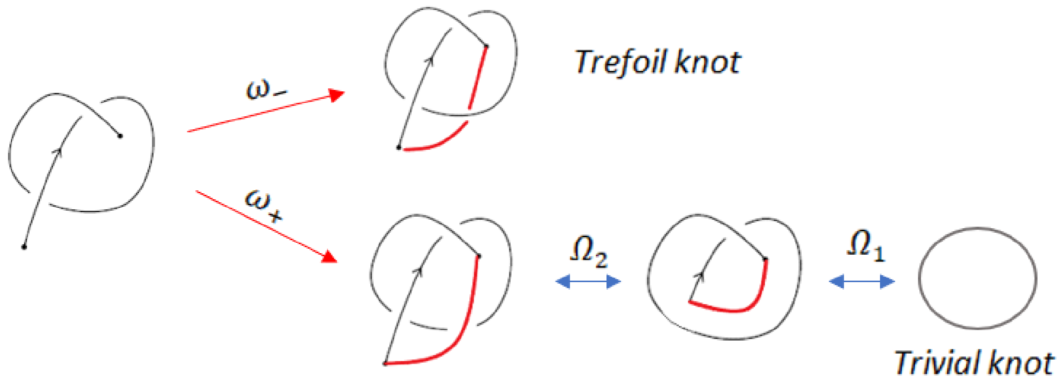


Figure 2.4: Example of overpass-underpass closure

Definition 2.2.2. Every classical knot can be represented by a knotoid diagram in S^2.
Let k^* be a knot in $\mathbb{R}^3$. We take an oriented diagram D of k^* in S^2. By cutting out an arc from D that doesn't contains crossing or that contains only crossing which are overcrossing (or undercrossing). Then we obtain a knotoid diagram.

Remark 2.2.2. By cutting out different arcs of the knot diagram D we may obtained non-equivalent knotoid diagrams.

For example

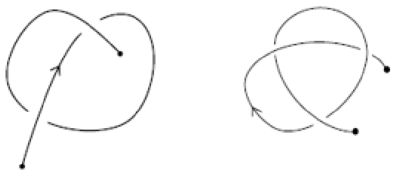


Figure 2.5: The images under ω_- of the two knotoids are both trefoil knot but the knotoids diagrams are not equivalent

Definition 2.2.3. Spherical knotoids extending classical knot theory There is an injective map:

$$\alpha : \text{Classical knots}_{/\langle\Omega_1,\Omega_2,\Omega_3\rangle} \to \text{Knotoids in } S^2$$

$\langle\Omega_1, \Omega_2, \Omega_3\rangle$ denotes the equivalence relation generated by the Reidemeister moves.
We consider an oriented knot diagram D in S^2, representing a classical knot k^*. The map α assigns to D the knotoid diagram in S^2 obtained by deleting an arc a of D which does not contain any crossings.
Then $K = D - a$ is a knotoid diagram in S^2 representing $k \in \mathcal{K}(S^2)$.
Therefore the map α is well-defined.
The diagram K may depend on the choice of a but the knotoid k does not depend on this choice: when a is pulled along D under (respectively over) a crossing of D, our procedure yields an equivalent knotoid diagram. The equivalence is achieved by pushing the strand of D transversal to a at the crossing in question over (respectively under) D towards ∞, then across ∞, and finally back over (respectively under) D from the other side of a. (This application expands as a composition of isotopies, moves $\Omega_2^{\pm 1}$, $\Omega_3^{\pm 1}$ and, at the very end, two moves Ω_1^{-1}).
That k does not depend on the choice od D is clear because for any Reidemeister move on D or a local isotopy of D, we can choose the arc a outside the disk where this move/isotopy modifies D.
For the injectivity of α, it is sufficient to see that underpass and overpass closures of any knotoid that is in the image of the map α, are equivalent knot diagrams.
A knotoid in S^2 that is in the image of α, is called a **knot-type knotoid** and it has both endpoints in the same region of its representative diagram.
A knotoid that is not in the image of α, is called a **proper knotoid** and the endpoints can be in any local region of its representative diagram.
The set of knotoids, $\mathcal{K}(S^2)$ can be regarded as the union of the set of knot-type knotoids and the set of proper knotoids.
If we consider the Figure 2.1 in S^2, the examples of knot-type knotoid diagrams are (1),(2),(5), and (3),(4) illustrate some examples of proper knotoid diagrams.

Remark 2.2.3. There is a 1-1 corrispondece between knot-type knotoids and classical knots, induced by the operation of closing the endpoints.

Definition 2.2.4. The *height* (or the complexity) of a knotoid diagram $K \subset S^2$ is the minimum number of crossings that a shortcut creates during the underpass closure. The height of a knotoid $k \in \mathcal{K}(S^2)$ is the minimum of the

heights of the diagrams of k and it is denoted by $h(k)$.
A knotoid in S^2 is of knot-type if and only if its height is zero or equivalently a knotoid in S^2 has nonzero height if and only it is a proper knotoid.

Definition 2.2.5. A **knotoid diagram** in $\mathbb{R}^2$ is said to be **normal** if its tail v_0 lies in the outermost region (the unbounded one) of the diagram. Any knotoid diagram in S^2 is in correspondence with normal knotoid diagram.

Definition 2.2.6. It is possible to connect the endpoints of a knotoid diagram in S^2 in the virtual fashion, this induces a well defined map from the set of classical knots to the set of virtual knots of genus at most 1. This map is called the **virtual closure map** and is denoted by $\bar{v}$. The endpoints of a knotoid diagram can be connected with an embedded arc in S^2 but this time a virtual crossing is created every time the connection arc crosses a strand of the diagram. The resulting virtual knot diagram can be represented in a torus by attaching a 1-handle to S^2 which holds the connection arc.

$$\bar{v} : \{Knotoids\ in\ S^2\} \to \{Virtual\ knots\ of\ genus \leq 1\}$$

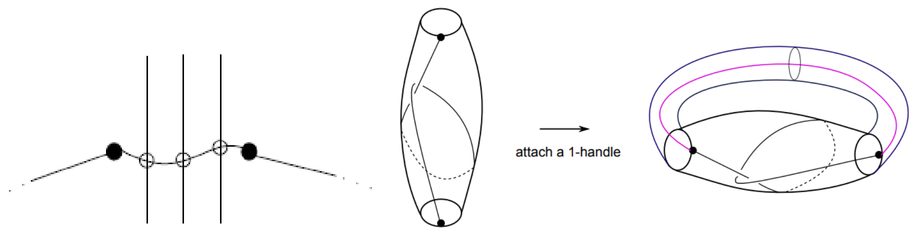
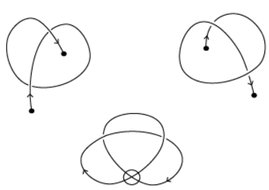


Figure 2.6: The virtual closure of a knotoid diagram

The virtual knot assigned to a knotoid K in S^2 via the virtual closure map is called the virtual closure of K, and is denoted by $\bar{v}(K)$.
An example of a pair of knotoid diagrams K_1, K_2, whose virtual closures are the same virtual knot.



We have already seen that the underpass closure of K_1 is the trefoil knot,

and the underpass closure of K_2 is the unknot (in Figure 2.4).
K_1 and K_2 are two non-equivalent knotoid diagrams, and so, the virtual closure map is not an injective map.

Remark 2.2.4. The virtual closure of a knot-type knotoid is a classical knot. It follows from Korablev and May [6] that the virtual closure will produce a genus 0 knot only if the knotoid is of knot-type, i.e. only if the knotoid has height 0.

2.3 Multiplication of knotoids

Multiplication of knotoids is the analogue for connected sum of knots.

Definition 2.3.1. Each endpoint of a knotoid diagram K in S^2 admits a 2-disk (a neighbourhood) D such that K intersect D precisely along one arc of D, i.e. a radius of D.
Given two diagrams K_1 and K_2 in S^2 representing the knotoids k_1 and k_2, we consider a 2-disk D_1 on the head v_1 of K_1 and a 2-disk D_2 on the tail v_0 of K_2.
The multiplication of knotoids $k = k_1 \cdot k_2$ is defined as follows.
We glue $S^2 - Int(D_1)$ to $S^2 - Int(D_2)$ through a homeomorphism taking ∂D_1 to ∂D_2 and carrying the single intersection point of $\partial D_1 \cap K_1$ to the single intersection point of $\partial D_2 \cap K_2$. Then $K_1 - Int(D_1)$ meets K_2- Int(D_2) at one point and form a knotoid diagram $K_1 \cdot K_2$ representing the knotoid $k_1 \cdot k_2$ in S^2. Note that the multiplication of spherical knotoids has a clear representation in terms of normal knotoid diagrams.

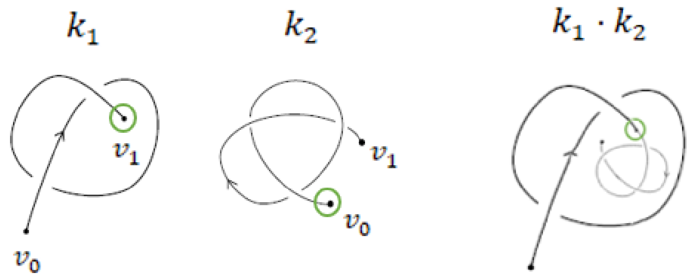


Figure 2.7: Example of multiplication of knotoids

Definition 2.3.2. A knotoid k in $\mathcal{K}(S^2)$ is called *prime* if it is not the trivial knotoid and $k = k_1 \cdot k_2$ implies that either k_1 or k_2 is the trivial knotoid.

2.4 Geometric interpretation of knotoids

2.4.1 Planar knotoids

A knotoid diagram gives rise to a multitude of embedded open curves in the three-dimensional space in the following way.

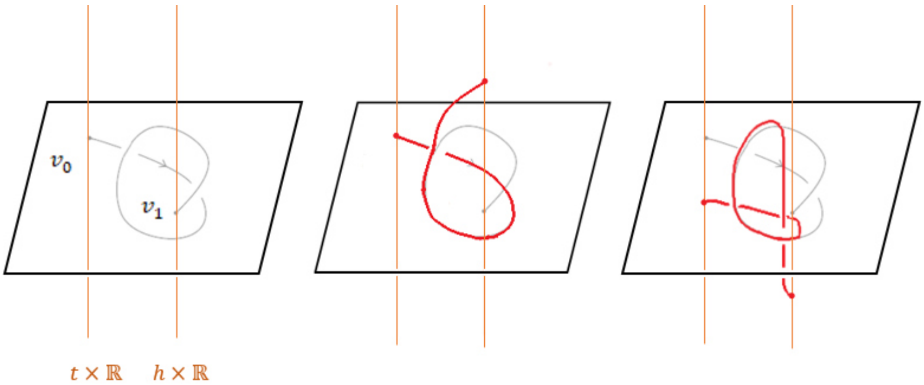


Figure 2.8: Examplex of open curves in the 3-dimensional space (in red) obtained by the knotoid diagram (in gray)

Let K be a knotoid diagram in $\mathbb{R}^2$. The plane of the diagram is identified with $\mathbb{R}^2 \times \{0\} \subset \mathbb{R}^3$.
K can be embedded into $\mathbb{R}^3$ by pushing the overpasses of the diagram into the upper half-space and the underpasses into the lower half-space, while keeping the endpoints attached to the two lines $\{t\} \times \mathbb{R}$ and $\{h\} \times \mathbb{R}$ that pass respectively through the tail and the head, the two lines are perpendicular to the plane of the diagram.
Moving the endpoints of K along these special lines gives rise to open oriented curves embedded in $\mathbb{R}^3$ with the two endpoints constrained to move along these lines.

Definition 2.4.1. Two open oriented curves embedded in $\mathbb{R}^3$ with the endpoints that are attached to two special lines, are said to be **line isotopic** if there is an (ambient) isotopy of the triple $(\mathbb{R}^3, \{t\} \times \mathbb{R}, \{h\} \times \mathbb{R})$, taking one curve to the other curve.

The other way around, let be given an open oriented embedded curve in $\mathbb{R}^3$ with a generic projection to the xy-plane.
The endpoints of the curve determine two lines passing through the endpoints and perpendicular to the plane. The generic projection of the curve

to the xy-plane along the lines with self-intersections endowed with over and under-crossing data, is a *knotoid diagram* in $\mathbb{R}^2$.
A **generic curve with respect to the xy-plane** is a smooth open embedded curve in $\mathbb{R}^3$ that has a generic projection to the xy-plane. Such a curve determines a line isotopy class as described before.

Theorem 2. *Two smooth open oriented curves in $\mathbb{R}^3$ that are generic with respect to the xy-plane are line isotopic with respect to the lines passing through the endpoints of the curves if and only if their generic projections to the xy-plane are equivalent knotoid diagrams, i.e. they are related by Reidemeister moves Ω_i $(i = 1, 2, 3)$ in the plane.*

Proof. Since everything is set in the smooth category, we can switch to the piecewise linear category.
Open curves are defined as piecewise linear curves in $\mathbb{R}^3$, that is, as a union of finitely many edges: $[p_1, p_2]$,...,$[p_{n-1}, p_n]$ such that each edge intersects one or two other edges at the points, p_i , $i = 2, ..., n-1$ and p_1 and p_n are the endpoints of the curve.
We define the triangle move in 3-dimensional space.
Given an open curve with endpoints on the lines, let $[p_i, p_{i+1}]$ be an edge of the curve and p_0 be a point in general position. The edge is transformed to two edges $[p_i$, $p_0]$ and $[p_0$,$p_{i+1}]$ which form a triangle, whenever this triangle is not pierced by another edge of the curve or by the lines.
In other words, a consecutive sequence of two edges may be transformed to one edge by a triangle move.
An ambient isotopy of a piecewise linear curve in the complement of the two lines can be expressed by a finite sequence of triangle moves. By using triangle moves we can subdivide the edges into smaller edges; we can see any triangle move can be factorited into a sequence of smaller triangular moves by subdividing the triangles and the edges accordingly.

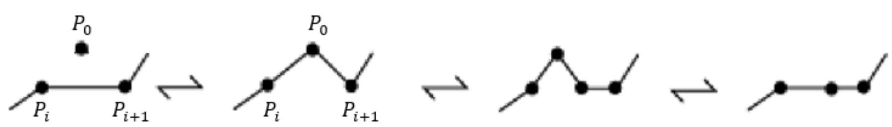


Figure 2.9: Subdivision of an edge

Consider the projection of a curve to the plane, the triangle where a triangular moves takes place is projected to a non-singular triangle.

This triangle can contain many strands which are the projection of other edges.

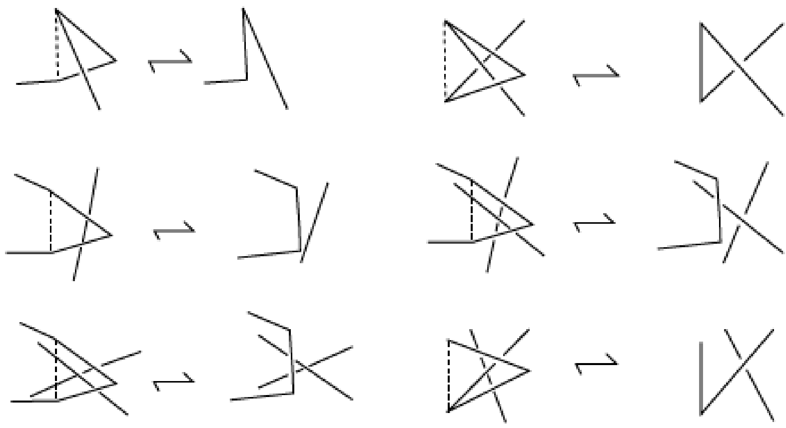


Figure 2.10: The strands in the triangle show that triangle moves are generated by Reidemeister moves. The right side of the figure shows some cases that are finite combinations of Reidemeister moves.

□

2.4.2 Spherical knotoids

In this subsection we present a geometric interpretation introduced by Turaev of spherical knotoids via θ-**curves**.

Definition 2.4.2. A **theta-curve** θ is a graph embedded in S^3 with two vertices v_0 and v_1 (the tail and the head of θ respectively) and three edges e_-, e_0, e_+ each of which joins v_0 to v_1.
Every vertex $v \in \{v_0, v_1\}$ of θ has a closed 3-dimensional ball neighborhood $B \subset S^3$ meeting θ along three radii of B.
B is called a *regular neighnorhood* of v.
The curves

$$\theta_- = e_- \cup e_0 \qquad \theta_0 = e_- \cup e_+ \qquad \theta_+ = e_+ \cup e_0$$

are knots in S^3. We orient θ_- and θ_+ coherently to e_0, while we can choose the orientation of $theta0$.
These knots are called **costituent knots** of θ.
Two θ-curves are *isotopic* if thery are related by an ambient isotopy that preserves the labels $0, 1$ of the vertices an the lables $-, 0, +$ of the edges.
A θ-curve is called **simple** if its constituent knot $\theta_0 = e_- \cup e_+$ is the *trivial knot*. Θ^s is the set of simple labelled θ-curves in S^3.

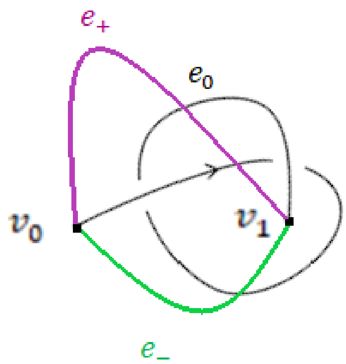


Figure 2.11: An example of a simple θ-curve

In general the set of θ-curves will be denoted by Θ and it has a binary operation called the *vertex multiplication*.

Definition 2.4.3. Vertex multiplication: Given θ-curves θ and θ', pick neighborhoods B and B' of the head of θ and of the leg of θ', respectively. Let us glue the closed 3-balls $S^3 - \text{Int}(B)$ and $S^3 - \text{Int}(B')$ through an orientation-reversing homeomorphism $\partial B \to \partial B'$ carrying the only point of ∂B lying on

the i-th edge of θ to the only point of $\partial B'$ lying on the i-th edge of θ' for $i = -, 0, +$.
The part of θ lying in $S^3 - (B)$ and the part of θ' lying in $S^3 - Int(B')$ meet in 3 points and form a θ-curve in S^3 denoted $\theta\theta'$.

Definition 2.4.4. θ is **standard** θ-curve if:
1) $\theta \subset \mathbb{R}^3$;
2) both vertices of θ lie in $\mathbb{R}^2 = \mathbb{R}^2 \times \{0\}$;
3) the edge e_+ lies in the upper half-space;
4) the edge e_- lies in the lower half-space;
5) e_-, e_+ project bijectively to the same embedded arc $a \subset \mathbb{R}^2$ connecting v_0 and v_1.

Remark 2.4.1. Any simple theta curve $\theta \subset S^3$ is isotopic to a standard theta-curve. To see this, we put θ away from $\infty \in S^3$ so that $\theta \subset R^3$, pick a disk for θ_0 and apply an isotopy this disk to a vertical one.

Theorem 3. *An orientation preserving diffeomorphism $f : S^3 \to S^3$ fixing pointwise an unknotted circle $S \subset S^3$ is isotopic to the identity in the class of diffeomorphisms $S^3 \to S^3$ fixing S pointwise.*

Remark 2.4.2. If two standard theta-curves $\theta, \theta' \subset R^3$ are isotopic, then they are isotopic in the class of standard theta-curves.
Indeed, we can deform θ' in the class of standard theta-curves so that θ and θ' share the same vertices and the same $\pm$-labeled edges.
Let S be the union of these vertices and edges. The set S is an unknotted circle in S^3.
Since θ is isotopic to θ', there is an orientation-preserving diffeomorphism $f : S^3 \to S^3$ carrying θ onto θ' and preserving the labels of the vertices and the edges. Then $f(S) = S$. Deforming f , we can assume that $f|_S = id$.
By the previous theorem, f is isotopic to the identity $id : S^3 \to S^3$ in the class of diffeomorphisms fixing S pointwise. This isotopy induces an isotopy of θ' to θ in the class of standard theta-curves.

2.5 Flat knotoids

Definition 2.5.1. A **flat knotoid diagram FKD** is a diagram in S^2 (or in R^2) with flat crossings and two endpoints that are distinct from each other and from any crossings. The *flat crossings* are the transversal intersections of strands without any under/over-crossing information. Endpoints are named the tail and the head of the diagram.
A FKD is called **trivial** if it has no crossings (i.e. if it is an embedding of [0,1]). A FKD can be viewed as a graph embedded into S^2.
A FKD has two univalent vertices (the endpoints) and all its other vertices (the crossings of the FDK) are 4-valent.
The edges of the graph are called the edges of the FKD. Two edges adjacent to the endpoints are called the **outer edges**.
Given a FKD $F \subset S^2$, connected components of the set $S^2 - F$ are called the **regions** of the FKD F.

Definition 2.5.2. A flat knotoid diagram F is called **prime** if:
(i)Every embedded circle meeting F transversely in exactly two points bounds a disk meeting F along a proper embedded arc or along two disjoint embedded arcs adjacent to the endpoints of F.
(ii) Every embedded circle meeting F transversely in exactly one point bounds a regular neighborhood of one of the endpoints of F.
Examples:

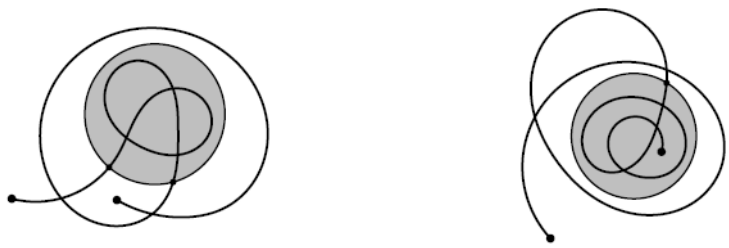


Figure 2.12: Two examples of non-prime FKD. The left FKD does not satisfy condition (i), the right FKD does not satisfy condition (ii)

Definition 2.5.3. Let F be a FKD with a shortcut a (i.e an edge that connects endpoints of F).
A shortcut a is called the **minimal shortcut** of F if the cardinality

$$|\,\mathrm{Int}\, a \cap F| = h(F)$$

where Int a denotes the interior of the shortcut and $h(F)$ is the height of F (see definition 2.2.4).
An edge e of F is called the a-**edge** of F if either e is an outer edge or $e \cap a \neq \emptyset$.
A connected component Δ of the set $S^2 - F$ is called the a-**region** of F if $\Delta \cap a \neq \emptyset$.

Example:

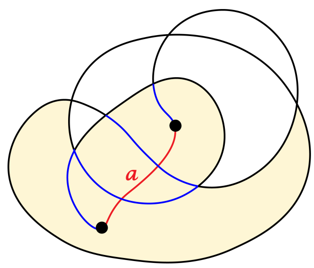
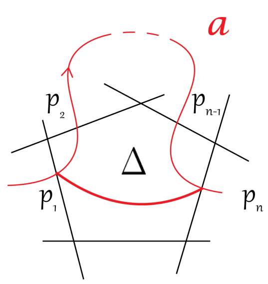


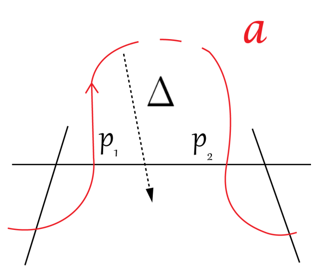
Figure 2.13: FKD with a shortcut a. The a-regions are orange, and the a-edges are drawn in blue

Theorem 4. *Let F be a non-trivial FKD with minimal shortcut a.*
(1) If Δ is a a-region then a intersects $\partial\Delta$ in exactly two points which are inside two distinct a-edges.
(2) If F is prime and both regions adjacent to an edge e are a-regions then e is the a-edge.

Proof. (1) The interior of a shortcut intersects with a FKD transversely in a finite number of points.
By definition of a a-region Δ is connected and $\partial\Delta \subset F$. The number of intersections of a with $\partial\Delta$ is finite and is greater than 1. Let $\partial\Delta \cap a = \{p_1, ..., p_n\}$ where $n \geq 2$ and the points $p_1, ..., p_n$ are numerated in the order in which a passes trought them.
If $n > 2$ the part of a between p_1 and p_n contains at least one intersection with F and this contradicts the minimality of the shortcut a.
In fact, if we replace the part $[p_1, p_n] \subset a$ with a simple arc in Δ that connects p_1 with p_n, then the resulting shortcut has less intersections with F than the initial one.



If $n = 2$, $a \cap \partial\Delta = \{p_1, p_2\}$ and we can show that p_1, p_2 there are not in the same a-edge.
We assume the contrary: there exists an edge e such that $p_1, p_2 \in e$.
If e is an outer edge then p_2 can not be the other endpoint of the edge e because, by definition, a shortcut does not passes through a crossings and, by hypothesis, F is non-trivial. So we can decrease by one the number of intersections of a with F by connecting p_1 with a point immediately after p_2.
If e is not an outer edge then crosses a in different directions (it comes into Δ in p_1 and then goes out in p_2) because otherwise $|a \cap \partial\Delta| \geq 3$. So we can decrease by 2 the number of intersection pushing the arc $[p_1, p_2] \subset a$ from Δ across the edge e.



(2) If the edge e is an outer edge then it is an a-edge by definition.
Let e is not an outer edge. We suppose that e is not a a-edge, i.e. $a \cap e = \emptyset$ and we denote a-regions adjacent to e by Δ_1, Δ_2.
If $\Delta_1 \neq \Delta_2$, the shortcut a is minimal and the regions Δ_1, Δ_2 are a-regions. By assumption, $a \cap e = \emptyset$ hence there exists an a-edge that we called e' such that a-regions adjacent to $e'$are the same Δ_1, Δ_2. Thus Δ_1 and Δ_2 have two different common edges. There exists an embedded circle which intersects F in exactly two points lying inside e and e'. Both disks bounded by the circle contain crossings of F (the endpoints of e and e'). The existence of such a circle contradicts to condition (i) of the definition of prime FKD.
If $\Delta_1 = \Delta_2$, it means that the endpoints of e do not coincide. In this situation

there exists an embedded circle which intersects with F in exactly one point that is in the edge e. Both disks bounded by the circle contain crossings of F (the endpoints of e). The existence of such a circle contradicts to the condition (ii) of the definition of prime FKD. □

Two consequences of the previous theorem:
1) If an edge e of a FKD F with a minimal shortcut a is an a-edge then e is not a loop.
2) The minimal shortcut a of a prime FKD F crosses through a-regions sequentially one-by-one without coming back to already visited regions. If we go from an a-region to the next a-region, a crosses a a-edge that is the only common edge of these two regions.
By the definition 2.2.4 of the height, the interior of a crosses F exactly $h(F)$ times, then there are $h(F)+1$ pairwise distinct a-regions. Each of these a-regions has common edges with two other a-regions, while the first and the last a-regions has common edge with only one other a-region. The first one and the last one coincide for FKD of the height 0. So there is a natural numbering of a-regions of a prime FKD F with fixed minimal shortcut a according to the order in which the shortcut a traverses the regions. $\Delta_0, \Delta_1, ..., \Delta_{h(F)}$ where Δ_0 and $\Delta_(h(F))$ are a-regions adjacent to the beginning and to the end of F.

Definition 2.5.4. Let x is a crossing of FKD F with a shortcut a.
We will say that **the crossing** x **is of the type** n, $0 \leq n \leq 4$, if x is adjacent to exactly n a-edges.
The type of a crossing depends on the choice of a shortcut.
Denote by $c_n(F, a)$ the number of crossings of FKD F having the type n with respect to the shortcut a.

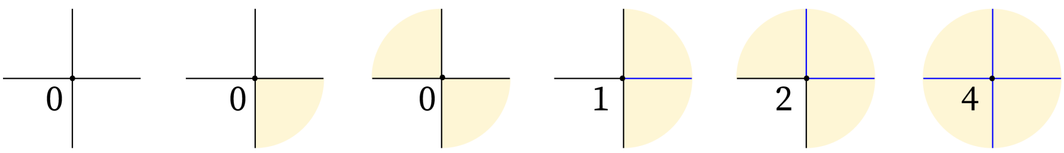
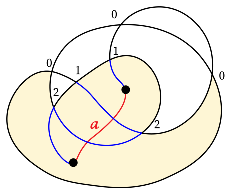


Figure 2.14: All types of crossing neighbourhoods. a-regions are orange and a-edges are drawn in blue

Example:



Lemma 1. If F is a prime FKD with a minimal shortcut a then $c_3(F,a) = c_4(F,a) = 0$.

Proof. Let x be a crossing of F.
We uppose that x is of the type 3, then exactly 3 of edges adjacent to x are a-edges while the fourth edge that we denote by e is not a-edge. By the statement (2) of the theorem 4 at least one of regions adjacent to e is not a a-region.
Hence at least one of regions adjacent to the crossing x is not an a-region and by statement (2) at least 2 of edges adjacent to x are not a-edges, then this contradicts our assumption that x is of the type 3.
We suppose a crossing x is of the type 4, then we denote by e_1, e_2, e_3, e_4 edges adjacent to x; by definition, all these edges are a-edges and none of them is a loop. Put $p_i = a \cap e_i$, $(i = 1, ..., 4)$. Note that in all possible situations we can connect p_1 either with p_3 or with p_4 by an arc not intersecting F.
Hence the shortcut a is not minimal. This contrads the hypothesis of the lemma. □

Theorem 5. *Let F be a prime FKD with a minimal shortcut a.*
Then following inequalities are equivalent:

$$c(F) \geq 2h(F)$$
$$\textit{and}$$
$$c_0(F,a) + 2 \geq c_2(F,a)$$

Proof. By the previous lemma

$$c(F) = c_0(F,a) + c_1(F,a) + c_2(F,a) \qquad (\diamond)$$

and a-edge has distinct endpoints because it is not a loop.
Then the total number of crossings (that are endpoints of a-edges) is equal to $2h(F)+2$, where $2h(F)$ are non-outer a-edges and $+2$ are the outer edges.
We can write:

$$2h(F) + 2 = c_1(F, a) + 2c_2(F, a) \qquad (\star)$$

Now ($\diamond$)-($\star$) gives

$$c(F) - 2h(F) - 2 = c_0(F, a) + c_1(F, a) + c_2(F, a) - c_1(F, a) - 2c_2(F, a)$$

and we get

$$c(F) - 2h(F) - 2 = c_0(F, a) - c_2(F, a).$$

Hence

$$c(F) - 2h(F) = c_0(F, a) - c_2(F, a) + 2$$

where in the left-hand side there is a difference between the left-hand side and the right-hand side of the first inequality of the theorem, while the right-hand there is a difference between the left-hand side and the right-hand side of the second inequality of the theorem. □

Definition 2.5.5. Let F be a FKD, and R_1,R_2 be two of its regions.
$\rho(R_1, R_2)$ is the **distance between two regions**, defined as the minimal number of intersections of a simple arc starting inside R_1, ending inside R_2 and along the way intersecting F transversely in points different from the crossings and the endpoints of F.

