Knotoids, Braidoids and Rail Knotoids

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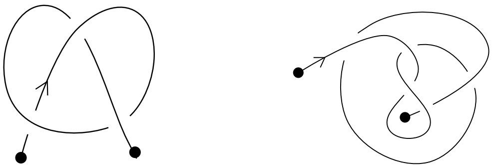
The theory of knotoids [Turaev, 2011]



A *knotoid diagram* in S^2 or in $\mathbb{R}^2$ is an open-ended knot diagram with two endpoints that can lie in different regions of the diagram.

- *Knotoids*, V. Turaev, *Osaka J. Math.* 49 (2012).
- *On a move reducing the genus of a knot diagram*, Daikoku, K., Sakai, K., and Takase, M., in *Indiana University Mathematics Journal* 61.3 (2012), pp. 1111–1127. ISSN: 00222518, 19435258. url: http://www.jstor.org/stable/24904076.

What is a knotoid diagram?

Definition

A *knotoid diagram* K in an oriented surface Σ is an immersion

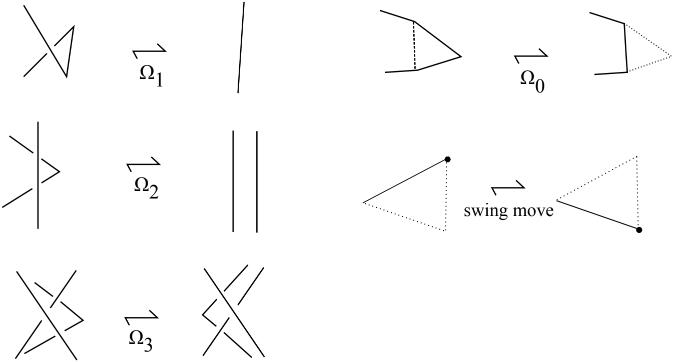
$$K : [0,1] \to \Sigma \text{ such that:}$$

1. finite double points, transversal and endowed with under/over data, the *crossings* of K,
2. the images of 0 and 1 are two disjoint points, the *endpoints* of K, called the *leg* and the *head* of K, respectively,
3. K is oriented from leg to head.

What is a knotoid?

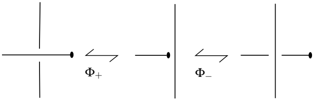
Definition

A *knotoid* in Σ is an equivalence class of knotoid diagrams in Σ up to the equivalence relation induced by the Ω-moves and isotopy of Σ.

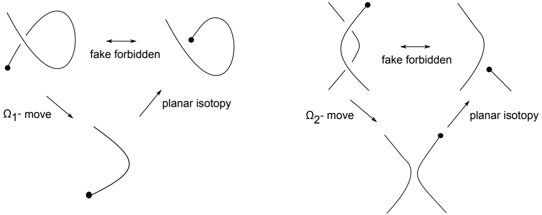


Knotoid moves

The forbidden moves



Forbidden moves for knotoids



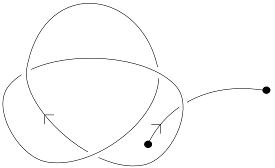
Fake forbidden moves

Extending the definition of a knotoid

Definition

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.

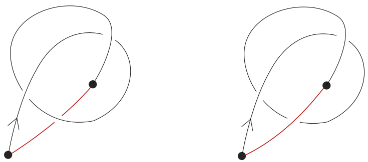
A *multi-knotoid* is an equivalence class of multi-knotoid diagrams determined by the equivalence relation generated by Ω-moves and isotopy of the surface.



A multi-knotoid diagram

We mostly focus on the cases $\Sigma = S^2$ and $\mathbb{R}^2$.

From knotoids to classical knots



There is a surjective map,

$$\omega_{-} : \{\text{Knotoids}\} \to \{\text{Classical knots}\}$$

induced by connecting the endpoints of a knotoid diagram with an underpassing arc (*the underpass closure*).
$\Rightarrow$ Invariants of classical knots can be computed on knotoid representatives.
$\Rightarrow$ Knot invariants computed on # of crossings have exponentially reduced computations (strong motivation).

Let κ be a classical knot and let K be any knotoid diagram representing κ, that is $\omega_-(K) = \kappa$.

Lemma (Tu)

$$\pi_1(\kappa) = \pi(K).$$

Lemma (Tu, DaSaTa)

Let D be an oriented diagram of κ. The Seifert genus of κ

$$g(\kappa) \leq (cr(K) - |\tilde{K}| + 1)/2 \leq (cr(D) - |\tilde{D}| + 1)/2$$

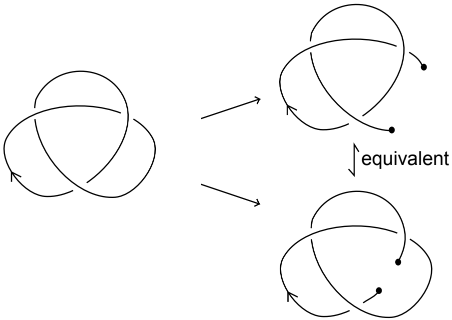
where $\tilde{K}, \tilde{D}$ are the 1-manifolds obtained by (oriented) smoothings of the crossings of K, D, $cr(K), cr(D)$ =# of crossings of K and D, $|\tilde{K}|, |\tilde{D}|$ = # of components of $\tilde{K}$and $\tilde{D}$.

From classical knots to knotoids

There is an injective map,

$$\alpha\colon\ \{\text{Classical knots}\} \to \{\text{Knotoids in } S^2\},$$

induced by deleting an open arc which does not contain any crossings from an oriented classical knot diagram.



$\Rightarrow$ The theory of knotoids in S^2 is an extension of classical knot theory.

