Bonded Knots and Braids: From Topology to Algebra and Protein Structure

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(Joint works with Louis H. Kauffman, U. Illinois Chicago; Sofia Lambropoulou, N.T. University of Athens; and Sonia Mahmoudi, Tohoku University)

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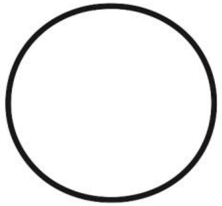
Outline

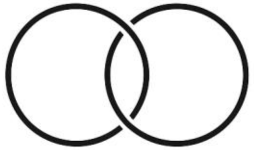
- Introduction to classical Knot Theory
- Bonded Knots (joint work with L. Kauffman & S. Lambropoulou)
- Bonded Braids (joint work with S. Lambropoulou)
- Bonded DP Tangles (joint work with S. Lambropoulou & S. Mahmoudi)

Classical knots and links

Definition

A *knot* is a smooth embedding of the circle $c : S^1 \hookrightarrow \mathbb{R}^3$ or S^3 . A *link* of k components is a smooth embedding of k copies of the circle S^1 in $\mathbb{R}^3$ or in S^3. A knot is a 1-component link.


Unknot

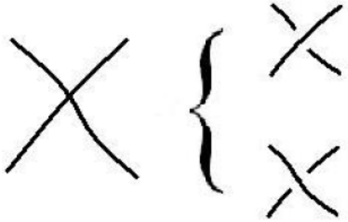

Hopf link

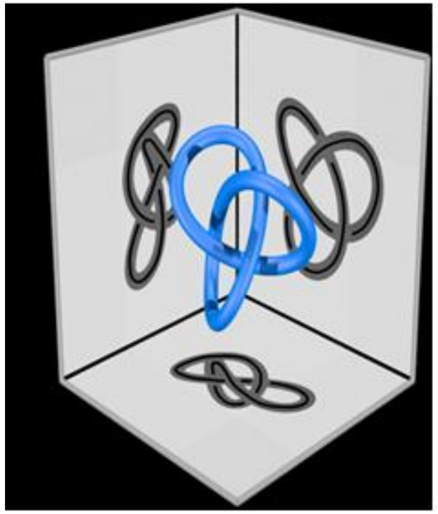
Definition

Two links are *isotopic* $L_1 \sim L_2 \iff \exists F : \mathbb{R}^3 \times [0,1] \to \mathbb{R}^3$ continuous s.t.: (i) F_0 is the identity, (ii) F_t is an o.p. homeomorphism $\forall t \in [0,1]$ and (iii) $F_1 \circ L_1 = L_2$.

Discretization of isotopy

A *knot diagram* is a projection on a plane, with only finitely many double points, the **crossings**, with extra ‘under/over’ information:

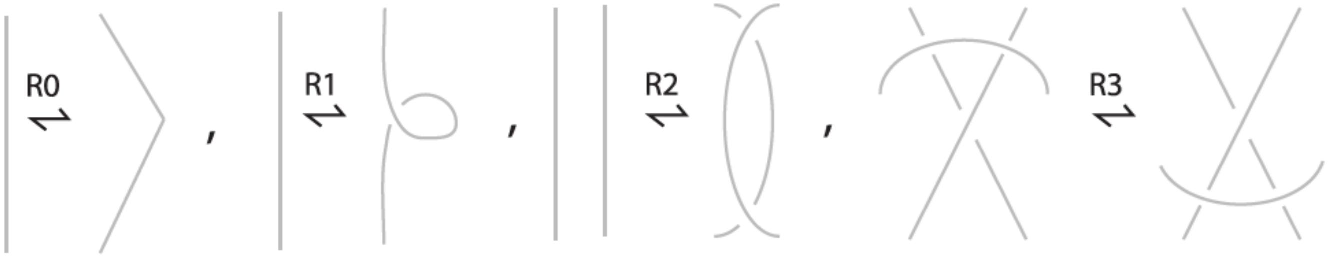




Theorem (Reidemeister, 1927)

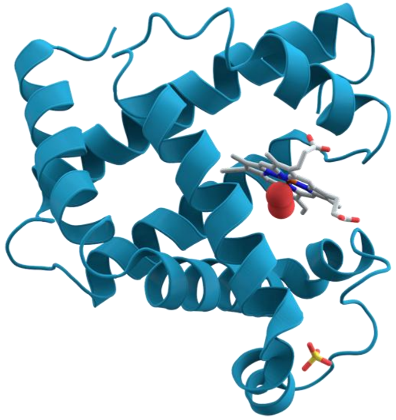
Two knots are isotopic iff any diagrams of theirs differ by finitely many planar isotopies and the Reidemeister moves RI, RII, RIII.

Regular isotopy is generated by planar isotopies and the Reidemeister moves RII, RIII.



Motivations from protein structure and function

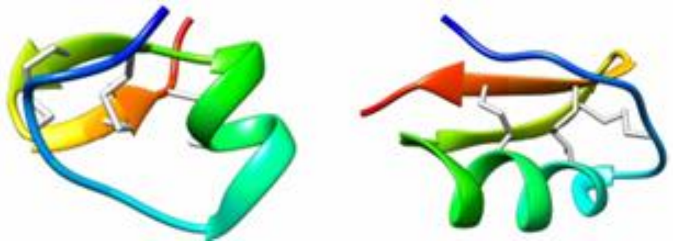
[*Wikipedia*]: Proteins are (***open-ended***) large biomolecules and macromolecules that comprise one or more long chains of amino acid residues.



Proteins perform a vast array of functions within organisms, including catalysing metabolic reactions, DNA replication, responding to stimuli, providing structure to cells and organisms, and transporting molecules from one location to another.

Proteins differ from one another primarily in their sequence of amino acids, which is dictated by the nucleotide sequence of their genes, and which usually results in protein folding into a specific 3D structure that determines its activity.

A linear chain of amino acid residues is called a polypeptide. A protein contains at least one long polypeptide. The individual amino acid residues are bonded together by peptide bonds and adjacent amino acid residues.



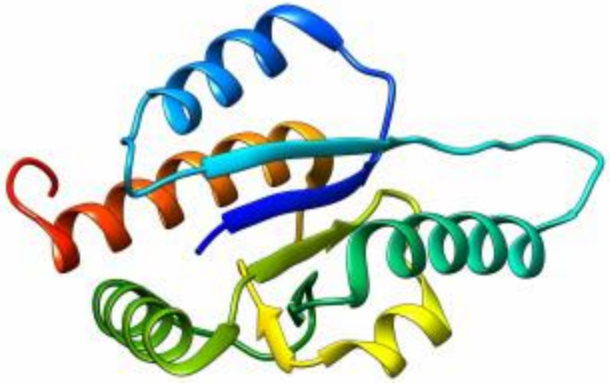
Knotted proteins

- Knots in proteins were first hypothesized in 1994 and identified shortly thereafter.
- Today, it is recognized that knotted proteins are relatively common, and approximately 1% of all entries in the Protein Data Bank (PDB) exhibit knotted structures.
- Although the functional role of these knots is not yet fully understood, it is suggested that knottedness enhances the molecule's thermal and kinetic stability.

To analyse the topology of a protein and detect possible knottedness, it was first considered necessary to represent its backbone as a closed loop.

Protein closures: the direct closure

- Direct segment closure: Connect the two endpoints of a protein chain and analyze the type of the resulting knot (sensitive to small movements).



(A) The YBEA methyltransferase from E. coli (PDB entry 1NS5).

(B) The corresponding topology of the backbone (closed by a direct segment).

An example of a knotted protein and its backbone topology forming an oriented right-handed trefoil knot via direct closure. Source: [B. Gabrovsek, An invariant for colored bonded knots, Studies in Applied Mathematics, Volume 146, Issue 3, 2020].

A direct approach to the protein topology

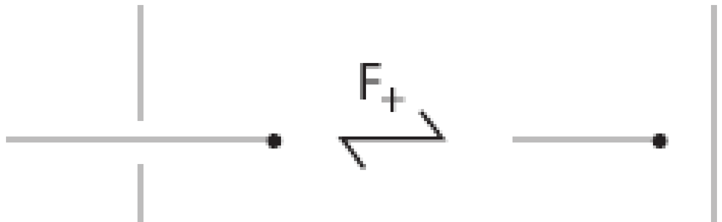
Recently, alternative models have been proposed that bypass the need for closure altogether, such as knotoids (open-knotted curves).

- **Knotoids**, V. Turaev, Osaka J. Math. 49 (2012), 195–223.

Definition

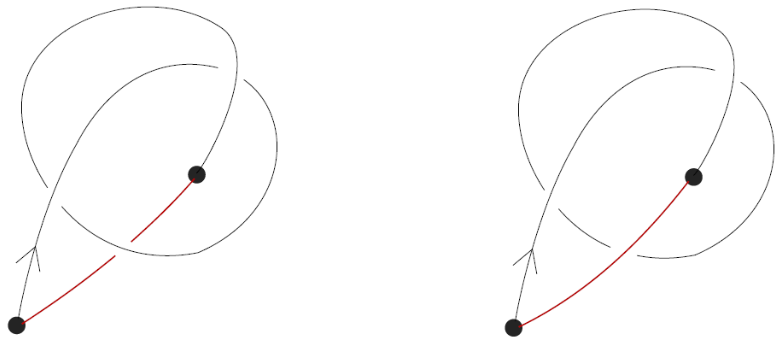
A knotoid diagram in S^2 or in $\mathbb{R}^2$ is an open-ended knot diagram with two endpoints that can lie in different regions of the diagram.
A knotoid is an equivalence class of knotoid diagrams up to the equivalence relation induced by the Reidemeister moves and planar isotopies, including the swing moves for the endpoints.

A knotoid



Forbidden moves

From knotoids to classical knots



Two types of closures resulting in different classical knots

[Turaev] There is a surjective map,

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

induced by connecting the endpoints of a knotoid diagram with an underpassing arc (<u>the underpass closure</u>).

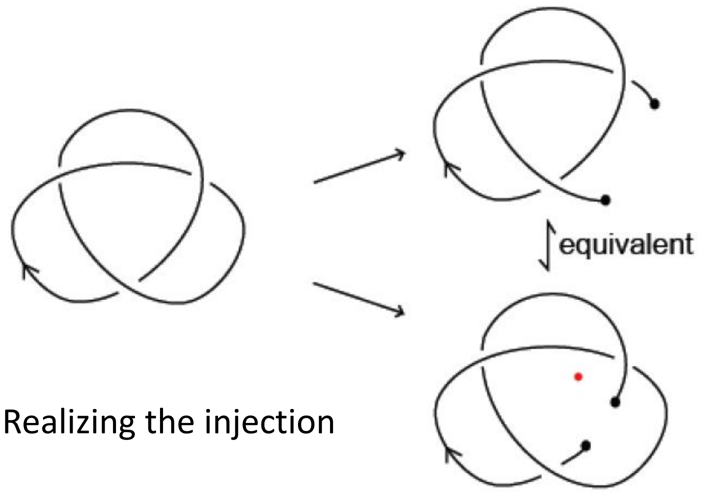
⇒ Invariants of classical knots can be computed on knotoid representatives.

[Turaev] There is an injective map,

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

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

⇒ The theory of knotoids in S^2 is an extension of classical knot theory.



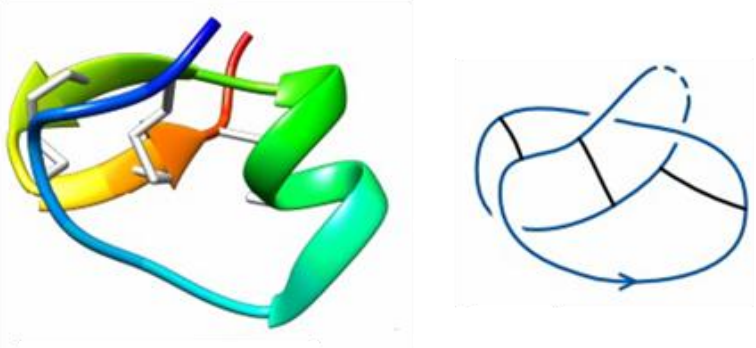
Realizing the injection

Reclaiming bonds: All proteins contain bonds

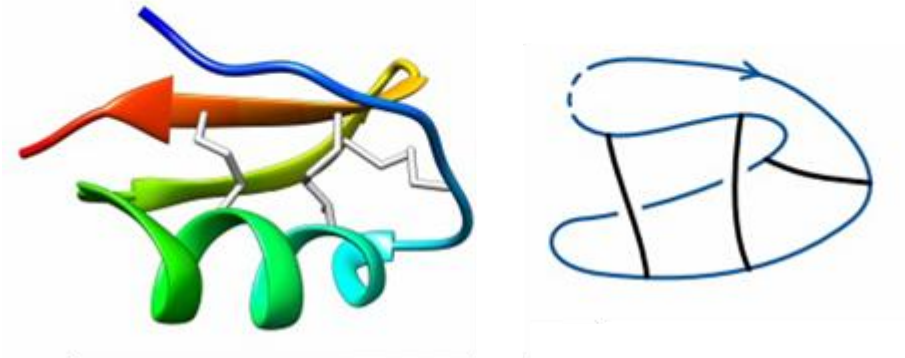
The three-dimensional structure of a protein also includes bonds that link parts of the peptide backbone. These bonds, which serve both structural and functional purposes, include hydrogen bonds, hydrophobic interactions, salt bridges, disulfide bonds, and others.