Lemma 2. Let F be a prime FKD with a minimal shortcut a, x is an exceptional crossing of the type 0 and Δ_1, Δ_2 are a-regions adjacent to x. Then:

$$\rho(R_1, R_2) = \begin{cases} 1 & \text{if } x \text{ is two-sided} \\ 2 & \text{if } x \text{ is one-sided} \end{cases}$$

Definition 2.5.6. Given a FKD F with a shortcut a. An edge e of F is called the **border edge** if exatly one of the regions adjacent to e is a a-regions. We can to partition the set of border edges into two disjoint subsets: the union of shortcut a with outer edges cuts each a-regions and its boundary into two connected parts, one of them lies to the left and the other lies to the right of the shortcut a; so a border edge e is called **a left boder edge** (resp. a **right border edg**e) if it is contained in the left (resp. the right) part of the boundare of an a-region adjacent to th edge e.
Denoted by R_a the **a-domain of** F which is defined to be the union of all a-regions with the interior of all a-edges and both endpoints of F.
The set $S^2 - R_a$ is the union of all regions which are not a a-regions with all edges which are not a-edges. ∂R_a consists of all border edges.
In the case of prime FKD we can regard ∂R_a as the closed path in F, which goes exactly one time along each border edge. We denote the path by P_a.
From the fact that the union of a with outer edges divides R_a and ∂R_a into

two parts, one of which lies on the left of a while the other one lies on the right, the path can be divided into two parts by two crossings which are connected by outer edges with the endpoints of F.
One of these parts is formed by all left border edges and other one is formed by all right border edges.
A **left** (resp.**right**) **border chain** is defined to be a sequence of the left (resp. the right) border edges, forming a connected subpath of P_a .
Below we denote such a chain by $E = \{e_1, ..., e_n\}$.
A left (resp. right) border chain E is called **true** if the endpoints of E are either of the type 2 or one-sided left (resp. right) exceptional crossing of the type 0.

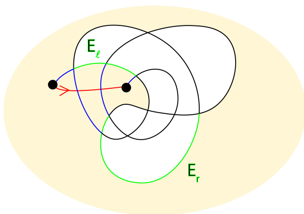


Figure 2.15: All types of crossing neighbourhoods. a-regions are orange, a-edges are drawn in blue, the left border chain E_l and the right border chain E_r of a FKD are green

Definition 2.5.7. A crossing x of the type 0 of a FKD F with a shortcut a is called:
- regular crossing: if at least one of edges adjacent to x is not a border edge;
- exceptional crossing: if all 4 edges adjacent to x are border edges;
- **left** (resp. **right**) **one-sided exceptional crossing**: if all 4 edges adjacent to x are left (resp. the right) border edges;

Lemma 3. Let F be a prime FKD with a shortcut a and E be a true border chain satisfying following conditions:
1. E do not contain a true border chain distinct from E;
2. None of the endpoints of E is adjacent to an outer edge;
3. E passes through not more than 1 two-sided exceptional crossing.
Then E passes through at least 1 regular crossing.

Proof. We omit the proof that is in the reference [12]. □

Remark 2.5.1. Lemma 3 can not be extended directly to border chains of which endpoints are adjacent to outer edges. To do this:

- we consider the crossing x of the type 2, that is adjacent to an outer edge of a FKD,
- we denote a-edges adjacent to x by e_1 and e_2, where e_1 is the outer edge of the FKD. The crossing x is called the **left-sided** (resp. the **right-sided**) **crossing of the type 2**, if starting at x and going along e_2 we arrive from the left (resp. from the right)

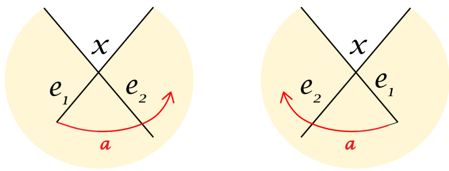


Figure 2.16: Left-sided crossing of the type two (on the left) and right-sided one (on the right)

Lemma 4. Let F be a prime FKD with a shortcut a, and E be a true border chain satisfying following conditions:
1. E do not contain a true border chain distinct from E;
2. If E is a left (resp. right) border chain and an endpoint of E is adjacent to an outer edge of F then the endpoint is a left-sided (resp. right-sided) crossing of the type 2;
3. E passes through no two-sided exceptional crossing.
Then E passes through at least 1 regular crossing.

Proof. Let E be a true left border chain (the proof in the case of the right border chain is completely analogous). Firstly consider the case in which both endpoints of E are adjacent to outer edges of F. We assume E does not pass through a regular crossing and show that it is impossible. By the first condition of Lemma 4, E does not pass through neither a crossing of the type 2 nor a one-sided exceptional crossing. By the third condition E does not pass through two-sided exceptional crossings. Hence all crossings in E except its endpoints are of the type 1.
By hypothesis, both endpoints of E are left-sided crossings of the type 2. Hence the union of E with outer edges of F forms a path, which goes from the beginning of F to its end and crosses the rest part of the diagram transversely. Thus the diagram (which, by definition, is a generic immersion of the segment into S^2) is indeed a generic immersion of a disconnected 1-manifold, i.e. in this case the diagram in question is not a FKD. If both endpoints of E are not adjacent to outer edges, then required property follows from Lemma 3.

So it is remains to consider the case, when exactly one of endpoints (say the beginning) is adjacent to an outer edge of F. Then, by hypothesis, the endpoint is left-sided crossing of the type 2. In such a situation we can use the same trick as in the case of $k = 0$ in the proof of Lemma 3. □

Lemma 5. Let F be a prime FKD with a minimal shortcut a , and E be a left (resp. right) border chain which starts and ends at the same one-sided exceptional left (resp. right) crossing of the type 0. Then
1. E passes through not more than one crossing of the type 2,
2. If E passes through an exceptional crossing of the type 0 distinct from its endpoints, then E passes through the crossing twice.

Proof. We omit the proof. You can find it in the reference [12]. □

2.6 Gauss code

Gauss codes encode the knotoid diagrams in a way that can be easily handled by a computer.
The standard notations for encoding *knotoid diagrams in* S^2 is the **oriented Gauss code**.

$$\text{Gauss code} = (\text{Crossings(or Gauss word)}, \text{Signs})$$

*Crossing*s (or Gauss word): it is a sequence of labels that are assigned to diagram's crossings starting from one end and proceeding to the other. When traveling along the diagram and we meet the crossings to label them we use strictly increasing non-negative integers. Each crossing appears twice, once as an undercrossing and once as an overcrossing. To indicate an undercrossing we add a "$-$" before the label and to indicate an overcrossing we add a "$+$". Therefore the length of this sequence is $2n$, where n is the number of crossings of the diagram.
Signs: it is a sequence of the signs of each of the crossings of the diagram. The length of this sequence is n.

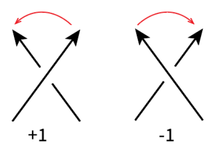


Figure 2.17: Signs of the crossings

A **positive crossing** with sign $+1$: to overlap the arc above the arc below (with the correct orientation) we need to turn counterclockwise.
A **negative crossing** with sign -1: to overlap the arc above the arc below (with the correct orientation) we need to turn clockwise.

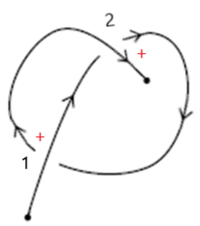


Figure 2.18: Example of Gauss code: $1 -2 -1\ 2 \quad ++$

For *planar knotoids*, we attach to the oriented Gauss code a third piece of information, that is the list of labels of arcs that are adjacent to the outer of the diagram. This part has no fixed lenght.

$$\text{Gauss code} = (\text{Crossings}, \text{Signs}, \text{Outside arcs})$$

The labels are assigned to the arcs by travelling around the diagram and labelling arcs as we meet them. The labelling of the arcs starts from 0 and each time we pass through a crossing it increases by one.

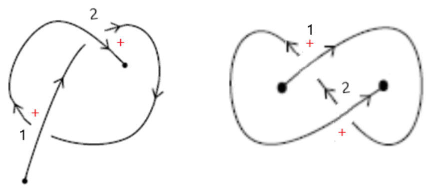


Figure 2.19: Example of planar knotoid diagrams that have the same oriented Gauss code: $1 - 2 - 1\ 2 \quad ++$

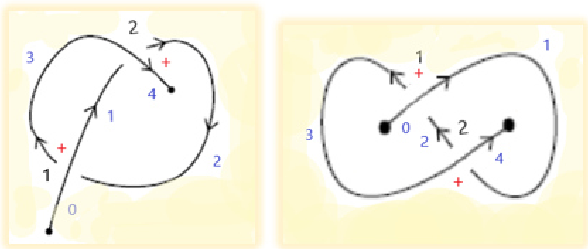


Figure 2.20: The black numbers correspond to the crossings while the blue ones to the arcs. The outer region is in yellow.

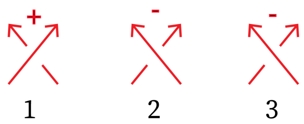
The extended oriented Gauss code of the left knotoid diagram is:
$1 - 2 - 1\ 2 \quad ++ \quad 0\ 2\ 3$.
The extended oriented Gauss code of the right knotoid diagram is:
$1 - 2 - 1\ 2 \quad ++ \quad 1\ 3$

Given a knotoid diagram we get a unique extended oriented Gauss code, by construction.
The extended oriented Gauss code allows the unique encoding of a planar knotoid diagram, up to plane isotopy.

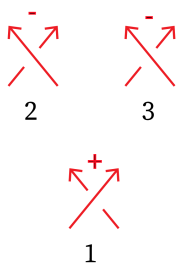
How we can recover the knotoid diagram from the extended oriented Gauss code?
We consider an extended oriented Gauss code, for example:

$$1 -2\ 2\ 3 -1 -3 \quad + - - \quad 2$$

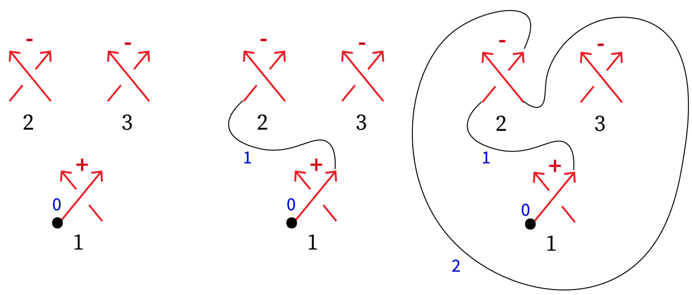
Step 1: We consider the second part of the extended oriented Gauss code: Signs. In this case we have three crossings (the first is positive and the others are negative) and we call these crossings 1 , 2, 3 respectivelly.

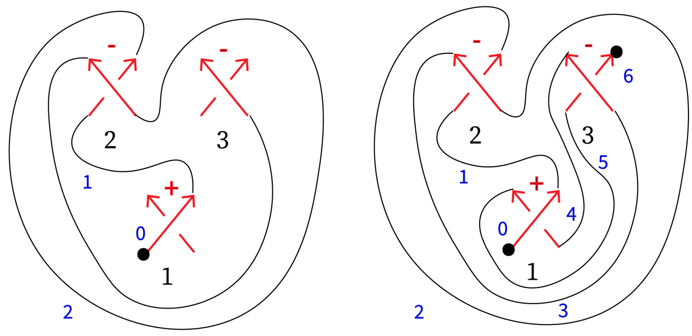


Step 2: We consider the first part of the code: Crossings.
"−" indicates an undercrossing while "+" indicates an overcrossing. So 1 indicates an overcrossing in the crossing 1, after we have −2 an undercrossing in the crossing 2 and so on.
By the first part of code we can see what crossings are adjacent and so they have a common arc.
In the our example we have that: 1 is adjacent to crossings 2 and 3, 2 is adjacent to crossings 3 and 4, 3 is adjacent to crossings 2 and 1.

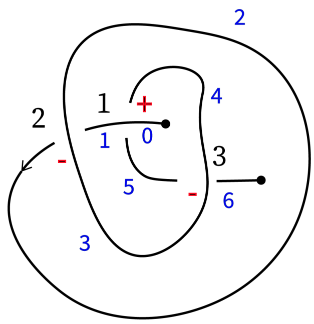


We connect crossings following the first part of code without creating new crossings. The starting point is the tail while the ending point is the head. From the tail to the head we label arcs starting from 0.

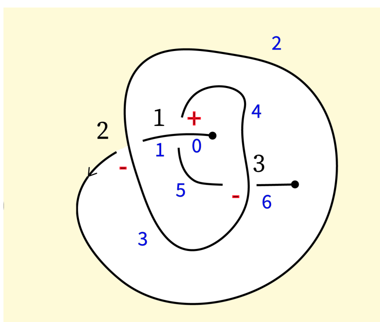




Step 3: By plane isotopy, we can stretching-bending arcs and we can move crossings (all without creating new crossings). Hence :



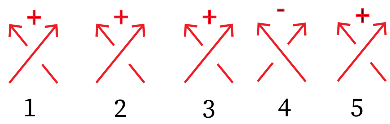
This is the planar knotoid 3_5. (see Appendix B)
Step 4: Now we can control the outside arcs looking the third part of code. The outside arcs are adjacent to the outside region. In the our example is the arc 2.



Another example: We consider the extended oriented Gauss code:

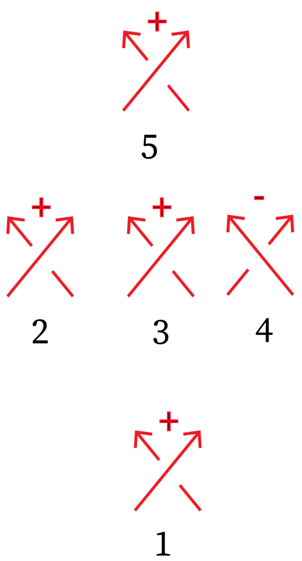
$$1\ -2\ 3\ \ -1\ \ -4\ \ -5\ 2\ \ -3\ 5\ 4\quad + + + - +\quad 0\ 3\ 4\ 5\ 8\ 10$$

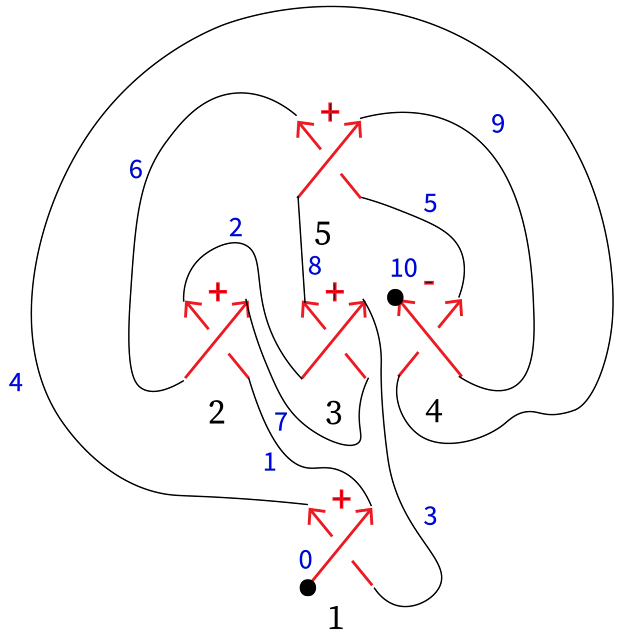
Step 1:



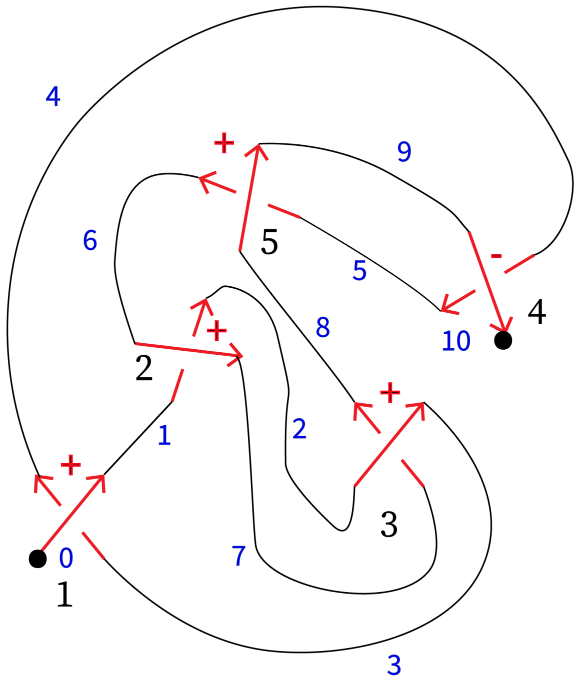
Step 2: By the first part of Gauss code we have that:

1 is adjacent to crossing 2, 3, 4;
2 is adjacent to crossings 1, 3, 5;
3 is adjacent to crossings 1, 2, 5;
4 is adjacent to crossings 1 and 5;
5 is adjacent to crossings 2, 3, 4.

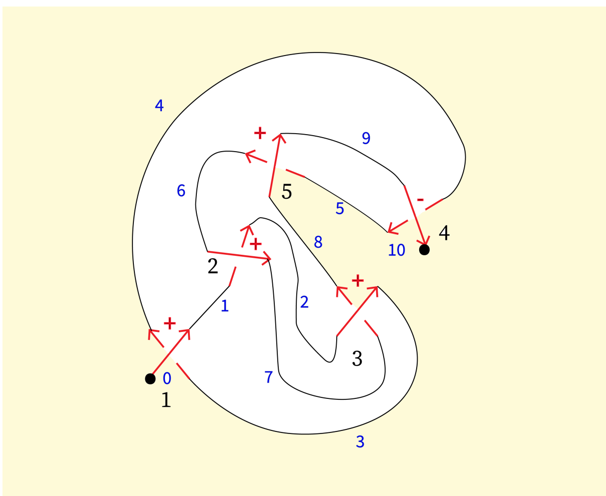




Step 3: By plane isotopy we have:

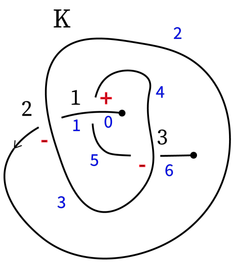


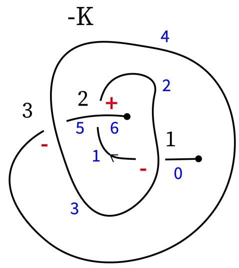
Step 4:



2.6.1 Extended oriented Gauss code and involutions

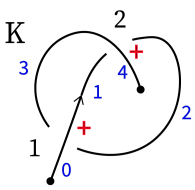
Applying each of the involutions on a knotoid diagram has the following effects on its extended oriented Gauss code.
Reversion: The reversion involution reverses and renumbers the Gauss word and reverses the list of signs. Finally, it reverses and renumbers the list of arcs the are adjacent to the outer region:

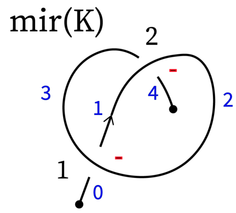




$1 -2\ 2\ 3 -1 -3 \quad + - - \quad 2$ $\qquad$ $-1 -2\ 1\ 3 \ -3\ 2 \quad - + - \quad 4$

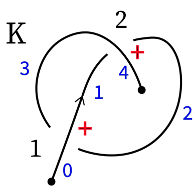
Mirror reflection: The mirror reflection involution changes the under-crossings to over-crossings and the other way around as well as the signs of the crossings in the second part of the extended oriented Gauss code:

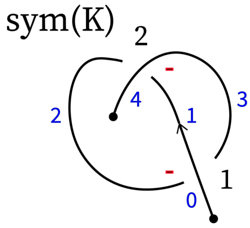




$1 -2 -1\ 2 \quad ++ \quad 0\ 2\ 3$ $\qquad$ $-1\ 2\ 1 \ -2 \quad -- \quad 0\ 2\ 3$

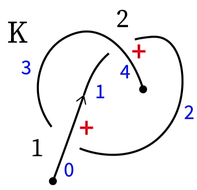
Symmetry: The symmetric involutions changes the signs of the crossings in the extended oriented Gauss code.



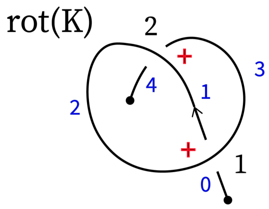


$1 \ -2 -1\ 2 \quad ++ \quad 0\ 2\ 3$ $\qquad$ $1 \ -2 \ -1\ 2 \quad -- \quad 0\ 2\ 3$

Rotation: The rotation involution changes under-crossings to over-crossings and the other way around.



$1\ -2\ -1\ 2\ \ {++}\ \ 0\ 2\ 3$



$-1\ 2\ 1\ -2\ \ {++}\ \ 0\ 2\ 3$

2.6.2 Gauss code and Reidemeister moves

KNOTOID DIAGRAMS IN S^2

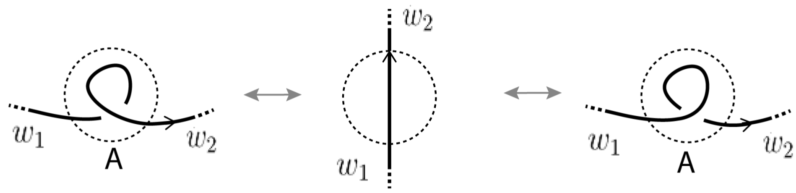
Using the oriented Gauss code, we can encode the application of Reidemeister moves on a knotoid diagram in S^2. We denote with:

- w the Gauss word;
- w_i, $i = 1, 2, ...$ the subword of the Gauss word;
- A, B, C, ... the crossings.

Then, applying or removing Reidemaister moves have the following effects:

(1) Ω_1-move

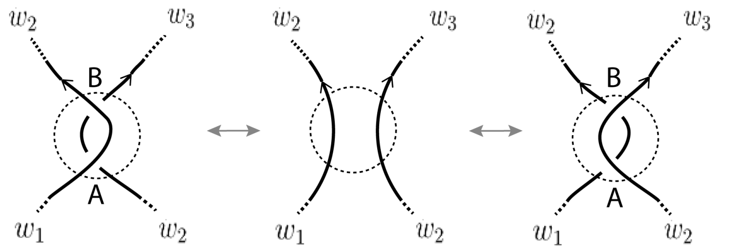
The set of signs: A positive or negative Ω_1-move on an arc, adds or removes a negative or positive crossing.



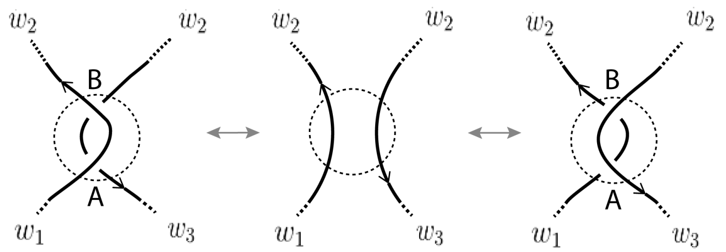
Gauss word $\quad w_1 w_2 \leftrightarrow w_1 \pm A \mp A w_2$

(2) Ω_2-move

There are two cases of Gauss word which depend on the orientation of the arcs that take part in the Ω_2-move.



Gauss word $\quad w_1w_2w_3 \leftrightarrow w_1 \pm A \pm Bw_2 \mp A \mp Bw_3$



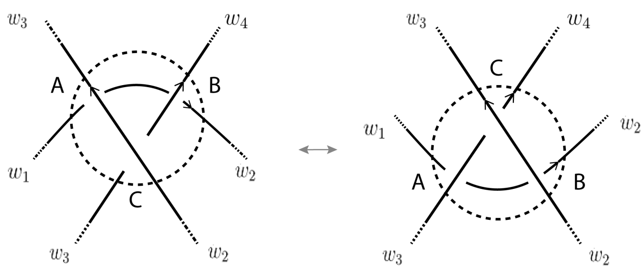
Gauss word $\quad w_1w_2w_3 \leftrightarrow w_1 \pm A \pm Bw_2 \mp B \mp Aw_3$

The set of signs: Ω_2-move adds or removes two consecutive opposing signs.

(3) Ω_3-move

There are different cases of Gauss word which depend on the orientation of the arcs and on the sign of crossings that take part in the Ω_3-move.

One case is:



Gauss word

$$w_1 - A - Bw_2 + C + Aw_3 - C + Bw_4 \leftrightarrow w_1 - A - Bw_2 + B + Cw_3 + A - Cw_4$$

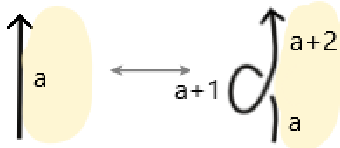
The set of signs: Ω_3-move reorders the set of signs.

KNOTOID DIAGRAMS IN $\mathbb{R}^2$

When performing Reidemeister moves on an extended oriented Gauss code, one must also take into account how the third part of the code is affected by the applied Ω -move; in the case when the arcs involved in the move bound the outer region.

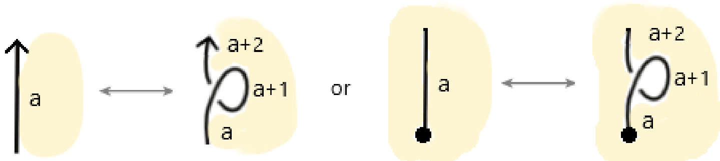
(1) Ω_1**-move** creates or removes a crossing and so divides an arc into three subarcs or unites them into a single arc. After the move the third part of the Gauss code can be:

- The kink that is introduced by the Ω_1-move doesn't touch the outer region (in yellow on the figure) and so the third part, after renumbering the arcs, becomes:



$$..., a, ... \leftrightarrow ..., a, a+2, ...$$

- The kink touches the outer region or an arc that contains an endpoint is involved and so the third part becomes:

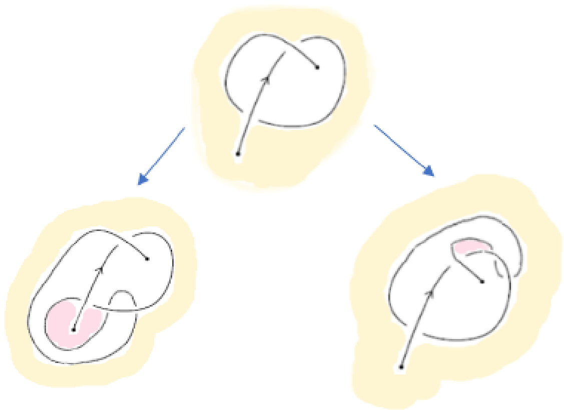


$$..., a, ... \leftrightarrow ..., a, a+1, a+2, ...$$

(2) Ω_2**-move** creates or removes two crossings and so divides each of the two arcs into three subarcs or unites them into the initial two arcs.

Observation

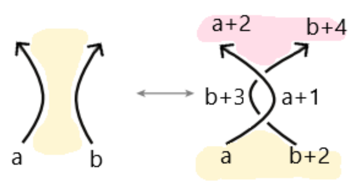
It may happen that when applying the Ω_2 -move two different regions are created, that both can be chosen as the outer region of the knotoid diagram.



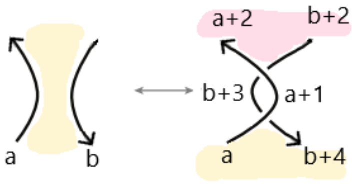
Example of the two different choices for the outside region of a knotoid diagram after an Ω_2-move

The original labels of the arcs following arc a are shifted by ± 2 and the arcs following arc b are shifted by additional ± 2.
For example, assume that the third part of a Gauss code contains the arcs a b c, with $a < b < c$, and that we apply an Ω_2-move between arcs a and b. The new arcs $a+1$ and $a+2$ shift the labels of both of the arcs b and c by 2. The Ω_2-move splits arc b into three subarcs with labels $b+2$, $b+3$ and $b+4$ then the label of c is shifted once more by 2 and therefore the third part of the Gauss code after the application of an Ω_2-move becomes: $a, a+1, a+2, b+2, b+3, b+4, c+4$.
After the Ω_2-move we have the following cases:

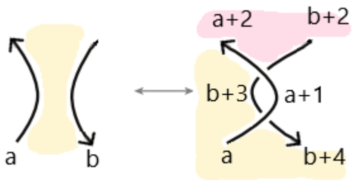
- **Both arcs touch the outer region.**
  - If the arcs are **parallel** we have the following two choices:
    Yellow outer region $..., a, b, ... \leftrightarrow ..., a, b+2, ...$
    Pink outer region $..., a, b, ... \leftrightarrow ..., a+2, b+4, ...$



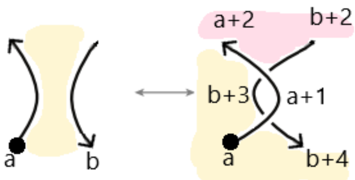
  - If the arcs are **antiparallel** we have the following two choices:
    Yellow outer region $..., a, b, ... \leftrightarrow ..., a, b+4, ...$
    Pink outer region $..., a, b, ... \leftrightarrow ..., a+2, b+2, ...$



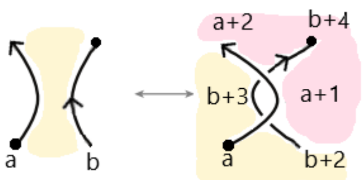
- **Both arcs touch the outer region and one of the arcs contains an endpoint**
  - If the arcs are **parallel** we have the following two choices:
    Yellow outer region $..., a, b, ... \leftrightarrow ..., a, a+2, b+2, b+3, ...$
    Pink outer region $..., a, b, ... \leftrightarrow ..., a+2, b+4$



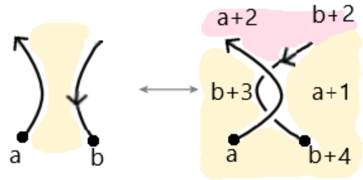
  - If the arcs are **antiparallel** we have the following two choices:
    Yellow outer region $..., a, b, ... \leftrightarrow ..., a, a+2, b+3, b+4, ...$
    Pink outer region $..., a, b, ... \leftrightarrow ..., a+2, b+2, ...$



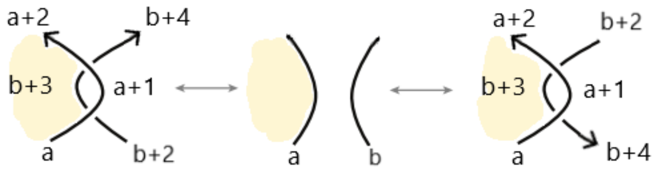
- **Both arcs touch the outer region and both contain endpoints**
  - If the arcs are **parallel** we have the following two choices:
    Yellow outer region $..., a, b, ... \leftrightarrow ..., a, a+2, b+2, b+3, ...$
    Pink outer region $..., a, b, ... \leftrightarrow ..., a+1, a+2, b+2, b+4$



– If the arcs are **antiparallel** we have the following two choices:
Yellow outer region $..., a, b, ... \leftrightarrow ..., a, a{+}1, a{+}2, b{+}2, b{+}3, b{+}4, ...$
Pink outer region $..., a, b, ... \leftrightarrow ..., a+2, b+2, ...$

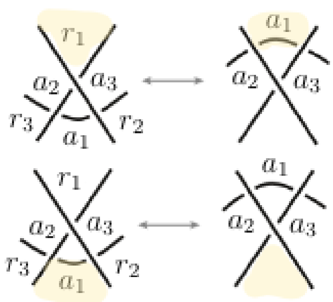


- **Only one arc touches the outer region**



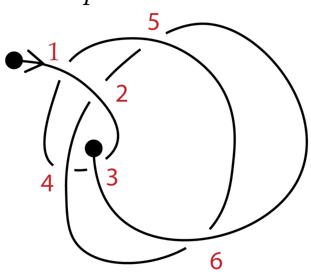
$$..., a, b, ... \leftrightarrow ..., a, a+2, b+3, ...$$

(3) Ω_3-move involves three arcs of the diagram that form a triangular region and let a_1, a_2, a_3 be those arcs. Opposite from an arc a_i i = 1, 2, 3 and adjacent to the intersection of the other two arcs, lies a local region of the diagram, r_i , i = 1, 2, 3 .
If $r_i \subseteq$ outer region $\leftrightarrow$ outer region $+a_i$.
If $r_i \subseteq$ outer region and $a_i \in$ outer region $\leftrightarrow$ outer region $-a_i$



Definition 2.6.1. A crossing of a knotoid diagram is called odd if there is an **odd** number of labels between the two appearances of the crossing otherwise it is called an **even** crossing.