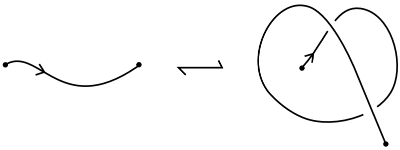
From classical knots to knotoids

Definition

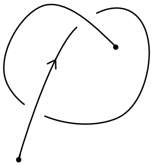
A knotoid in S^2 that is in the image of α, is called a *knot-type* knotoid.
A knotoid that is not in the image of α, is called a *proper* knotoid.

$$\{\text{Knotoids in } S^2\} = \{\text{Knot-type knotoids}\} \cup \{\text{ Proper knotoids}\}$$

Knot-type knotoids carry the same topological information as the corresponding classical knots.



A knot-type knotoid



A proper knotoid

Invariants of knotoids

Definition

Let M denote a set of mathematical objects. An *invariant of knotoids* is a mapping

$$I:\{\text{Knotoids}\} \to M,$$

assigning the same value to equivalent knotoid diagrams.

Knotoid invariants defined by Turaev:

- The bracket polynomial.
- 2-variable extended bracket polynomial: Using this invariant Bartholomew classified knotoids in S^2 up to 5 crossings:
- *Knotoids*, A. Bartholomew's mathematical page, http://www.layer8.co.uk/maths.knotoids/index.htm, Jan. 2015.

The complexity or height of a knotoid

Definition

The *complexity* of a knotoid diagram (Tu), renamed to *height* (GüKa), is the minimum number of crossings created by the underpass closure. The *complexity or height* of a knotoid K is defined as the minimum of the complexities (or heights), taken over all equivalent knotoid diagrams to K.

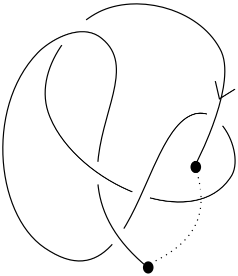
The complexity is a knotoid invariant.

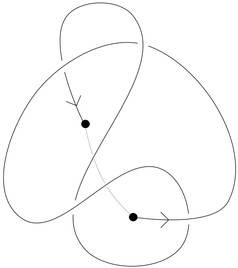
A knotoid has zero complexity if and only if it is a knot-type knotoid.

$$\equiv$$

A knotoid has non-zero complexity if and only if it is a proper knotoid.

Computing complexity can be tricky



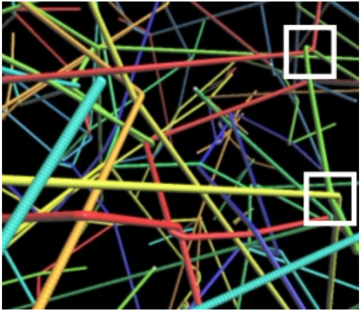


Question

The first diagram has complexity 1 and the second one has complexity 2. But are there some equivalent diagrams to the knotoid diagrams above with less complexity?

Knotoids revisited

- In May 2011 Turaev presented his theory of knotoids at the Lake Thun.
- At the time I was working with my ex-student Eleni Panagiotou and Ken Millett on the study of topological entanglements of open polymer chains. So, I could see immediately the applicability of the theory.



Knotoids revisited

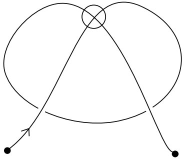
- In 2014 I proposed the subject to my new student Neslihan Gügümcü. Lou Kauffman was the Visiting Researcher of the big research grant Thalis of my research team.
- *New invariants of knotoids*, N. Gügümcü, L.H. Kauffman, *Europ. J. Combinatorics* 65C (2017).
- *On knotoids, braidoids and their applications*, Gügümcü, N., *PhD thesis*, National Technical U. Athens, 2017.

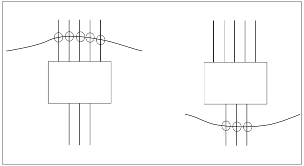
Virtual knotoids [Turaev, GüKa]

The notions of virtual knot theory naturally extend to knotoids.

Definition

A *virtual knotoid diagram* is a knotoid diagram in S^2 (or in $\mathbb{R}^2$) with classical and virtual crossings.
A *virtual knotoid* is an equivalence class of virtual knotoid diagrams up to the equivalence relation generated by the Ω-moves and the detour move.





The following theorem was stated by Turaev.

Theorem (Gügümcü,Kauffman)

The theory of virtual knotoids is equivalent to the theory of knotoid diagrams in higher genus surfaces considered up to Ω-moves in the surfaces, isotopy of the surfaces and addition/removal of handles in the complement of knotoid diagrams.

Definition

The *genus* of a virtual knot is the minimum genus among the surfaces for which the knot has a diagram without any virtual crossings.

From knotoids to virtual knots

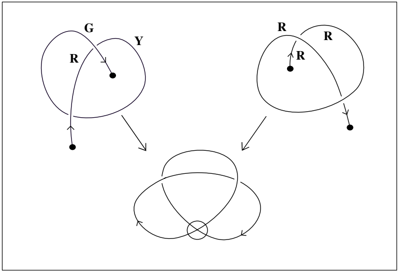
There is a well-defined map called the *virtual closure map*,

$$\overline{v}\colon \{\text{Knotoids in } S^2\} \to \{\text{Virtual knots of genus} \leq 1\},$$

induced by associating a knotoid diagram to the virtual knot diagram obtained by connecting virtually the endpoints of the knotoid diagram.

The virtual closure map

- The virtual closure map is not injective:



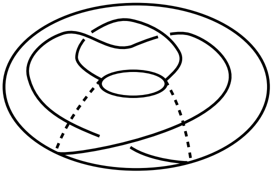
A pair of non-equivalent knotoids with the same virtual closure

The virtual closure map

Proposition (Gügümcü,Kauffman)

The virtual closure map is not surjective.

The virtual knot below is a genus 1 knot that is not in the image of $\overline{v}$.



- They showed this by examining the surface-state curves of the diagram in torus.

- Yet, since the virtual closure map is well-defined, any virtual knot invariant can define an invariant of knotoids through this map.