From a knot-theoretic perspective, it is crucial that such bonds are incorporated into the topological representation of the protein structure.

Including bonds in the protein model



CN29 toxin.

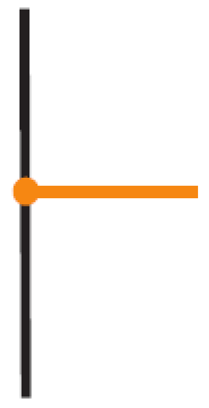


ADWX-1 toxin.

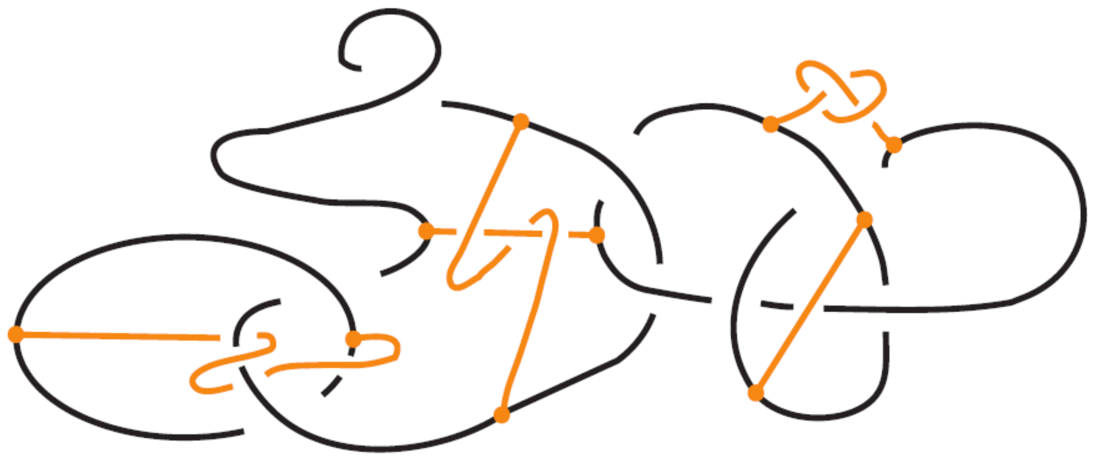
Bonded knots and links

Definition

A *(oriented) bonded link* is a pair (L, B), where L is a (oriented) knot/link embedded in S^3 and B is a finite set of k pairwise disjoint embedded arcs called *bonds*, whose interiors are properly embedded in the complement of L in S^3, $S^3 \backslash L$, such that the boundaries of the k bonds intersect the link transversely in $2k$ distinct points, the bonding sites, called *nodes*. If $B = \emptyset$, then $(L, B) = L$ a classical link in S^3.



A neighbourhood of a node



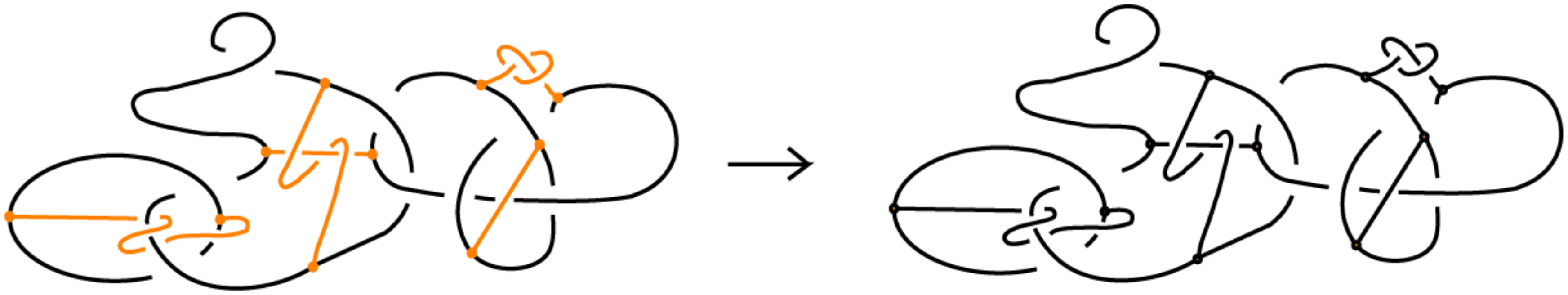
A bonded link

Bonded knots and embedded graphs

- The theory of bonded knots is based theoretically on the studies of *embedded graphs* of Conway-Gordon (1983); Kauffman (1989, Transactions AMS); Kauffman-Vogel (1992); Jaeger (1993); et al.

- The theory of embedded graphs has been applied in Chemistry in the study of polymers [Flapan, Simons, et al.] and in Biology in the study of RNA [Kauffman et al.].

- Bonded knots/links can be viewed as special cases of embedded trivalent graphs, where there are two types of edges: ordinary edges and bonds (orange). Bonds always start and terminate at a classical edge and the nodes are the vertices.

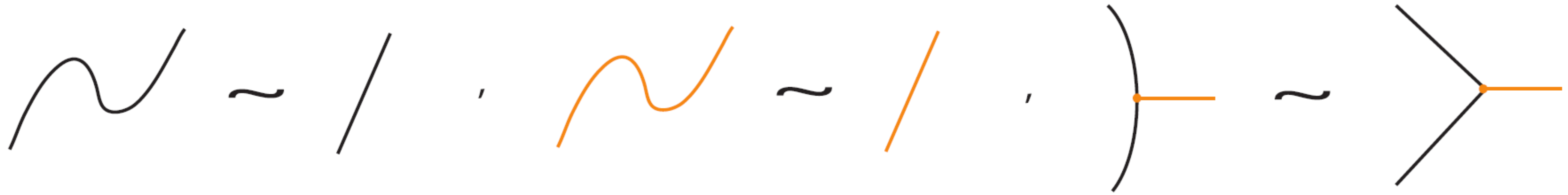


Topological and rigid vertex isotopy for bonded links

Adapting [Kauffman] we then have:

Theorem

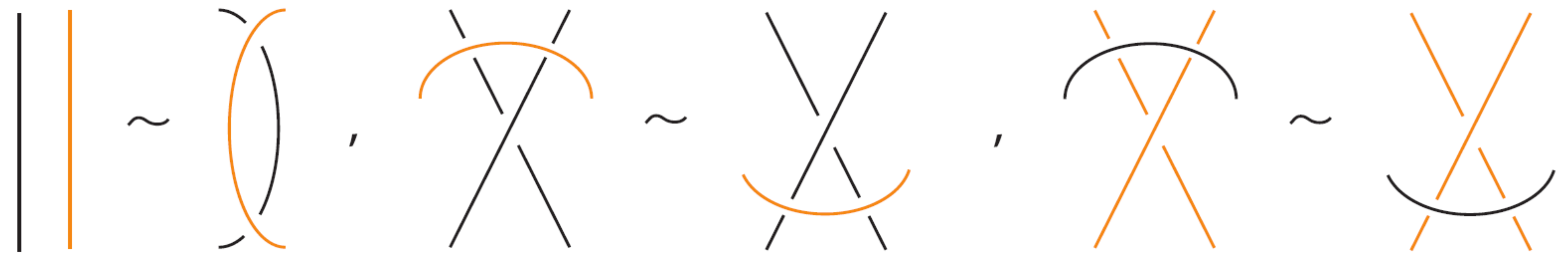
Two (oriented) bonded links (L_1, B_1) and (L_2, B_2) are equivalent via *topological vertex isotopy* resp. *rigid vertex isotopy* if and only if any diagrams of theirs differ by a finite sequence of the basic moves illustrated in Figs.



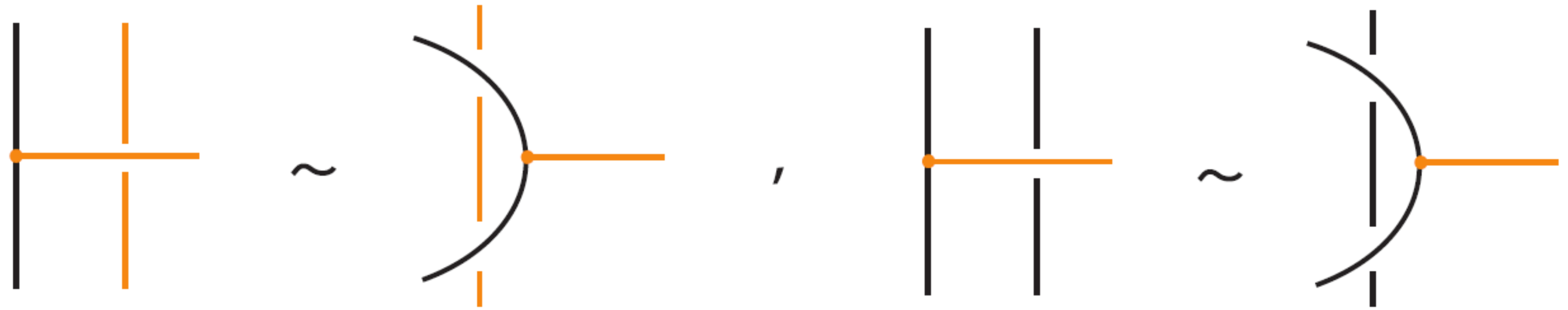
The planar isotopy moves

Reidemeister moves on link arcs.

Reidemeister moves on bonded arcs.

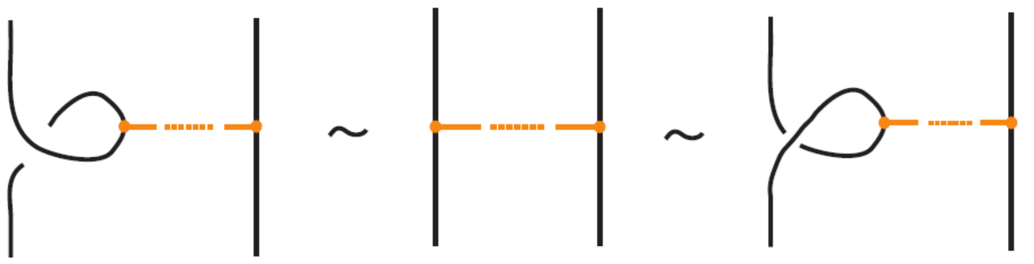


Reidemeister moves between link and bonded arcs.

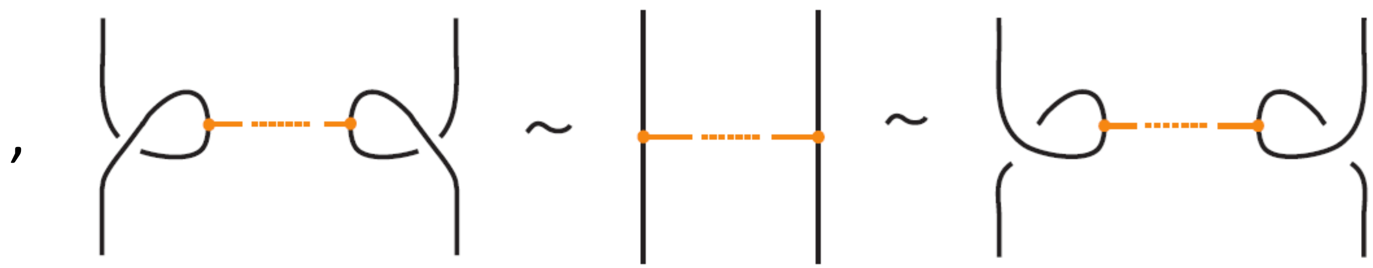


Vertex slide (VS) moves.

Topological versus rigid vertex isotopy moves



Topological vertex twists (TVT).



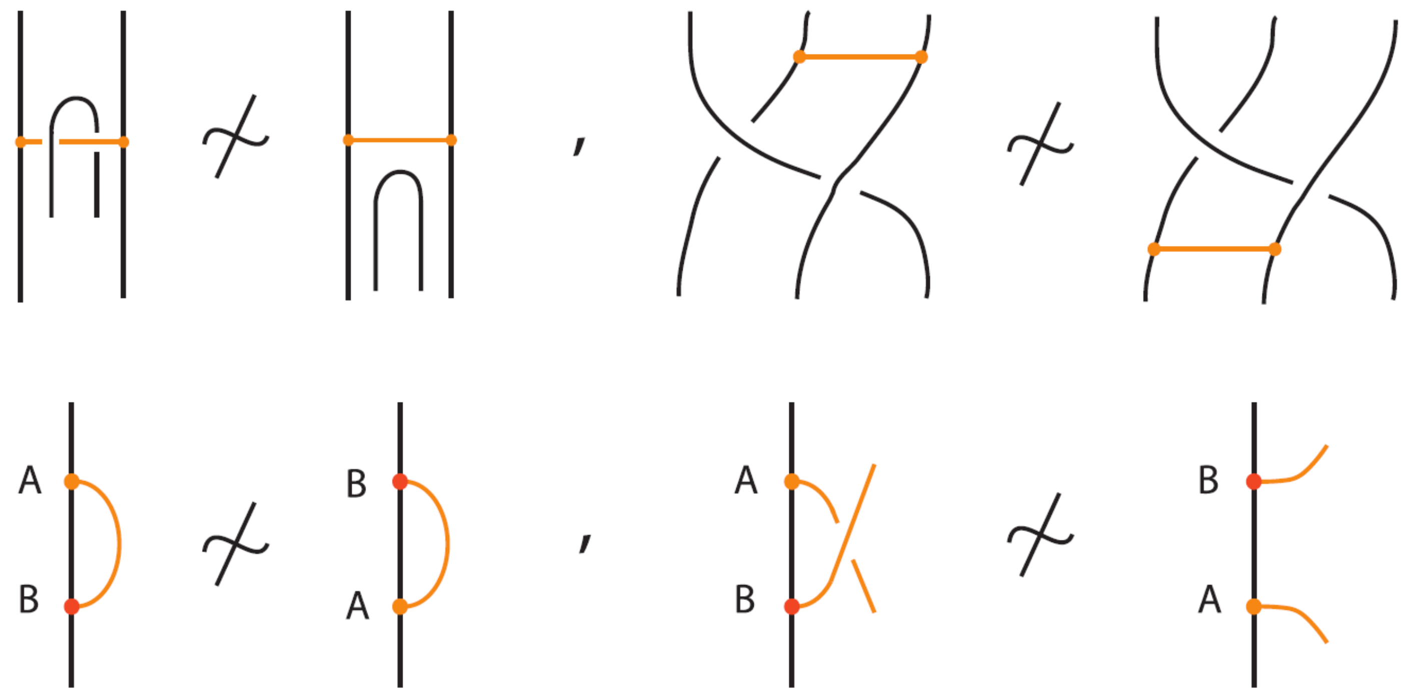
Rigid vertex twists (RVT).