Example 1:



Gauss code: $1\ 2\ -3\ -4\ -1\ 5\ -6\ 4\ -2\ -5\ 6\ 3$ $++++++++++++$
The crossings $1, 4, 5$ and 6 of the knotoid diagram are odd, and the crossings $2, 3$ are even.

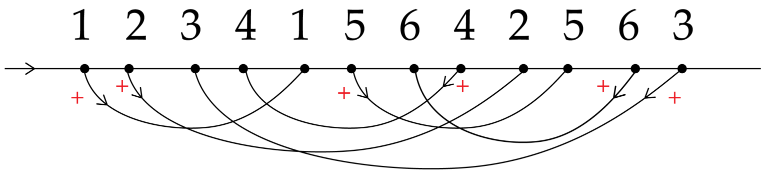
Definition 2.6.2. Gauss code of a knotoid diagram is said to be **evenly intersticed** if there is an even number of labels between two appearances of any label.

Theorem 6. *The Gauss code of a knotoid diagram in S^2 is evenly intersticed if and only if it is a knot-type knotoid diagram.*

Proof. The loop at a crossing of a knotoid diagram in S^2 is defined to be the path obtained by traversing the knotoid diagram starting and ending at that crossing. There is a loop at each crossing of a knotoid diagram.
Let K be a proper knotoid diagram then one of the endpoints is located inside at least one loop, i.e. endpoints of K are separated by at least one loop at a crossing of K.
All the strands entering the loop except the one that is adjacent to the endpoint, leave the loop and each such strand contributes with a pair of labels to the Gauss code of the diagram. We consider the crossing "1" that forms the loop, the Gauss code of K along this loop is: ...$1\ 2\ 5\ 7\ -5\ -7\ -1$..., where 2 represents the crossing of the strand adjacent to the endpoint with the loop, and $5, -5$ and $7, -7$ for the pairs of crossings created by the transversally intersecting strands which enter and leave the loop. We can see that between the two appearances of the label 1, we have an odd number of labels (five labels) so that the Gauss code of K is not evenly-intersticed.
For a knot-type diagram K, we can assume that the tail and head lie in the outermost region of the diagram so that none of the loops at crossings encloses them. All the strands passing through any of the loops of K enter and leave the loop so that they contribute with a pair of labels to the Gauss code of K. This shows that each crossing is even, i.e. the Gauss code of K is evenly-intersticed. □

Definition 2.6.3. Gauss codes have a diagrammatic representation called **chord diagram**.
We consider a segment which is oriented from left to right, each label in the Gauss code is represented by 2 points on this segment.
The points are labeled as the corresponding labels in the code.
A signed and oriented chord connects each pair of the labeled points. The orientation of a chord heads from the overcrossing to the undercrossing.
Starting from the tail, during a travel along the knotoid diagram K, if the first time that we meet a crossing is an overcrossing then the arrow of the corresponding chord heads towards the second appearance of the label.
The sign of the chord is the sign of the associated crossing.
For flat knotoid diagrams, we have the notion of right and left at each flat crossing. If we meet for the fist time a crossing that goes to the right then the head of the arrow on the corresponding chord heads towards the first appearance of the label. We call such a diagram with chords that represents the Gauss code of a knotoid diagram the chord diagram of the knotoid diagram.
Each knotoid diagram has a unique Gauss code and chord diagram.

Example 2: Recall the *Example 1*
The chord diagram of Gauss code
$1\ 2\ -3\ -4\ -1\ 5\ -6\ 4\ -2\ -5\ 6\ 3$ $++++++++++++$



Chapter 3

Invariants of knotoids

Given two knotoid diagrams K and K', if K and K' are equivalent then they have the same invariants. The invariants can be numbers, polynomial...
In this chapter we will consider polynomial invariants, in particular the Jones polynomial and the arrow polynomial for spherical knotoids, while for planar knotoids we will consider the Turaev loop bracket polynomial and the loop arrow polynomial. We will see the definitions of height of knotoids, of the crossing number and their relation.
Knotoids invariants can be used to classify knotoids, in particular in Appendix B it is possible to find a table (taken from [5]) of all distinct knotoids in the sphere up to four crossings.

3.1 Invariants of spherical knotoids

3.1.1 The Jones polynomial

Before giving a definition of the Jones polynomial it is necessary to introduce some preliminary notions.

Definition 3.1.1. Let $K \subset S^2$ be a knotoid diagram (not-oriented). A **state s** of a knotoid diagram is a simple curve in S^2 obtained by smoothing each crossing in one of two different ways in Figure 3.1.
We have the crossing c_i and it determines four angles. We orient each angle starting from the arc that passes above to arrive at the arc that passes below.
If we cut clockwise angles (horizontally cutting) we get the negative smoothing and the sign of this smoothing of the i-th crossing c_i is $\sigma_i(s) = -1$
If we cut counterclockwise angles (vertically cutting) we get the positive smoothing and the sign of this smoothing of the i-th crossing c_i is $\sigma_i(s) = +1$

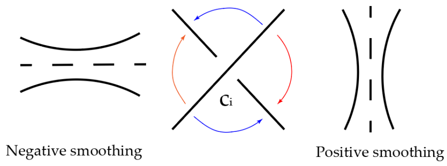


Figure 3.1: Smoothings of the crossing c_i

Definition 3.1.2. Let $S(K)$ be the set of all states of K and let $C(K)$ be the crossing number of the knotoid diagram.
For every state $s \in S(K)$ the *sum of signs of all smoothings of state* s is

$$\sigma(s) = \sigma_1(s) + ... + \sigma_{C(K)}(s)$$

Remark 3.1.1. The state depends on the choice made at each crossing, therefore the cardinality of the set of all states is $|S(D)| = 2^{C(D)}$.

Definition 3.1.3. Once smoothed all crossings of the knotoid diagram we get a (possibly empty) finite set of loops and an arc. Then, we put

ρ(s) = number of components of the state s (once smoothed all crossings).

Definition 3.1.4. BRACKET POLYNOMIAL
Let $K \subset S^2$ be a knotoid diagram (not-oriented).
The **bracket polynomial** is given by:

$$\langle K \rangle = \sum_{s \in S(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\rho(s)-1} \in \mathbb{Z}[A^{\pm 1}]$$

The orientation is not used to calculate this polynomial.

Rules to construct the polynomial:

1. $\langle \hat{K} = K \sqcup S^1 \rangle = (-A^2 - A^{-2})\langle K \rangle$

Proof.

Given $\hat{K} = K \sqcup S^1$ then $S(\hat{K}) \leftrightarrow S(K)$ and $\sigma(\hat{s}) = \sigma(s)$ because the number of crossings is the same, while the number of components is different $\rho(\hat{s}) = \rho(s) + 1$ (there is an other component: a circle S^1).

$$\langle \hat{K} \rangle = \sum_{\hat{s} \in S(\hat{K})} A^{\sigma(\hat{s})}(-A^2 - A^{-2})^{\rho(\hat{s})-1} =$$

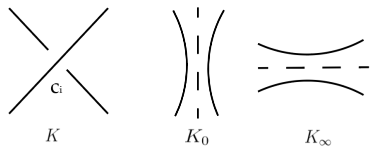
$$= \sum_{s \in S(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\rho(s)+1-1} = (-A^2 - A^{-2})\langle K \rangle \qquad \square$$

2. $\langle$  $\rangle = 1$

Proof.

$\langle$$\rangle = A^{\sigma(s)}(-A^2 - A^{-2})^{\rho(s)-1} = A^0(-A^2 - A^{-2})^{1-1} = 1$ $\square$

3. $\langle K\rangle = A\langle K_0\rangle + A^{-1}\langle K_\infty\rangle$



Proof.

Let K, K_0, K_∞ be three identical diagrams that differ only in the crossing c_i.
States of K is the disjoint union of states where c_i is smoothed as in K_0 and states where c_i is smoothed as in K_∞.

$$\begin{array}{ccccc} S(K) = & S_0(K) & \sqcup & S_\infty(K) \\ & \updownarrow & & \updownarrow \\ & S(K_0) & & S(K_\infty) \end{array}$$

Considering $s \in S_0(K)$ and $s_0 \in S(K_0)$ we obtain $\sigma(s) = \sigma(s_0) + 1$ ($+1$ because the crossing c_i is been smoothed in positive way) and $\rho(s) = \rho(s_0)$.
Considering $s \in S_\infty(K)$ and $s_\infty \in S(K_\infty)$ we obtain $\sigma(s) = \sigma(s_\infty) - 1$ (-1 because the crossing c_i is been smoothed in negative way) and $\rho(s) = \rho(s_\infty)$.

$$\langle K\rangle = \sum_{s\in S(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\rho(s)-1} =$$

$$= \sum_{s\in S_0(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\rho(s)-1} + \sum_{s\in S_\infty(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\rho(s)-1} =$$

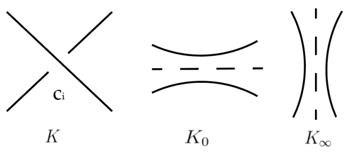
$$= \sum_{s_0\in S(K_0)} A^{\sigma(s_0)+1}(-A^2 - A^{-2})^{\rho(s_0)-1} + \sum_{s_\infty\in S(K_\infty)} A^{\sigma(s_\infty)-1}(-A^2 - A^{-2})^{\rho(s_\infty)-1} =$$

$$= A \sum_{s_0\in S(K_0)} A^{\sigma(s_0)}(-A^2 - A^{-2})^{\rho(s_0)-1} + A^{-1} \sum_{s_\infty\in S(K_\infty)} A^{\sigma(s_\infty)}(-A^2 - A^{-2})^{\rho(s_\infty)-1} =$$

$$= A\langle K_0\rangle + A^{-1}\langle K_\infty\rangle$$

$\square$

4. Rotating the crossing c_i (in the case 2.) 90 degree we obtain

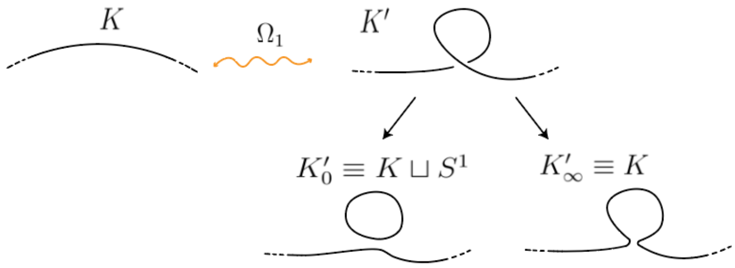


$$\langle K\rangle = A\langle K_0\rangle + A^{-1}\langle K_\infty\rangle$$

Proposition 1. The bracket polynomial is invariant under the second and the third Reidemeister moves but not under the first Reidemeister move.

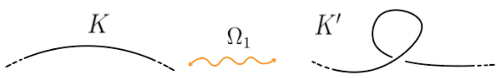
Proof.

Let K and K' be two diagrams related by an Ω_1-move.



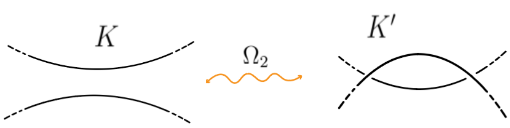
$$\begin{aligned}\langle K'\rangle &= A\langle K'_0\rangle + A^{-1}\langle K'_\infty\rangle = A\langle K \sqcup S^1\rangle + A^{-1}\langle K\rangle = \\ &= A(-A^2 - A^{-2})\langle K\rangle + A^{-1}\langle K\rangle = \\ &= (-A^3 - A^{-1} + A^{-1})\langle K\rangle = -A^3\langle K\rangle\end{aligned}$$

Similarly if we have the other crossing:

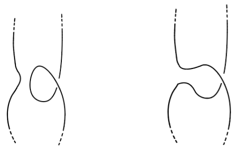


$$\langle K'\rangle = -A^{-3}\langle K\rangle$$

Let K and K' be two diagrams related by an Ω_2-move.



$\langle K' \rangle = A\langle K'_0 \rangle + A^{-1}\langle K'_\infty \rangle =$



$= A(A\langle K'_{00} \rangle + A^{-1}\langle K'_{0\infty} \rangle) + A^{-1}(A\langle K'_{\infty 0} \rangle + A^{-1}\langle K'_{\infty\infty} \rangle) =$

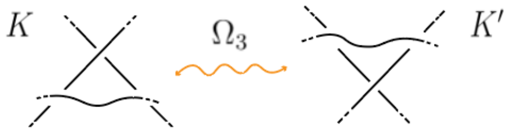
$\uparrow$ they are equal, we call them K'' $\uparrow$

$= A^2\langle K'' \rangle + \langle K'_{0\infty} \rangle) + \langle K'_{\infty 0} \rangle + A^{-2}\langle K'' \rangle) =$

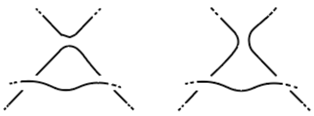
$= A^2\langle K'' \rangle + \langle \hat{K''} = K'' \sqcup S^1 \rangle) + \langle K \rangle + A^{-2}\langle K'' \rangle) =$

$= (A^2 + A^{-2})\langle K'' \rangle + (-A^2 - A^{-2})\langle K'' \rangle + \langle K \rangle = \langle K \rangle$

Let K and K' be two diagrams related by an Ω_3-move.



$\langle K \rangle = A\langle K_0 \rangle + A^{-1}\langle K_\infty \rangle$

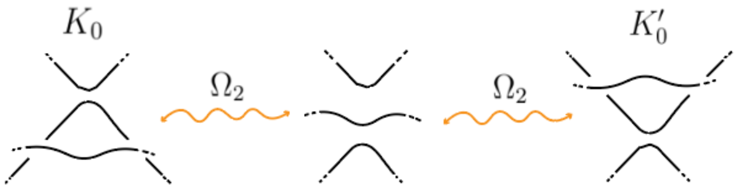


$\|$ $\|$

$\langle K' \rangle = A\langle K'_0 \rangle + A^{-1}\langle K'_\infty \rangle$

We can see that $\langle K_\infty \rangle = \langle K'_\infty \rangle$ up to isotopy because they have same crossings but displaced.

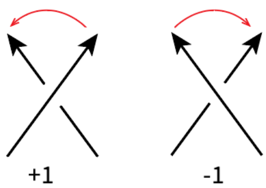
We have seen that the bracket polynomial is invariant by Ω_2-move. Appling the Ω_2-move we have $\langle K_0 \rangle = \langle K'_0 \rangle$.



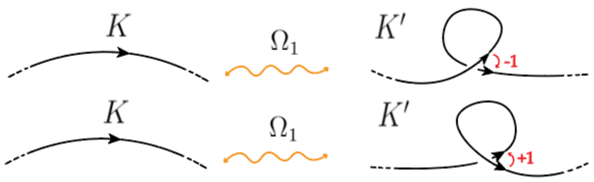
So we get $\langle K\rangle = \langle K'\rangle$. $\square$

The bracket polynomial is not an invariant of knotoid diagram because it is not invariant by all Reidemeister moves so it is necessary to apply a *correction factor* in order to obtain an invariant: the **Jones polynomial**.

In order to establish invariance under the first move, we *choose an orientation* for the given knotoid diagram. The crossings in an oriented diagram can be positive $+1$ or negative -1:



The correction factor is given by the sum of signs of all crossing of oriented knotoid diagram K. This sum is called *writhe* of K and denoted by $\mathrm{wr}(K)$. The first Reidemeister move:



$\mathrm{wr}(K') = \mathrm{wr}(K) - 1$

$\mathrm{wr}(K') = \mathrm{wr}(K) + 1$

The second Reidemeister move generates two new crossings that are opposite (independently of the orientation choice) then the *writhe* does not change. The third Reidemeister move only changes the positions of crossings, then the *writhe* does not change.

Definition 3.1.5. THE JONES POLYNOMIAL
Let K be an oriented knotoid diagram in S^2.
The **Jones polynomial** is given by:

$$J_K(A) = (-A^{-3})^{\mathrm{wr}(K)}\langle K\rangle \in \mathbb{Z}[A^{\pm1}]$$

where $\langle K \rangle$ is bracket polynomial.
The correction factor $(-A^{-3})^{wr(K)}$ ensures that the Jones polynomial is invariant under first Reidemeister move:

$$J_{K'}(A) = (-A^{-3})^{\text{wr}(K')}\langle|K'|\rangle = (-A^{-3})^{\text{wr}(K)-1}(-A^{-3})\langle|K|\rangle =$$
$$= (-A^{-3\,\text{wr}(K)+3-3})\langle|K|\rangle = (-A^{-3})^{\text{wr}(K)}\langle|K|\rangle = J_K(A)$$

$$J_{K'}(A) = (-A^{-3})^{\text{wr}(K')}\langle|K'|\rangle = (-A^{-3})^{\text{wr}(K)+1}(-A^{3})\langle|K|\rangle =$$
$$= (-A^{-3\,\text{wr}(K)-3+3})\langle|K|\rangle = (-A^{-3})^{\text{wr}(K)}\langle|K|\rangle = J_K(A)$$

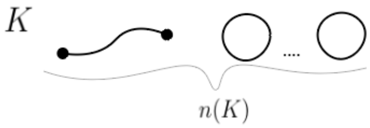
Properties of Jones polynomial:

1. $J_K(A)$ is invariant under all Reidemeister moves.

2. K trivial knotoid diagram $\Rightarrow J_K(A) = (-A^2 - A^{-2})^{n(K)-1}$
where $n(K)$ is the number of components of knotoid diagram K.

Proof.

Let K be a knotoid diagramm with $n(K)$ components.



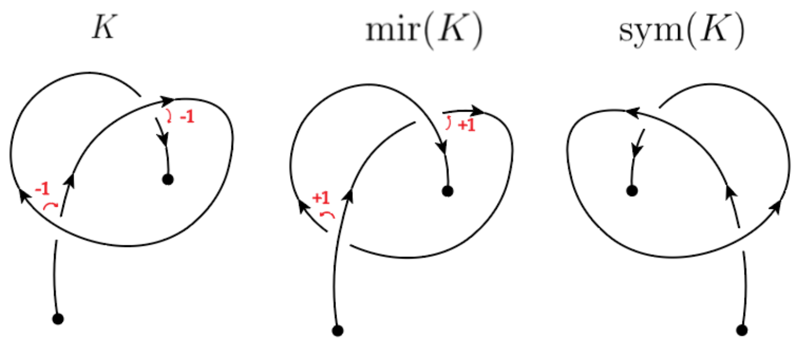
This diagram has only one state because it's a diagram without crossings $wr(K) = 0$ $\sigma(s) = 0$.

$$\langle K \rangle = \sum_{s \in S(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\rho(s)-1} = A^0(-A^2 - A^{-2})^{n(K)-1}$$

$$J_K(A) = (-A^{-3})^{\text{wr}(K)}\langle K \rangle = (-A^{-3})^0\langle K \rangle = (-A^2 - A^{-2})^{n(K)-1} \qquad \square$$

3. If K is *connected* $J_K(A)$ it does not depend on the orientation because it only has an orientation and the opposite one.
$J_{-K}(A) = J_K(A)$
$-K$ is the knotoid diagram with inverted orientation.

4. $J_{mir(K)}(A) = J_K(A^{-1})$ where $mir(K)$ is the **mirror reflection** of the knotoid diagram, it is the same diagram with inverted crossings.
Example



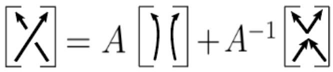
wr$(K) = -2$ wr(mir$(K)) = +2$ wr(sym$(K)) = -$ wr(K)
because each crossing changes sign, then there is an exchange between K_0 and K_∞ in the formula $\langle K\rangle = A\langle K_0\rangle + A^{-1}\langle K_\infty\rangle$ but it is like to exchange A and A^{-1}.
The bracket polynomial of mir(K) valuated in A corresponds to bracket polynomial of K valuated in A^{-1}. $\langle |\,\text{mir}(K)|\rangle(A) = \langle |K|\rangle(A^{-1})$.

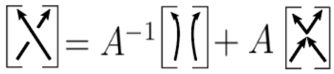
Remark 3.1.2. The knotoid diagram is symmetric $\Rightarrow J_K(A) = J_K(A^{-1}) = J_{\text{mir}(K)}(A)$

3.1.2 The arrow polynomial

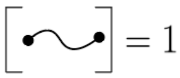
To give the definition of the arrow polynomial, it is necessary to give a definition of bracket polynomial for oriented states.

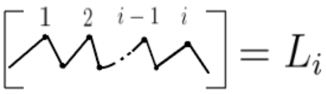
Definition 3.1.6. BRACKET POLYNOMIAL for oriented states
Rules to construct the polynomial:

1a. 

1b. 

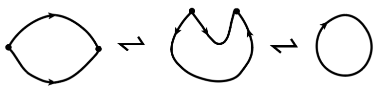
2. $[K \sqcup \bigcirc] = -A^2 - A^{-2}[K]$

3. 

4. 

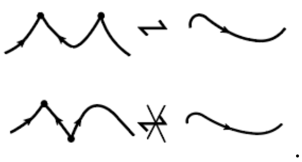
Each oriented state is composed by a finite number of closed components and an arc with endpoints, both can contain consecutive cusps that we get by construction of the polynomial, in particular by the rules **1a.** and **1b.**.
Each cusp has two arcs either going into the cusp or going out from the cusp. We call "inside of the cusp" the part of the acute angle and "outside of the cusp" the part of the obtuse angle.
Rules which reduce the number of cusps in a state:
- two consecutive cusps on a closed component can be canceled if they have insides in the same region;

(c1)



- two consecutive cusps which have insides on the same side of the arc can be canceled;

(c2)



Let $K \subset S^2$ be an **oriented** knotoid diagram.
The **bracket polynomial for oriented state** is given by:

$$[K] = \sum_{s \in S(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\rho(s)-1} L_{i(s)} \in \mathbb{Z}[A^{\pm 1}, L_1, L_2, ...]$$

where: $S(K)$ is the set of states of knotoid diagram, $\sigma(s)$ is the sum of signs of all smoothings of state s, $\rho(s)$ is the number of components of the state s (once smoothed all crossings) and $L_{i(s)}$ is the variable assigned to each arc of a state with $i(s)$ surviving cusps.

Proposition 2. The bracket polynomial is invariant under the second and the third Reidemeister moves but not under the first Reidemeister move.

Proof. Similar proof to that of the Proposition **??**. □

Definition 3.1.7. THE ARROW POLYNOMIAL
Let K be an **oriented** knotoid diagram in S^2.
The **arrow polynomial** is given by:

$$\mathbb{A}(K) = (-A^{-3})^{\text{wr}(K)}[K] \in \mathbb{Z}[A^{\pm 1}, L_1, L_2, ...]$$

where $[K]$ is bracket polynomial for oriented states.
The arrow polynomial is invariant under Reidemeister moves. (The correction factor $(-A^{-3})^{\text{wr}(K)}$ ensures that the arrow polynomial is invariant under first Reidemeister move.)

Remark 3.1.3. The arrow polynomial gives nontrivial information about the height (definition 2.2.4). See chapter 3.7.

3.2 Invariants for planar knotoids

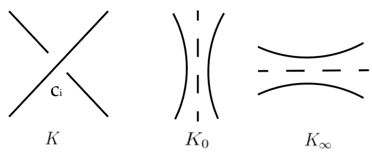
3.2.1 The Turaev loop bracket polynomial

The Turaev loop bracket polynomial is an extention of Jones polynomial for the case of planar knotoids. To give a definition of Turaev polynomial, it is necessary to give a definition of loop bracket polynomial.

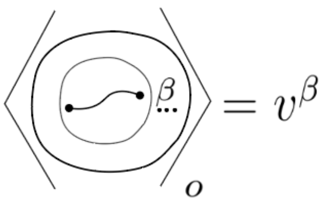
Definition 3.2.1. LOOP BRACKET POLYNOMIAL
When we have studied the bracket polynomial we have seen that when all crossings of the knotoid diagram are smoothed we get a finite number of disjoint loops and an arc.
Rules to construct the polynomial:

1. $\langle \hat{K} = K \sqcup S^1 \rangle_o = (-A^2 - A^{-2})\langle K \rangle_o$

2. $\langle K \rangle_o = A\langle K_0 \rangle + A^{-1}\langle K_\infty \rangle_o$



3. Rotating the crossing c_i (in the case 2.) 90 degree we obtain
$\langle K \rangle = A\langle K_0 \rangle + A^{-1}\langle K_\infty \rangle$

4. 

where $\beta > 0$ is the number of copies of loops that contain the arc.

If the arc remains inside a circle in $\mathbf{S^2}$ we can always take it out by moving an arc of circle around the surface of the sphere but if we work in $\mathbb{R}^2$ with planar knotoids, we cannot do this and it is necessary to keep track of this information.
For this reason we add an other variable v to the bracket polynomial that indicates the situation in which the segment is inside a finite number of circles.
Let $K \subset \mathbb{R}^2$ be a knotoid diagram (not-oriented).
The **loop bracket polynomial** is given by:

$$\langle K \rangle_o = \sum_{s \in S(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\alpha(s)} v^{\beta(s)} \in \mathbb{Z}[A^{\pm 1}, v]$$

where: $S(K)$ is the set of states of knotoid diagram, $\sigma(s)$ is the sum of signs of all smoothings of state s, $\alpha(s)$ is the number of circular components which do not contain the arc, v is the variable assigned to the situation in which the arc is inside a finite number of loops ($\beta(s)$ is the number of closed components that contain the arc). $\alpha(s) + \beta(s) = \rho(s) - 1$

The orientation is not used to calculate this polynomial.

Definition 3.2.2. THE TURAEV LOOP BACKET POLYNOMIAL
Let K be an oriented knotoid diagram in $\mathbb{R}^2$.
The **Turaev loop bracket polynomial** is given by:

$$\hat{J}_K(A, v) = (-A^{-3})^{\text{wr}(K)} \langle K \rangle_o \in \mathbb{Z}[A^{\pm 1}, v]$$

where $\langle K \rangle_o$ is loop bracket polynomial.
The Turaev loop bracket polynomial is invariant under Reidemeister moves. (The correction factor $(-A^{-3})^{\text{wr}(K)}$ ensures that the Turaev loop bracket polynomial is invariant under first Reidemeister move.)

3.2.2 The loop arrow polynomial

The loop arrow polynomial is an extention of arrow polynomial for the case of planar knotoids. To give a definition of loop arrow polynomial, it is necessary to give a definition of loop bracket polynomial for oriented states.

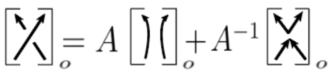
Definition 3.2.3.

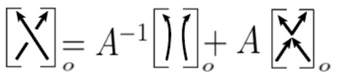
LOOP BRACKET POLYNOMIAL for oriented states
When we smooth all crossings we can have these situations:
- an arc which remains inside of a finite number of circles (like in the loop bracket polynomial),
- there are two type of zig-zag segments, they are formed by a finite number of surviving cusps (the rules to remove cusps are the same seen in the bracket polynomial for oriented states)

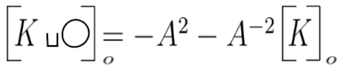
Type 1  Type 2 

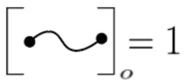
- a type 1 (type 2) zig-zag segment remains inside of a finite number of circles.

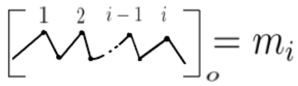
Rules to construct the polynomial:

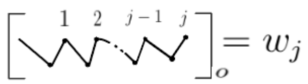
1a. 

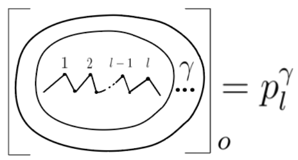
1b. 

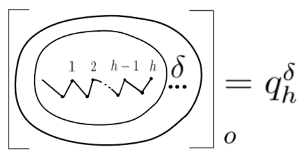
2. 

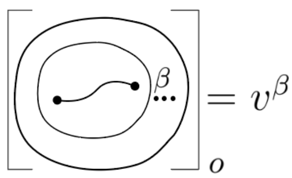
3. 

4a. 

4b. 

5a. 

5b. 

6. 

Let $K \subset \mathbb{R}^2$ be an oriented knotoid diagram.
The **loop bracket polynomial for oriented states** is given by:

$$[K]_o = \sum_{s \in S(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\alpha(s)} v^{\beta(s)} m_{i(s)} w_{j(s)} p_{l(s)}^{\gamma(s)} q_{h(s)}^{\delta(s)}$$
$$\in \mathbb{Z}[A^{\pm 1}, v, m_1, m_2, ...w_1, w_2, ..., p_1, p_2, ..., q_1, q_2, ...]$$

where: $S(K)$ is the set of states of knotoid diagram;
$\sigma(s)$ is the sum of signs of all smoothings of state s; $\alpha(s)$ is the number of circular components which do not contain the arc;
v is the variable assigned to the situation in which the arc is inside a finite number of loops ($\beta(s)$ is the number of closed components that contain the arc);
$m_{i(s)}$ is the variable assigned to each arc of a state with $i(s)$ surviving cusps that create the type 1 zig-zag;
$w_{j(s)}$ is the variable assigned to each arc of a state with $j(s)$ surviving cusps that create the type 2 zig-zag;
$p_{l(s)}$ is the variable assigned to the situation in which the arc of a state with $l(s)$ surviving cusps (that create the type 1 zig-zag) is inside a finite number of loops ($\gamma(s)$ is the number of closed components that contain the arc);
$q_{h(s)}$ is the variable assigned to the situation in which the arc of a state with $h(s)$ surviving cusps (that create the type 2 zig-zag) is inside a finite number of loops ($\delta(s)$ is the number of closed components that contain the arc).

Definition 3.2.4. THE LOOP ARROW POLYNOMIAL
Let K be an oriented knotoid diagram in $\mathbb{R}^2$.
The **loop arrow polynomial** is given by:

$$\hat{\mathbb{A}}(K) = (-A^{-3})^{\mathrm{wr}(K)}[K]_o \in \mathbb{Z}[A^{\pm 1}, v, m_1, m_2, ...w_1, w_2, ..., p_1, p_2, ..., q_1, q_2, ...]$$

where $[K]_o$ is loop bracket polynomial for oriented states.
The loop arrow polynomial is invariant under Reidemeister moves.
(The correction factor $(-A^{-3})^{\mathrm{wr}(K)}$ ensures that the loop arrow polynomial is invariant under first Reidemeister move.)

3.3 The affine index polynomial

Given a knotoid diagram K, the **affine index polynomial** of knotoid, is based on an integer labeling assigned to flat knotoid diagram (definition 2.5.1) of K in the following way:
- the labeling of each arc of knotoid diagram of K begins with the first arc which connects the tail and the first flat crossing,
- at each crossing, the labels of the arcs change by one; if the incoming arc labeled by $a \in \mathbb{Z}$ crosses the crossing towards left then the next arc is labeled by $a + 1$, if the incoming arc crosses the crossing towards right then it is labeled by $a - 1$.