Indeed, let *Inv* denote an invariant of virtual knots.
Define an invariant of knotoids I by the following formula,

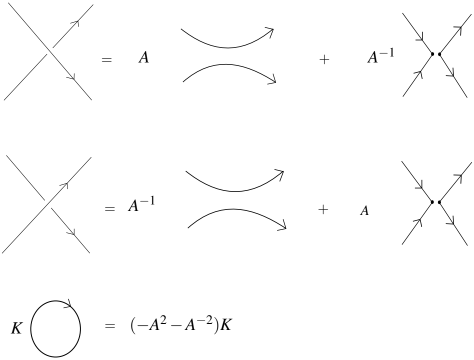
$$I(K) = Inv(\overline{v}(K)),$$

where K denotes a knotoid in S^2.

- Many virtual knot invariants can be constructed directly on knotoids.

An extension of the bracket polynomial: The arrow polynomial

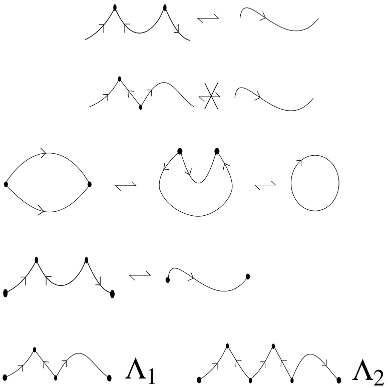
The construction of the arrow polynomial for knotoids is based on the *oriented state expansion* of the bracket polynomial.



Oriented state expansion

Reduction rules for the arrow polynomial

To reduce the number of cusps in a state component we have the following rules:



The arrow polynomial

Definition (Gügümcü,Kauffman)

The *arrow polynomial* of a knotoid diagram K is defined as,

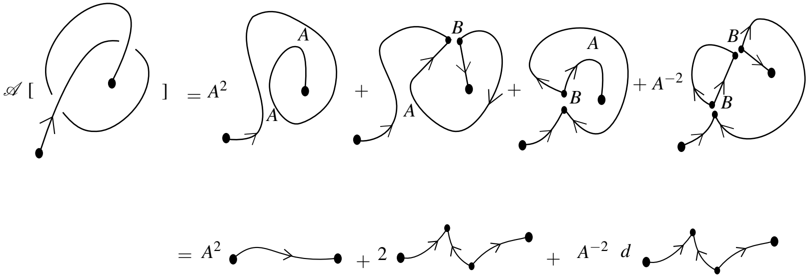
$$\mathscr{A}[K] = \sum_S < K|S > (-A^2 - A^{-2})^{||S||-1}\Lambda_i$$

where $< K|S >$ is the usual vertex weights of the bracket polynomial, $||S||$ is the number of components of the state S and Λ_i is the variable associated to the long segment component of S with irreducible zig-zags.

Theorem (Gügümcü,Kauffman)

The normalization of the arrow polynomial (multiplication by $(-A^{-3})^{-\mathrm{wr}(K)}$) is a knotoid invariant.

An example for computing the arrow polynomial



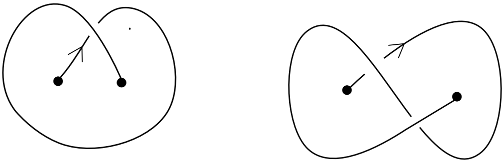
$$= A^2 + (1 - A^4)\Lambda_1$$

Comparing knotoids in S^2 and in $\mathbb{R}^2$

There is a surjective map,

$$\iota : \{\textit{knotoids in } \mathbb{R}^2\} \to \{\textit{knotoids in } S^2\}$$

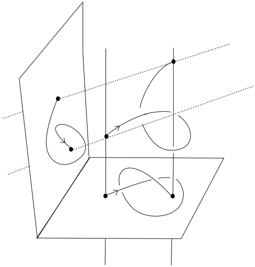
which is induced by $\iota : \mathbb{R}^2 \hookrightarrow S^2$. This map is not injective.



Nontrivial and nonequivalent planar knotoids which are both trivial in S^2

A lifting in space for planar knotoids

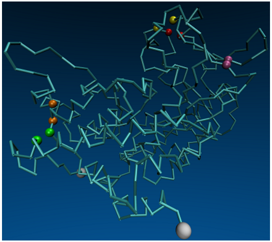
Two open space curves with their ends attached on two parallel lines are *line isotopic* (GüKa) or *rail isotopic* (KoLa) if there is an ambient isotopy taking one curve to the other in the complement of the lines and keeping the ends on the lines.



Theorem (Gügümcü, Kauffman)

There is a bijection between the set of knotoids in $\mathbb{R}^2$ and the set of line isotopy classes of smooth open oriented curves in $\mathbb{R}^3$.

Analyzing the topology of open protein chains



Previous approaches:

1. **Direct closure**: Connect the two endpoints of a protein chain and analyze the type of the resulting knot.
2. **Uniform closure**: Enclose the protein chain in a ball, choose a point on the boundary of the ball, connect the two endpoints to this point and analyze the resulting knot type.
3. **Virtual closure**: Project the protein chain on several planes, connect the two endpoints virtually and analyze the resulting virtual knot types.

Analyzing open protein chains using knotoids

In 2015, at the dissemination workshop of our grant Thalis, my ex-student Dimos Goundaroulis told me he was applying for a post-doc at Lausanne with Andrzej Stasiak and asked me if he could propose the use of knotoids for the study of proteins.