Definition

- Bonded links subjected to topological vertex isotopy shall be called *topological bonded links*.
- Bonded links subjected to rigid vertex isotopy shall be called *rigid bonded links*.

Forbidden moves for bonded links

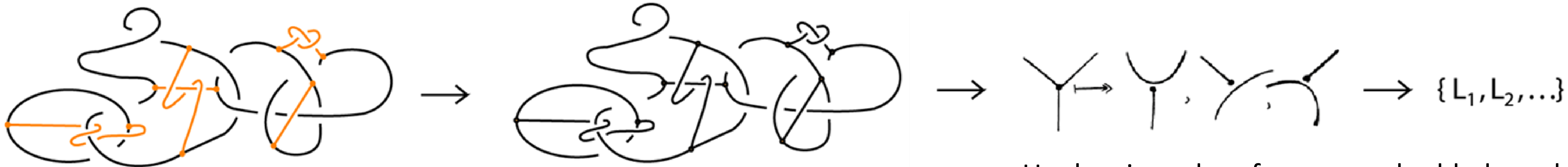
Rigid vertex isotopic bonded links are also topologically vertex isotopic. But TVT is forbidden in the theory of rigid bonded links. Other moves forbidden in either category are:



Forbidden moves in the theory of bonded links.

Topological vertex isotopy invariants: unplugging

For a bonded link (K,B), consider the bonds and the link arcs as graph edges invariantly and perform ‘unpluggings’ at the vertices:



Unplugging edges from an embedded graph.

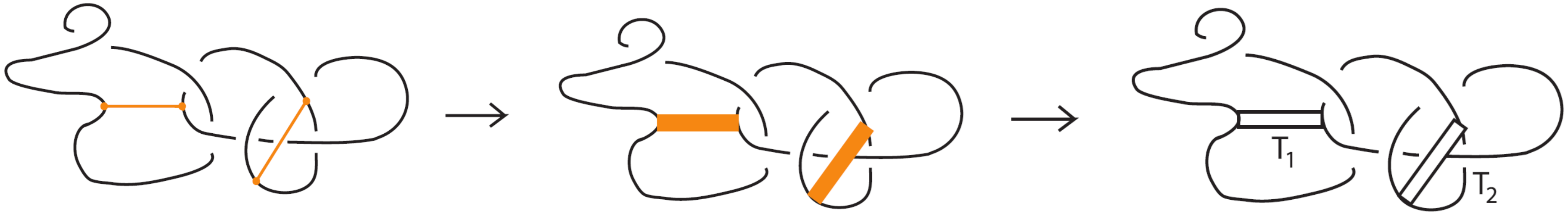
Theorem [Kauffman]

Let (K, B) be a bonded link. Then, considering the bonds and the link arcs as graph edges *invariantly*, we have that:

- *The set $\mathcal{L}_{(K,B)}$ of classical links derived from all possible vertex unpluggings is a topological vertex isotopy invariant of (K, B).*
- Consequently: *Any ambient isotopy invariant applied on $\mathcal{L}_{(K,B)}$ is also a topological vertex isotopy invariant of (K, B).*

Rigid vertex isotopy invariants: tangle insertion

For a bonded link (K,B), replace the bonds by properly embedded bands and perform 'tangle insertions' at the bands:



Theorem [Kauffman]

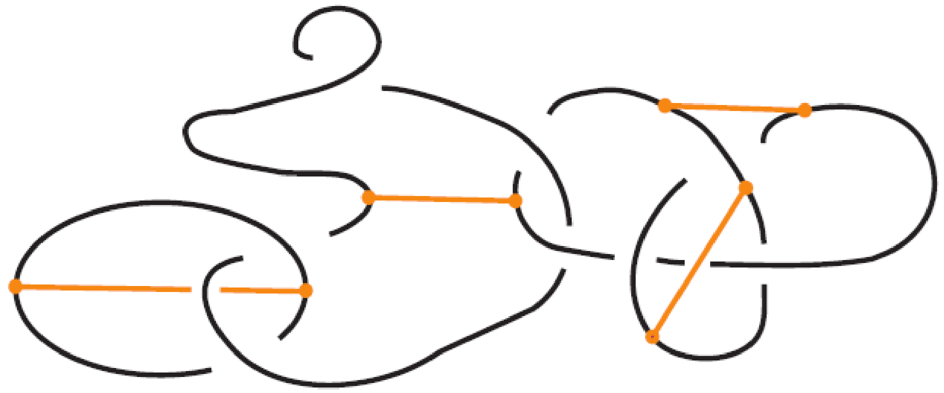
Let (K, B) be a bonded link and let *the bonds be replaced by* properly embedded discs in the form of *bands*. Then, inserting any embedded 2-tangles in place of the bands, we have that:

- *The set $\mathcal{T}_{(K,B)}$ of classical links derived from all possible tangle insertions is a rigid vertex isotopy invariant of (K, B).*
  In particular, for a given choice of tangles:
- *Any ambient isotopy invariant applied on the classical link $L_{(K,B)}$ after tangle insertions is also a rigid vertex isotopy invariant of (K, B).*

Intermediate category: regular bonded knots

Definition

A *regular bonded knot/link diagram* is a bonded knot/link diagram that contains no crossings or self-crossings of bonded arcs.
(Bonds can be long but not knotted. Needed for bonded braids.)

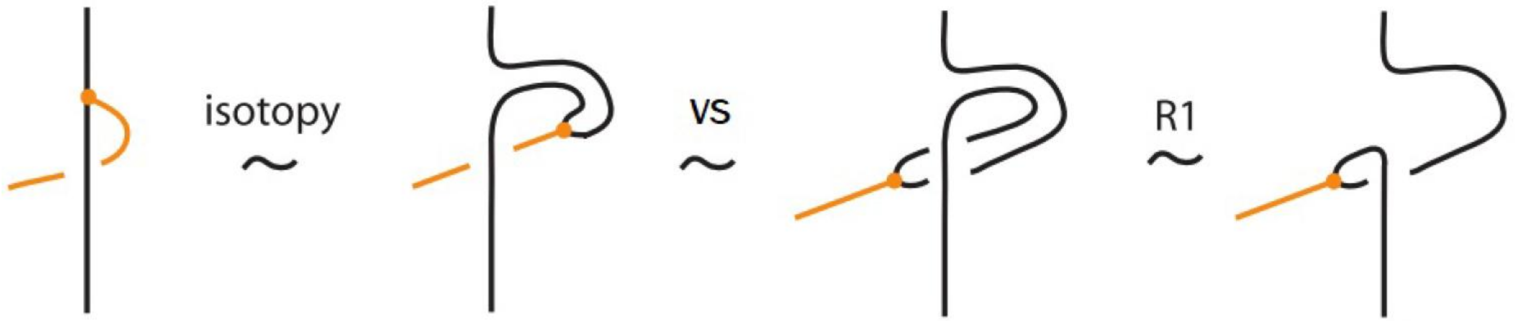


A regular bonded link.

A neighbourhood of a regular bond.

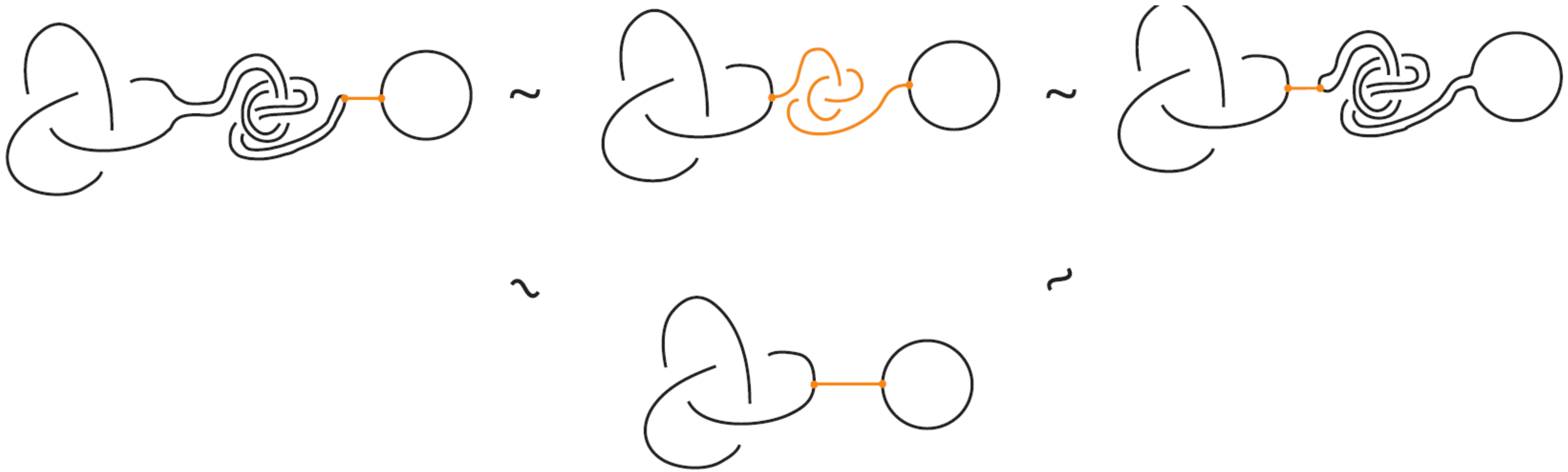
Proposition

A (topological or rigid) bonded link diagram can be transformed isotopically into a regular bonded link diagram.



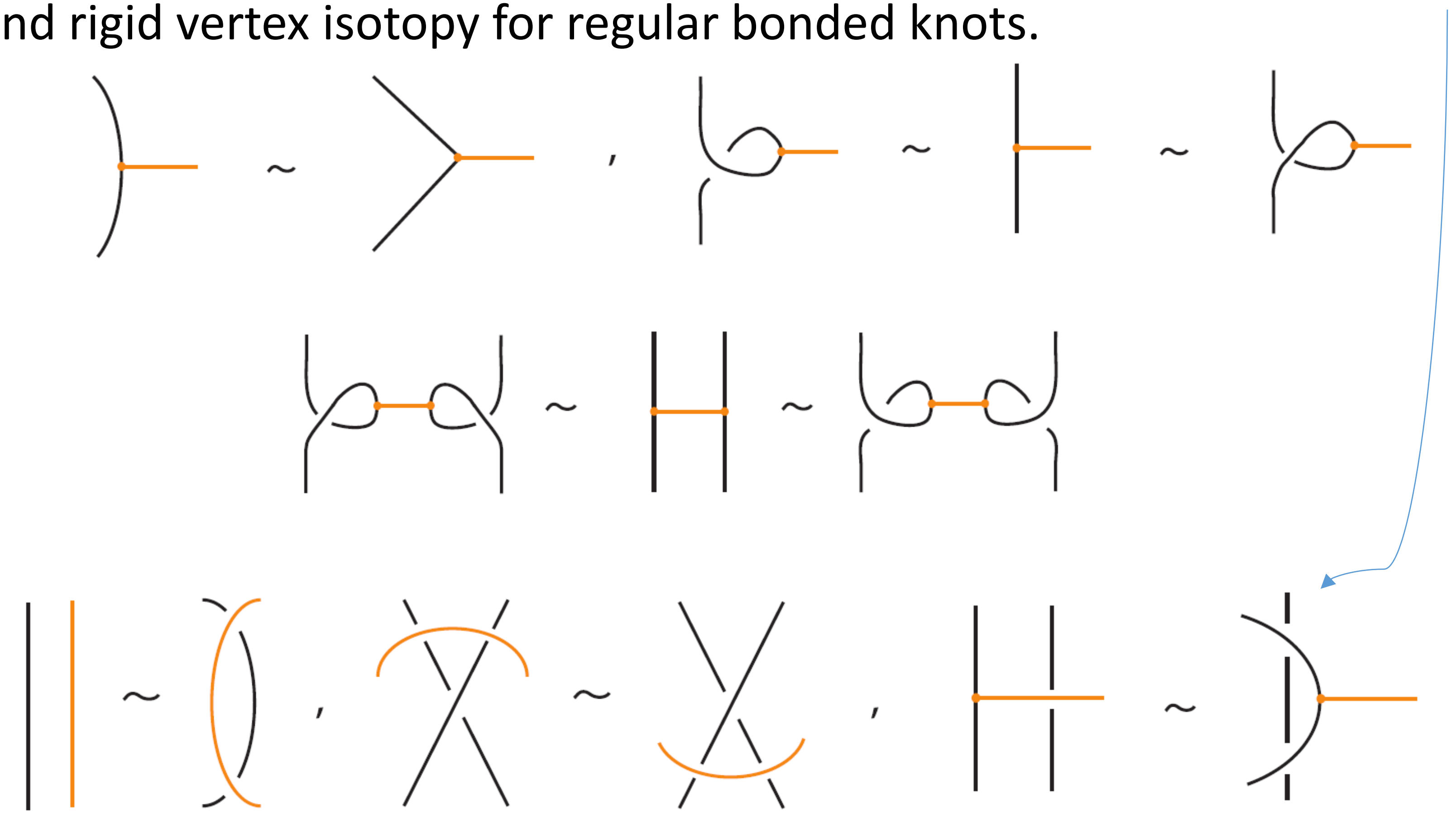
Bringing a bonded link to regular form.