Let c be a classical crossing of K, we define two numbers at c resulting by the labeling:

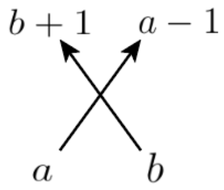


Figure 3.2: Integer labeling at a flat crossing

$w_+(c) = a - (b+1)$ positive weight
$w_-(c) = b - (a-1)$ negative weight
where a and b are the labels for the left and the right incoming arcs of the corresponding flat crossing c, respectively.
The weight of c is defined as

$$w_K(c) = \begin{cases} w_+(c); & \text{if the sign of } c \text{ is a positive crossing} \\ w_-(c); & \text{if the sign of } c \text{ is a negative crossing} \end{cases}$$

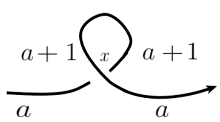
Definition 3.3.1. THE AFFINE INDEX POLYNOMIAL
Let K be an oriented knotoid diagram in S^2. The **affine index polynomial** of classical knotoid diagram K is defined by:

$$P_K(A) = \sum_c \operatorname{sgn}(c)(A^{w_K(c)} - 1)$$

where the sum is taken over all classical crossings of a diagram K and $sgn(c)$ is the sign of c.

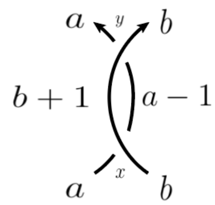
The affine index polynomial is invariant under Reidemeister moves, it can be seen that:

Ω_1-**move** adds a crossing with zero weight



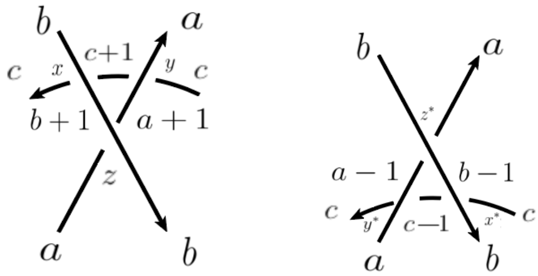
$$w(x) = w_+(x) = 0$$

Ω_2-**move** adds/removes two crossings with opposite signs but with same



$$w(x) = w_-(x) = b - (a-1) = -a + b + 1$$
$$w(y) = w = +(y) = (b+1) - a = -a + b - 1$$

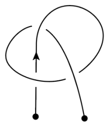
Ω_3-move does not change weights or signs of the three crossings in the move pattern $x^*y^*z^*$



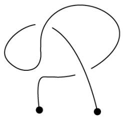
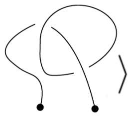
$$w_-(x) = b - c = w_-(x^*)$$
$$w_+(y) = a - c = w_+(y^*)$$
$$w_+(z) = b - a = w_+(z^*)$$

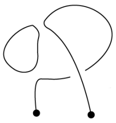
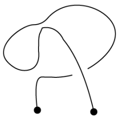
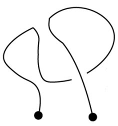
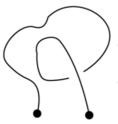
Remark 3.3.1. When we have given the definition 2.2.4 of *height* of a knotoid diagram $K \subset S^2$, we have seen that a knotoid in S^2 is of knot-type if and only if its height is zero or equivalently a knotoid in S^2 has nonzero height if and only it is a proper knotoid.
1) Knot-type knotoids have trivial affine index polynomial.
2) Proper knotoids may have nonzero affine index polynomial.
⇒If a given knotoid diagram has nonzero affine index polynomial, then the knotoid diagram represents a proper knotoid. It is often hard to compute the height with an attempt of direct computation, for we should take into account all the equivalent knotoid diagrams.
The affine index polynomial provides the estimation for the height that we seen in the subchapter 3.7 .

3.4 Example: The invariant polynomials of the spherical knotoid 3_1

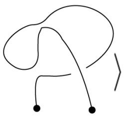
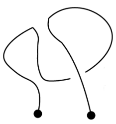
We consider the spherical knotoid 3_1: 

We consider the not-oriented knotoid diagram 3_1 and the computation of *bracket polynomial* is:

$\langle 3_1 \rangle = A\langle$  $\rangle + A^{-1}\langle$  $\rangle =$

$= A\Big[A\langle$  $\rangle + A^{-1}\langle$  $\rangle\Big] + A^{-1}\Big[A\langle$  $\rangle + A^{-1}\langle$  $\rangle\Big] =$

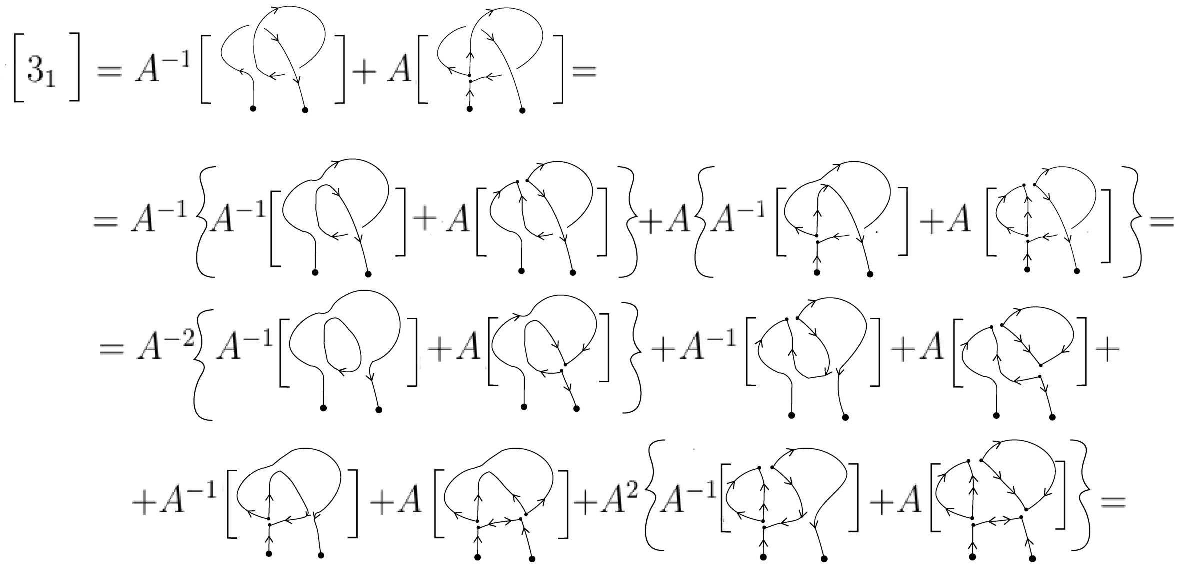
(using **1.**)

$= A\Big[A(-A^2 - A^{-2})\langle$  $\rangle + A^{-1}\langle$  $\rangle\Big] + A^{-1}\Big[A\langle$  $\rangle + A^{-1}\langle$  $\rangle\Big] =$

$= A[A(-A^2 - A^{-2})(-A^{-3}) + A^{-1}(-A^3)] + A^{-1}[A(-A^3) + A^{-1}(-A^{-3})] =$
$= [(-A^4 - 1)(-A^3) - A^3] + [-A^3 - A^{-5}] =$
$= A^7 + A^3 - 2A^3 - A^{-5} = A^7 - A^3 - A^{-5}$

Now we consider the orientation of 3_1 and the computation of **Jones polynomial** is:
$\mathrm{wr}(3_1) = -3$
$J_{3_1}(A) = (-A^{-3})^{\mathrm{wr}(3_1)}\langle 3_1 \rangle = (-A^{-3})^{-3}(A^7 - A^3 - A^{-5}) = -A^{16} + A^{12} + A^4$

We consider the oriented knotoid diagram 3_1 and the computation of *bracket polynomial for oriented states* is:



(simplifying with **(c1)**, **(c2)** and using **2.**)

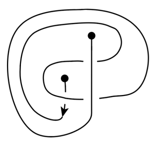
$= A^{-3}(-A^2 - A^{-2}) + A^{-1} + A^{-1} + A(-A^2 - A^{-2}) + A^{-1} + A(-A^2 - A^{-2}) +$
$\quad +A(-A^2 - A^{-2}) + A^3(-A^2 - A^{-2})(-A^2 - A^{-2}) =$
$= -A^{-1} - A^{-5} + A^{-1} + A^{-1} - A^3 - A^{-1} + A^{-1} - A^3 - A^{-1} - A^3 - A^{-1} +$
$\quad +(-A^5 - A)(-A^2 - A^{-2}) =$
$= -A^{-5} - 3A^3 - A^{-1} + A^7 + A^3 + A^3 + A^{-1} = -A^{-5} + A^7 - A^3$

The computation of **Arrow polynomial** is:

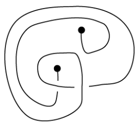
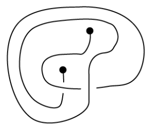
$\mathrm{wr}(3_1) = -3$

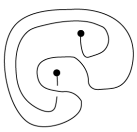
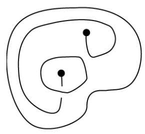
$\mathbb{A}(3_1) = (-A^{-3})^{\mathrm{wr}(3_1)}[3_1] = -A^9(A^7 - A^3 - A^{-5}) = -A^{16} + A^{12} + A^4$

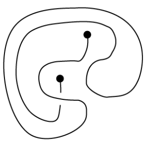
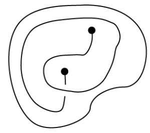
3.5 Example: The invariant polynomials of the planar knotoid 3_3

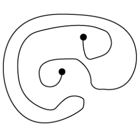
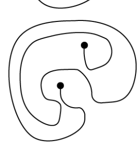
We consider the planar knotoid 3_3: 

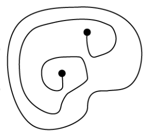
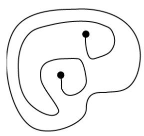
We consider the not-oriented knotoid diagram 3_3 and the computation of *loop bracket polynomial* is:

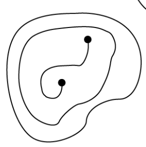
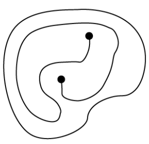
$\langle 3_3 \rangle_o = A\langle$  $\rangle_o + A^{-1}\langle$  $\rangle_o =$

$= A\Big[A\langle$  $\rangle_o + A^{-1}\langle$  $\rangle_o\Big] +$

$+ A^{-1}\Big[A\langle$  $\rangle_o + A^{-1}\langle$  $\rangle_o\Big] =$

$= A^2\Big[A\langle$  $\rangle_o + A^{-1}\langle$  $\rangle_o\Big] +$

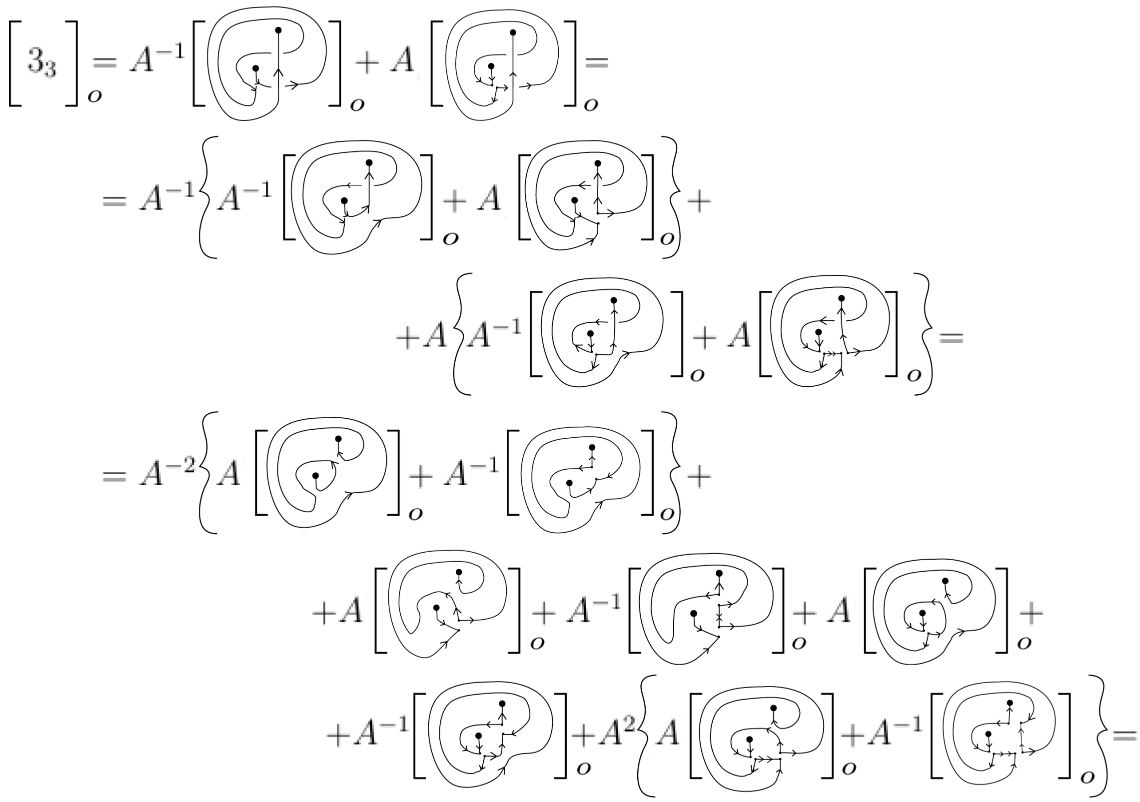
$+ A\langle$  $\rangle_o + A^{-1}\langle$  $\rangle_o - A^3 +$

$+ A^{-2}\Big[A\langle$  $\rangle_o + A^{-1}\langle$  $\rangle_o\Big] =$

$= A^2(A + A^{-1}) + Av + A^{-1}v - A^3 + A^{-1}v^2 + A^{-3}v =$
$= A^3 + A + Av + A^{-1}v - A^3 + A^{-1}v^2 + A^{-3}v =$
$= A + Av + A^{-1}v + A^{-1}v^2 + A^{-3}v$

Now we consider the orientation of 3_3 and the computation of **Turaev loop bracket polynomial** is:
$\text{wr}(3_3) = -1$
$\hat{J}_{3_3}(A, v) = (-A^{-3})^{\text{wr}(3_3)}\langle 3_3 \rangle_o = -A^3(A + Av + A^{-1}v + A^{-1}v^2 + A^{-3}v) =$
$= -A^4 - A^4v - A^2v - A^2v^2 - v$

We consider the oriented knotoid diagram 3_1 and the computation of *loop bracket polynomial for oriented states* is:



(simplifying with **(c1)**, **(c2)** and using **2.**)

$$= A^{-1}v + A^{-3}p_1 + A + A^{-1}m_1 + Ap_1 + A^{-1}p_1^2 + A^3m_1 + A(-A^2 - A^{-2})m_1 =$$
$$= A^{-1}v + A^{-3}p_1 + A + A^{-1}m_1 + Ap_1 + A^{-1}p_1^2 + A^3m_1 - A^3m_1 - A^{-1}m_1 =$$
$$= A^{-1}v + A^{-3}p_1 + A + Ap_1 + A^{-1}p_1^2$$

Now we consider the orientation of 3_3 and the computation of **loop arrow bracket polynomial** is:

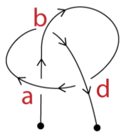
$\mathrm{wr}(3_3) = -1$

$\hat{\mathbb{A}}(3_3) = (-A^{-3})^{\mathrm{wr}(3_3)}[3_3]_o = (-A^3)(A^{-1}v + A^{-3}p_1 + A + Ap_1 + A^{-1}p_1^2)$

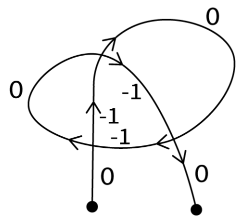
$= -A^2v - p_1 - A^4 - A^4p_1 - A^2p_1^2$

3.6 Examples of calculation of the affine index polynomial

We consider the spherical knotoid 3_1:



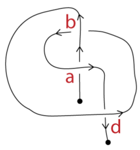
where a,b,c are crossings: sng(a)$= -1$, sng(b)$= -1$, sng(d)$= -1$
We consider the flat knotoid of 3_1 with integer labels:



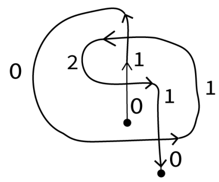
We compute the weight of crossings:
$w_{3_1}(a) = w_-(a) = -1 - (-1) = 0$
$w_{3_1}(b) = w_-(b) = -1 - (-1) = 0$
$w_{3_1}(d) = w_-(d) = -1 - (-1) = 0$
The affine index polynomial is given by:

$$P_{3_1}(A) = \sum_{c \in \{\text{crossings of } 3_1\}} \text{sgn}(c)(A^{w_{3_1}(c)} - 1) =$$
$$= -(A^0 - 1) - (A^0 - 1) - (A^0 - 1) = 0$$

We consider the spherical knotoid 3_2:



where a,b,c are crossings: sng(a)$= +1$, sng(b)$= +1$, sng(d)$= -1$
We consider the flat knotoid of 3_2 with integer labels:



We compute the weight of crossings:
$w_{3_2}(a) = w_+(a) = 2 - 1 = 1$
$w_{3_2}(b) = w_+(b) = 1 - 2 = -1$
$w_{3_2}(d) = w_-(d) = 0$
The affine index polynomial is given by:

$$P_{3_2}(A) = \sum_{c \in \{\text{crossings of } 3_2\}} \operatorname{sgn}(c)(A^{w_{3_2}(c)} - 1) =$$
$$= +(A-1) - (A^{-1} - 1) - (A^0 - 1) = A - 1 + A^{-1} - 1 = A + A^{-1} - 2$$

3.7 Height of spherical knotoids

Definition 3.7.1. The **height** of a knotoid diagram $K \subset S^2$ is the minimum number of crossings that a shortcut creates in the underpass closure. The height of a knotoid $k \in \mathcal{K}(S^2)$ is the minimum of the heights of the diagrams of k and it is denoted by $h(k)$ (i.e the height of a knotoid K in S^2 is defined as the minimum of the heights, taken over all equivalent classical knotoid diagrams to K).
A knotoid in S^2 is of knot-type if and only if its height is zero, or equivalently a knotoid in S^2 has nonzero height if and only it is a proper knotoid.

3.7.1 The affine index polynomial and the height of spherical knotoids

Theorem 7. *Let k be a knotoid in S^2. The height of k is greater than or equal to the maximum degree of the affine index polynomial of k.*

Proof. Let K be a knotoid diagram representing k. We label the knotoid diagram of K with respect to the labeling rule given in figure 3.2.
Each crossing of a knotoid diagram determines a unique loop (the continous path obtained by traversing the diagram starting and ending at that crossing according to the orientation of the diagram). The loop determined by a crossing C is called the *loop at the crossing* C and we indicate it with $l(C)$.
The algebraic intersection number of the loop at a crossing C with a strand of K is defined to be the total number of times that the strand intersects the loop from right to left minus the total number of times that the strand intersects the loop from left to right.
The algebraic intersection number of a loop at a crossing C, with other strands of the diagram is equal to either the positive weight or the negative weight of that crossing, depending to the orientation of the loop.

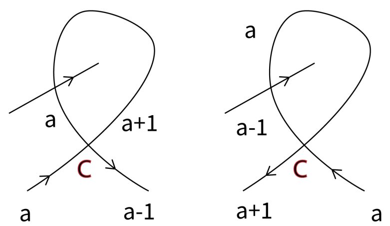
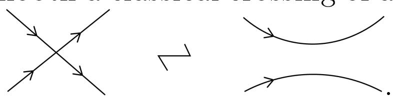
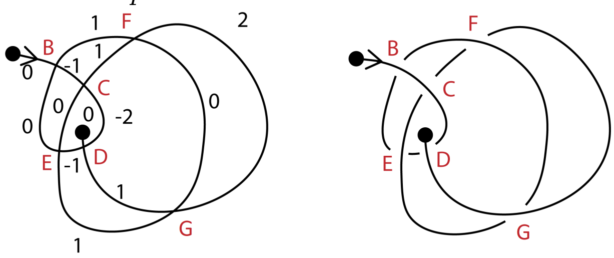


Figure 3.3: Two possible types of loops at the crossing C, one is oriented in the counterclockwise and the other in the clockwise direction.

The algebraic intersection numbers of the loop at C with the piece of strand shown in the figure 3.3, are $+1$ and -1, respectively. We can see that $w_-(C) = +1$ for the first loop that is oriented counterclockwise and $w_+(C) = -1$ for the second loop that is oriented clockwise. If the sum of the algebraic intersection numbers of the loop $l(C)$ at the crossing C with intersecting strands is equal to n, then n is equal to either $w_-(C)$ or $w_+(C)$, depending on the orientation of the loop $l(C)$.
Let m be the maximum degree of the affine index polynomial of k. Then there exists a crossing of K with weight m. In fact, m is the maximal weight among the weights of crossings of K. Let $\hat{C}$ be one of the crossings of K with weight m and $l(\hat{C})$ be the loop at $\hat{C}$.
The way to smooth a classical crossing of a knotoid diagram according to the orientation is .
Each crossing which are met twice while traversing along the loop $l(\hat{C})$, are all smoothed accordingly to the orientation. This implies that each self-intersection of the loop $l(\hat{C})$ is smoothed. Smoothing the self-intersections of the loop $l(\hat{C})$ results in oriented embedded circles (in S^2) and an oriented arc containing the tail and the head of K.
The arc may intersect the resulting circles and itself. The algebraic intersection number of one of the resulting circles with the arc is defined as the total times of the segment intersects the circle from left to right minus the total times of the segment intersects the circle from right to left. Let I_K denote the sum of the algebraic intersection numbers of the resulting circles with the arc. None of the crossings of K that contributes non-trivially to the total algebraic intersection number, is smoothed since such a crossing is met only once. As a result, I_K is equal to the sum of algebraic intersection numbers of the loop at the crossing $\hat{C}$ with the strands intersecting $l(\hat{C})$. This shows that the sum of algebraic intersection numbers of the circles with the arc is equal to either $w_-(\hat{C})$ or $w_+(\hat{C})$. Thus, the absolute value of I_k is m. On the other hand, it is easy to verify that the number $|I_k|$ can be at most as large as the number of the circles that are enclosing the endpoints (the tail or the head). In particular, $|I_k|$ is equal to the number of the circles if all intersections are positive. Thus we have that m is at most the number of circles enclosing the endpoints.
The height of the diagram K is at least as large as the number of the circles enclosing the endpoints, by the Jordan curve theorem. Then $h(K) \geq m$. So m turns out to be the maximum degree of the affine index polynomial of any classical knotoid diagram equivalent to K. This implies that there is a crossing with weight m in each representative knotoid diagram of k. Applying the

same procedure explained above applied to the loops of the crossings with weight m in each representative diagram gives us the inequality, $h(k) \geq m$ for any representative classical diagram of k. $\square$

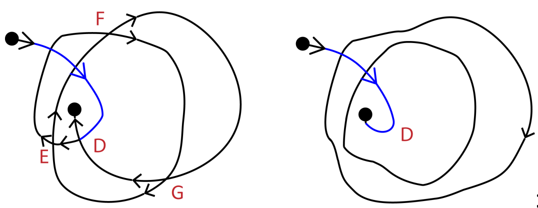
Example:



	w_+	w_-
B	-1	1
C	-2	2
D	2	-2
E	1	-1
F	-1	1
G	1	-1

;

Now we see loop of the crossing D and resulting circles and the arc:

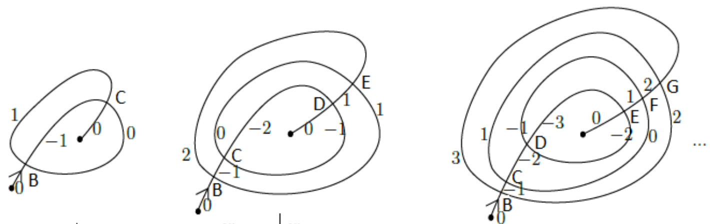


;

The height of knotoid is the minimum of all heights of diagrams, one consequence of the previous theorem is that we can get the minimum of all height of diagrams by means of a spiral diagram with positive crossings.

The knotoids each represented by a diagram overlying the flat diagrams with positive crossings:

K_1 K_2 K_3



	w_+	w_-
B	−1	+1
C	+1	−1

	w_+	w_-
B	−2	+2
C	−1	+1
D	+2	−2
E	+1	−1

	w_+	w_-
B	-3	+3
C	-2	+2
D	-1	+1
E	+3	-3
F	+2	-2
G	+1	-1

Figure 3.4: Example

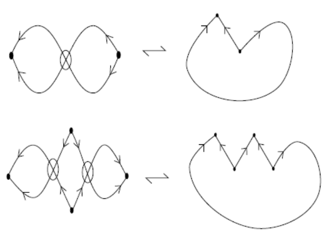
We have the following affine index polynomials:
$P_{K_1}(A) = A + A^{-1} - 2$
$P_{K_2}(A) = A^2 + A + A^{-1} + A^{-2} - 4$
$P_{K_3}(A) = A^3 + A^2 + A + A^{-1} + A^{-2} + A^{-3} - 6.$
The heights of the given diagrams are 1, 2 and 3, respectively by the previous theorem.
Generalization: The affine index polynomial of a classical knotoid represented by an n-fold spiral knotoid diagram has a term of the form $A^n + A^{-n}$ if all crossings of the diagram are positive. The maximum degree of the affine index polynomial is n and the height of the spiral diagram is n. By the previous theorem we conclude that the height of the knotoid is n. This shows that we have an infinite set of knotoids whose height is given by the affine index polynomial.
If we consider the flat knotoid K_3 with C, D, E negative crossings and B, F, G positive crossings, it has trivial affine index polynomials.
$P_{K_3}(A) = +(A^{-3}-1)-(A^2-1)-(A-1)-(A^{-3}-1)+(A^2-1)+(A-1) = 0$
There are examples of proper knotoids with trivial affine index polynomial so that the affine index polynomial gives trivial lower bound for the height of knotoids.
So the polynomial gives trivial information about the height of the knotoid represented. An other knotoid invariant that gives a non trivial information about the height is the arrow polynomial. Using the arrow polynomial we

can see that K_3 has height 3.

3.7.2 The arrow polynomial and the height of spherical knotoids

The arrow polynomial can be used for estimating the height of a knotoid in S^2.

Remark 3.7.1. The arrow polynomial of virtual knot is computed in a similar way of the arrow polynomial of classical knotoid (see the subsection 3.1.2) but when we calculate the arrow polynomial of virtual knot we have the variables K_i that are assigned to the closed components with surviving cusps (see articles [3]and [4] of references).
In other words, a closed component with two cusps forming a zig-zag contributes as K_1 to the polynomial. In general, a closed component with zig-zags formed by $2i$ alternating cusps, contributes as a variable, K_i to the arrow polynomial.



Definition 3.7.2. A closed component with $2i$ irreducible cusps contributes as a K_i-variable to the arrow polynomial. The arrow polynomial of virtual knot k^* is given by:

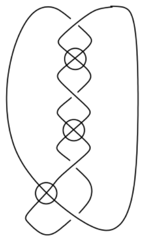
$$\mathbb{A}(k^*) = (-A^{-3})^{\mathrm{wr}(k^*)}[k^*] = (-A^{-3})^{\mathrm{wr}(k^*)} \sum_{s \in S(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\rho(s)-1} K_{i(s)}$$

where: $S(K)$ is the set of states of virtual knot diagram, $\sigma(s)$ is the sum of signs of all smoothings of state s, $\rho(s)$ is the number of components of the state s (once smoothed all crossings) and $K_{i(s)}$ is the variable assigned to each closed component of a state with $i(s)$ surviving cusps.
Notice that the addends of the arrow polynomial have the form: $A^m K_{i_1}^{j_1} K_{i_2}^{j_2} ... K_{i_n}^{j_n}$.
The K-degree of the addend is:

$$i_1 \times j_1 + ... + i_n \times j_n.$$

The maximum K-degree of the arrow polynomial is the maximum K-degree of the addends.

Example:



$$\mathbb{A}(k^*) = A^2K_3 + 1 - A^{-2}K_1K_2 - A^2K_1K_2 + A^{-2}K_1$$

K-degree of the 1° addend is 3 because $3 \times 1 = 3$.
K-degree of the 2° addend is 0 because there is not K_i.
K-degree of the 3° addend is 3 because $1 \times 1 + 2 \times 1 = 3$.
K-degree of the 4° addend is 3 because $1 \times 1 + 2 \times 1 = 3$.
K-degree of the 5° addend is 1 because $1 \times 1 = 1$.
So the maximum K-degree is 3.
(For other examples see the reference [16]).

Definition 3.7.3. The virtual crossing number of a virtual knot/link is the minimum number of virtual crossings over all representative diagrams.

The problem of determining the virtual crossing number of a virtual knot or link is a fundamental problem in virtual knot theory. We have the following theorem:

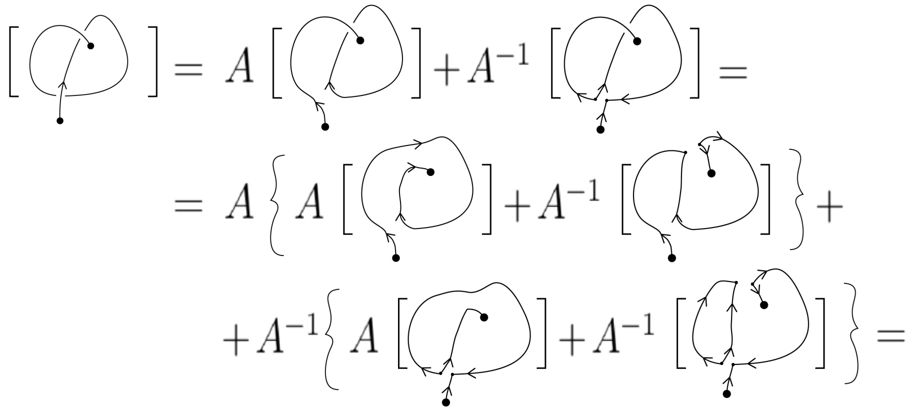
Theorem 8. *The virtual crossing number of a virtual knot/link is greater than or equal to the maximum K-degree of the arrow polynomial of that virtual knot/link. (see references [2], [14] and [15])*

Definition 3.7.4. In the arrow polynomial we have the variables $L_{i(s)}$ that is assigned to each arc of a state with $i(s)$ surviving cusps. The L-degree of the arrow polynomial is the maximum of $i \in \mathbb{N}$ assigned to $L_{i(s)}$ appearing in the arrow polynomial.