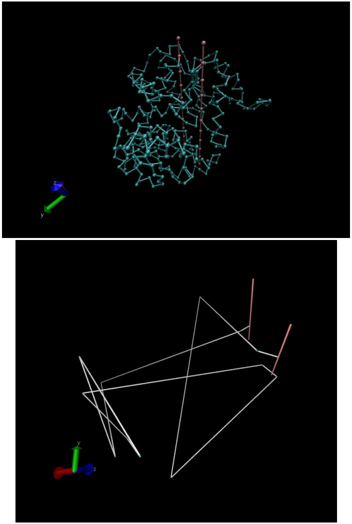
- *Studies of global and local entanglements of individual protein chains using the concept of knotoids*, D. Goundaroulis, J. Dorier, F. Benedetti, A. Stasiak, *Sci. Reports 7* (2017), 6309.
- *Topological models for knotted bonded open protein chains using the concept of knotoids and bonded knotoids*, D.Goundaroulis, N.Gügümcü, S.Lambropoulou, J.Dorier, A.Stasiak and L.H.Kauffman, *Polymers* 9(9), (2017).
- *KnotProt 2.0: a database of proteins with knots and other entangled structures*, Dabrowski-Tumanski, P., Rubach, P., Goundaroulis, D., Dorier, J., Sukowski, P., Millett, K.C., Rawdon, E.J., Stasiak, A., and Sukowska, J.I., *Nucleic Acids Research* **1** (2018). DOI: 10.1093/nar/gky1140.

Analyzing open protein chains using knotoids

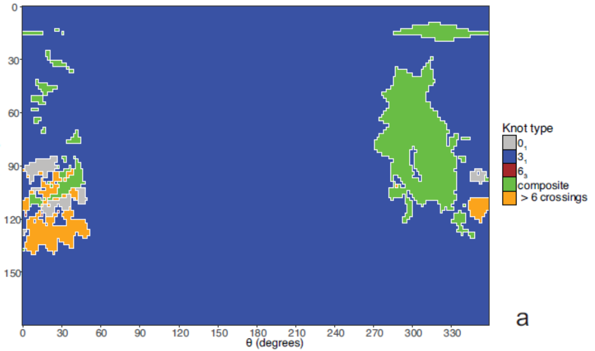
The knotoid approach (thanks to the lifting!):

1. The protein chain is assumed to lie in a ball of sufficiently large radius.
2. Each point on the boundary determines a projection plane for the protein chain.
3. Choose one plane and introduce the lines passing through the termini and are perpendicular to the plane.
4. Simplify the chain by an algorithm eliminating triangles never crossing through the lines.
5. Project the chain to the plane, along the lines.
6. The resulting diagram is a knotoid diagram. Determine the knotoid type by using knotoid invariants (the bracket polynomial for spherical and the arrow polynomial for planar knotoids).

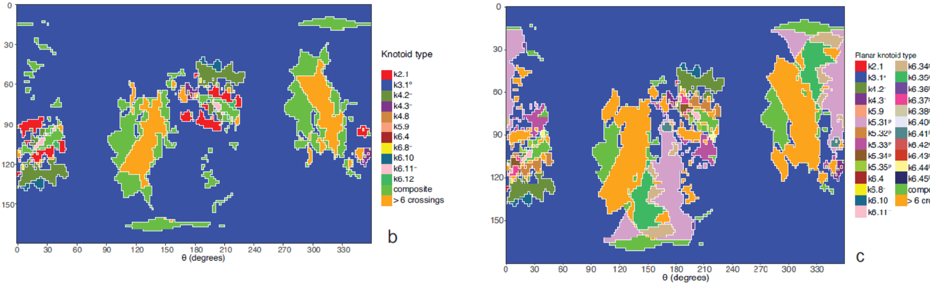
Analyzing the protein 3KZN



The protein 3KZN



Detecting 3KZN via uniform closure



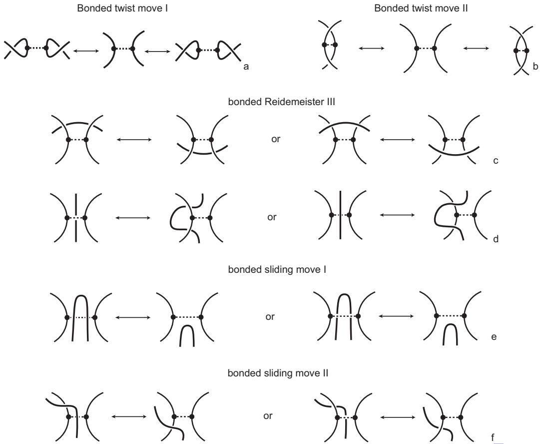
Detecting 3KZN via knotoids, b:spherical knotoids, c: planar knotoids

Conclusions

- Spherical knotoids render as much information as the virtual closure.
- Analyzing open protein chains as planar knotoids reveals more details of their topology.

A topological model for bonded protein chains

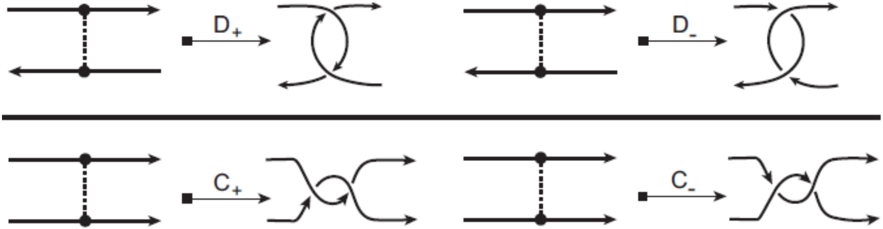
Definition: A *bonded knotoid diagram* is a knotoid diagram with finitely many edges connecting any two strands of the diagram.
A *bonded knotoid* is an equivalence class of bonded knotoid diagrams up to the equivalence relation generated by the *bonded moves*:



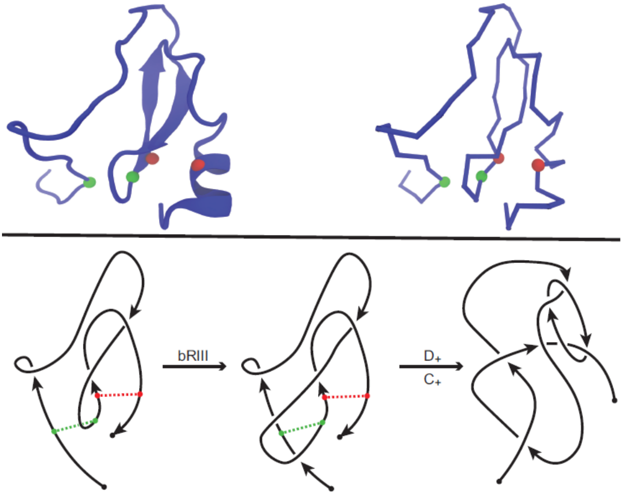
A topological model for bonded protein chains

1. Determine a projection direction for the chain with bonds.
2. Draw the two lines passing through the endpoints of the chain and are perpendicular to the projection plane. Simplify the chain accordingly to the lines.
3. Project the chain to the plane along the lines. The bonds of the protein are projected as edges between the corresponding points. The resulting diagram is a bonded knotoid diagram.
4. Replace the bonding site by a full-twist along the edge if the neighbouring strands are directed anti-parallel. Otherwise replace the bonding site by a full-twist. The resulting diagram is a planar (multi-)knotoid diagram. Determine its type via knotoid invariants.