Example:



Topological/rigid vertex isotopy for regular bonded knots

Here we exclude any move involving bonded crossings or adapt them in the regular setting. Hence, bonded planar isotopy moves, the mixed Reidemeister moves, the Vertex Slide (VS) moves, are valid in both topological and rigid vertex isotopy for regular bonded knots.



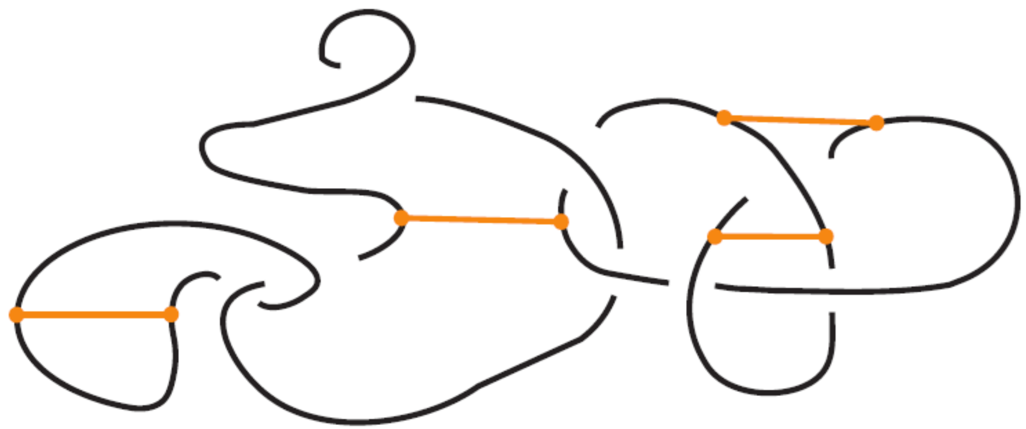
Moves between link and bonded arcs.

Tight bonded knots

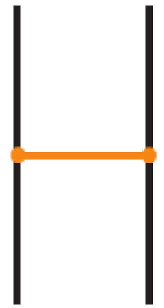
For invariants with **local rules**, we need the bonds free of other arcs.

Definition

A *tight bonded knot/link diagram* is a simply bonded knot/link diagram such that the region of any bond is free of arcs.



A tight bonded link.



A neighbourhood of a tight bond.

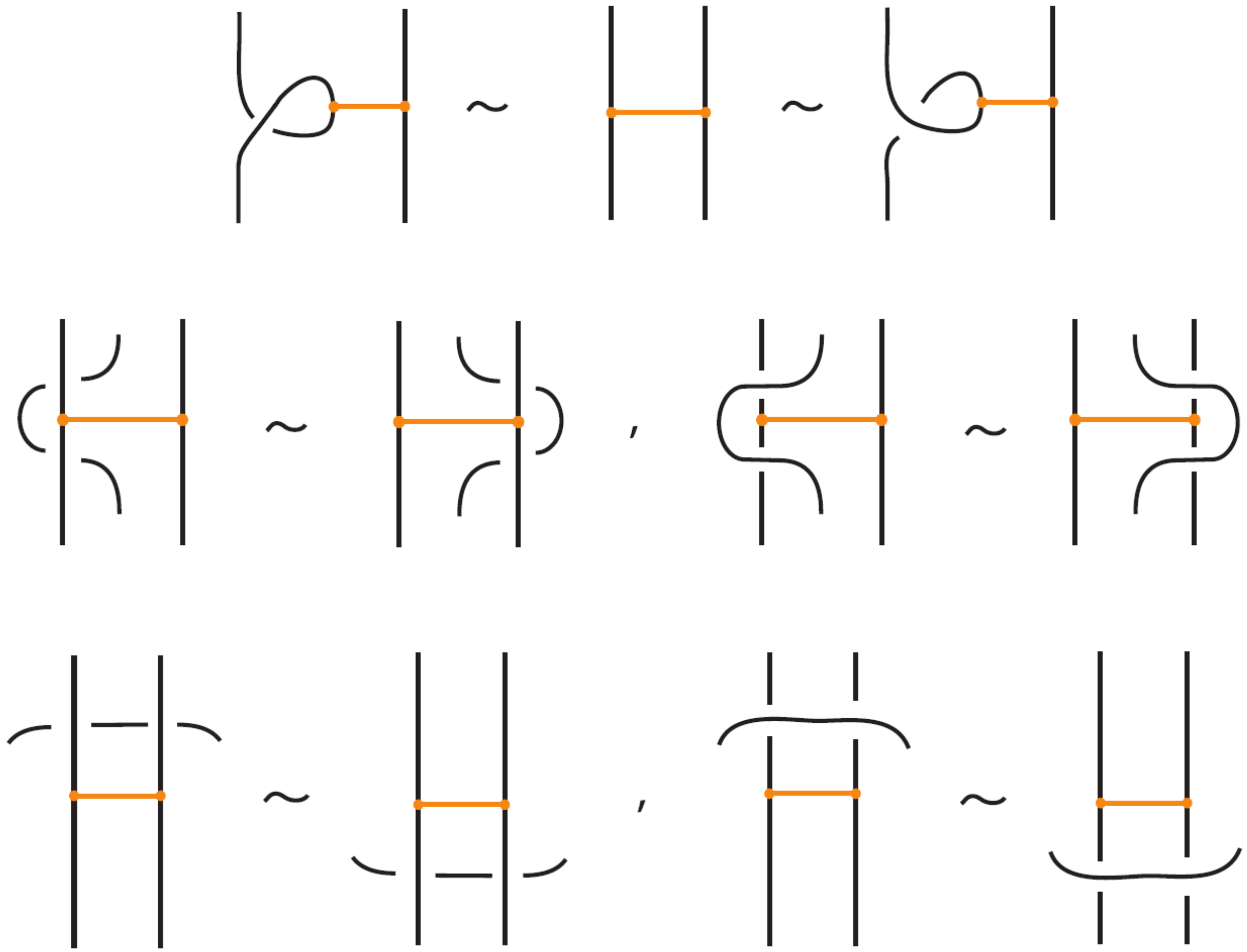
Tight bonded knots

Proposition

A regular bonded link diagram can be transformed isotopically (topologically and rigidly) into a tight bonded link.

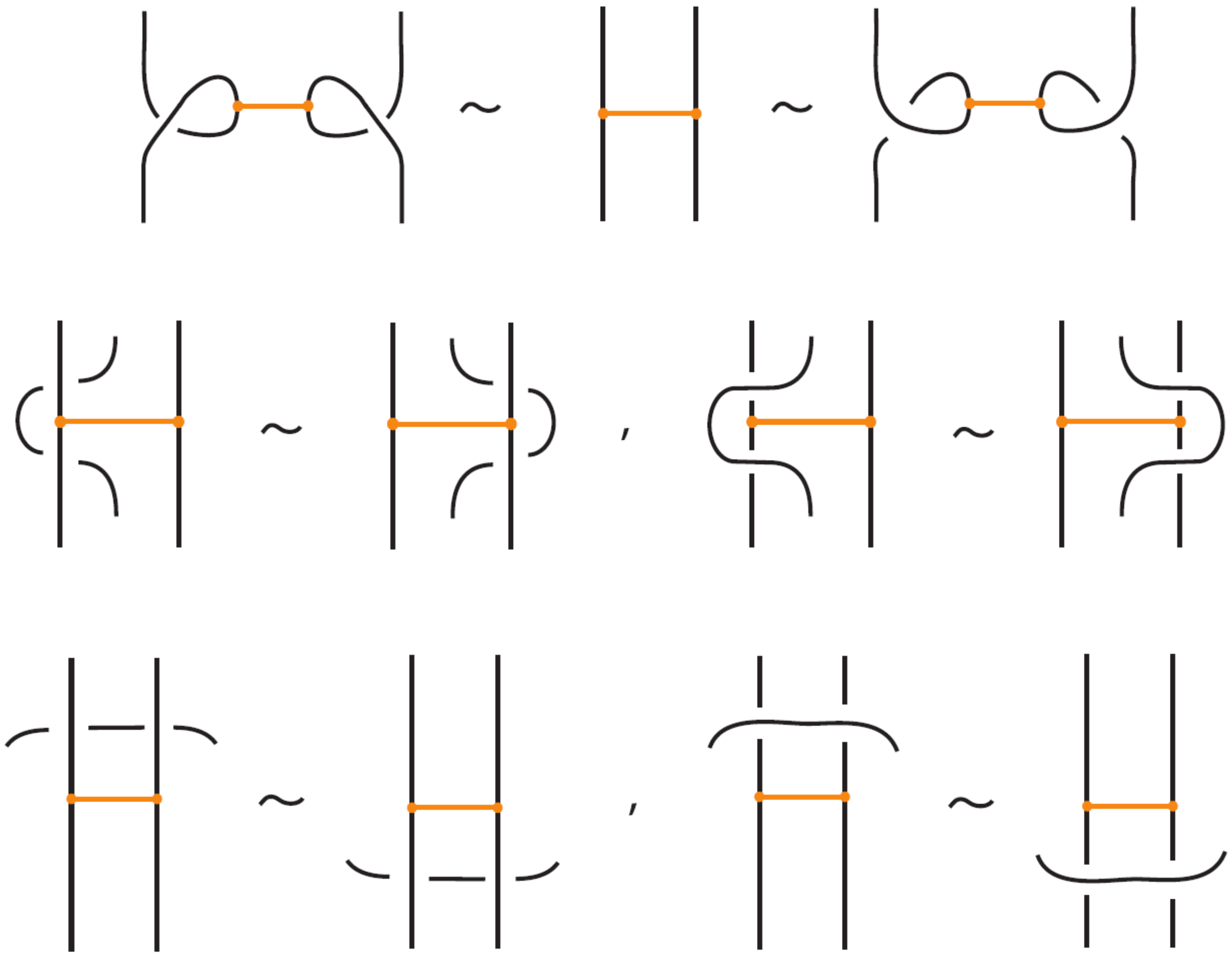
Basic moves for bringing to tight form.

Topological vertex isotopy moves for tight bonded knots



Topological vertex tight isotopy moves.

Rigid vertex isotopy moves for tight bonded knots

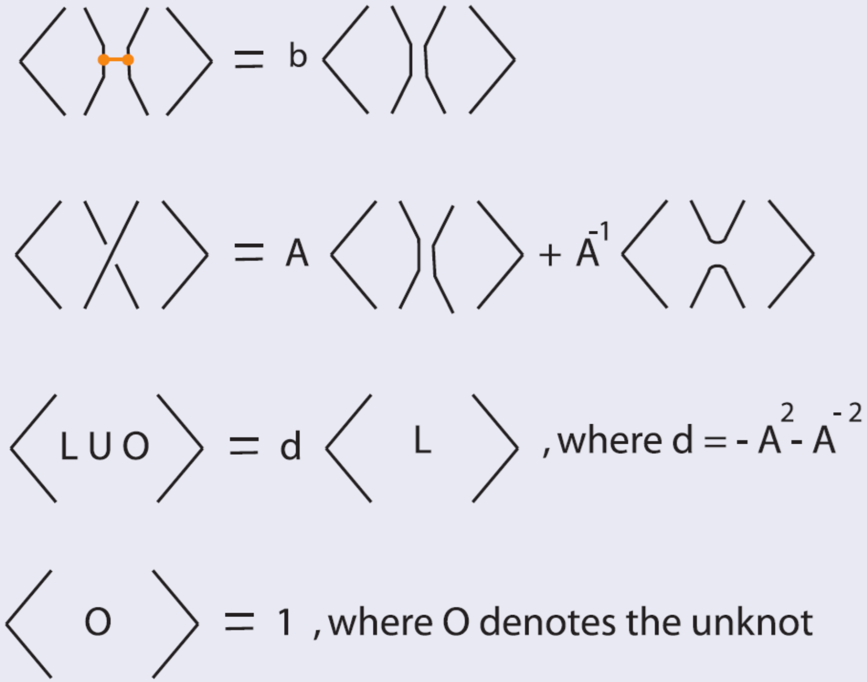


Rigid vertex tight isotopy moves.