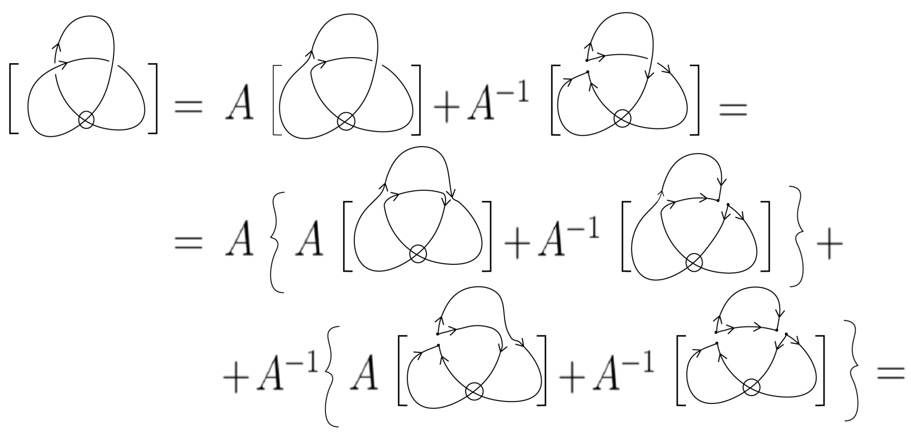
Let K be a knotoid diagram in S^2.
A closed component with $2i$ irreducible cusps contributes as a K_i-variable to the arrow polynomial.
Since circular components of an oriented state of knotoid are cusp-free, no

K_i-variables occur in the arrow polynomial of a knotoid in S^2.
However, closing the endpoints of a knotoid diagram via the virtual closure map turns L_i-variables into K_i-variables that are assigned to the closed components obtained via this closure.
Using this idea, we show that the L-degree of the arrow polynomial can be used as a lower bound for the height of knotoids in S^2.
So we have:
$L -$ degree of $\mathbb{A}(k) \leq$ virtual crossing number of the virtual knot $\bar{v}(K)$ $(\diamondsuit)$

Example: arrow polynomials of a knotoid and of its virtual closure
We compute the bracket polynomials for oriented states of a knotoid diagram K.



$= A^2 + L_1 + L_1 + A^{-2}(-A^2 - A^{-2})L_1 =$
$= A^2 + (2 + A^{-2}(-A^2 - A^{-2}))L_1 =$
$= A^2 + (1 - A^{-4})L_1$
Closing the endpoints of a knotoid diagram K via the virtual closure map we get a virtual knot $\bar{v}(K)$. Now we compute the bracket polynomials for oriented states of virtual knot $\bar{v}(K)$.



$= A^2 + K_1 + K_1 + A^{-2}(-A^2 - A^{-2})K_1 =$
$= A^2 + (2 + A^{-2}(-A^2 - A^{-2}))K_1 =$
$= A^2 + (1 - A^{-4})K_1$
So the arrow polynomials are:
$\mathbb{A}(K) = (-A^{-3})^{\mathrm{wr}(K)}[K] = (-A^{-3})^2[A^2 + (1 - A^{-4})L_1] =$
$= A^{-6}[A^2 + L_1 - A^{-4}L_1] = A^{-4} + A^{-6}L_1 - A^{-10}L_1$
$\mathbb{A}(\bar{v}(K)) = (-A^{-3})^{\mathrm{wr}(\bar{v}(K))}[\bar{v}(K)] = (-A^{-3})^2[A^2 + (1 - A^{-4})K_1] =$
$= A^{-6}[A^2 + K_1 - A^{-4}K_1] = A^{-4} + A^{-6}K_1 - A^{-10}K_1$
The lower bound on the virtual crossing number is 1.

Theorem 9. *The height of a knotoid K in S^2 is greater than or equal to the L-degree of its arrow polynomial.*

Proof. Let $\tilde{K}$ be a classical knotoid diagram representing K. The height of the knotoid diagram $h(\tilde{K})$ is equal to the number of virtual crossings of $\bar{v}(\tilde{K})$, in other words, the minimum number of virtual crossings obtained by closing a classical knotoid diagram in virtual way is equal to the height of that diagram. By $(\diamondsuit)$ we get: $L - \text{degree of } \mathbb{A}(K) \leq h(\tilde{K})$.
The inequality above holds for any classical knotoid diagram equivalent to K since the L-degree of the polynomial is invariant under the Ω-moves.
So we have:

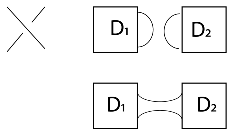
$$L - \text{degree of } \mathbb{A}(K) \leq h(K)$$

where $h(K)$ denotes the height of the knotoid K. □

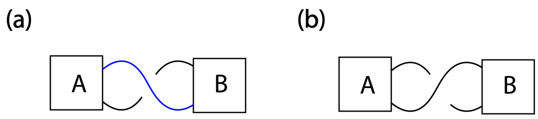
Example: Using the arrow polynomial we can see that K_3 (figure 3.4), with C, D, E negative crossings and B, F, G positive crossings, has height 3. The arrow polynomial of the knotoid:
$\mathbb{A}(K) = 1 + (-A^{-3} + A^{-2} + A^2 + A^6)\,\mathrm{L}_1 + (-2A^{-4} - 2A^4 + 4)\,\mathrm{L}_2 + (-A^{-6} + A^{-2} + A^2 + A^6)\,\mathrm{L}_3$. The L-degree of the arrow polynomial is 3 so by the previuous theorem, the height of the knotoid K is at least 3. It is not difficult to see that the height of the given diagram is also 3. Thus the height of the knotoid K is 3.

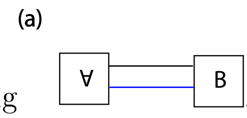
3.7.3 Alternating knots and alternating knotoids

Definition 3.7.5. Given D a knot diagram, the **separator crossing** is defined: if we cut a diagram in the separator crossing in one of these two ways we get a disconneted diagram.



Definition 3.7.6. Let $D \subset \mathbb{R}^2$ be a knot diagram.
D is **alternating knot diagram** *if and only* under- and over-crossings alternate along D. D is **reduced alternating knot diagram** *if and only* if there are no if there are no separating crossings, i.e. D is not:



Note that, if we overturn A we can eliminate the crossing 

.
If D is an alternating knot diagram, after the overturning the diagram is still alternating. We can eliminate the crossing in between A and B by either overturing A in the suitable sense or overturing B in the opposite one.

Definition 3.7.7. Let $k^* \subset \mathbb{R}^3$ **alternating knot** *if and only if* it admits an alternating diagram.
If k^* is a prime knot with $c(k^*) \leq 7 \Rightarrow k^*$ is alternating knot.

Definition 3.7.8. If $k^* \subset \mathbb{R}^3$ alternating knot $\Rightarrow$ there exists a reduced alternating knot diagram D of k^*.

($\Leftarrow$Tait conjecture)

(If the diagram is not "reduced" we can simplify it and each time the number of crossings decreases by one. This process ends and we get a reduced alternating knot diagram because we cannot make any further reductions.)

Definition 3.7.9. Tait conjecture
If D is a reduced alternating knot diagram of k^* then $c(D)$ is minimal, i.e. $c(D) = c(k^*)$

Definition 3.7.10. A **knotoid diagram** is **alternating** if traversing the diagram from the head to the tail one meets under- and over-crossings in an alternating order.

Proposition 3. All alternating knotoid diagrams in S^2 have height 0.

Proof. For a diagram K of positive height consider the region of $S^2 - K$ adjacent to the head of K. This region is not adjacent to the tail of K. Analyzing the over/under-passes of the edges of this region, we can observe that K cannot be alternating. $\square$

3.8 Crossing number of spherical knotoids

Definition 3.8.1. Given a knot $k^* \subset S^3$, the **crossing number** $c(k^*)$ is the minimal number of crossings in a knot diagram of k^*.
One can use knotoid diagrams to define two similar invariants $c_\pm(k^*)$ that by definition they are the minimal numbers of crossings of a knotoid diagram K such that $K_\pm = k^*$.
Note that $c_\pm(k^*) \leq c(k^*) - 1$ because the knotoid diagram of k^* can be obtained from a knot diagram of k with minimal number of crossings by cutting out an overpass (underpass) containing one crossing.
If a minimal diagram of k^* has an overpass (underpass) with $N \geq 2$ crossings, then $c_\pm(k^*) \leq c(k^*) - N$.

Definition 3.8.2. Given a knot k^*, we can construct a Seifert surface of a knotoid diagram K of k^* in this way: every crossing of K admits a unique smoothing compatible with the orientation (see figure 1.2.2) of K from the leg to the head. Applying these smoothings to all crossings, we obtain an oriented 1-manifold $\tilde{K} \subset S^2$.
This $\tilde{K}$ consists of an oriented arc $J \subset S^2$ (with the same endpoints of K) and several disjoint simple closed curves. The closed curves bound a system of disjoint disks in S^3 lying above S^2. We add a band $J \times [0,1]$ lying below S^2 and meeting S^2 along $J \times \{0\} = J$. The union of these disks with the band and with half-twisted strips at the crossings is a compact connected orientable surface in S^3 bounded by $K_- = k^*$. The genus of this surface is equal to $g(S) = \dfrac{c(K) - |\tilde{K}| + 1}{2}$ where $c(K)$ is the number of crossings of K and $|\tilde{K}|$ is the number of components of $\tilde{K}$.
So $g(k^*) \leq \dfrac{c(D) - |\tilde{D}| + 1}{2}$

Definition 3.8.3. Turaev conjecture Minimal diagrams (with respect to the crossing number) of knot-type knotoids have zero height.

To proof the Turaev conjecture we need of one definition and two theorems:

Definition 3.8.4. $K_1 < K_2$ means that K_1 is obtained by deleting some chords in the chord diagram of Gauss code (see definition 2.6.3) of K_2. This means that some classical crossings of K_1 are made virtual to obtain K_2.

Theorem 10. ***(Nikonov)***
There is a map pr from minimal genus virtual knot diagrams to classical knot

diagrams such that for every virtual knot diagram K we have $pr(K) < K$ and if two diagrams K_1 and K_2 are related by a Reidemeister move then their images $pr(K_1)$, $pr(K_2)$ are related to each other by a Reidemeister move

Theorem 11. ***(Manturov)***
For every virtual knot diagram K there exists a classical knot diagram D, such that $D < K$ and K admits the same Gauss diagram of D if and only if K is classical.

Proof. (Turaev conjecture) Let k be a knot-type knotoid and by absurd we assume that i.e: there is a minimal diagram of k, K_1 that has a non-zero height.
Let n be the number of crossings of K_1.
The virtual closure of K_1, $\bar{v}(K_1)$ is a virtual knot diagram with n classical crossings and a number of virtual crossings that is at least equal to the height of K_1. We know that k is a knot-type knotoid then the virtual closure of k, $\bar{v}(k)$ is a classical knot, and the virtual knot diagram $\bar{v}(K_1)$ lies in the virtual equivalence class of $\bar{v}(k)$ since the virtual closure map $\bar{v}$ is a well-defined map on the set of knotoids in S^2.
Now we compute the Euler characteristic in this way:

$$\chi(F(K_1)) = \#vertices - \#edges + \#discks = (n+2) - (2n+1) + \delta = -n + 1 + \delta$$

The genus of the closed connected orientable surface $F(K_1)$ obtained by attaching 2-disks to the boundary components of the abstract knotoid diagram surface associated to K_1 (to more details see [4]) is given by:

$$g(F(K_1) = \frac{2 - \chi(F(K_1))}{2} = 1 + \frac{(n-1) - \delta}{2} = 0$$

where n is the crossing number of K_1 and δ is the number of boundary components of the abstract knotoid diagram. This is equal zero because K_1 has only classical crossings.
The number of boundary components of the associated abstract knotoid diagram (i.e δ) is equal to the number of planar regions (see definition 2.1.7) determined by the diagram K_1. We can see that the boundary components that are adjacent to the endpoints of K_1, are distinct since the endpoints of K_1 are in different regions.
Furthermore, connecting the endpoints of K_1 virtually we get $\bar{v}(K_1)$ and it does not change the number of classical crossings but reduces the number of boundary components by 1 (i.e. $\delta - 1$)).
In a similar way as above the genus of the closed connected orientable surface $F(\bar{v}(K_1))$ obtained by attaching 2-disks to the boundary components of the abstract knot diagram surface associated to $\bar{v}(K_1)$ is given by the following formula:

$$g(F(\bar{v}(K_1)) = 1 + \frac{n - (\delta - 1)}{2} = g(F(K_1) + 1 = 1$$

By Nikonov's theorem, any minimal diagram of $\bar{v}(k)$ has strictly less than n classical crossings. Let $\bar{K}$ be any minimal diagram of $\bar{v}(k)$, and $\bar{K}$ has m classical crossings, then $m < n$.
The image of $\bar{K}$ under the map α (definition 2.2.3) is a knot-type knotoid diagram K with m crossings.
The underpass closures of knotoids diagrams K and K_1 are isotopic to knot $\bar{v}(k)$, this implies that K and K_1 are equivalent to each other since the underpass closure is a bijective map on the knot-type knotoids.
We have assumed that K_1 is a minimal diagram of k, then $n < m$ and this contradicts the above inequality. So, the assumption is wrong and the theorem follows.

□

Remark 3.8.1. Turaev conjecture gives the following result: The crossing number of a knot-type knotoid is equal to the crossing number of the knot that is the closure of the knotoid.

The problem of determining the exact value of the crossing number of a knotoid is very complicated. Any diagram gives an upper bound of the value but not many lower bounds are known.

3.8.1 The bracket polynomial and the crossing number

When defining the bracket polynomial, we have seen the notion of state of a knotoid diagram that is a simple curve in S^2 obtained smoothing each crossing in two different ways in figure 3.1. This yields a single arc (with endpoints) and several disjoint circles.

Definition 3.8.5. Given a bracket polynomial

$$\langle K \rangle = \sum_{s \in S(K)} A^{\sigma(s)}(-A^2 - A^{-2})^{\rho(s)-1} \in \mathbb{Z}[A^{\pm 1}],$$

the span of a knotoid diagram K is defined by

$$\text{spn}(K) = \text{spn}(\langle K \rangle) = \max\ \exp(\langle K \rangle) - \min\ \exp(\langle K \rangle)$$

Lemma 6. Let $K \subset \Sigma$ a knotoid diagram with n crossings then:
1) $\max \exp(\langle K \rangle) \leq n + 2\rho(s_+) - 2$
2) $\min \exp(\langle K \rangle) \leq -n - 2\rho(s_-) + 2$

Proof. The bracket polynomial is $\langle K \rangle = \sum_{s \in S(K)} A^{\sigma(s)} (-A^2 - A^{-2})^{\rho(s)-1}$, so

$$\max \exp(\langle K \rangle) = \sigma(s) + 2(\rho(s) - 1)$$
$$\min \exp(\langle K \rangle) = \sigma(s) - 2(\rho(s) - 1)$$

If we consider $s \in S(K)$, it is a state where there are some positively smoothed and some negatively smoothed crossings.
We can pass from state s to state s_+ through a sequence of states $s = s_0, s_1, ..., s_r = s_+$ where we change only one smoothing between one state and the next.
We immage to change all the negative smoothings of the state s to positive smoothings one by one.
The sum of signes of s_i is $\sigma(s_i) = \sigma(s_{i+1}) - 2$.
The number of components is $\rho(s_i) = \rho(s_{i+1}) \pm 1$.
Each time we reverse a smoothing, the number of components can increase or decrease by one.
We consider the maximum exponent

$$\sigma(s_i) + 2\rho(s_i) - 2 \leq \sigma(s_{i+1}) + 2\rho(s_{i+1}) - 2$$

this is true for every step, then

$$\sigma(s) + 2\rho(s) - 2 \leq \underbrace{\sigma(s_+) + 2\rho(s_+) - 2}_{= \, n}$$

Then, we get 1).
Similarly, to see 2) we have a sequence from s to s_-, we immage to change positive smoothings of the state s to negative smoothings one by one. □

Proposition 4. Let $K \subset \Sigma$ be a connected knotoid diagram (that is the flat knotoid diagram associated to K is connected).
Let $s_\pm \in S(K)$ the unique state of K such that $\sigma(s_\pm) = \pm c(K)$ then

$$\rho(s_+) + \rho(s_-) \leq c(K) + 2.$$

If K is alternating : $\rho(s_+) + \rho(s_-) = c(K) + 2$

Proof. By induction on the number of crossings :
If $c(K) = 0$ then we have trivial knotoid $K =$ .
In this case the states s_+ and s_- are equal because there are no a crossings to be smoothed then $\rho(s_+) = \rho(s_-) = 1$ and hence $\rho(s_+) + \rho(s_-) \leq c(K) + 2$ is true, it will be $2 \leq 2$.
Suppose we have $c(K) > 0$. We consider an any crossing and its smoothings.
If K is connected then K_0 or K_∞ must be connected and we call the connected one $K' = K_0$ or K_∞. We get $c(K') = c(K) - 1 < c(K)$ then we

$K \quad K_0 \quad K_\infty$

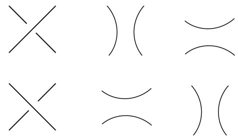


Figure 3.5: Smoothings of crossing

apply the induction Suppose to solve all crossings of K' in positive way (K_0) and we get s'_+.

$$K' = \begin{cases} K_0 & \rho(s'_+) = \rho(s_+) \quad , \quad \rho(s'_-) = \rho(s_-) \pm 1 \\ \text{or} & \\ K_\infty & \rho(s'_+) = \rho(s_+) \pm 1 \quad , \quad \rho(s'_-) = \rho(s_-) \end{cases}$$

If $K' = K_0$ then the crossing is positively smoothed. Now if we take the state in which the other crossings are positively smoothed, we obtain the state of K where all the crossings are positively smoothed s_+.
So we have $s'_+ = s_+$ and $\rho(s'_+) = \rho(s_+)$.
Therefore if we smooth the first crossing in positive way, we obtain s'_- where the first crossing is positively smoothed an the other crossings are negatively smoothed.
The state s'_- is different from s_- because s_- is the state where all crossing are negativly smoothed.
To pass from s'_- to s_-, we must change the smoothing of the first crossing and in this case the number of components increase or decrease by 1.
Similarly if $K' = K_\infty$ then the crossing is negatively smooth. We get:

$$\rho(s_+)+\rho(s_-) \leq \rho(s'_+) = \rho(s'_-)+1 \leq c(K')+2+1 = c(K)-1+2+1 = c(K)+2$$

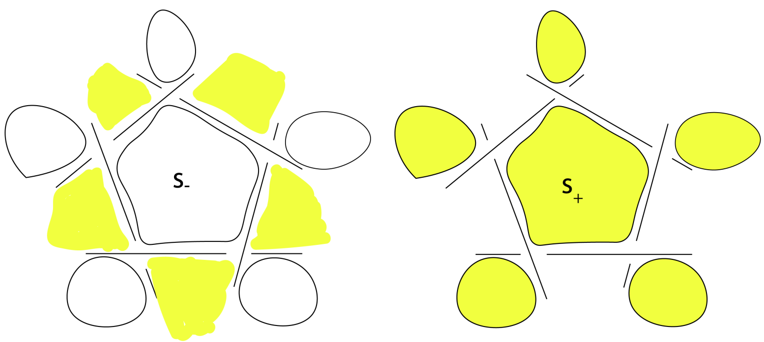
If K is alternating then (by proposition 3 and the Turaev conjecture) K is a diagram of knot-type knotoid; we can close the knotoid diagram and we obtain an alternating knot diagram.
So, if $h(K) = 0$ we can close the knotoid diagram we get a knot diagram D and we can see that there is a one-to-one correspondence:

state $s_\pm \longleftrightarrow$ white and yellow regions of a checkerboard coloring of the diagram D

When we draw a diagram and we think it as a graph (or flat diagram), it divides a surface Σ in a finite number of regions. At each crossing we have 4 regions and we color them one yellow, the next white,...in altertating way.

Suppose we consider in any region bounded by the alternating diagram D of knot:

(A) (B)



In the Figure (A): turning in a counterclockwise way, each edge of the region begins with an overpass and it ends with an underpass.
In Figure (B): turning in a counterclockwise way, each edge of the region begins with an underpass and it ends with an overpass.
If we consider the negative smoothing in all crossing of the region diagram (A), s_- is the number of the white regions while s_+ is the number of the yellow regions.
If we consider the positive smoothing in all crossing of the region diagram (B), s_+ is the number of the white regions while s_- is the number of the yellow regions.
The idea is $\rho(s_+) + \rho(s_-) =$ number of white and yellow regions
Now, using the Euler theorem (For every polygonation of S^2 we have $\#\{\text{polygons}\} - \#\{\text{edges}\} + \#\{\text{vertices}\} = 2$), we get

$$\#\{\text{polygons}\} = \#\{\text{regions}\} = \rho(s_+) + \rho(s_-),$$

and so

$$\#\{\text{vertices}\} = \#\{\text{crossings}\} = c(D).$$

At every vertex there are 4 edges, every edge has 2 vertices then

$$\#\{\text{edges}\} = 4\#\{\text{vertices}\}/2 = 2\#\{\text{vertices}\} = 2c(D).$$

So we get

$$\rho(s_+) + \rho(s_-) - 2c(D) + c(D) = 2,$$

hence $\rho(s_+) + \rho(s_-) = c(D) + 2$.

$\square$

Theorem 12. *Let Σ be an oriented surface. For any knotoid diagram $K \subset \Sigma$ with n crossings,*

$$\operatorname{spn}(\langle K \rangle) = \operatorname{spn}(J_K(A)) \leq 4n \qquad (\star)$$

Proof. By the previous lemma and $\rho(s_+) + \rho(s_-) \leq 2 + n$:

$$\begin{aligned}\operatorname{spn}(K) = \operatorname{spn}(\langle K \rangle) = \max\exp(\langle K \rangle) - \min\exp(\langle K \rangle) \leq \\ \leq (n + 2\rho(s_+) - 2 + n + 2\rho(s_-) - 2) \leq 4n\end{aligned}$$

$\square$

Remark 3.8.2. The factor $(-A^{-3})^{\mathrm{wr}(K)}$ of the Jones polynomial appears in all terms of the polynomial and when we calculate the maximum degree minus the minimum degree, this factor is irrelevant.

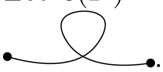
Remark 3.8.3. The theorem implies that for any knotoid k in Σ,

$$\operatorname{spn}(\langle K \rangle) \leq 4c(k),$$

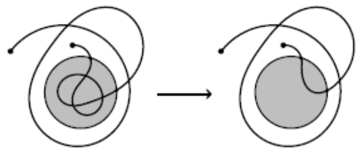
where $c(k)$ is the crossing number of k defined as the minimal number of crossings in a diagram of k.

Remark 3.8.4. $\operatorname{span}(\langle K \rangle) = 4n$ if the knotoid diagram is alternating.

Lemma 7. For an arbitrary FKD F, the inequality $c(F) \geq 2h(F)$ is valid.

Proof. We proceed by induction on $c(F)$.
Let $c(F) = 1$. There exists exactly one FKD F for which $c(F) = 1$, i.e. . The height of FKD is equal to 0 then $c(F) \geq 2h(F)$ is holds.
Let $c(F) > 1$.
If F is not prime, then at least one of conditions (i) and (ii) in the definition 2.5.2 of a prime FKD does not hold.
(i)Every embedded circle meeting F transversely in exactly two points bounds a disk meeting F along a proper embedded arc or along two disjoint embedded arcs adjacent to the endpoints of F.
(ii) Every embedded circle meeting F transversely in exactly one point bounds a regular neighborhood of one of the endpoints of F.
So, there is an embedded circle C which intersects F in 1 or 2 points and such that each disk bounded by C contains at least one crossing. If the circle

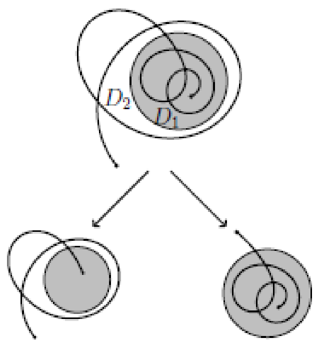
C intersects F in exactly 2 points (i.e. the condition (ii) does not hold) then one of disks bounded by C (denote it by D) does not contain the endpoints of F. Consider the FKD F' obtaining from F by contracting the disk D to a point or, equivalently, by replacing the fragment inside D with a simple arc connecting the same point in ∂D.



Then we have $c(F) > c(F')$ and $h(F) = h(F')$.
By induction assumption $c(F) \geq 2h(F')$, hence

$$c(F) > c(F') \geq 2h(F') = 2h(F)$$

If the circle C intersects F in exactly 1 points (i.e. the condition (i) does not hold), then C cuts F into two non-trivial FKD F_1 and F_2 which lie inside different disks bounded by C. F_1 and F_2 are obtained as a result of a contracting into a point the disks D_1 and D_2 respectively. In these disks the circle C cuts the sphere S^2.



Then

$$c(F) = c(F_1) + c(F_2)$$
$$c(F) > c(F_i) \quad i = 1, 2$$
$$h(F) = h(F_1) + h(F_2)$$

By induction assumption $c(F_i) \geq 2h(F_i)$, $i = 1, 2$, hence

$$c(F) = c(F_1) + c(F_2) \geq 2h(F_1) + 2h(F_2) = 2h(F)$$

If F is prime, then for the following Theorem 13 the inequality $c(F) \geq 2h(F)$ is true. □

Theorem 13. *If F is a prime FKD then*

$$c(F) \geq 2h(F)$$

We omit the proof that you can find in the reference [12]).

Now, the following theorem is fundamental to find a lower bound for the crossing number of knotoid.

Theorem 14. *For a knotoid K*

$$c(K) \geq 2h(K)$$

and there exists an infinite family of knotoids for which the inequality becomes equality.

Proof. Given a knotoid K and a minimal diagram D of it, that is c(D)=c(K). Consider a FKD F (see definition 2.5.1) that is obtained from D as a result of forgetting over/under-crossing information in all crossings. By definition the height of knotoid is the minimum of the height over all representative diagram $h(F) \geq h(K)$ and using the Lemma 7, we get:

$$c(K) = c(F) \geq 2h(F) \geq 2h(K).$$

□

3.8.2 A lower bound for the crossing number of a knotoid via the extended bracket polynomial

Definition 3.8.6. EXTENDED BRACKET POLYNOMIAL of knotoids
Let K be a knotoid diagram in S^2. Let $a \subset S^2$ be a shortcut for K.
Given a state $s \in S(K)$, consider the smoothed 1-manifold $K_s \subset S^2$ and its arc component k_s (the smoothing of K is effected in small neighborhoods of the crossings disjoint from a).
Then, k_s coincides with K in a small neighborhood of the endpoints of K.
In particular, the set $\partial k_s = \partial a$ is formed of the endpoints of K.
We orient K, k_s and a from the leg of K to the head of K.
Let $k_s \cdot a$ be the algebraic number of intersections of k_s with a, that is the number of times k_s crosses a from the right to the left minus the number of times k_s crosses a from the left to the right (the endpoints of k_s and a are not counted). Similarly, let $K \cdot a$ be the algebraic number of intersections of

K with a.
The extended bracket polynomial is given by:

$$\langle\langle K\rangle\rangle = (-A^3)^{-w(K)} u^{-K\cdot a} \sum_{s\in S(K)} A^{\sigma(s)} u^{k_s\cdot a} (-A^2 - A^{-2})^{\rho(s)-1} \in \mathbb{Z}[A^{\pm 1}, u^{\pm 1}]$$

Lemma 8. The polynomial $\langle\langle K\rangle\rangle$ does not depend on the choice of the shortcut a and it is invariant under the Reidemeister moves on K.

Proof. Any two shortcuts for K are isotopic in the class of embedded arcs in S^2 connecting the endpoints of K. Therefore to verify the independence of a it is enough to analyze the following local transformations for a:
(1) pulling a across a strand of K (this adds two points to $a \cap K$);
(2) pulling a across a double point of K;
(3) adding a curl to a near an endpoint of K (this adds a point to $a \cap K$).
The transformations (1) and (2) preserve the numbers $K \cdot a$ and $k_s \cdot a$ for all states s of K.
The transformation (3) preserves $k_s \cdot a - K \cdot a$ for all s.
So, $\langle\langle K\rangle\rangle$ is preserved under these transformations and does not depend on a. Now we consider the 'unnormalized' version $\langle\langle K, a\rangle\rangle$ of $\langle\langle K\rangle\rangle$ i.e.

$$\langle\langle K, a\rangle\rangle = \sum_{s\in S(K)} A^{\sigma(s)} u^{k_s\cdot a} (-A^2 - A^{-2})^{\rho(s)-1}$$

The polynomial $\langle\langle K, a\rangle\rangle$ depends on a but does not depend on the orientation of K (to compute $k_s \cdot a$ one needs only to remember which endpoint is the leg and which one is the head). The polynomial $\langle\langle K, a\rangle\rangle$ satisfies the relation:

$$\langle\langle K, a\rangle\rangle = A\langle\langle K_0, a\rangle\rangle + A^{-1}\langle\langle K_\infty, a\rangle\rangle$$

where K_0 and K_∞ are obtained from K by the smoothings of a certain crossing(see figure 3.5).
$\langle\langle K, a\rangle\rangle$ is invariant under the second and third Reidemeister moves and it is multiplied by $-A^{\pm 3}$ under the first Reidemeister moves. Such moves preserve the number $K \cdot a$ and therefore they preserve $\langle\langle K\rangle\rangle$. Since the polynomial does not depend on a, it is invariant under all Reidemeister moves on K. □

Definition 3.8.7. The A-span and the u-span
Let $F \in \mathbb{Z}[A^{\pm 1}, u^{\pm 1}]$ be a polynomial.
We consider F as a finite sum $\sum_{i,j\in\mathbb{Z}} F_{i,j} A^i u^j$, where $F_{i,j} \in \mathbb{Z}$.
If $F \neq 0$, we define two numbers:

(1)$\text{spn}_A(F) = i_+ - i_-$ where i_+ (i_-) is the maximal (the minimal) integer i such that $F_{i,j} \neq 0$ for some j;
(2) $\text{spn}_u(F) = j_+ - j_-$ where j_+ (j_-) is the maximal (the minimal) integer j such that $F_{i,j} \neq 0$ for some i.
For a knotoid k in S^2, set $\text{spn}_A(k) = \text{spn}_A(\langle\langle k \rangle\rangle)$ and $\text{spn}_u(k) = \text{spn}_u(\langle\langle k \rangle\rangle)$. Both these numbers are even (non-negative) integers. So we get:

$$\text{spn}(k) \leq \text{spn}_A(k) \leq 4c(k)$$
and
$$\text{spn}_u(k) \leq 2(k_s \cdot a) = 2h(k)$$

where $c(k)$ is the crossing number of knotoid and $h(k)$ is the height of knotoid. So we obtained a *lower bound for the height of a knotoid* via the extended bracket polynomial. These inequalities are proved similarly to ($\star$).

By the theorem 14 we obtain the following statement

Corollary 1. For a knotoid K

$$c(K) \geq \text{spn}_u(\langle\langle k \rangle\rangle)$$

3.8.3 A lower bound for the crossing number of a knotoid via the affine index polynomial and the arrow polynomial

Recall the following theorems:
Theorem 7 Let K be a knotoid in S^2. The height of K is greater than or equal to the maximum degree of the affine index polynomial of K.
Theorem 9 The height of a classical knotoid K is greater than or equal to the L-degree of its arrow polynomial.
By the theorem 14 we obtain the following statement

Corollary 2. For a knotoid K

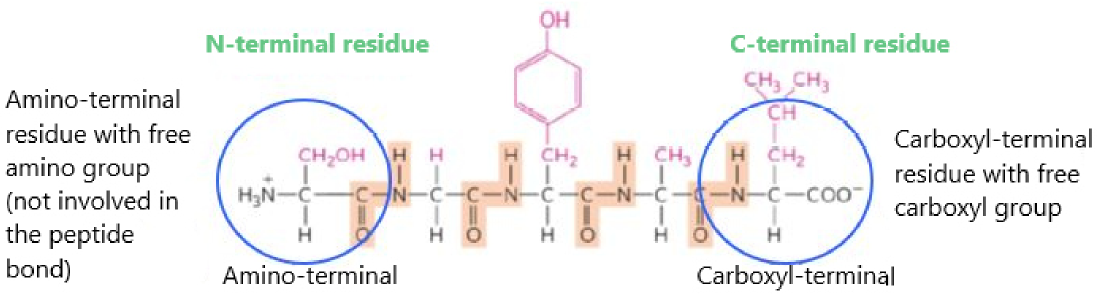
$$c(K) \leq 2 \max\exp(P_K(A))$$
and
$$c(K) \leq 2 \max\exp(\mathbb{A}(K))$$

where $\max\exp(P_K(A))$ and $\max\exp(\mathbb{A}(K))$ denote respectively the maximum degree of the affine index polynomial and L-degree of the arrow polynomial of K.