Twist Insertions



An application



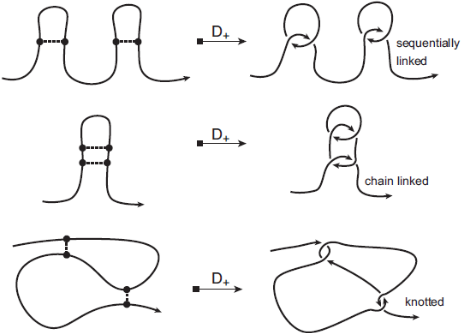
A projection of the protein chain 2LFK

Conclusion

With this model, we are able to detect three types of protein bonds

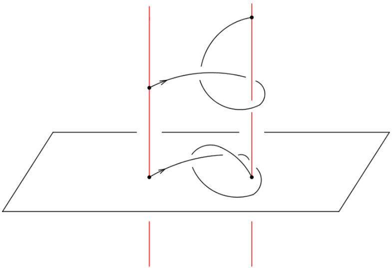
- sequential bonds
- nested bonds
- pseudoknot-like bonds

via knotoid invariants, such as the Turaev loop polynomial and the arrow polynomial.



The theory of rail knotoids [Kodokostas & SL]

Recall the open space curves (GüKa) or rail arcs (KoLa) lifting knotoids:



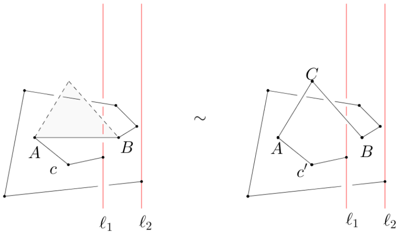
Definition

A *rail arc* is any oriented, connected, embedded arc c in $\mathbb{R}^3$ with its interior in $\mathbb{R}^3 - (\ell_1 \cup \ell_2)$, its first endpoint on ℓ_1 and the last on ℓ_2.

Rail isotopy

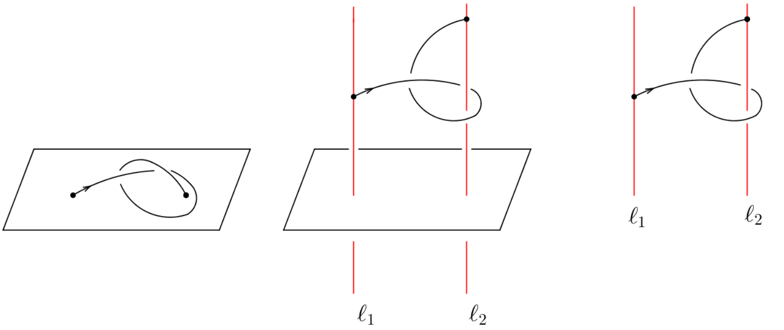
Definition

Rail isotopy between two rail arcs c_1, c_2 is an isotopy of $\mathbb{R}^3$ taking one onto the other, so that each rail maps onto itself (not necessarily pointwise) throughout the isotopy. So, throughout the isotopy, the image of the arc is a rail arc, and each endpoint remains on the same rail, but with the freedom to slide along it.



Δ-moves for p.l. rail arcs

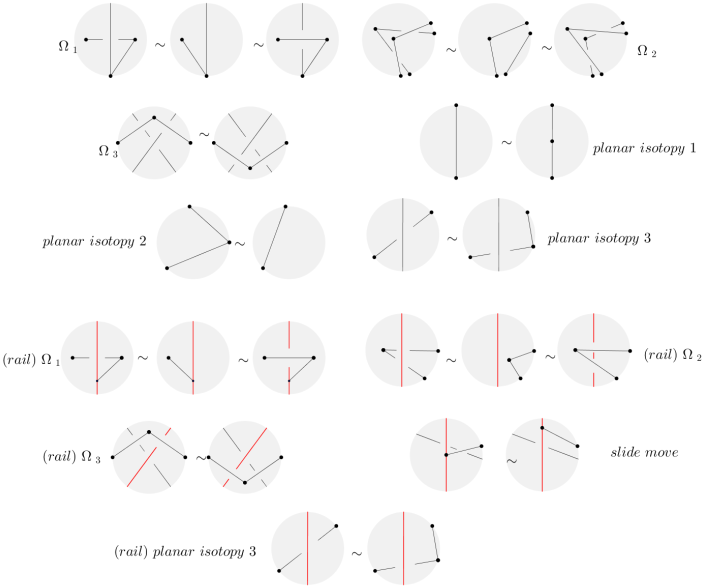
Rail knotoids



Planar knotoid, lifting rail arc, corresponding rail knotoid

- *Rail knotoids*, Kodokostas, D., Lambropoulou, S., to appear in *J. Knot Theory & Ramif.* (2019), arXiv:1812.09493.