A Kauffman bracket for tight bonded knots

Proposition

Let L be a bonded link. The *bonded bracket polynomial* of L defined by means of the following relations:

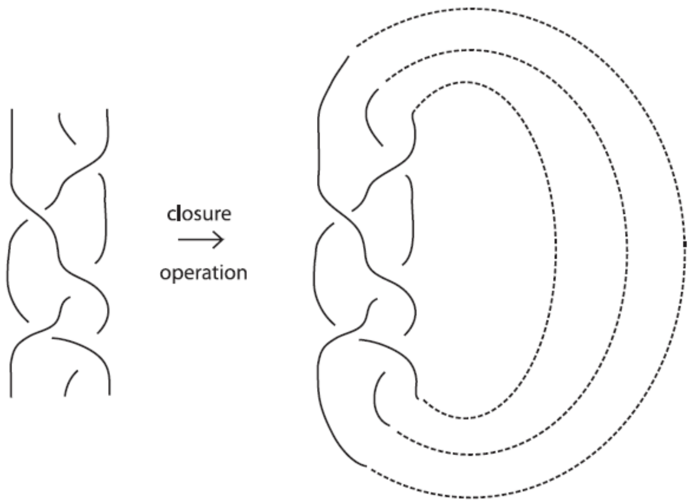


where b is a formal coefficient, *is an invariant of topological vertex isotopy.*

Braids

Definition (Artin; 1926)

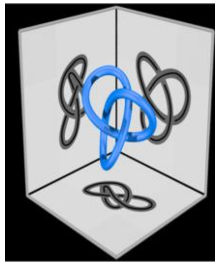
Braids are links with an organized boundary, consisting of two bars which may be assumed to be top and bottom, and strings which tie the two bars, such that they are strictly decreasing.

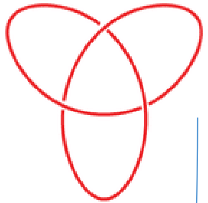


Theorem (Alexander; 1923)

Any oriented knot or link can be represented as a closed braid.

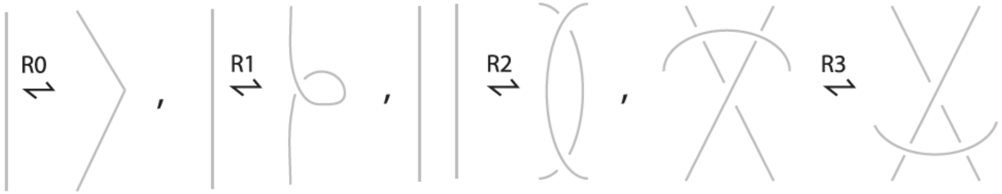
$K: S^1 \to S^3$





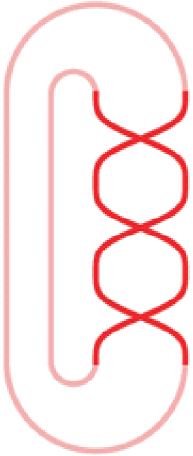
Reidemeister; 1927

Isotopy

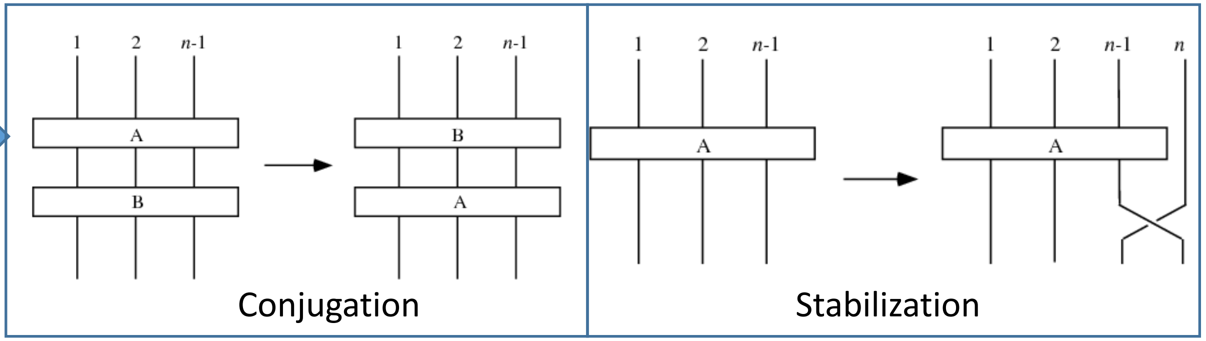


Alexander; 1923

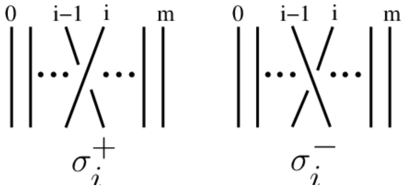
$\forall K \in S^3 \; \exists b : \hat{b} \sim K$



Markov; 1936



Artin; 1926



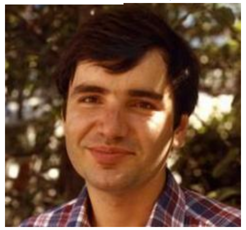
2 – variable
Jones polynomial

HOMFLYPT; 1986

$$\mathrm{tr}(ab) = \mathrm{tr}(ba)$$
$$\mathrm{tr}(1) = 1$$
$$\mathrm{tr}(ag_n) = z\,\mathrm{tr}(a)$$

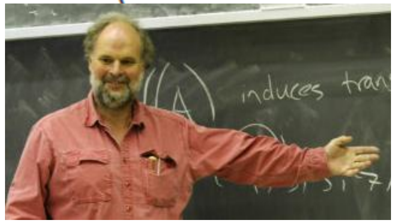
Ocneanu; 1982

$$\mathrm{tr} : \bigcup_{n=1}^{\infty} \mathrm{H}_n(q) \to \mathbb{C}$$



$$B_n = \left\langle \sigma_1, \ldots, \sigma_{n-1} \;\middle|\; \begin{array}{ll} \sigma_i\sigma_{i+1}\sigma_i = \sigma_{i+1}\sigma_i\sigma_{i+1}, & 1 \leq i \leq n-2 \\ \sigma_i\sigma_j = \sigma_j\sigma_i, & |i-j| > 1 \end{array} \right\rangle$$

$$\mathrm{H}_n(q) = \frac{\mathbb{C}\left[q^{\pm 1}\right] B_n}{\langle \sigma_i^2 - (q-1)\sigma_i - q \rangle}$$



Jones; 1984

$$\frac{knots}{Reidemeister's\ theorem} = \frac{braids}{Markov's\ theorem}$$

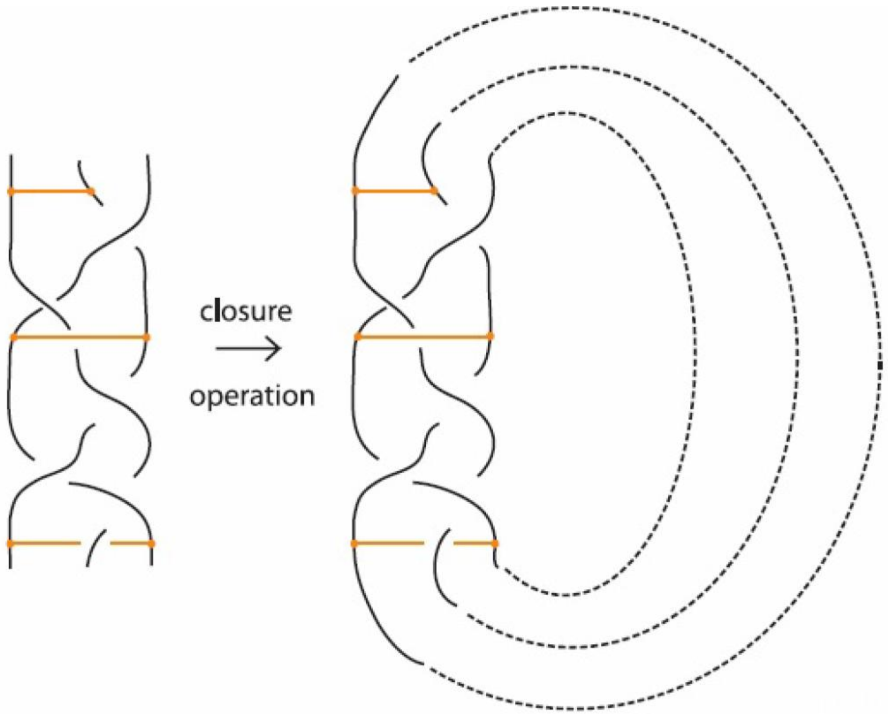
$$\mathrm{H}_n(q) = \left\langle g_1, \ldots, g_{n-1} \;\middle|\; \begin{array}{ll} g_i g_{i+1} g_i = g_{i+1} g_i g_{i+1}, & 1 \leq i \leq n-2 \\ g_i g_j = g_j g_i, & |i-j| > 1 \\ {g_i}^2 = (q-1) g_i + q, & i = 1, \ldots, n-1 \end{array} \right\rangle$$

$\sigma \mapsto g_i$

Bonded Braids

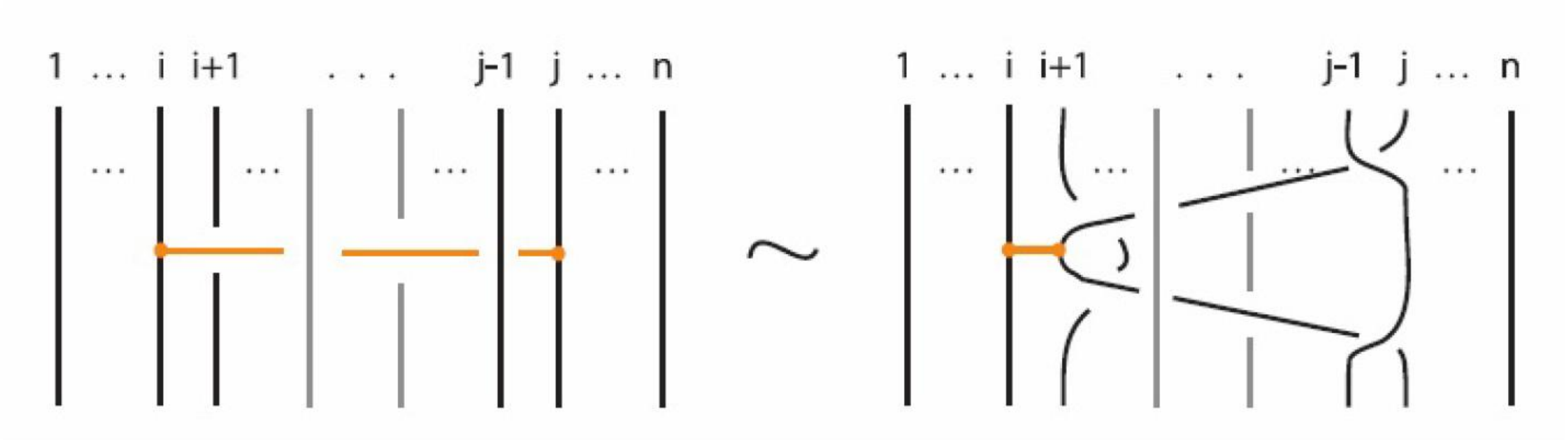
Definition

Bonded braids are classical braids equipped with embedded horizontal simple arcs, which we call *bonds*. The bond $b_{i,j}$ threads through the strands between the i^{th} and j^{th} strand of the braid, which it crosses transversely, with over/under information.



Bonded Braids

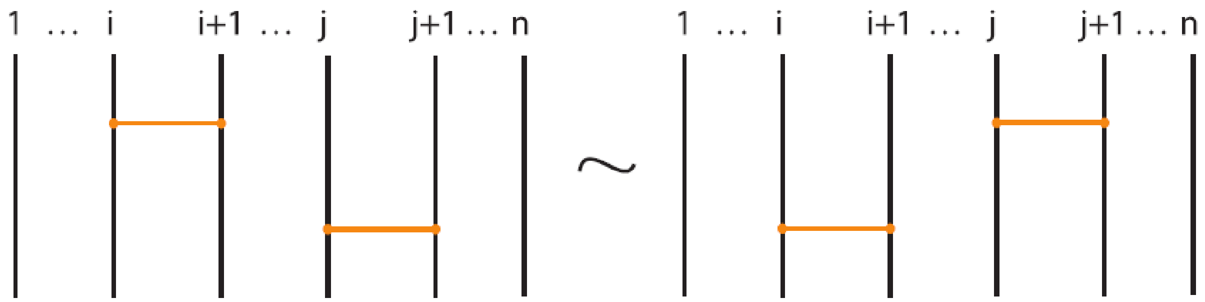
$b_{i,j}$ denotes a bond between the i^{th} and j^{th} strands. The endpoints of the bond $b_{i,j}$, $\partial b_{i,j}$, lie on the braid strands i and j and have local neighborhoods that are 3-valent graphs.
A bond joining two consecutive strands i and $i+1$ shall be called *elementary bond*, denoted by b_i.