Chapter 4

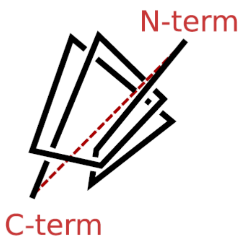
Knotoids and protein chains

A protein chain is a polymer formed by the union of **amino acids** and the bond between two amino acids is the **peptide bond**. We can imagine a protein as a pearl necklace where each pearl is an amino acid. (see Appendix C)

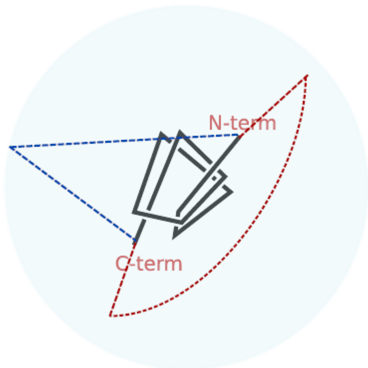


In the last twenty-five years numerous studies have revealed that there are proteins whose main chain fold into non-trivial topologies and this implies the presence of knots in their conformation.
The precise nature of the structural and functional advantages created by the presence of knots in the protein backbone is a subject of high interest from both experimental and theoretical point of view. To better understand this open problem, several attempts have been made towards the characterization and classification of the protein chains based on their knot type.
A protein chain, to perform its biological function, has to reach first its native folded state. Proteins in their native folded structure are frequently quite rigid and a continuous deformation from protein chain to a straight line is not allowed.
So the analysis of their knottedness has to be done for their open chains with fixed geometry. A protein is represented as an open polygonal chain.

Early approaches to the study the knottedness of protein chain required closure of the protein polypeptide because available mathematical tools that could be used to determine the knot type could only analyse closed curves. With the word *closure* we mean an artificial extension of the open polygonal curve representing the polymer chain that we want to study, so that its ends are connected and we get a closed curve. Various methods of chain closure have been proposed, for example:
(A)*Direct closure:* The polygonal is closed by connecting its ends with a straight line;



(B)*Stochastic closure:* This approach is based on a "statistical definition of knottedness", by which a set of closures is defined. Two variants of this scheme have been defined:



-(In blue on the figure)We consider a sphere that enclose the whole curve (the protein chain). We generate a set of N points r_i, uniformly distributed on this sphere. N different closures of the curve are then defined by connecting each r_i to both ends. This gives us a spectrum of topologies, in which the most populared state is chosen as the topology of protein chain.
In those cases in which no clear dominant state emerges, no knot type is assigned. The randomized direction of the chain extensions implies that interference with the polymer can occur in a relevant number of cases.

-(In red on the figure) In the second variant, proposed by Mansfield, the procedure is the same, with the difference that N pairs of points r_i are generated on the sphere that encloses the protein chain. Each point of the pair is connected by a straight segment to one of the two curve ends, and then they are joined with an arc on the enclosing sphere.
After closure, formed knots identification is achieved via computation of a knot polynomial; all knots that are encountered within the backbone of a protein are relatively simple and thus they can be identified by polynomial invariants of knots such as the Jones polynomial for example.

Example of stochastic closure:

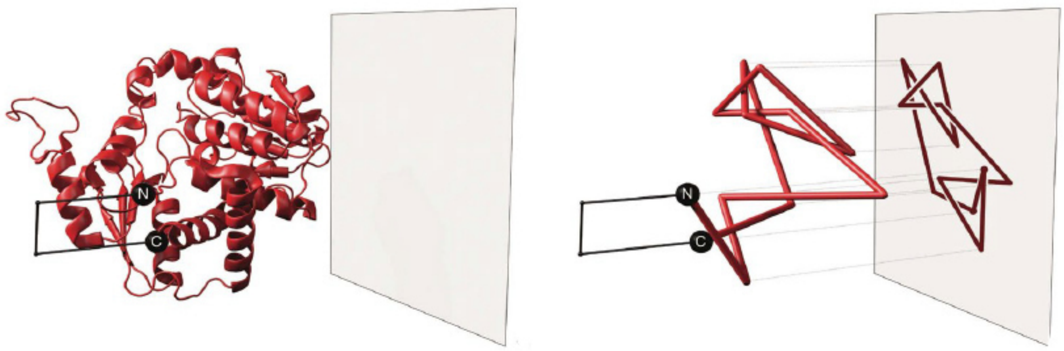


Figure 4.1: We consider a closing direction and two rays extending (paralleling to closing direction) from the ends to the sphere's surface that enclose the protein chain. On the right of the figure, we can see the resulting knot diagram.

With the discovery of the *concept of knotoids* we have a big news: the topology of open chains can be analyzed using just projections of these chains without the need to close them.
Hence, we consider that the protein chain is a knotoid where the N-terminal of the chain is the "tail" of knotoid and the C-terminal is the "head" of knotoid.

Example:

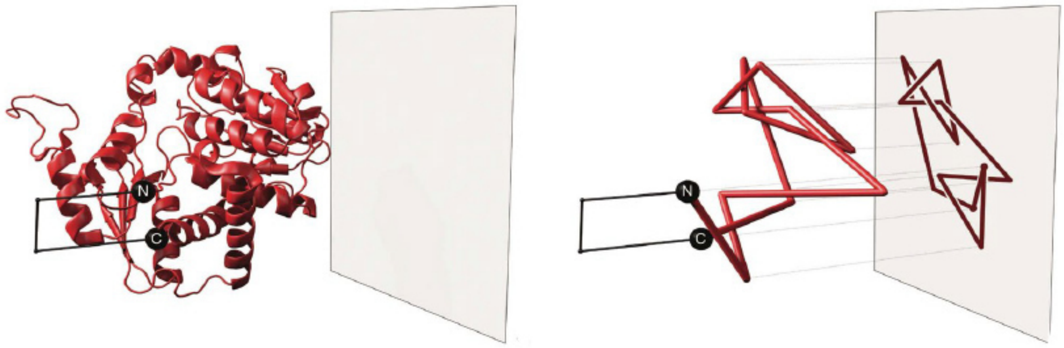


Figure 4.2: We consider a plane and two black infinite lines that pass through the N-terminal and C-terminal of the protein chain. These two lines are perpendicular to the chosen plane. On the right of the figure we can see the resulting knotoid diagram.

4.1 Database KnotProt 2.0

The KnotProt 2.0 is an online database that collects information about proteins using the concepts of knot and knotoid.
We will focus on how it uses the **knotoid approach** to analyse knottedness of entire protein chains and of their all possible subchains.

4.1.1 The study the global entanglement of protein chains

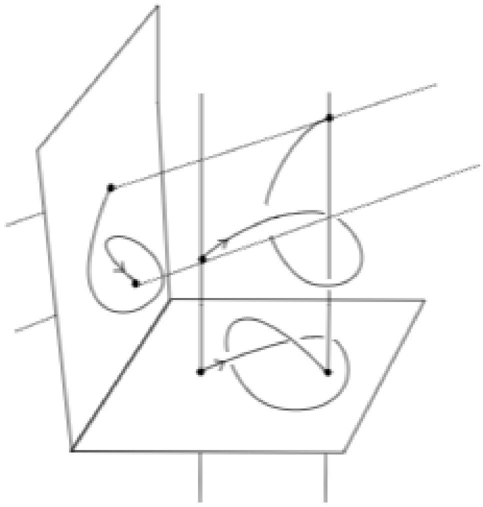
KnotProt 2.0 is based on the results of a software KNOTO-ID.
Now we want to describe the implementation of this software.
Each protein chain in space is considered as a polygonal curve, we trace the coordinates of its essential contituents, that is the carbon atoms that are contained in the amino acids that form the protein (also called C_α atoms) (to see the structure of the amino acid in appendix C) The coordinates of the C_α atoms of the protein backbone can be extracted from a pdb file downloaded from the PDB (www.rcsb.org).
Proteins appear in various, often very complicated, conformations and the study of their topology is very difficult.
The projection of protein chain is simplified using Reidemaister moves and

the **triangle elimination** (or KMT (Koniaris-Muthukumar-Taylor) algorithm):
- we choose a projection plane and then we take consecutive triples of points of the curve;
- we check if the surface of the triangle that the three points form is pierced by any other part of the curve or by any of the two infinite lines that pass through the endpoints: if it isn't pierced, we remove the middle point of the triplet;
- we repeat the process with the next triplet and so on.
The protein chain lies into a large enough sphere. In this case each point of the sphere corresponds to a projection direction on a surface that lies outside the sphere.
When the projection direction is determined, we consider the two infinite lines and we apply the simplification KMT algorithm on the chain.
We projecte the protein chain on a perpendicular sphere to the chosen direction and we obtain a specific knotoid.
Each knotoid type is assegned a color and, hence we color the point of the sphere's surface that corrisponds to a chosen direction with the corrispondent color of the knotoid that we obtain projecting in this direction.

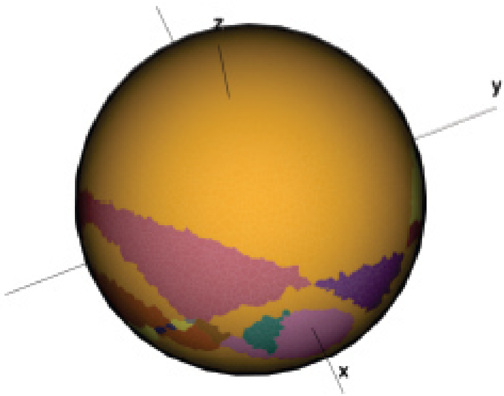
Each distinct region corresponds to the projection directions that produce the same knotoid type.
In the section 2.2, we have seen the differences between planar and spherical knotoids. We can further refine the projection globe of an open protein chain, by forbiding to push arcs around the surface of the sphere and considering projections of the chain on a plane instead. This will allow projections that were previously detected as unknotted to emerge as non-trivial planar knotoids.
Finally, a topological invariant is evaluated on the knotoid diagram.
In particular the Jones polynomial and the arrow polynomial is evalueted for curve projected on a sphere, while for curves projected on a plane we will consider the Turaev loop bracket polynomial and the loop arrow polynomial.
The knotoid type corresponding to the resulting polynomial can be obtained using the list knotoid types distributed with Knoto-ID.
The spectrum of knotoid types can be visualized using projection maps generated by Knoto-ID.

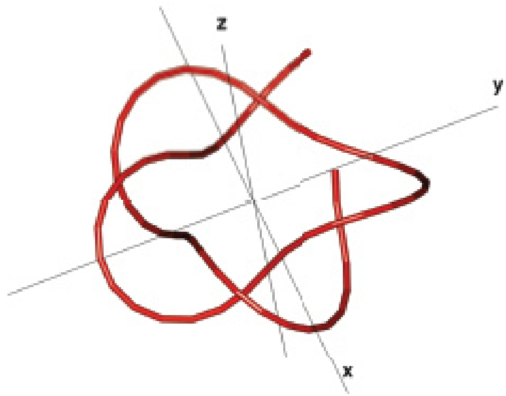
Remark 4.1.1. A three-dimensional curve corresponds to many different knotoid diagrams since different projection directions may yield different

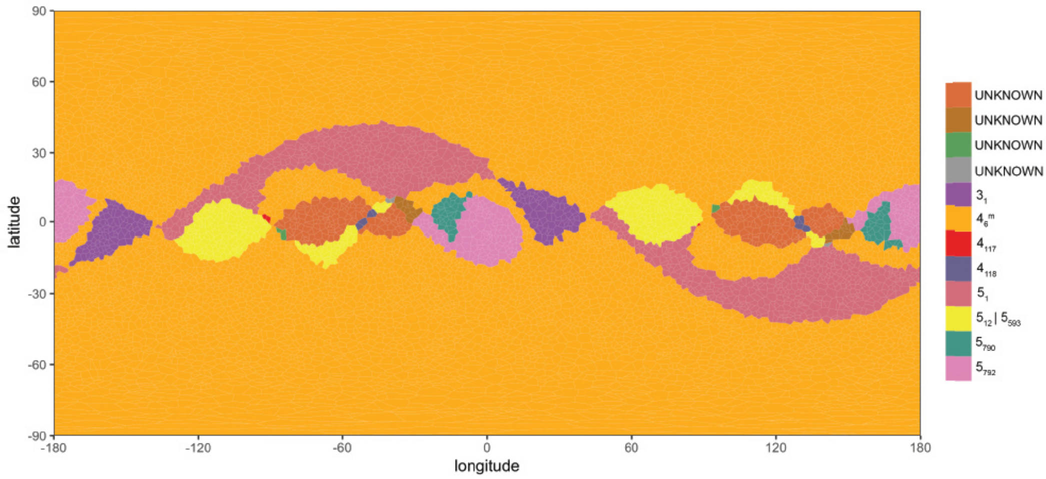
and non-equivalent diagrams. The knottedness of an embedded curve in the 3-dimensional space is a probability distribution over all of its possible projections.
Sampling the distribution allows one to approximate the **dominant knotoid**, i.e. it is the knotoid that appear with the highest probability.
The dominant knotoid type corresponds to the region that occupies the largest area in the projection map, which is usually easily identified.



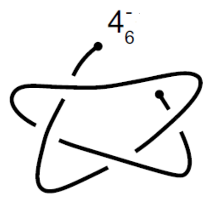
Example of generical open curve:







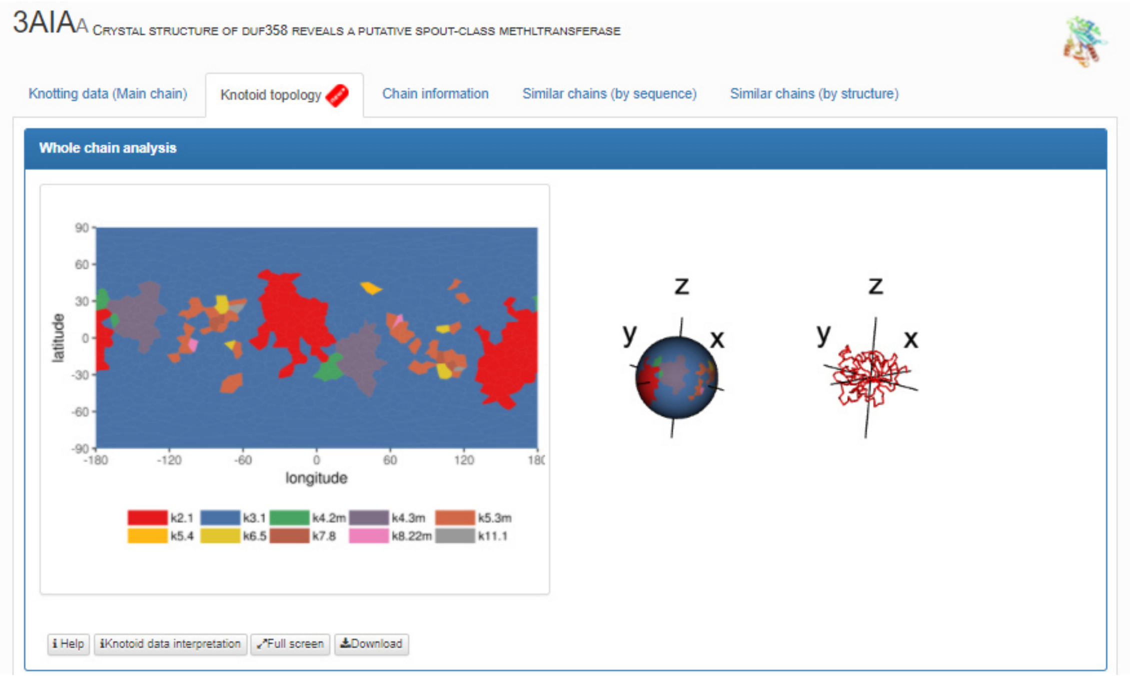
On below of the figure we see the stereografic projection of the sphere. In this particular example it was sampled 10000 projections of the open curve.

In this case the dominant knotoid is: 

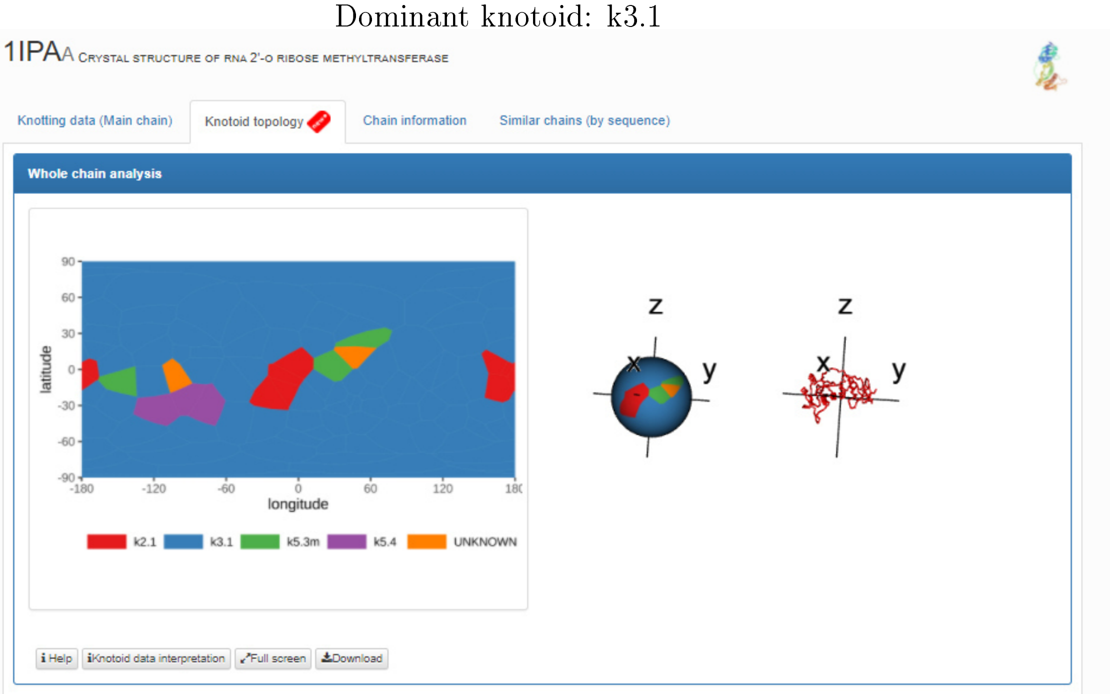
.

Remark 4.1.2. Regarding the symmetry, in principle, knotoids in S^2 exhibit antipodal symmetry in their projection maps while planar knotoids don't. In this example we can see the symmetry of the spherical knotoids 3_1, 5_1 and we don't see the simmetry of planar knotoid for example 4_1

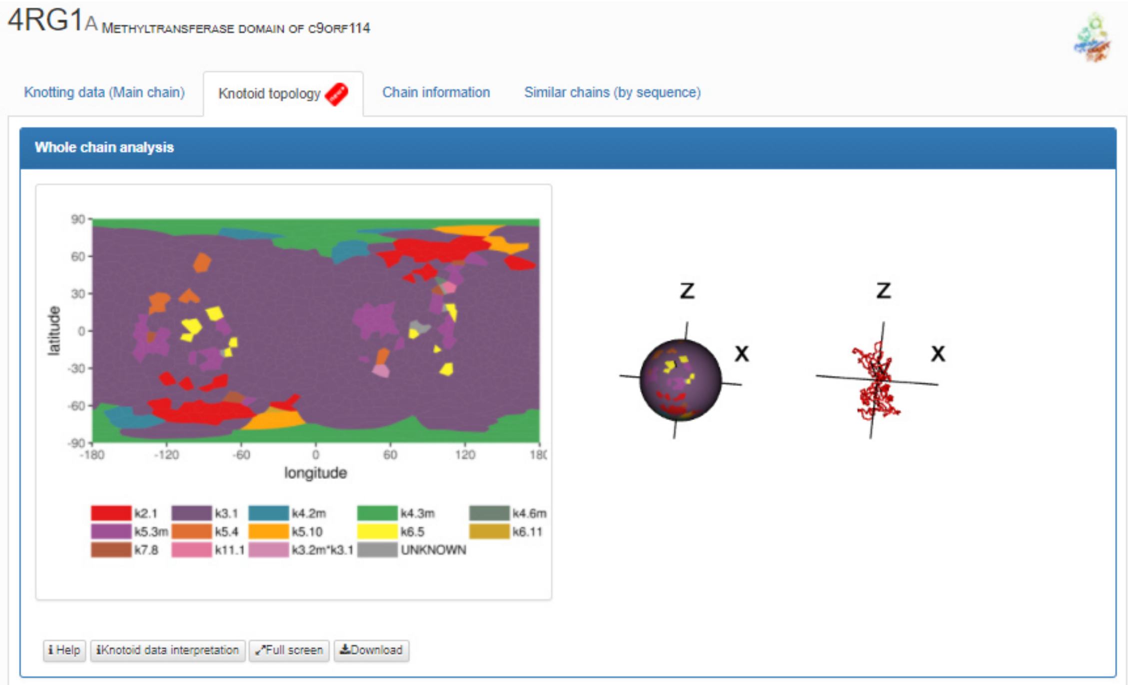
Now we see some examples of projection maps that we can find in the KnotProt 2.0:



Dominant knotoid: k3.1



Dominant knotoid: k3.1



Why we don't see the symmetry of spherical knotoids?
KnotProt 2.0 considers the probability distribution of knotoid types over 100 uniformly distributed projection directions, a larger number would improve precision, but makes computations slower.

What's the optimal number of projection?
In the article [10] Agnese Barbensi and Dimos Goudaroulis give an answer to this question using the following concept:

Definition 4.1.1. Given two knotoids k_1 and k_2, their forbidden move-distance or **f-distance** $d_f(k_1, k_2)$ is the minimal number of forbidden moves, across all representatives of k_1 and k_2, needed to transform k_1 into k_2.

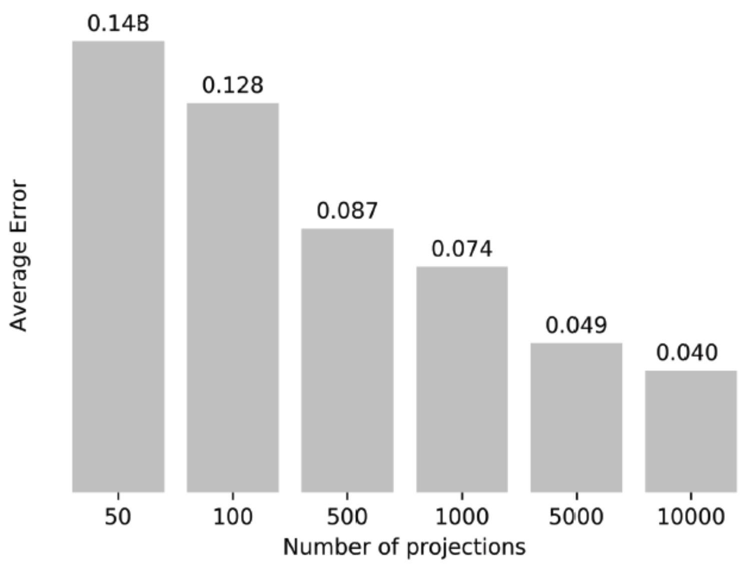
Consider a generic projection of a protein chain on some plane and let k be the corresponding knotoid. If we continuously perturb the projection direction until the knotoid type changes to k', we will obtain a pair of knotoids with $d_f(k, k') = 1$.
The spectrum of a protein chain depends on the number of projections. Therefore, there is a higher chance for regions corresponding to knotoids with $d_f > 1$ to appear next to each other.
Since the predominate knotoid corresponds to the largest region of the projection map, it is sufficient to focus on the discrepancies between the region of the predominate and its immediate neighbours.

Definition 4.1.2. The **spectrum** Spec(s) of a projection map is the number of distinct knotoids in the approximated knotoid distribution obtained considering s randomic projections.

Definition 4.1.3. The **interface error** er(s) associated to a sample set of size s of a projection map is the ratio of the number of regions that are adjacent to the region of the predominate knotoid k_0 that correspond to knotoids k_i for which $d_f(k_0, k_i) > 1$, over the number of all adjacent regions to k_0.

Agnese Barbensi and Dimos Goudaroulis wanted to see how these two coefficients were related to each other.

In particular, they analysed all the proteins with predominate knotoid type 3_1 (there are 517 such proteins in total deposited in the Protein Data Bank), using an increasing number of random projections: 50, 100, 500, 1000, 5000 and 10000 projections. Each time er(s) and Spec(s) were calculated for the respective projections map.
They computed the average interface error for one each of the six cases of projections sample size.

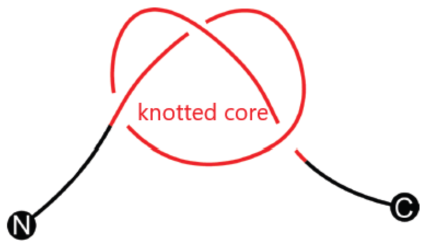


By gradually increasing the number of projections, regions will become progressively finer and so the possibility of having pairs of adjacent cells with $d_f > 1$ will effectively decrease, hence the error er(s) will decrease.

Throught 10000 projections they had the most accurate overview of the topology of the protein chain.
Another aspect found out by the authors is that the differences between results obtained using 5000 and 10000 projections respectively were not significant, so analysing a protein with 5000 projections may provide the best compromise between computational speed and accuracy.

4.1.2 The study of the protein subchains

Now we want to know:
-how large is the knotted core;

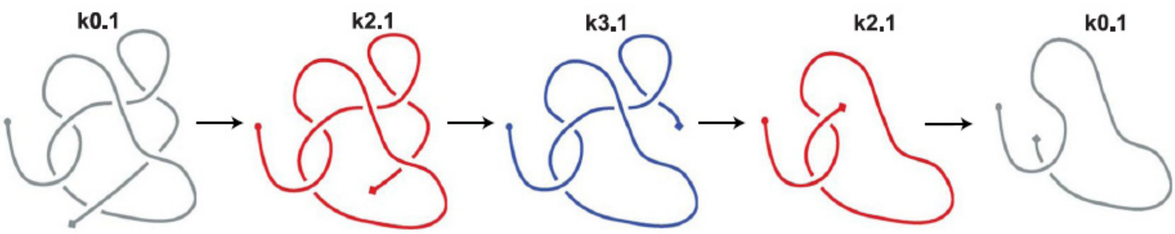


-if a given polypeptide chain contains subknots, i.e. they are less complex knots located inside more complex knots.
This information can be provided through when one analysis knottedness of every possible subchain of a given protein.

Given a protein chain, the analysis of every subchain provides the knotting **fingerprint**, which is usually presented in a form of triangular matrix where every point in the matrix informs what is the dominant knotoid type for a given subchain.

Given a protein chain, we start studying its local entanglement behaviour by clipping the chain one α-Carbon atom at a time, starting from one of endpoints of the chain.
Each time we obtain a shorter chain, which we analyze in terms of the knotoid technique that is, by projecting the trimmed chain along random directions and then computing the Jones polynomial of each projection.

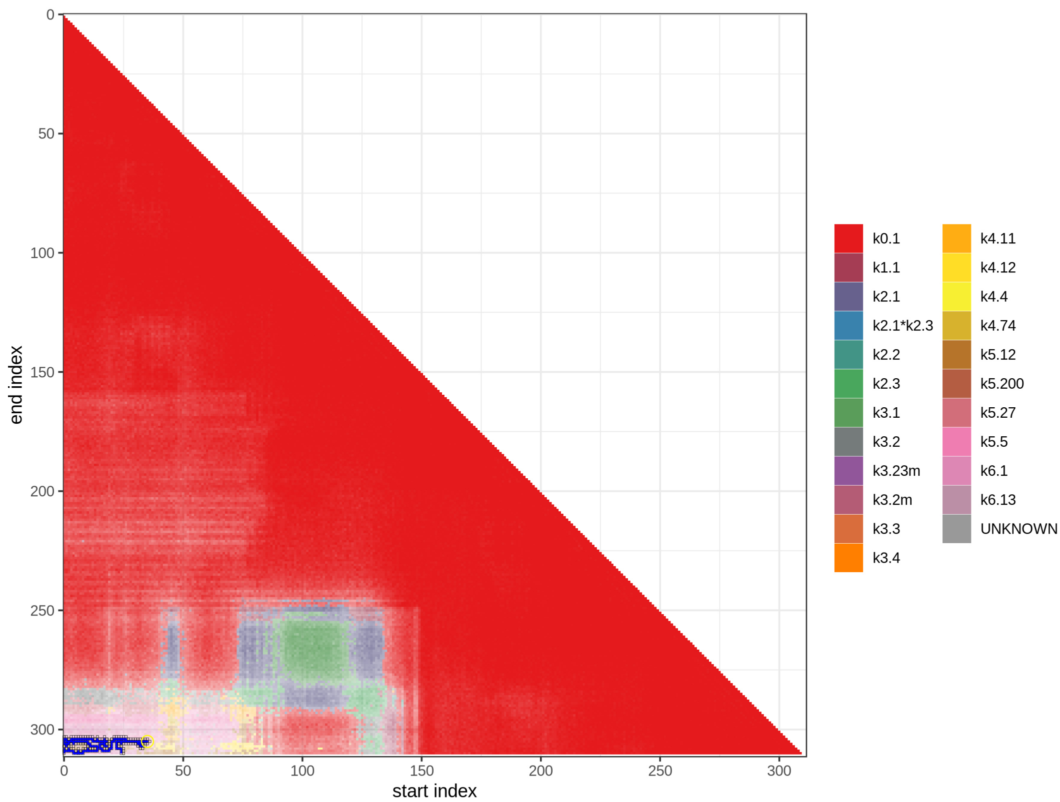
Example



(only one end of projected chain is progressively trimmed)

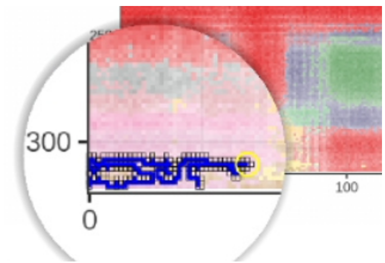
Notice that as we trim the chain, we observe that the knotoids types change.

Example 3KZN protein chain:
The knotoid fingerprint matrix obtained from KnotProt 2.0:



Each point in this matrix corresponds to the dominant knotoid type for a subchain of the protein chain.
The x-axis goes from N-terminal to C-terminal of the protein chain, while the y-axis goes from C-terminal to N-terminal.

The point in lower left corner corresponds to the whole chain.
Moving to the right along the x-axis, we cut the chain starting from one endpoint (the N-terminal) while moving up the y-axis we are cutting vertices from the other endpoint (C-terminal) of the chain.
KnotProt 2.0 use a colour code to indicate the dominant knotoid types appearing in this fingerprint matrix.
In the fingerprint matrix we also identify the 'knotted core', i.e. the shortest subchain whose knotoid type is the same as the knotoid type of the whole chain. On the figure the yellow circles are centered on knotted core.