Rail knotoid equivalence



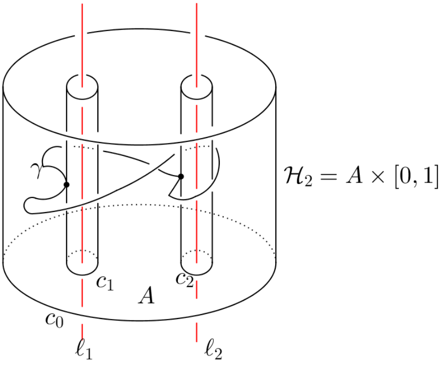
Rail knotoid equivalence

Theorem

Two rail arcs in $\mathbb{R}^3$ are rail isotopic iff their rail knotoid diagram projections on the plane of the rails are rail equivalent. In other words, rail arcs are isotopic iff they correspond to the same rail knotoid.

- Hence, planar knotoids correspond bijectively to rail knotoids.

Connection with the handlebody of genus 2



Proposition

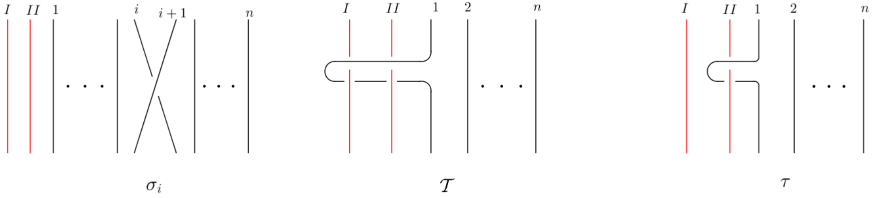
Rail isotopies in $\mathbb{R}^3$ are in one to one correspondence with rail isotopies in $\mathscr{H}_2$.

Knots in the handlebody of genus 2

Proposition

Knot isotopies in $\mathscr{H}_2$ are in one to one correspondence with matching rail isotopies of two rail arcs with the same endpoints.

The knot theory in the handlebody of genus 2 has been approached in terms of mixed braids and quotient Hecke-type algebras:



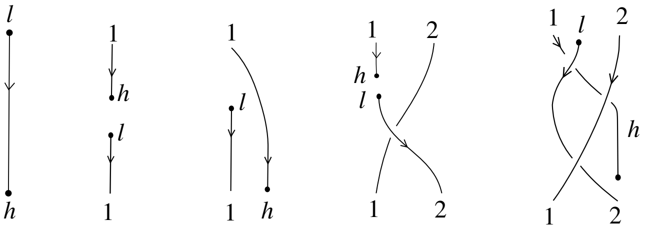
Mixed braid generators for knots in the handlebody of genus 2

- *Braid structures in knot complements, handlebodies and 3–manifolds*, S. Lambropoulou, in Proceedings of the Conference *Knots in Hellas '98*, Series on Knots and Everything **24**, pp. 274–289, 2000.
- *Some Hecke-type algebras derived from the braid group with two fixed strands*, D. Kodokostas, S. Lambropoulou, in Springer PROMS Series, Volume: *Algebraic Modeling of Topological and Computational Structures and Applications*, L.H. Kauffman et al. Eds, 2017.
- *Braid groups in handlebodies and corresponding Hecke algebras*, V. G. Bardakov, in Springer PROMS Series, Volume: *Algebraic Modeling of Topological and Computational Structures and Applications*, L.H. Kauffman et al. Eds, 2017.
- *A spanning set and potential basis of the mixed Hecke algebra on two fixed strands*, Kodokostas, D., Lambropoulou, S., *Mediterranean J. Math.* (2018), **15:192**, https://doi.org/10.1007/s00009-018-1240-7.

The theory of braidoids [N. Gügümcü & SL]

In parallel to revisiting knotoids, the theory of braidoids was established.

- *Knotoids, braidoids and applications*, N.Gügümcü, S.Lambropoulou, *Symmetry* 9(12):315, (2017).
- *Braidoids*, Gügümcü, N., Lambropoulou, S., submitted for publication.

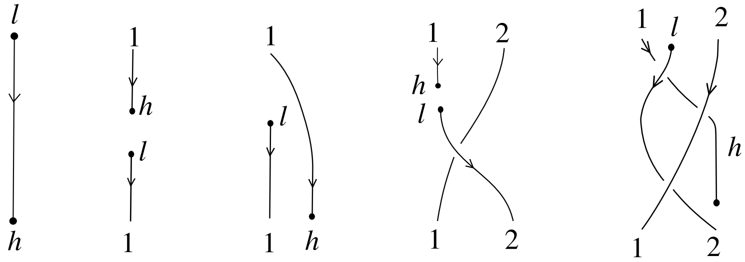


What is a braidoid diagram?

Definition

A *braidoid diagram* B is a system of a finite number of arcs embedded in $[0,1] \times [0,1] \subset \mathbb{R}^2$ that are called the *strands* of B.

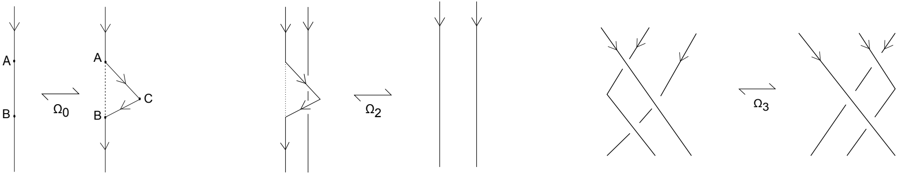
1. There are only finitely many intersection points among the strands, which are transversal double points endowed with over/under data, and are called *crossings*.
2. Each strand is naturally oriented downward, with no local maxima or minima, so that it intersects a strand horizontal line at most once.
3. A braidoid diagram has two types of strands, the classical strands and the free strands. A *free strand* has one or two ends that are not necessarily at $[0,1] \times \{0\}$ and $[0,1] \times \{1\}$. Such ends of free strands are called the *endpoints* of B.