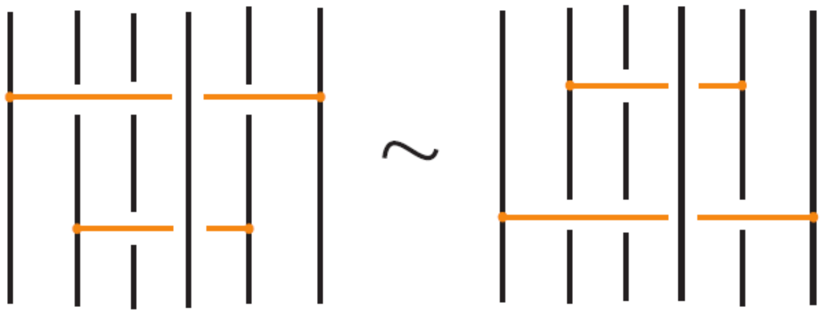
The bond $b_{i,j}$ expressed as a combination of classical braid generators and an elementary bond.

Definition Two bonded braids are isotopic if and only if they differ by classical braid isotopy that takes place away from the bonds, together with moves depicted in Figures

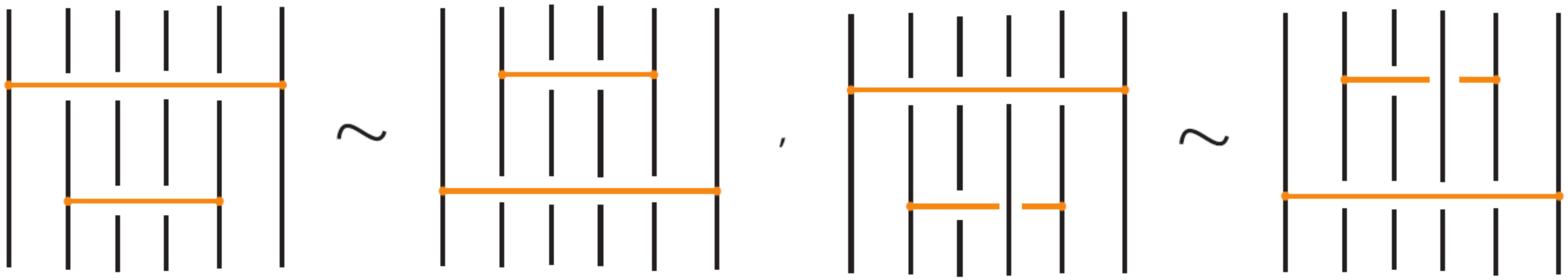
An equivalence class of isotopic bonded braid diagrams is called a *bonded braid*.



Interactions between two bonds that are far away from each other.

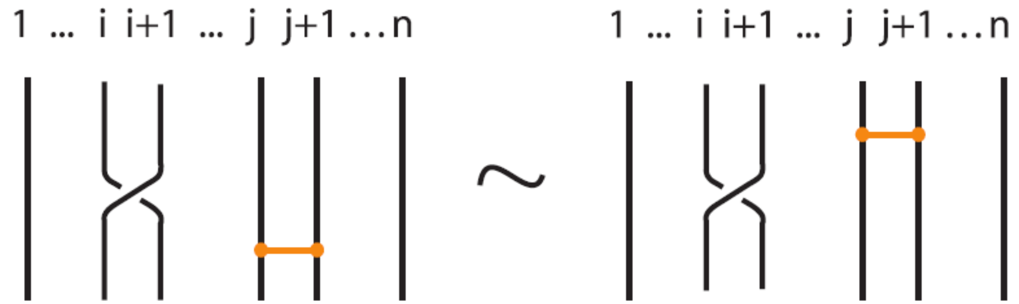


Interactions between two bonds: Matching crossing sequences.

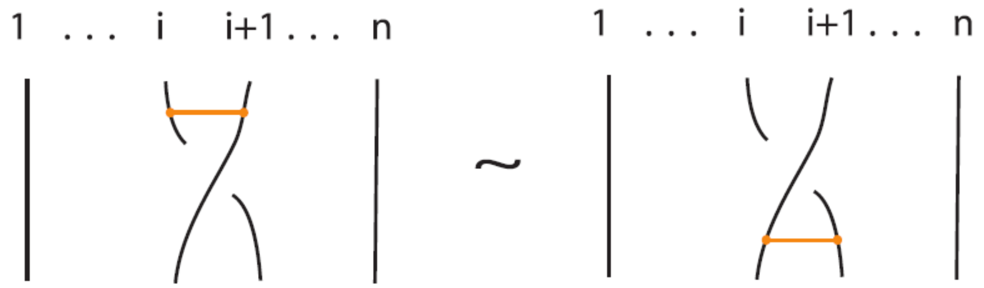


Interactions between two bonds: Uniform over/under configuration.

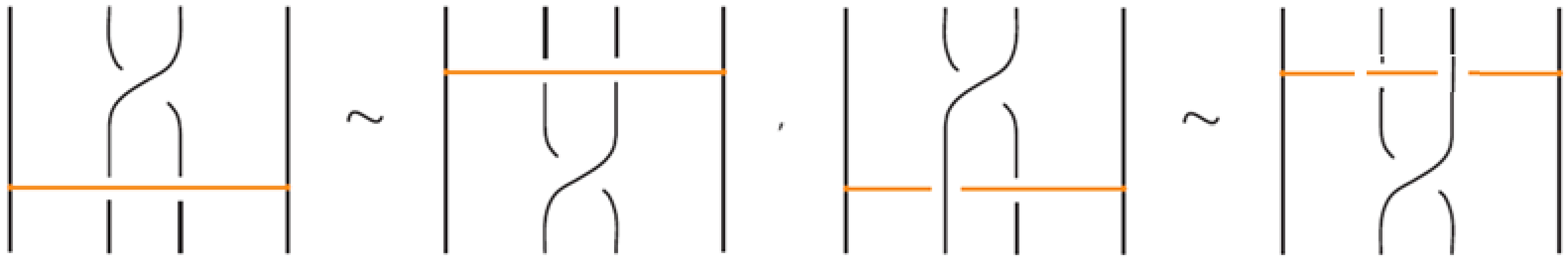
Definition Two bonded braids are isotopic if and only if they differ by classical braid isotopy that takes place away from the bonds, together with moves depicted in Figures



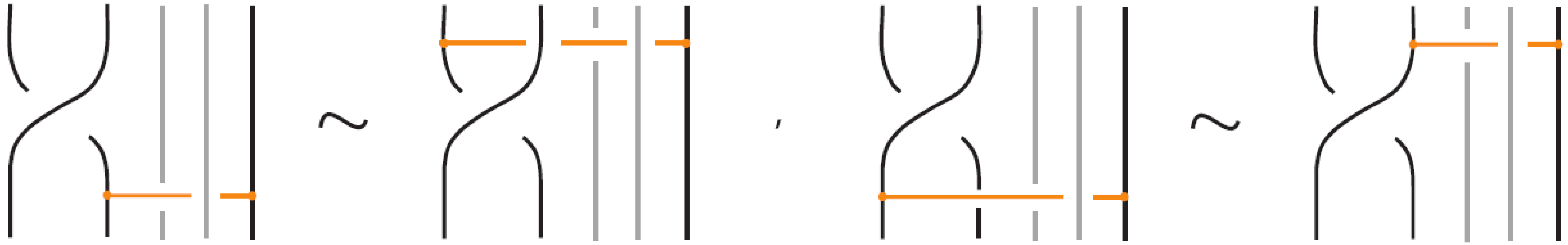
A crossing not involving a bond.



A crossing between strands that contain the boundaries of a bond.



Equivalence moves describing interactions between a bond and a crossing in the bonded braid.



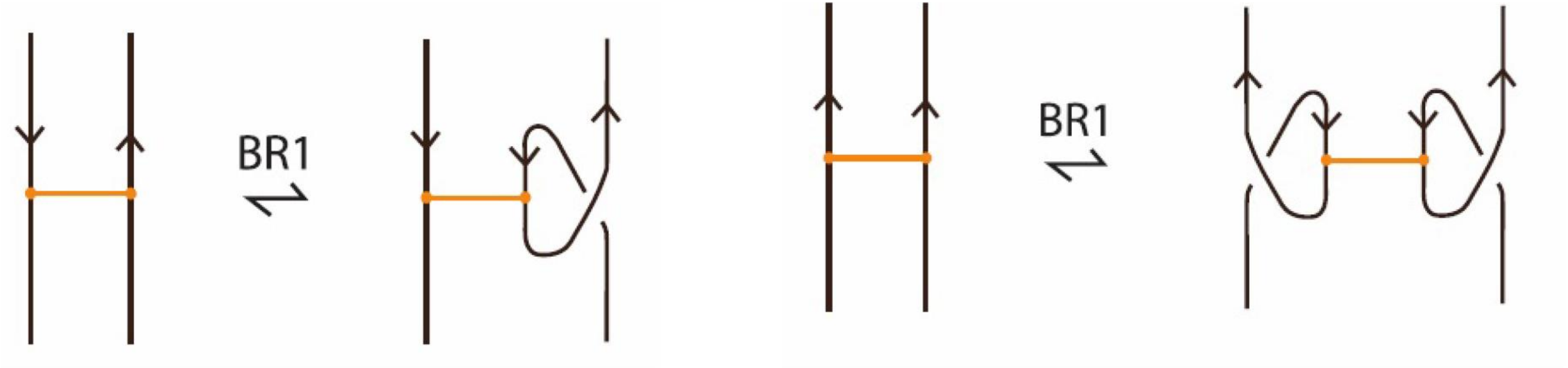
Equivalence moves describing interactions between a bond and a crossing in the bonded braid.

Braiding topological bonded links

Theorem

Every topological bonded link can be represented isotopically as the closure of a bonded braid.

The main idea is to keep the arcs of the oriented link diagrams that go downwards unaffected and replace arcs that go upwards with braid strands.



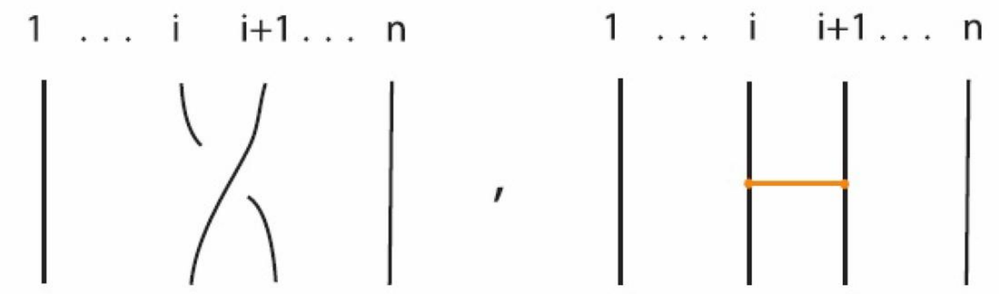
(a) Braiding two anti-parallel bonded strands

(b) Braiding two parallel bonded strands oriented upward

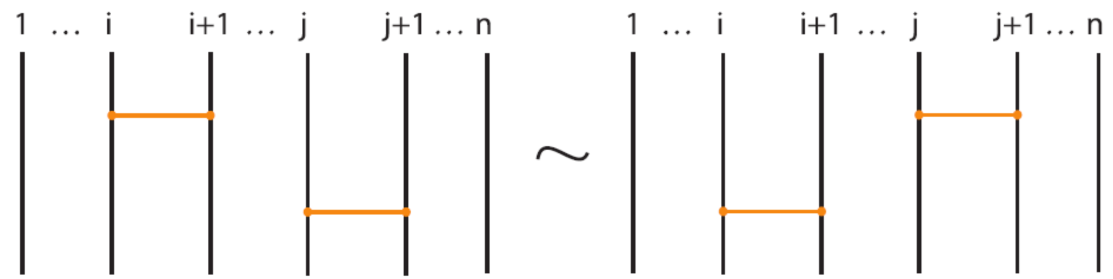
The bonded braid monoid

Definition

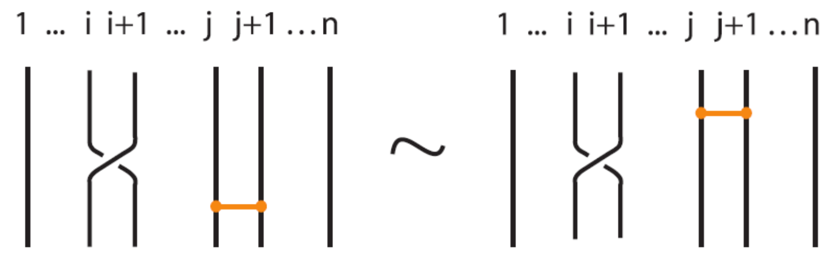
The *bonded braid monoid* BB_n is generated by the *elementary crossings* $\sigma_1, \ldots, \sigma_{n-1}$ of the Artin braid group B_n and the *elementary bonds* $b_1, \ldots, b_{n-1}$, with operation the usual braid concatenation. The generators satisfy the braid relations of B_n together with the relations:



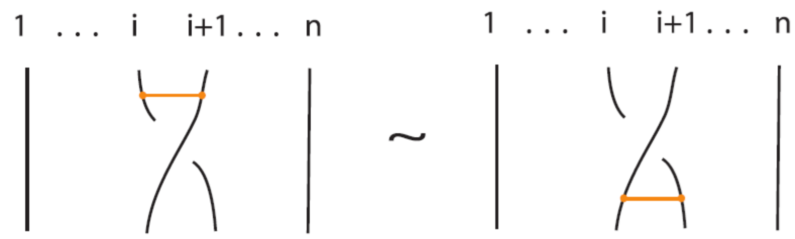
σ_i b_i



The relation $b_i b_j = b_j b_i$ for $|i - j| > 1$.