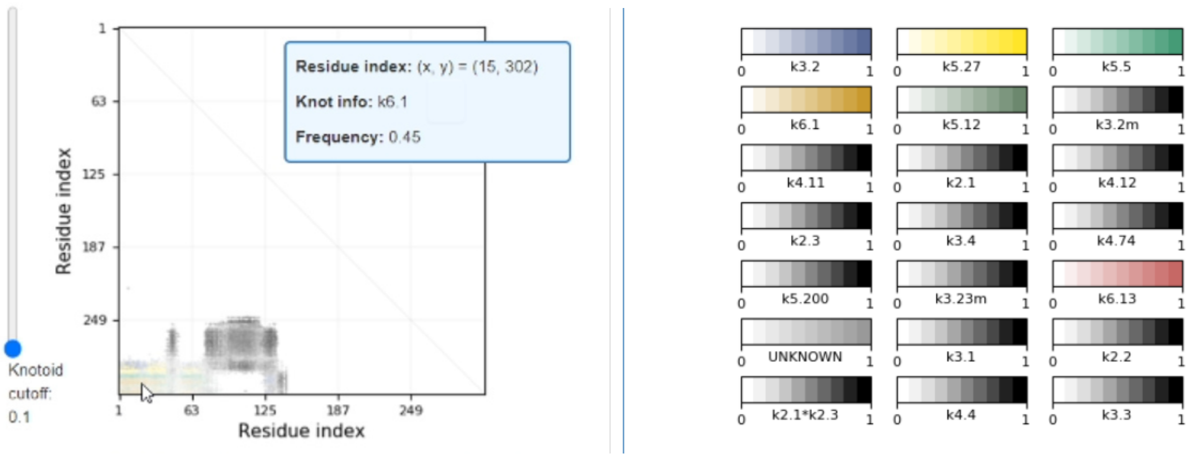


In this case the dominant knotoid is 6_1: KnotProt 2.0 gives us this information throught the projection map (the dominant knotoid type corresponds to the region that occupies the largest area in the map) and throught a row data.

Row data:

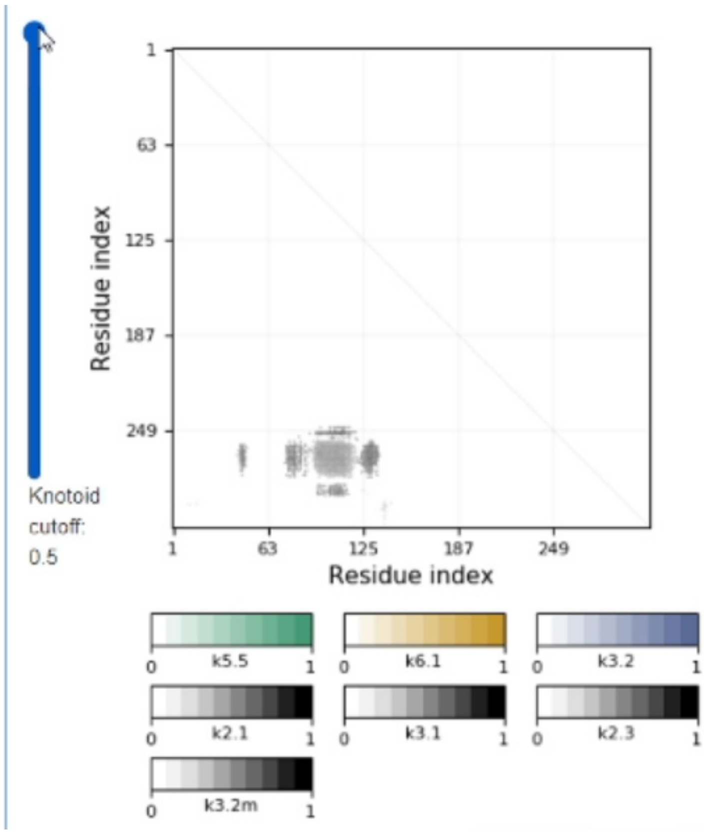
index_first	*index_last*	*length*	*frequency*	*knotoid_type*
35	305	270	0.22	$k6.1$

KnotProt 2.0 gives us an other visualization of knotoid fingerprint matrix:

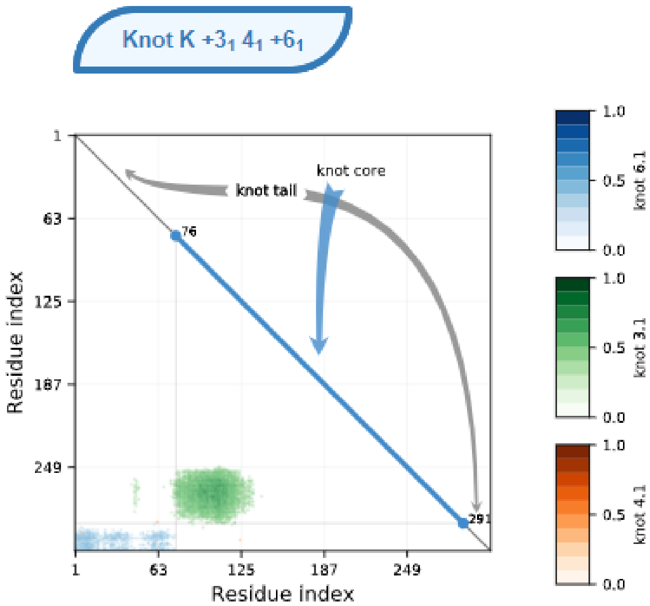


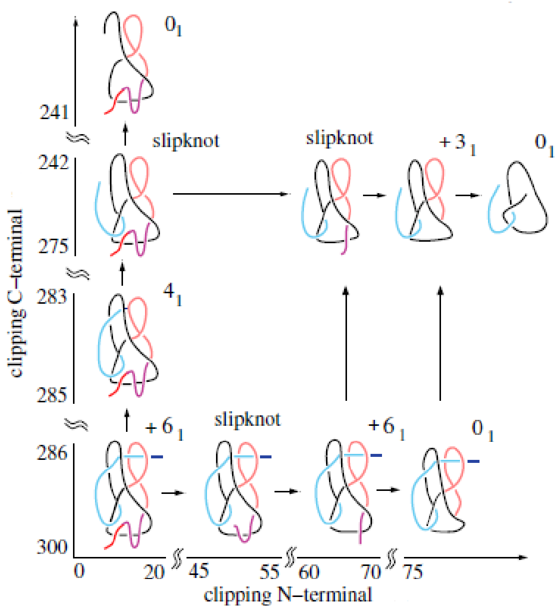
If we point the cursor at a point corresponding to some knotoid, KnotProt 2.0 shows in a blue box: the x- and y-coordinates of knotoid, the type

and the frequency of knotoid.
Color corresponds to dominant knotoid type of the subchain and transparency corresponds to its frequency.
*Remarck:*The knotoid distribution usually includes many different types of knotoids. It is possible that many of those types in the distribution to have a very small probability of appearing in a projection. This means that if we plot the knotoid matrix of the subchain analysis, we will have a very big list of different colors that may be confusing or not useful for that particular application. The "knotoid cutoff" is a lower bound that simplifies the visualization of data. For example "knotoid cutoff"=0.5: we get only those projections that appear more than 50% of the times.
If we set the cutoff to 0.5 the knotoid matrix of the example becomes:



The knot fingerprint matrix of the 3KZN protein chain:





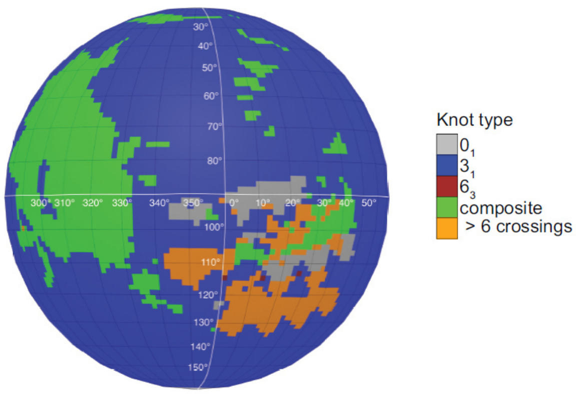
In the knot fingerprint all subchains of the protein chain were analyzed using the stochastic closure technique. The knot core on the figure, is the shortest subchain for which a dominant knot is detected (i.e. after cutting an

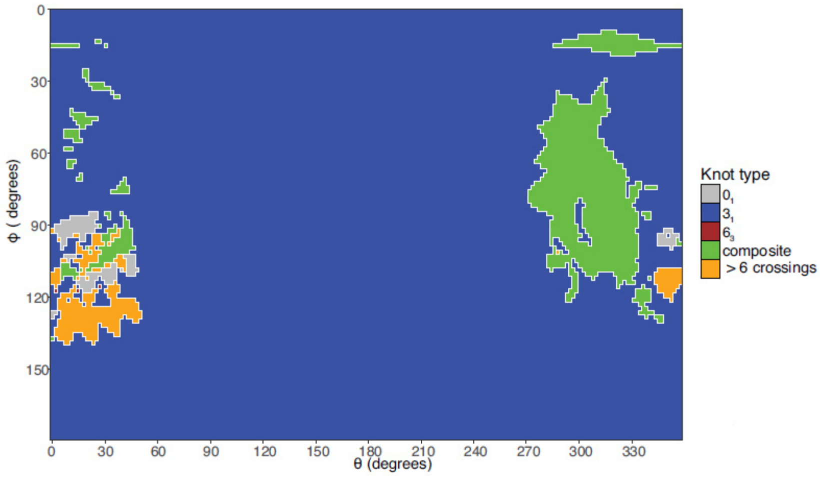
aminoacid from any terminal of such a subchain, just a trivial knot would be detected).
In the knot fingerprint it observs that, in addition to the 6_1 dominant knot formed by the entire protein, the smaller subchains form 4_1 and 3_1 knots.

Now comparing the knotoid fingerprint to knot fingerprint we observe that the knotoid approach gives us more details on the different topological forms.
We can see that the regions of non-trivial knots of the knot fingerprint of protein are contained inside regions of the knotoid fingerprint.
There are new regions in knotoid fingerprints that correspond to non-trivial proper knotoids that either border regions of knot-type knotoids (e.g. the regions of knotoid 2.1 that encircle the knot-type knotoid 3.1) or show up within trivial knotoids (the small slices of 2.1 and 3.2). The knotoids approach produces more refined fingerprints of the protein chains.

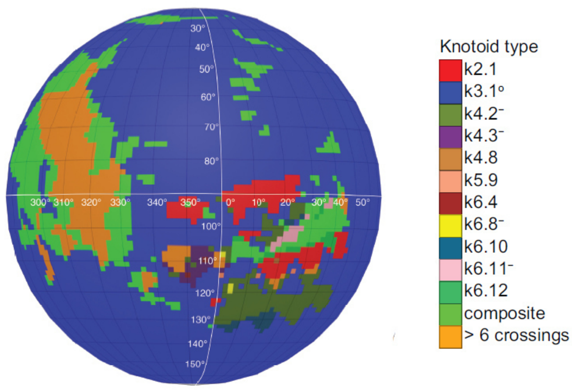
4.1.3 Comparation of the projection globes of protein chain

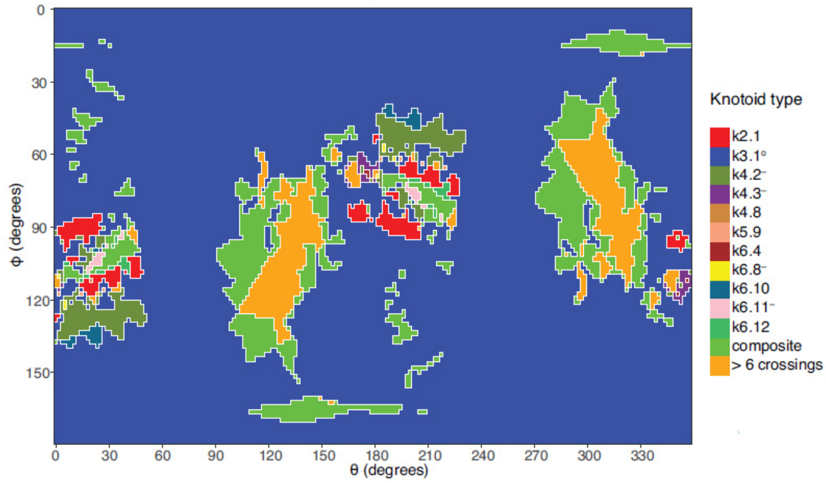
We consider 3KZN protein and we want to compare the projection globe obtained from the planar knotoids approach, to the one derived from the spherical knotoids approach and to the one that is derived from the uniform closure technique.
We can see that, from knots to spherical knotoids and then to planar knotoids, we have a gradually emerging of new regions.
The reason behind this is that the number of classes of planar knotoids is larger than the number of classes of spherical knotoids.
We can conclude that analyzing open protein chains as planar knotoids reveals more details of their topology.
The projection globe and map for the uniform closure technique:



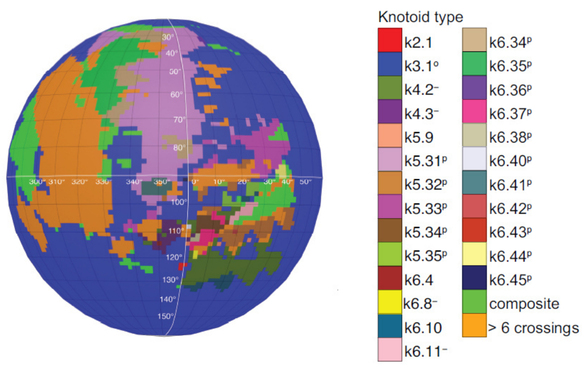


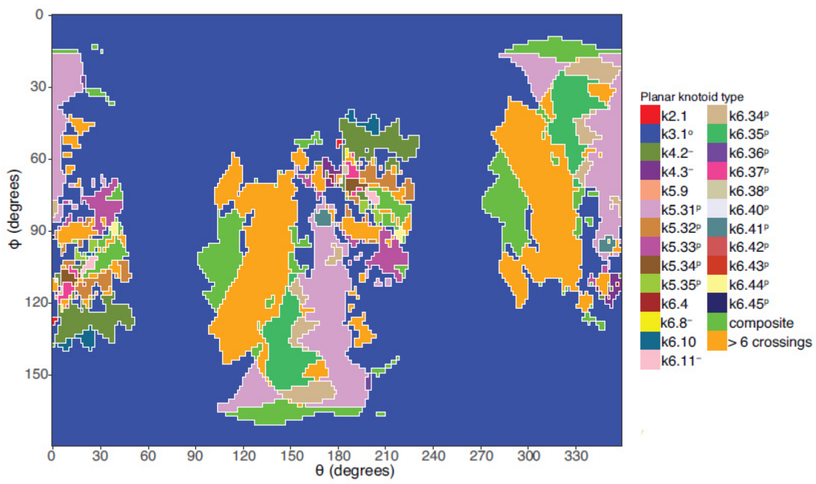
The projection globe and map for the spherical knotoids technique:





The projection globe and map for the planar knotoids technique:





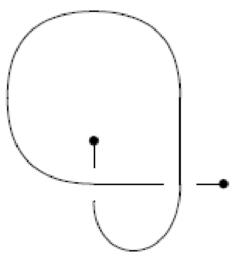
Notation on the figures: a knotoid is represented by kX.Y where:
X is the number of crossings of the knotoid diagram in question,

Y corresponds to the position of the knotoid in the table of knotoids with the same number of crossings,
$^{\circ}$ indicates a knot-type knotoid,
^{p} indicates a planar knotoid,
$^{-}$ a knotoid with its crossings inverted.
There is no wrong way to study the global entanglement of protein chain, it depends that what we want to see.
So, we can to work with knots if we just want to see quickly what is the dominant entanglement but if we want to see the real topology of a protein, planar knotoids is the way to go because we get the full spectrum of all possible entanglements.

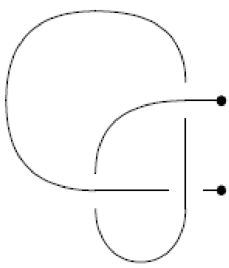
Appendix A

Table of knotoids in S^2

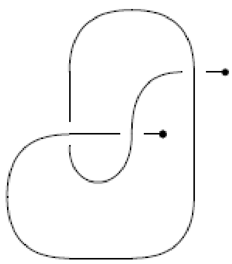
We consider the table of all distinct knotoids in the sphere S^2 with minimal number of crossings of a knotoid diagram up to five crossings.
These knotoids have been distinguished by the use of some knotoids invariants.
The notation follows the one in [5], that uses the scheme X_Y , where X is the minimal number of crossings of the knotoid and Y is the relative position among all knotoids with the same number of crossings.
Labels in red correspond to knot-type knotoids.



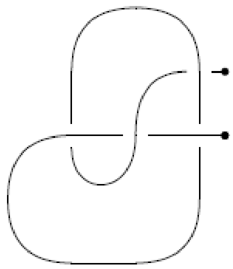
2_1



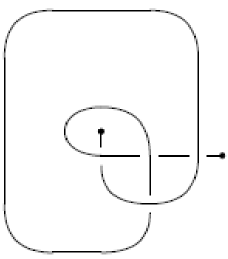
3_1



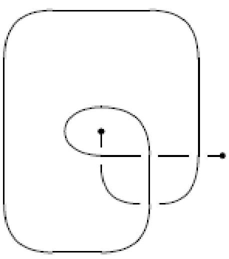
3_2



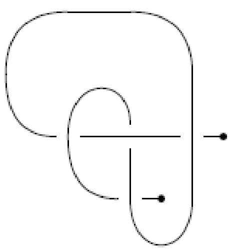
4_1



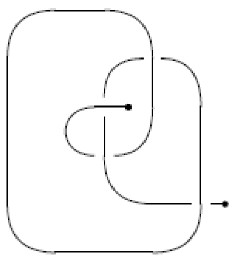
4_2



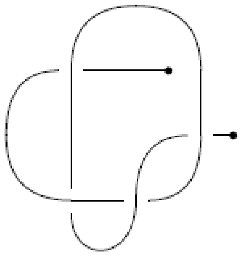
4_3



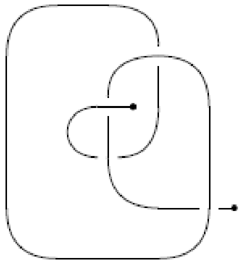
4_4



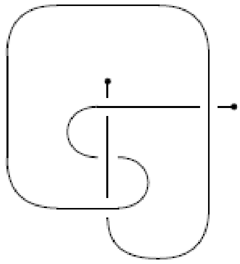
4_5



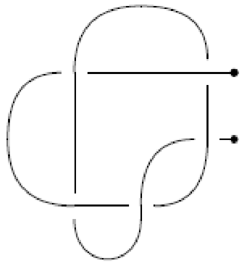
4_6



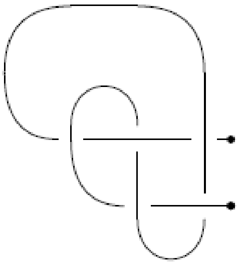
4_7



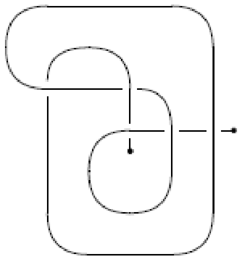
4_8



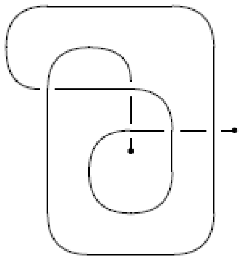
5_1



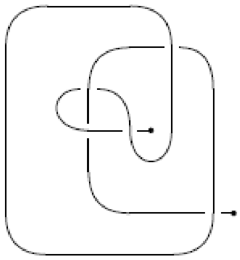
5_2



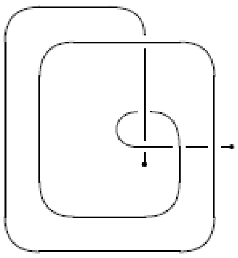
5_3



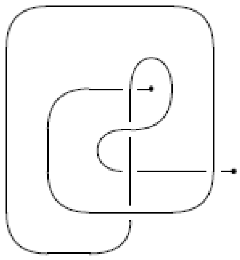
5_4



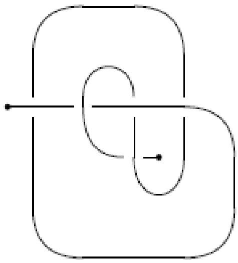
5_5



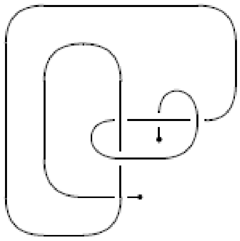
5_6



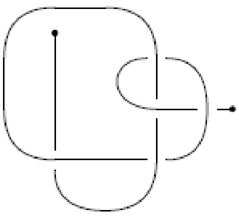
5_7



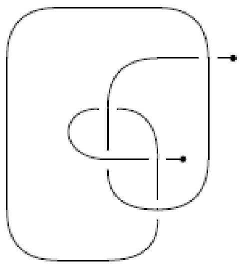
5_8



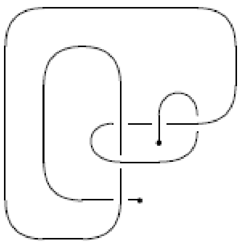
5_9



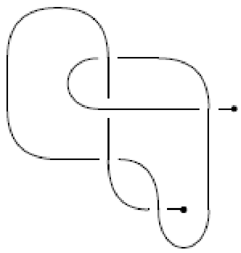
5_{10}



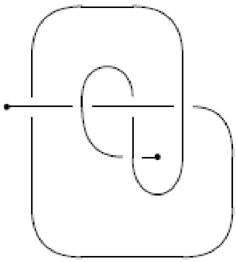
5_{11}



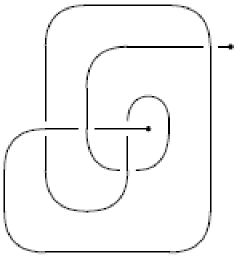
5_{12}



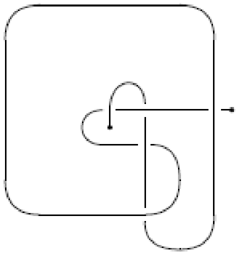
5_{13}



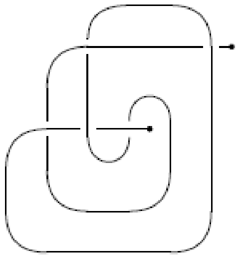
5_{14}



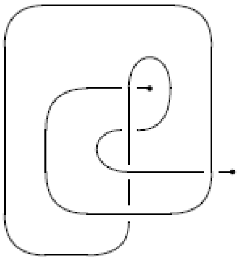
5_{15}



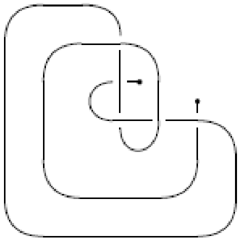
5_{16}



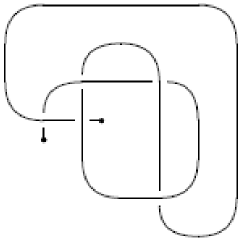
5_{17}



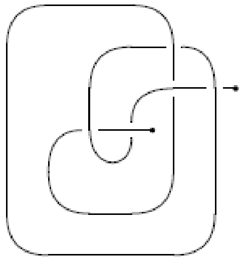
5_{18}



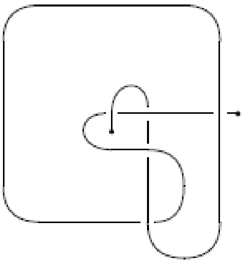
5_{19}



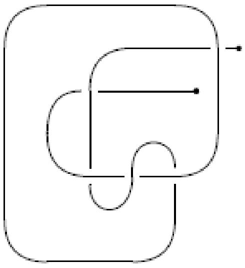
5_{20}



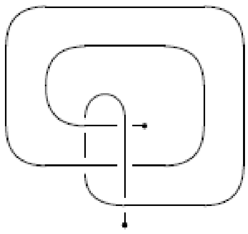
5_{21}



5_{22}



5_{23}

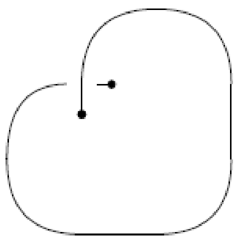


5_{24}

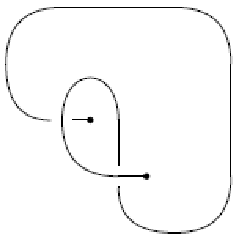
Appendix B

Table of knotoids in $\mathbb{R}^2$

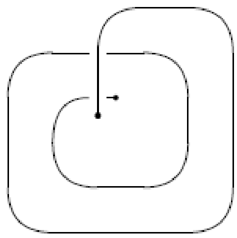
We consider the table of all distinct knotoids in the sphere $\mathbb{R}^2$ with minimal number of crossings of a knotoid diagram up to three crossings.



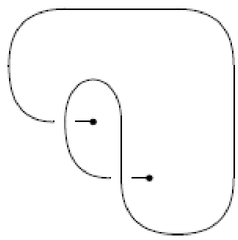
1_1



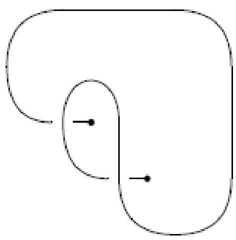
2_2



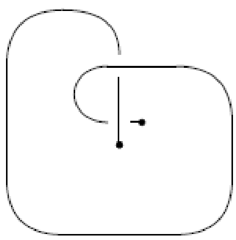
2_3



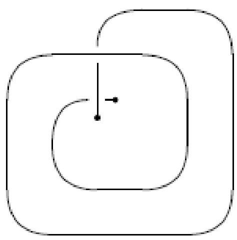
2_4



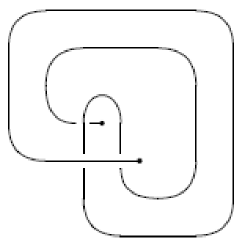
2_4



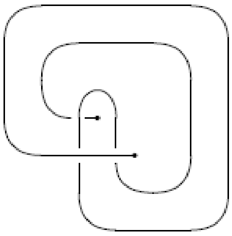
2_5



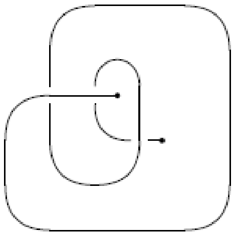
2_6



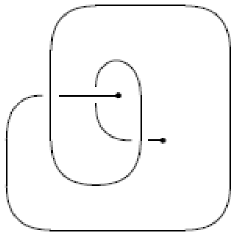
3_3



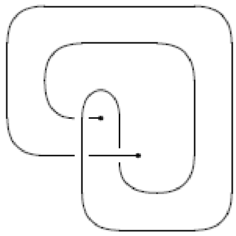
3_3



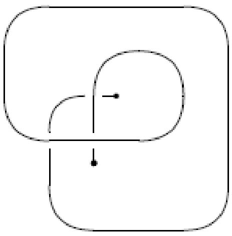
3_4



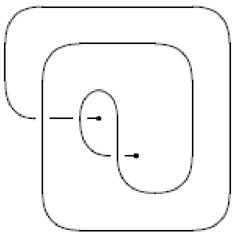
3_5



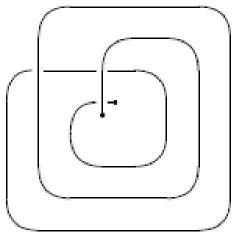
3_6



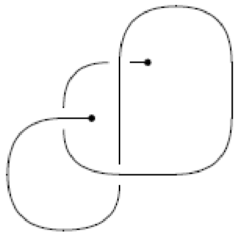
3_7



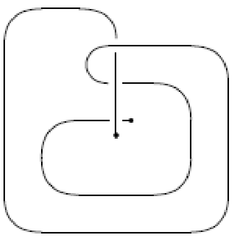
3_8



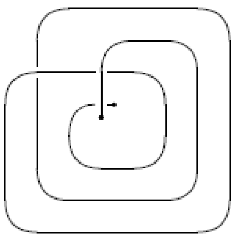
3_9



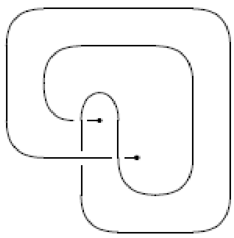
3_{10}



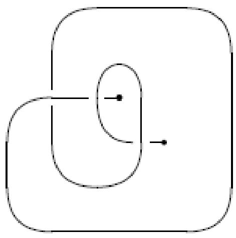
3_{11}



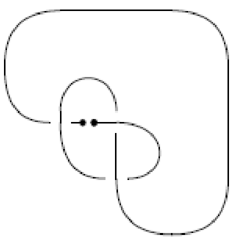
3_{12}



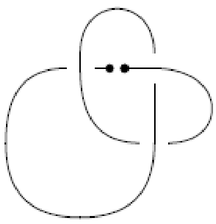
3_{13}



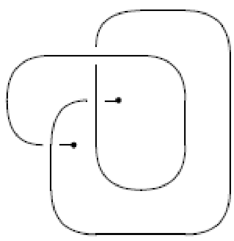
3_{14}



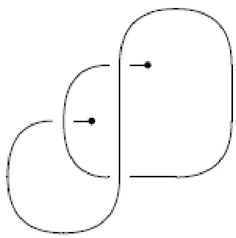
3_{15}



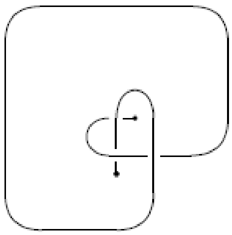
3_{16}



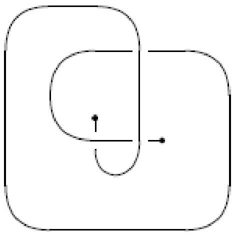
3_{17}



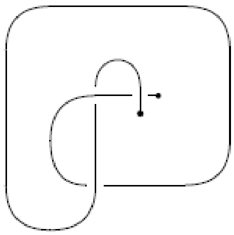
3_{18}



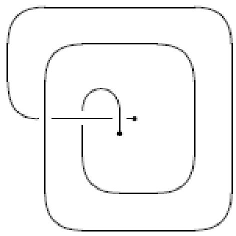
3_{19}



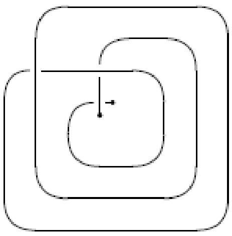
3_{20}



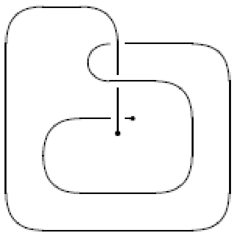
3_{21}



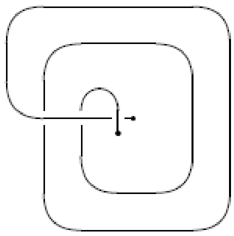
3_{22}



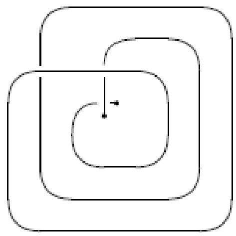
3_{23}



3_{24}



3_{25}

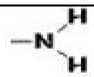


3_{26}

Appendix C

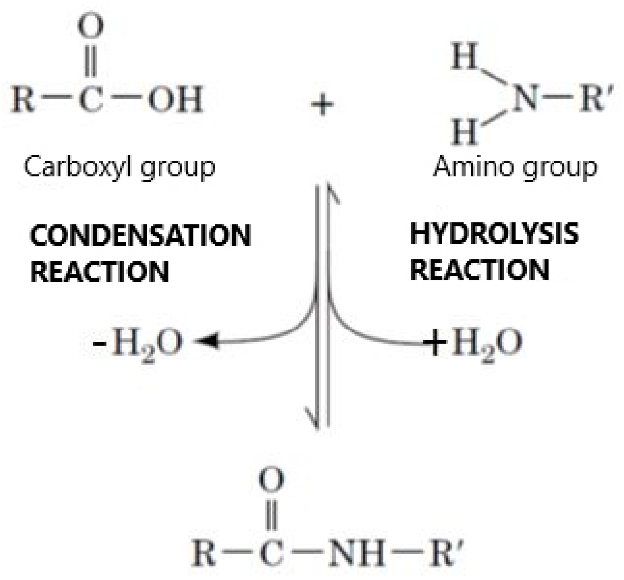
Biological macromolecules

Biochemistry is the science that describes the structures, reactions and chemical processes that characterize living organisms.
The fundamental unit that constitutes the organism is the ***cell***; more cells organize themselves to form tissues, organs ...up to more complex organisms.
Inside the single cells there are continuously thousands of *reactions* that allow to produce energy that the cell will then use for other reactions.
There are four main classes of biological macromolecules in the cell: *proteins, nucleic acids, carbohydrates and lipids.*
Macromolecules are made up of a limited number of *chemical elements* (mainly carbon C, nitrogen N, oxygen O, hydrogen H) which join together through chemical bonds; moreover, there are also *functional groups* which are characterized by atoms that interact with each other and which often determine the function of the molecule in which they are found.
Some examples:

Functional Group	**General formula**
Amino	$-NH_2$ 
Carboxyl	$-COOH$ 
Hydroxyl	$-0H$ **—OH**

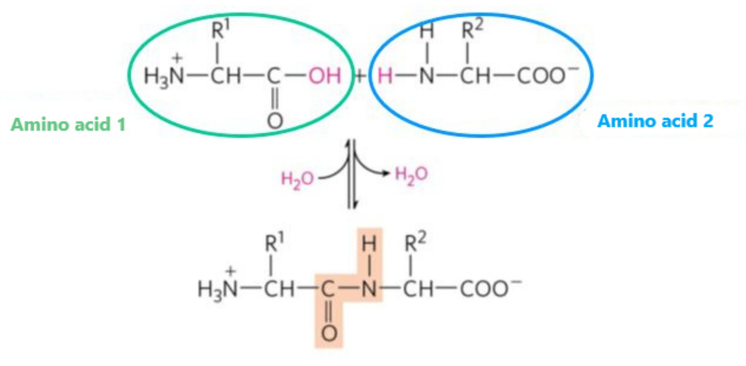
In macromolecules the fundamental unit is the *monomer*.
The union of monomers forms the *polymer*.