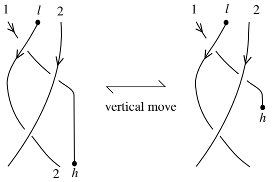
Examples of braidoid diagrams

Moves on braidoid diagrams

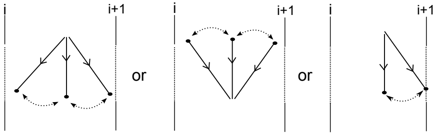
Δ-Moves:



Vertical Moves:



Swing Moves:



Braidoids

Definition

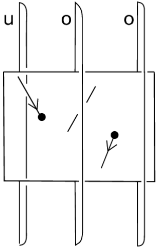
Two braidoid diagrams are said to be *isotopic* if one can be obtained from the other by a finite sequence of Ω-moves, vertical moves and swing moves. An isotopy class of braidoid diagrams is called a *braidoid*.

Definition

A *labeled braidoid diagram* is a braidoid diagram whose braidoid ends are labeled with o or u.
A *labeled braidoid* is an isotopy class of labeled braidoid diagrams up to the isotopy generated by the Ω-moves.

From braidoids to planar knotoids

- We define a closure operation on labeled braidoid diagrams by connecting each pair of corresponding ends accordingly to their labels and within a 'sufficiently close' distance:



The closure operation induces a well-defined map from the set of labeled braidoids to the set of planar multi-knotoids.

The analogue of the Alexander theorem for braidoids

Theorem (The classical Alexander theorem)

Any classical knot/link diagram is isotopic to the closure of a classical braid diagram.

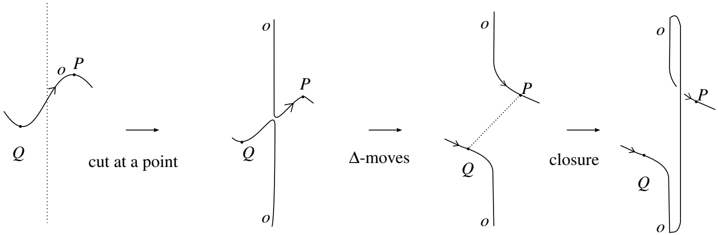
Theorem

Any multi-knotoid diagram in $\mathbb{R}^2$ is isotopic to the closure of a labeled braidoid diagram.

From a knotoid diagram to a braidoid diagram

We describe two braidoiding algorithms to prove our theorem.

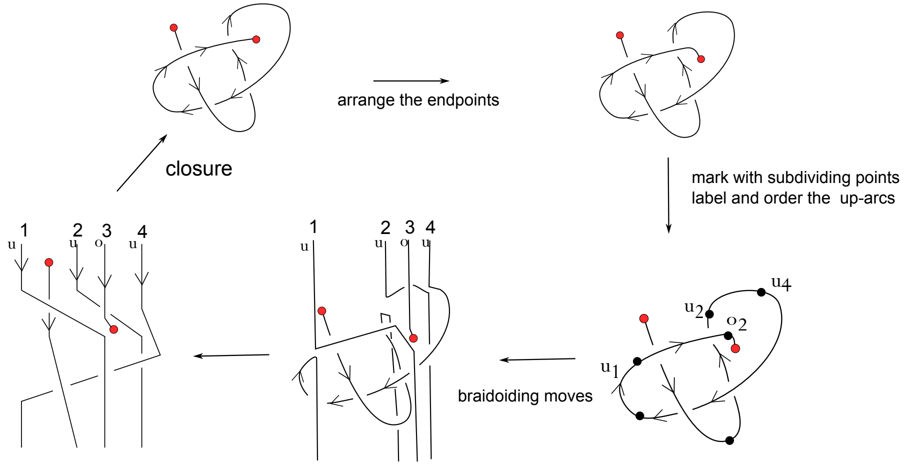
The idea of the algorithms: To eliminate the up-arcs of a (multi)-knotoid diagram. We do this by the *braidoiding moves*:



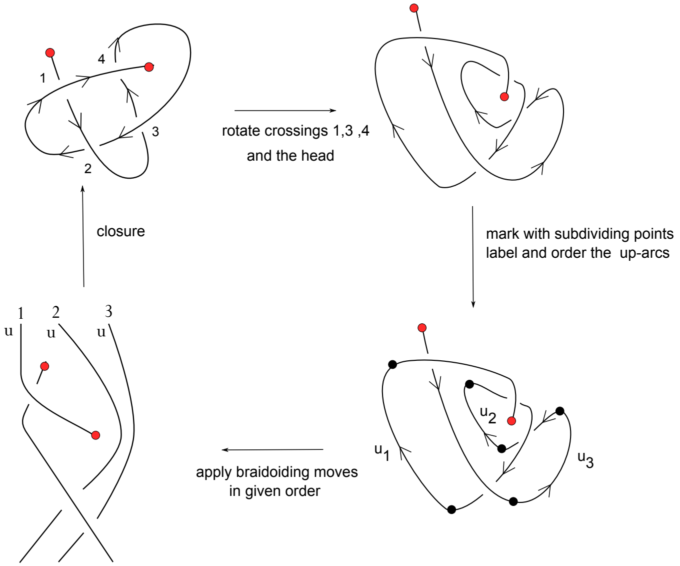
The L-braidoiding move and its closure

- Observe that the closure of each resulting labeled strand is isotopic to the initial up-arc.

Braidoiding algorithm I (based on SL):



Braidoiding algorithm II (based on Kauffman & SL):



A corollary of the braidoiding algorithm II

Definition

A *u-labeled braidoid diagram* is a labeled braidoid diagram whose ends are labeled all with u.

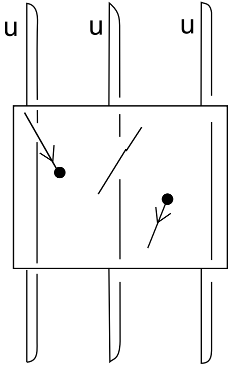
There is a bijection:

$$Label_u : \{\text{Braidoids}\} \rightarrow \{u\text{-labeled braidoids}\}$$

induced by assigning to a braidoid diagram a u-labeled braidoid diagram.

A sharpened version of the theorem

The uniform closure:



Theorem

Any multi-knotoid diagram $\mathbb{R}^2$ is isotopic to the uniform closure of a braidoid diagram.