The relation $b_i \sigma_j^{\epsilon} = \sigma_j^{\epsilon} b_i$ for $|i - j| > 1$.

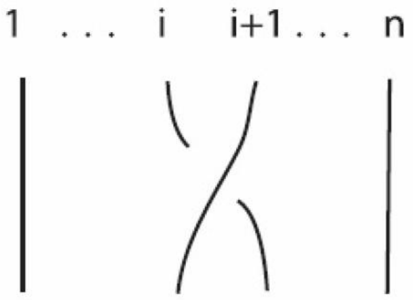


The relation $b_i \sigma_i^{\epsilon} = \sigma_i^{\epsilon} b_i$ for $\epsilon = 1$.

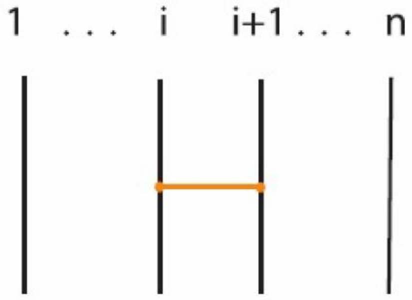
The bonded braid monoid

Definition

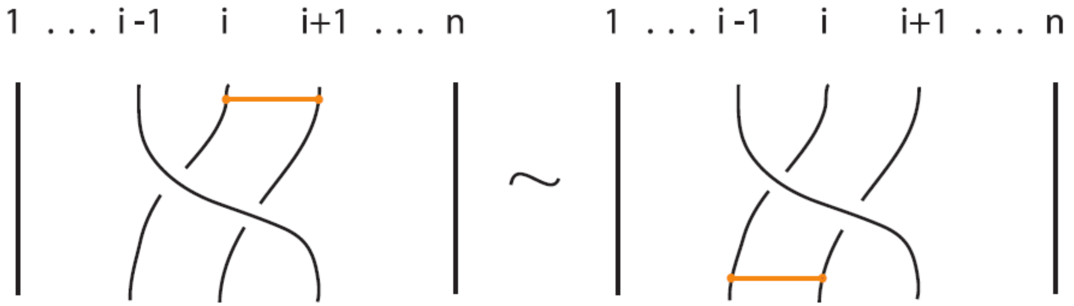
The *bonded braid monoid* BB_n is generated by the *elementary crossings* $\sigma_1, \ldots, \sigma_{n-1}$ of the Artin braid group B_n and the *elementary bonds* $b_1, \ldots, b_{n-1}$, with operation the usual braid concatenation. The generators satisfy the braid relations of B_n together with the relations:



σ_i



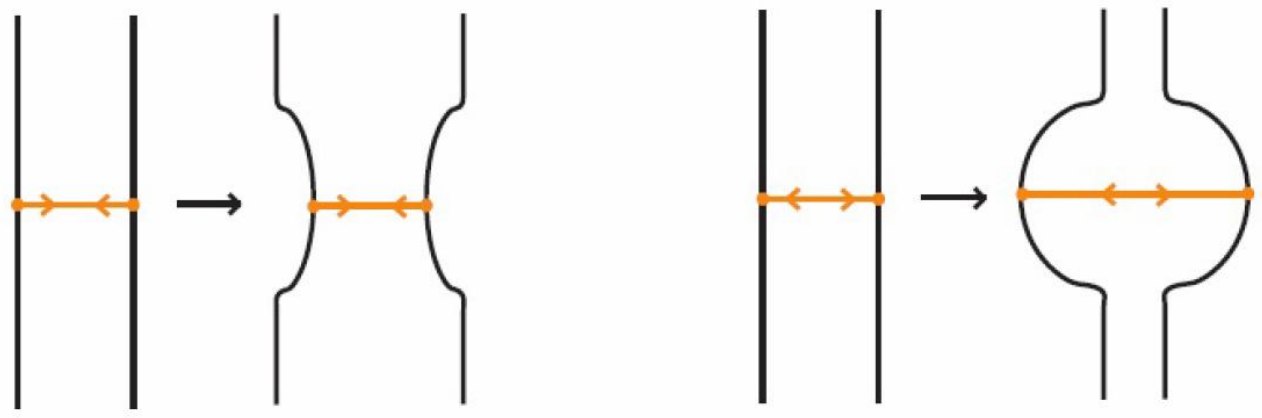
b_i



The relation $b_i \sigma_j^{\epsilon} \sigma_i^{\epsilon} = \sigma_j^{\epsilon} \sigma_i^{\epsilon} b_j$ for $\epsilon = 1$.

Bonded braids enhanced with 'forces'

Enhanced bonded braids are classical braids equipped with two different types of bonds. One type corresponds to attracting forces and the the other type to repelling forces.



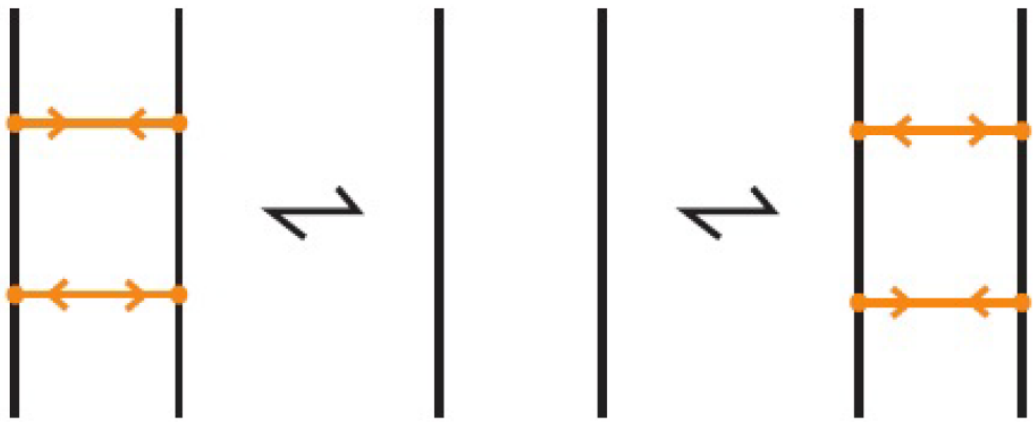
The bonded braid monoid embeds to a group, the *enhanced bonded braid group*.

The enhanced bonded braid group

Definition

The *enhanced bonded braid group* EB_n is the group generated by $\sigma_1, \ldots, \sigma_{n-1}$, the generators $b_1^{\pm 1}, \ldots, b_{n-1}^{\pm 1}$, called *enhanced bonds*, with operation the usual braid concatenation. The generators satisfy the relations of the bonded braid monoid, together with the following relations:

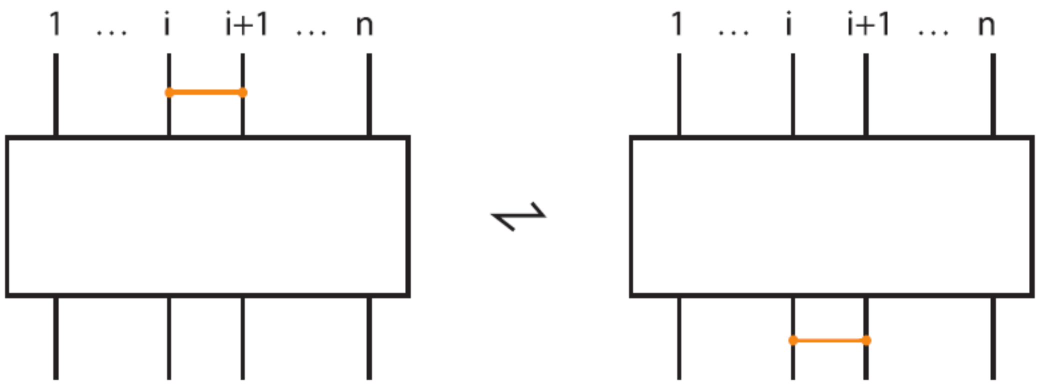
$$b_i \, b_i^{-1} \; = \; 1 \; = \; b_i^{-1} \, b_i, \text{ for all } i.$$



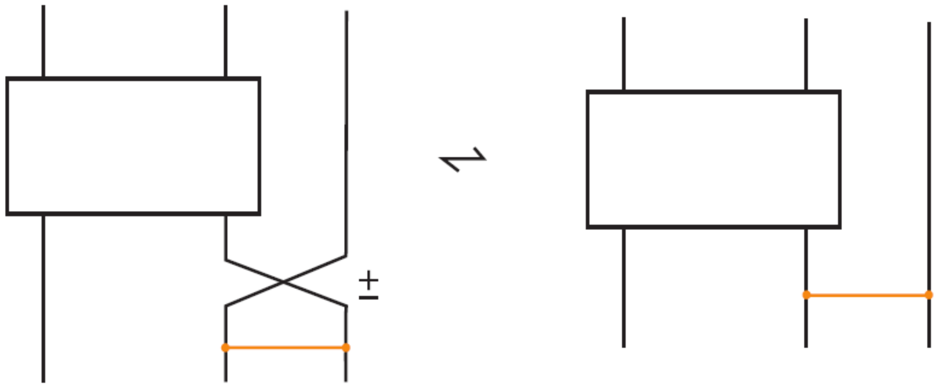
Markov's Theorem

Theorem (Markov equivalence for bonded braids). *Two bonded braids have isotopic closures if and only if one can be obtained from the other by a finite sequence of the following moves:*

$$
\begin{array}{llcll}
1. & \text{Markov Conjugation}: & \alpha & \sim & \sigma_i^{\pm 1}\,\alpha\,\sigma_i^{\mp 1}, & \text{for } \alpha,\, \sigma_i \in BB_n, \\
2. & \text{Bond Commuting}: & \alpha\, b_i & \sim & b_i\,\alpha, & \text{for } \alpha,\, b_i \in BB_n, \\
3. & \text{Markov Stabilization}: & \alpha & \sim & \alpha\,\sigma_n^{\pm 1}, & \text{for } \alpha \in BB_n,
\end{array}
$$



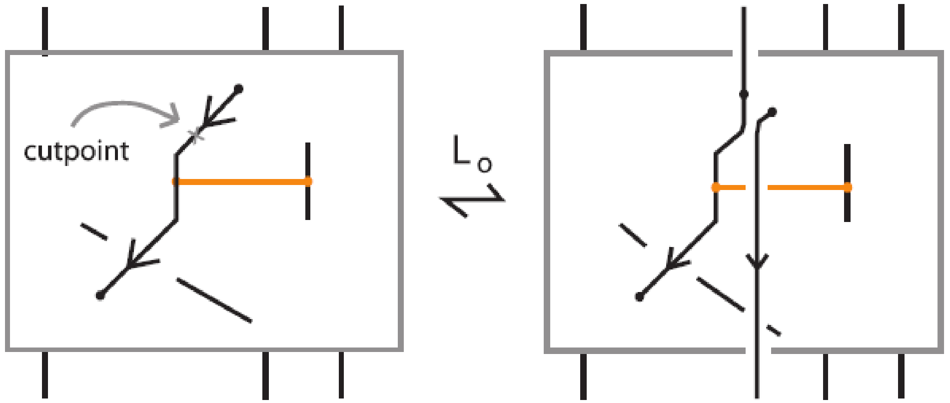
Bond Commuting.



Markov stabilization moves involving bonds.