To pass from simpler molecules (monomers) to more complex molecules (polymers), a textit condensation reaction is required which eliminates a water molecule H_2O. Conversely, to pass from more complex molecules to simpler molecules, a *hydrolysis reaction* is required which adds a water molecule H_2O. *Example*:



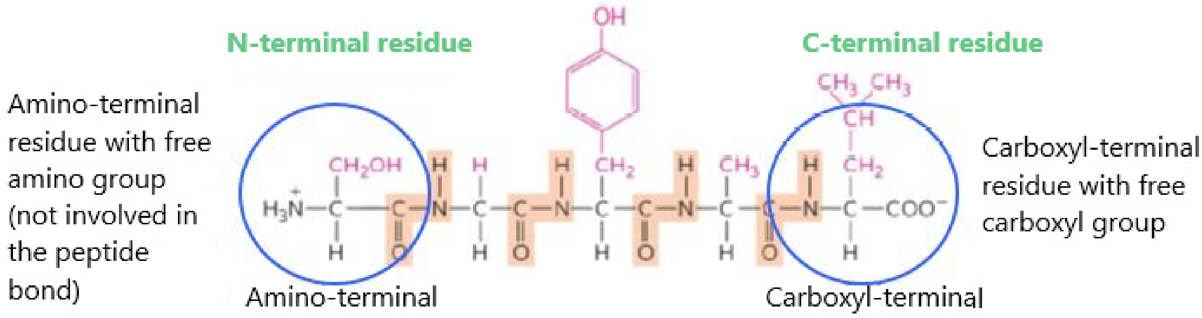
C.1 Protein and amino acids

The protein or polypeptide chain is a polymer formed by the union of **amino acids** (monomers).
The bond between two amino acids is the **peptide bond**; amino acids involved in the peptide bond are called amino acid residues.

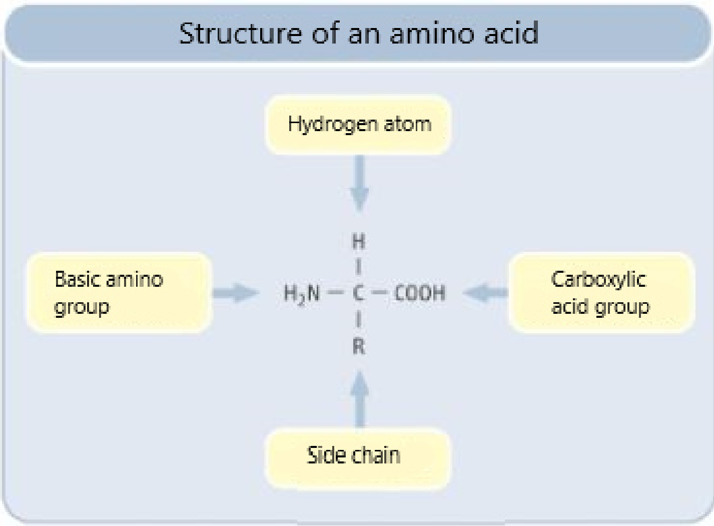


Dipeptide

In the peptide bond, the amino group of amino acid 2 reacts with the hydroxyl group (OH) of the carboxyl of amino acid 1.
The peptide bond is formed from the condensation reaction and a water molecule is released.
Proteins are polymers consisting of at least 50 amino acid residues (up to over 1000), while **peptide** is defined as the polymer consisting of less than 50 amino acid residues.
Based on the number of peptide bonds we will have: dipeptides (2 residues), tripeptides (3 residues), tetrapeptides, pentapetides etc.

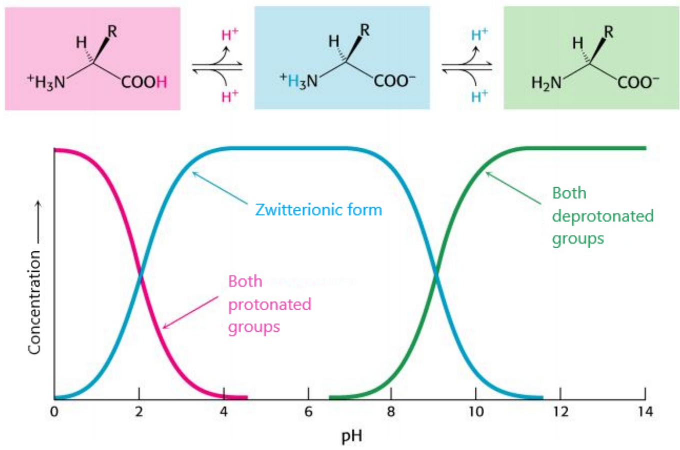


In nature there are 20 standard amino acids, which have a common structure that differs only at the level of their side chain (R group).

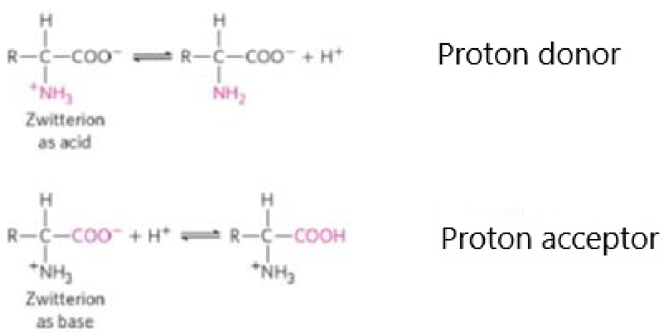


Each amino acid has a central carbon involved in four bonds with:
1- Amino group
2- Carboxyl group
3- Hydrogen atom
4- Group R or side chain (which differentiates the 20 standard amino acids)

The charge of the amino acid depends on the pH of the solution in which it is found. The pH indicates the concentration of protons (of H^+ ions) that occur in a given solution.
Considering R non-ionizable (i.e. once in water do not produce any charge), by changing the pH of the solution, the charge of the amino group will change and the charge of the carboxyl group will change, then the charge of the amino acid will change and the charge of the protein in which the amino acid is present will change.



At NEUTRAL pH (around 7) the carboxyl group is deprotonated (it loses a proton) and the amino group is protonated (it buys a proton): the amino acid charge is balanced, the overall charge is neutral.
The amino acid with neutral pH is called zwitterion and can behave as either acid (proton donor) or base (proton acceptor).



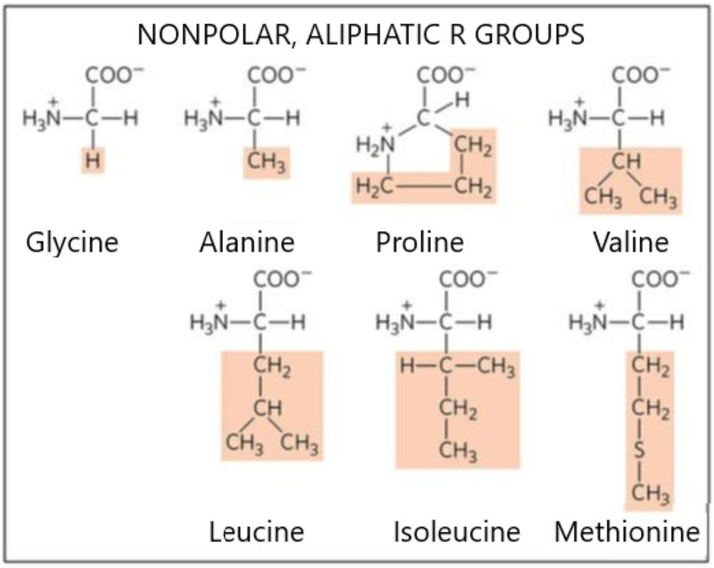
At $0 <$ ACID pH < 7 the carboxylic group and the amino group are both protonated: the amino acid charge is positive.

At BASIC pH > 7 the carboxylic group and the amino group are both deprotonated: the amino acid charge is negative.

C.2 R groups of amino acids

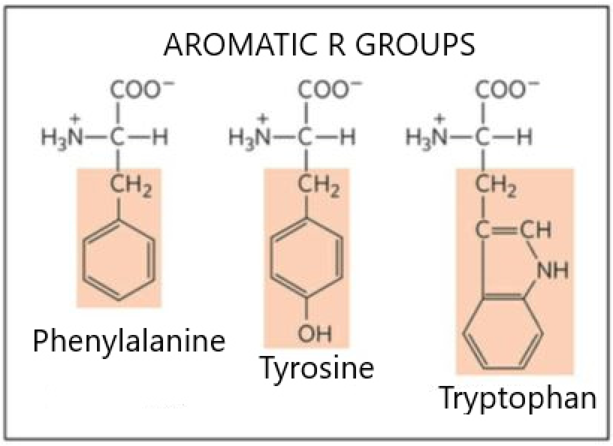
According to the characteristics of the R groups there is a different polarity of the amino acid.
Polarity is the tendency to interact with water at physiological (natural) pH, the polarity of the R groups is highly variable.

NONPOLAR, ALIPHATIC R GROUPS
The aliphatic R groups contain more or less branched carbon sequences, they not form ring-like chemical structures (except the Proline).
These groups are non-polar, hydrophobic, i.e. insoluble in water (they do not interact with water). The amino acids that have such R groups are:



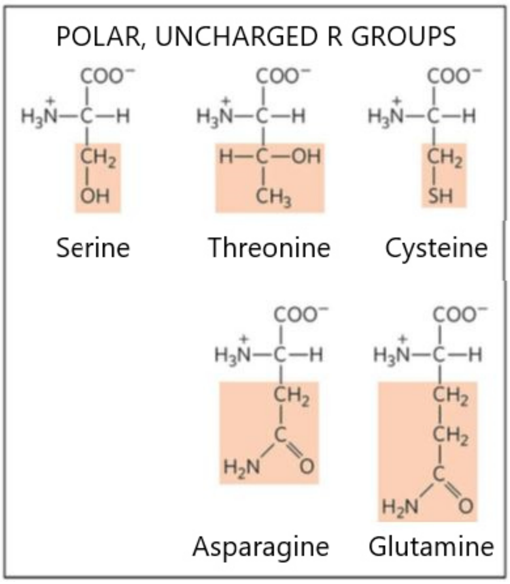
Curiosity: When the protein wraps itself in space, acquiring their three-dimensional structure, the hydrophobic R groups are positioned inside while the groups that interact more easily with water are positioned outside. If the protein is damaged and therefore its three-dimensional structure changes , the hydrophobic parts will be on the outside, then the hydrophobic regions of damaged proteins will interact with each other forming toxic aggregates, typical of neurodegenerative diseases.

AROMATIC R GROUPS
Aromatic groups have ring-like chemical structures.



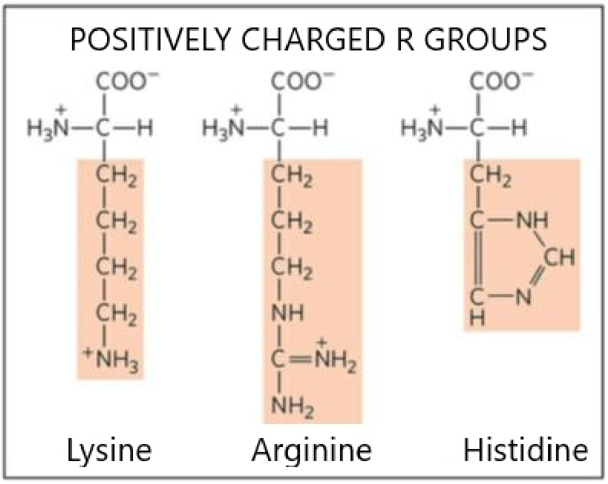
These three amino acids are relatively non-polar and can intervene in hydrophobic interactions. Tyrosine and tryptophan are more polar than phenylalanine.
Curiosity: Tryptophan, tyrosine and, to a lesser extent, phenylalanine absorb UV light. This is why the protein has an absorption peak at 280 nm.

POLAR, UNCHARGED R GROUPS
These groups are not charged neither positively nor negatively, moreover they interact in aqueous solution forming hydrogen bonds with water.



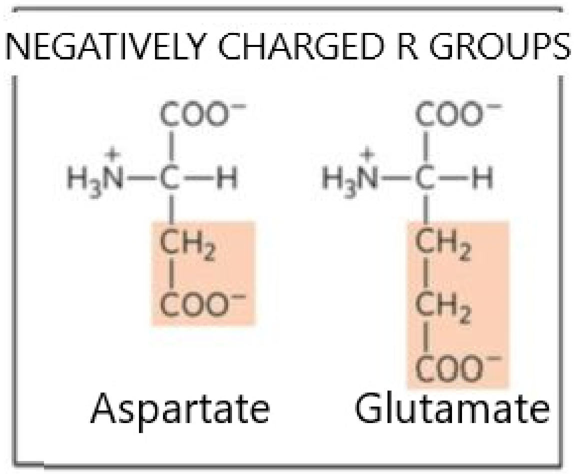
R GROUPS WITH POSITIVE CHARGE (BASIC)

Amino acids with these groups have a side chain with a net positive charge at pH 7.0.
They are proton acceptors.



R GROUPS WITH NEGATIVE CHARGE (ACIDS)

Amino acids with these groups have a side chain with a net negative charge at pH 7.0.
They are proton donors.



C.3 Protein structure

Proteins are said to be **monomeric** if they are costituited by a unique polypeptide chain. In this case they will have: primary, secondary and tertiary structure.
If they are made up of several polypeptide chains they are called **multimeric** and will also have the quaternary structure.

PRIMARY STRUCTURE
The primary structure of the protein is given by the sequence of amino acids linked together by peptide bonds. It is important to study it because:
1) The R groups of the individual amino acids that form the protein determine its function
2) To synthetically produce proteins, such as hormones and antibodies, in the laboratory, in this way we will have greater quantities available
3) Changes in the primary sequence can produce anomalies of the function and/or disease.

Example 1

Oxytocin and vasopressin are two peptides with very similar primary structures and very different biological functions and uses:

Oxytocin

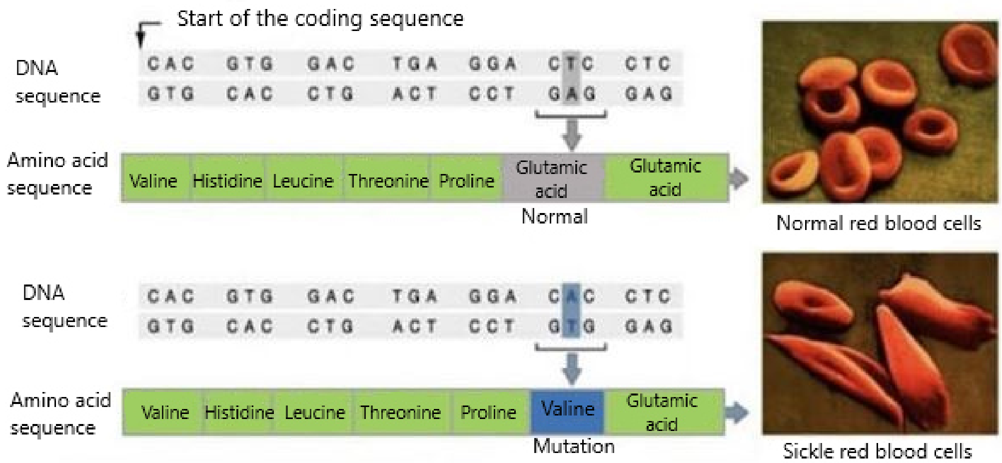
Primary structure: Cys-Tyr-**Ile**-Gln-Asn-Cys-Pro-**Leu**-Gly-NH2
Function: It causes contraction of the uterus and it is administered to induce childbirth

Vasopressin
Primary structure: Cys-Tyr-**Phe**-Gln-Asn-Cys-Pro-**Arg**-Gly-NH2
Function: It regulates the reabsorption of water from the urine and it is administered in the treatment of diabetes

Example 2

Sickle cell anemia
Hemoglobin consists of 4 polypeptide chains:
2 chains α of 141 amino acid residues
2 β chains of 146 amino acid residues
In patients with sickle cell disease, a residue of (polar) glutamic acid in the β chain is replaced by a (non-polar) valine residue due to a genetic error.

Section of the β chain of hemoglobin:
Normal hemoglobin .... Val-His-Leu-Thr-Pro- **Glu** -Gly-Lys ....
Abnormal hemoglobin .... Val-His-Leu-Thr-Pro- **Val** -Gly-Lys ....



Amino acids can be indicated with the whole name, with three letters or with a single letter.

SECONDARY STRUCTURE

The secondary structure describes how regions of the protein are distributed in space with each other. They are of two types: α-helix and pleated sheet-β.

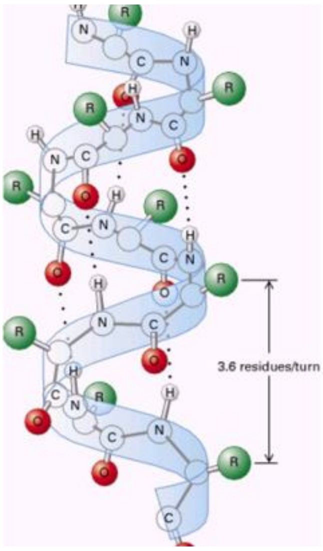
In the α**-helix** structure, amino acids wrap around an imaginary axis forming a helix. The helix skeleton is made up of carbon C and nitrogen N atoms which form the peptide bonds while the R groups are located outside the skeleton. The helix can have a right-handed or left-handed course.

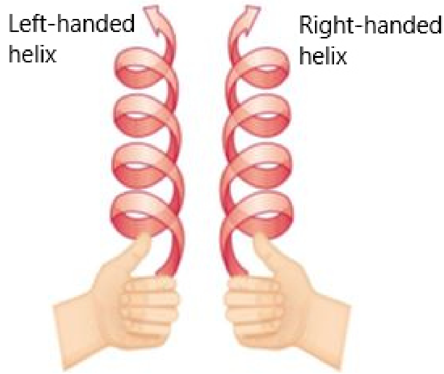
A round of helix is 5.4 A (Angstrom) long and contains 3.6 amino acid residues.

$1A = 0.1nm = 1 * 10^{-10}m$

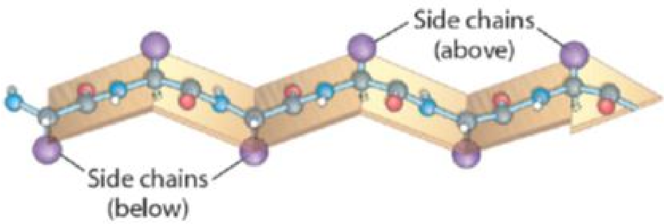
This structure is stabilized by the presence of *hydrogen bonds* between the oxygen atom O of the carboxylic group of the first amino acid residue and the hydrogen H bonded to nitrogen N (involved in the peptide bond) of the fourth amino acid residue.

The α-elics are positioned in the outer regions of the proteins.



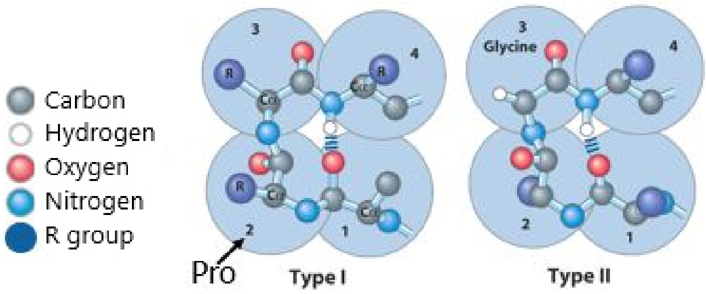


In the structure a **sheet-β** the skeleton is a zig-zag plane.
The R groups protrude from the zig-zag structure alternating above-below.

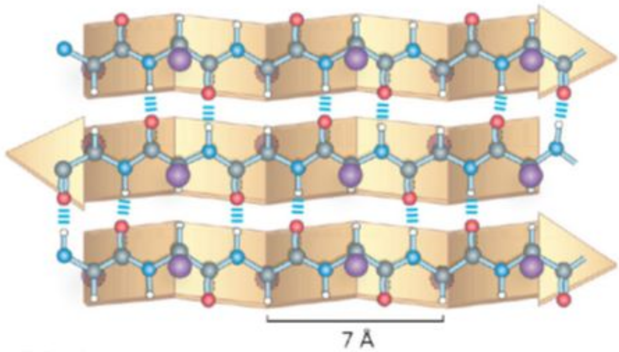


The sheets -β are positioned in the inner regions of the proteins because they are hydrophobic regions.
When several segments with configuration-β are arranged next to each other, the sheet-β can be **antiparallel** or **parallel**.

- **Antiparallel**: there are folds of 180° formed from 4 amino acid residues.
  Foldings of *Type I*: Proline is present in position 2 of amino acid residues.
  Folding of *Type II*: Glycine is present in position 3 of amino acid residues.

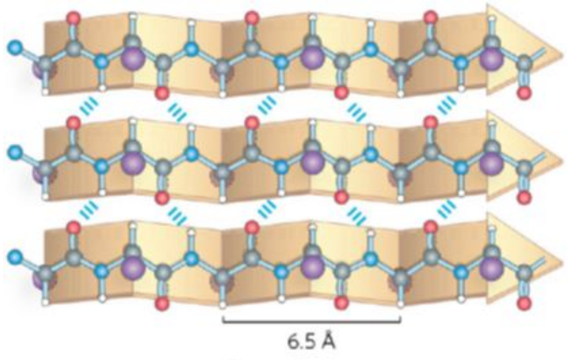


The formation of these curves means that each subsequent sheet has an opposite trend compared to the previous sheet.
The fundamental unit is 7 A long and the hydrogen bonds are straight (in the figure they are blue).



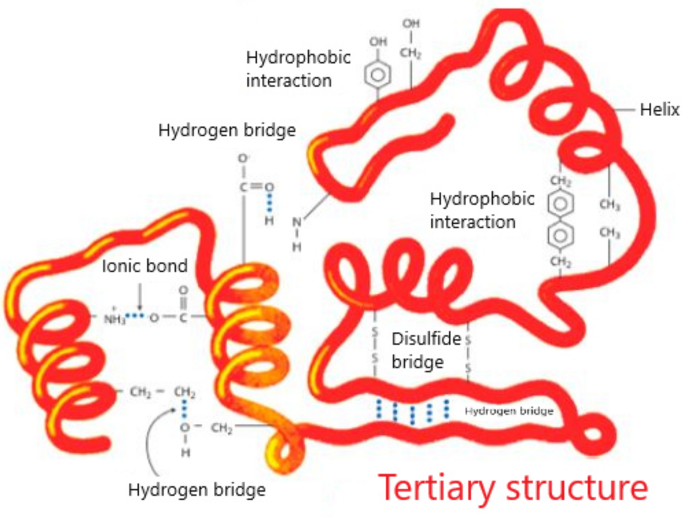
The first sheet goes from left to right (N-terminal, C-terminal), the next one goes from right to left (N-terminal, C-terminal).

- **Parallel**: the regions are arranged parallel, the sheets have the same trend.
  The fundamental unit is 6.5 A long and the hydrogen bonds are slightly distorted.



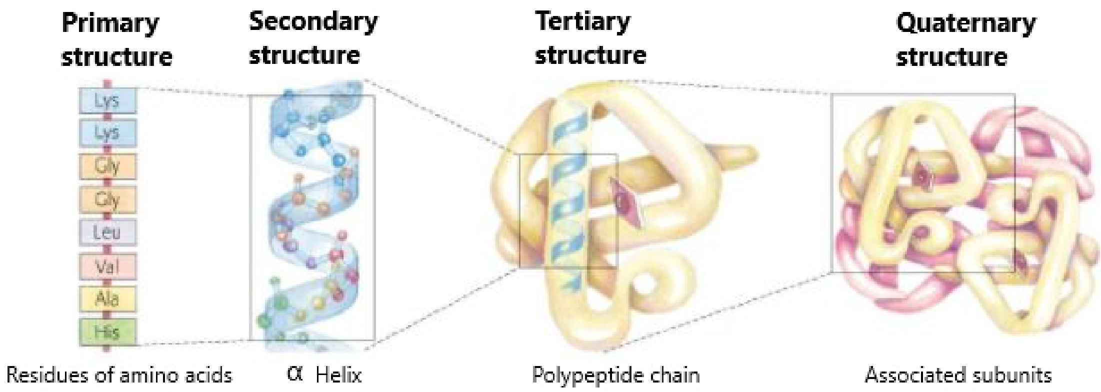
TERTIARY STRUCTURE

The tertiary structure describes how the whole protein is organized in space. The protein can assume different tertiary structures but assume the one that gives it more stability from an energetic point of view.
The tertiary structure is stabilized by bonds between R groups of amino acid residues that are spatially close together.
ION BOND: between groups that have a net negative charge (residues of lysine, arginine, histidine) and groups that have a net negative charge (residues of glutamic acid, aspartic acid).
HYDROPHOBIC BOND: tendency of non-polar R groups to unite with each other. Example: side chains of alanine, valine, leucine, isoleucine, phenylalanine.
DISULFIDE BRIDGE: A cysteine has a -SH group in R group.
After that the protein has assumed the tertiary structure, it may happen that two -SH groups of two different cysteines are spatially close; they oxidize and they form S-S bridges.



QUATERNARY STRUCTURE

The quaternary structure describes how the different polypeptide chains organize and interact with each other in space through chemical bonds. Proteins are classified into two main groups:
Fibrose: peptic chains arranged in long bundles or sheets.
(Examples: keratin, collagen)
Globular: folded chains with spherical or globular shapes.
(Examples: myoglobin and hemoglobin)
Structural differences: fibrous proteins have only one secondary structure (this is always a α-elic) and the tertiary one is very simple, while the globular ones have different secondary structures.
Functional differences: fibrous proteins determine the resistance, form and external protection of vertebrate cells, while globular ones have a regulatory function.



References

[1] V. Turaev, "Knotoids", Osaka Journal of Mathematics, 49, (2012)

[2]H.A. Dye and L.H.Kauffman, "Virtual Crossing Number and the Arrow Polynomial", J. Knot TheoryRamifications, 18, (2009)

[3] N. Gügümcü and L. H. Kauffman, "Parity in Knotoids", (2019)

[4] N. Gügümcü and L. H. Kauffman, "New invariants of knotoids", European Journal of Combinatorics, vol. 65, (2017)

[5] J. Dorier D. Goundaroulis and A. Stasiak. "A systematic classification of knotoids on the plane and on the sphere", (2019)

[6] Ph. G. Korablev, K.Ya. May. "Knotoids and knots in the thickened torus", Siberian Mathematical Journal, vol.78,(2017)

[7] N. Gügümcü and L. H. Kauffman, "On the height of knotoids", (2017).

[8] Claudio Perego and Raffaello Potestio, "Computational methods in the study of self-entangled proteins: a critical appraisal", (2019)

[9] Dorier J, Goundaroulis D, Benedetti F and Stasiak A "Knoto-ID: a tool to study the entanglement of open protein chains using the concept of knotoids",(2018)

[10] Barbensi A. and Goundaroulis D., "f-distance of knotoids and protein structure", (2021)

[12]Philipp Korablev and Vladimir Tarkaevy, "A relation between the crossing number and the height of a knotoid", (2020)

[13] Dabrowski-Tumanski Pawel, Rubach Pawel, Goundaroulis Dimos, Dorier Julien, Sulkowski Piotr, Millett Kenneth, Rawdon Eric, Stasiak Andrzej, Sulkowska Joanna. "KnotProt 2.0: a database of proteins with knots and other entangled structures. Nucleic Acids Research", (2018)

[14] Louis H. Kauffman, "Introduction to Virtual Knot Theory", (2012)

[15] Louis H. Kauffman, "Virtual Knot Theory", (2006)

[16] Kumud Bhandari, H. A. Dye and Louis H. Kauffman, "Lower Bounds on Virtual Crossing Number and Minimal Surface Genus", (2018)

[17] J. Green. A Table of Virtual Knots, http://www.math.toronto.edu/ drorbn/ Students/ GreenJ

[18] Goundaroulis D., Dorier J., Benedetti F., Stasiak A ."Studies of global and local entanglements of individual protein chains using the concept of knotoids", Scientific Reports, (2017)

[19] Goundaroulis D., Gügümcü N., Lambropoulou S., Dorier J., Stasiak A. and Kauffman LH, "Topological Models for Open-Knotted Protein Chains Using the Concepts of Knotoids and Bonded Knotoids", (2017)

[20] Dorier J., Goundaroulis D., Benedetti F., Stasiak A., "Knoto-ID: a tool to study the entanglement of open protein chains using the concept of knotoids", (2018).