Markov theorem for classical braids

Theorem (*Markov theorem*)

The closures of two braid diagrams b, b' in $\cup_{n=1}^{\infty} B_n$, represent isotopic links in $\mathbb{R}^3$ if and only if these braids are equivalent by the following operations.

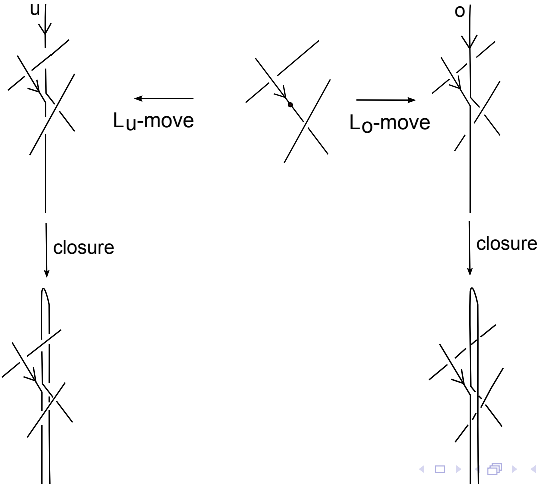
- *Conjugation: For $b, b' \in B_n$, $b' = gbg^{-1}$ for some $g \in B_n$.*
- *Stabilization: For $b \in B_n$, $b' \in B_{n+1}$, $b' = \sigma_n^{\pm} b$.*

Theorem (*One move Markov theorem*, SL & Rourke)

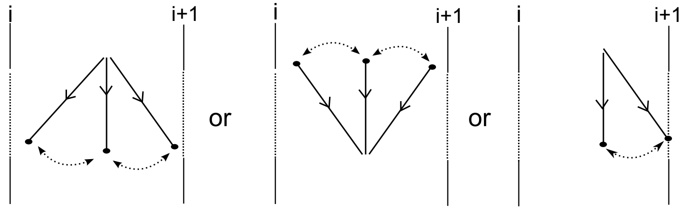
There is a bijection between the set of L-equivalence classes of braids and the set of isotopy classes of (oriented) link diagrams.

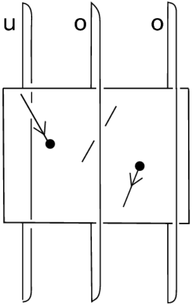
From knotoids to braidoids: Braidoid equivalence

An *L-move* on a labeled braidoid diagram B is the following operation:



Recall the swing moves for braidoids, due to the closure:

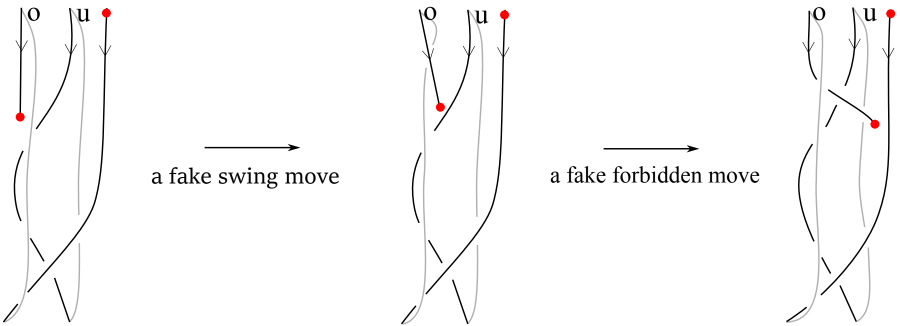




Fake forbidden and fake swing moves

Definition

A *fake forbidden move* on a labeled braidoid diagram B is a forbidden move on B which upon closure induces a fake forbidden move on the (multi-)knotoid diagram.



An L-move analogue theorem for braidoids

Lemma

A fake forbidden move on a labeled braidoid diagram can be obtained by a sequence of L-moves, fake swing moves and planar isotopy.

Definition

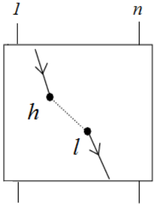
The L-moves together with braidoid isotopy moves and fake swing moves generate an equivalence relation on labeled braidoid diagrams that is called the *L-equivalence*.

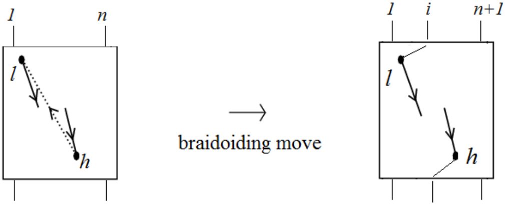
Theorem

The closures of two labeled braidoid diagrams are isotopic (multi-)knotoids in $\mathbb{R}^2$ *if and only if the labeled braidoid diagrams are L-equivalent.*

From braidoids to braids

The underpass closure: In order to receive as outcome a braid diagram we must also ensure the braid monotonicity condition.





Two examples of the underpass closure

Proposition

The underpass closure is a well-defined surjective map from the set of braidoids to the set of L-equivalence classes of classical braids.

Further references

1. Biquandle coloring invariants of knotoids, Gügümcü, N., Nelson, S., to appear in *J. Knot Theory Ramifications*, arXiv preprint: https://arxiv.org/abs/1803.11308.
2. A survey on knotoids, braidoids and their applications, Gügümcü, N., Kauffman, L.H., and Lambropoulou, S., in "Knots, Low-dimensional Topology and Applications" with subtitle "Proceedings of the International Conference on Knots, Low-dimensional Topology and Applications - Knots in Hellas 2016", *Springer Proceedings in Mathematics & Statistics (PROMS)*; 2019; C. Adams et al, Eds.
3. Classification of low complexity knotoids, Korablev, P.G., May, Y.K., Tarkaev, V, *Siberian Electronic Mathematical Reports* (2018), **15**, 1237-1244. [Russian, English abstract]. DOI: 10.17377/semi.2018.15.100.
4. Knots related by knotoids, Adams, C., Henrich, A., Kearney, K., and Scoville, N., to appear in *American Mathematical Monthly*

Thank you for your attention!