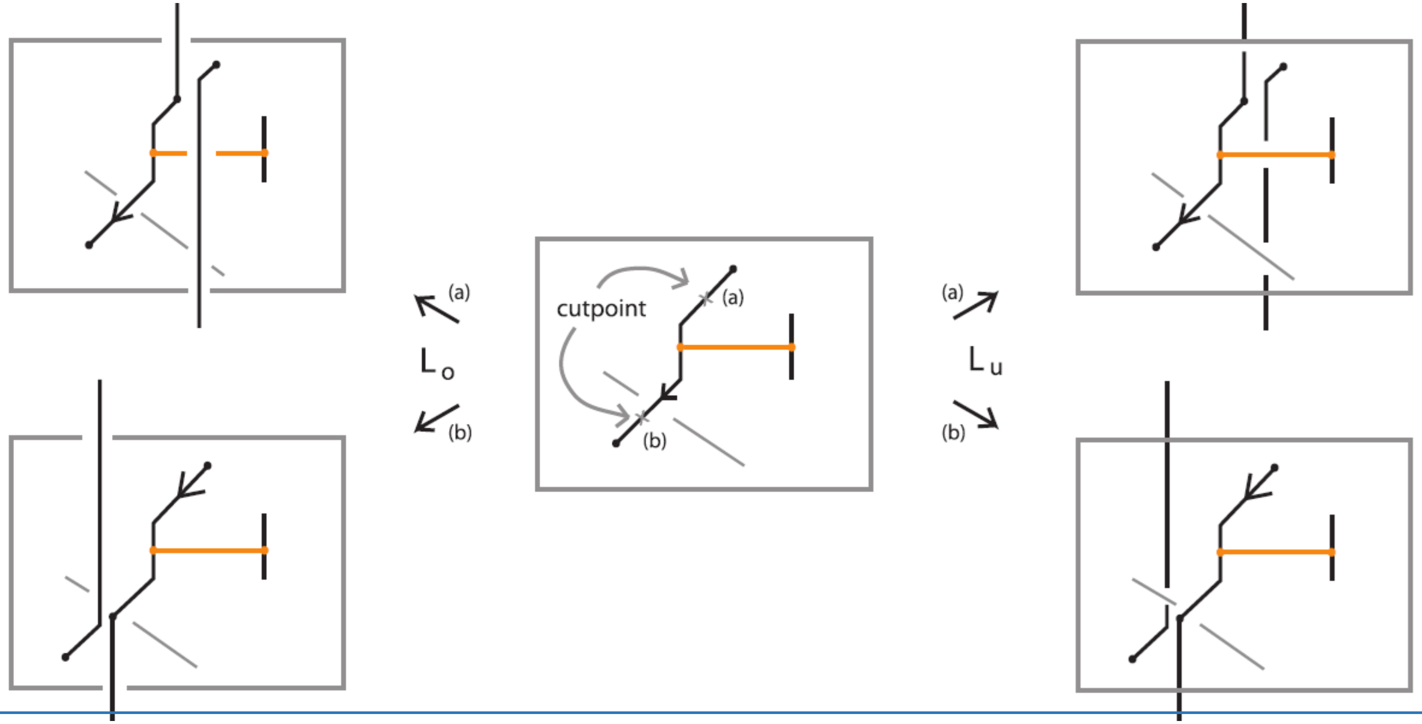
L-moves

Definition. An *L-move* on a bonded braid β, consists in cutting an arc of β open and pulling the upper cutpoint downward and the lower upward, so as to create a new pair of braid strands with corresponding endpoints (on the vertical line of the cutpoint), and such that both strandscross entirely over or entirely under the rest of the braid (including the bonds). Stretching the new strands over will give rise to an L_o-move and under to an L_u-move.



L-Moves

If an arc of β contains the boundary ∂b_i of a bond, then the cutpoint should be different from ∂b_i.



Theorem (***L*-move equivalence for bonded braids**). *Two bonded braids have isotopic closures if and only if one can be obtained from the other by a finite sequence of the following moves:*

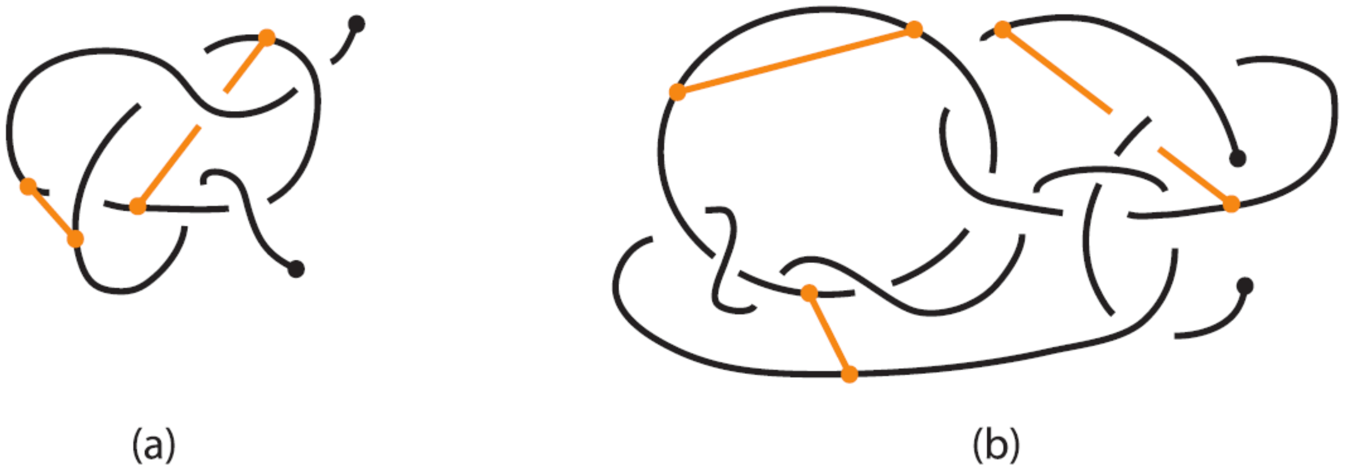
1. L – moves

2. Bond Commuting : $\alpha\, b_i \;\sim\; b_i\, \alpha,\quad \text{for } \alpha,\, b_i \in BBM_n$

Bonded Knotoids

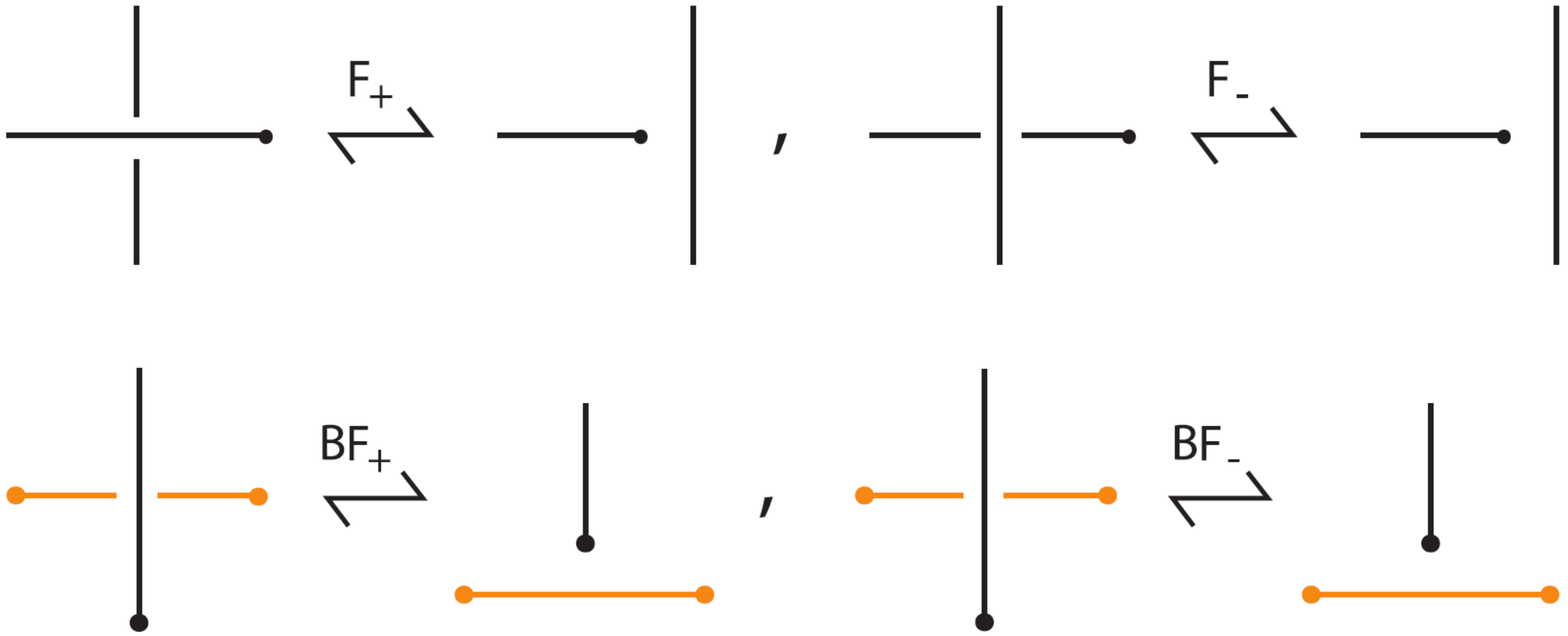
Definition

A *bonded knotoid diagram* is a classical knotoid equipped with (regular) bonds. A *bonded knotoid* is an equivalence class of bonded knotoid diagrams up to the equivalence relation generated by the knotoid and bonded moves.



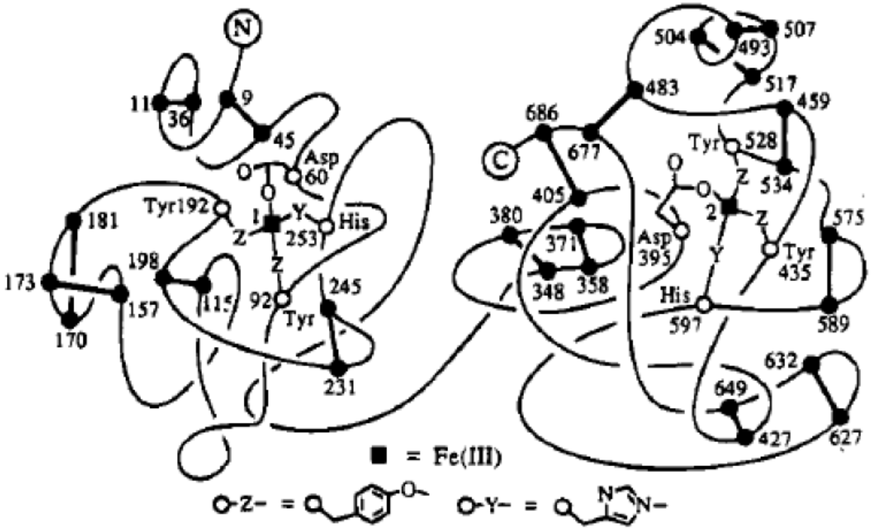
(a) A bonded knotoid; (b) a bonded multi-knotoid.

Forbidden Moves

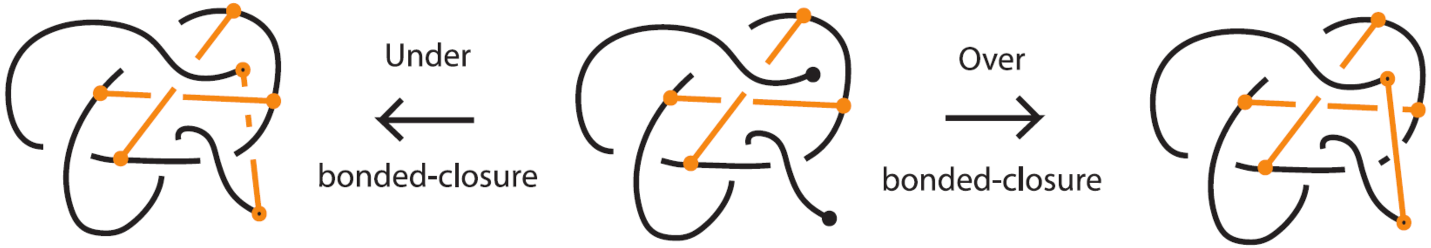


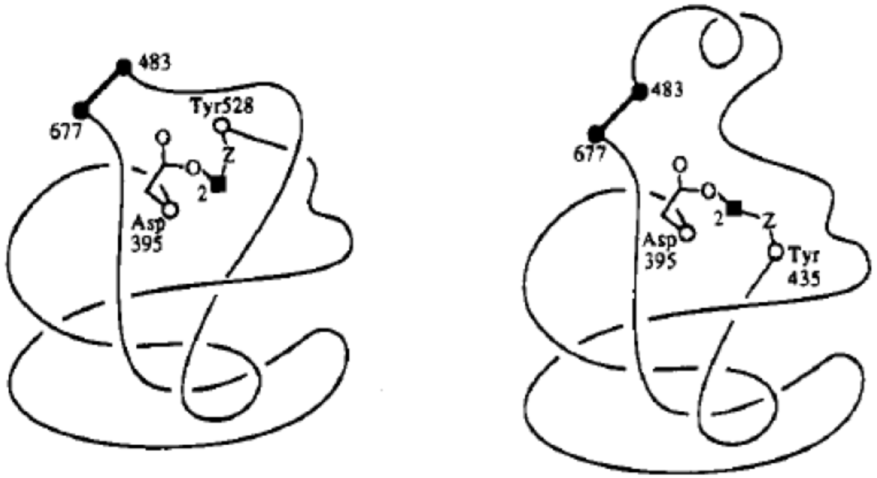
Bonded closure

Inspired by the molecules in [Liang & Mislow, 1994]:



we (SL, Kauffman) propose a new type of closure, the *under/over bonded closure* for bonded knotoids:





(Bonded) Doubly Periodic Tangles/Tangloids

- Doubly periodic tangles are entanglements of curves embedded in the thickened plane that are periodically repeated in two transversal directions.
- Such entangled networks are useful in many scientific fields for the study of physical systems, and inspire **new mathematical developments**.
- A better understanding of their **geometry and topology**, often associated to some **physical properties**, could allow the prediction of functions during the design process.
- No universal **mathematical study** and many **open questions**.

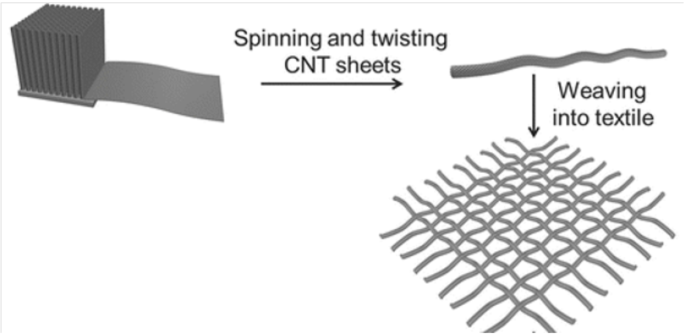
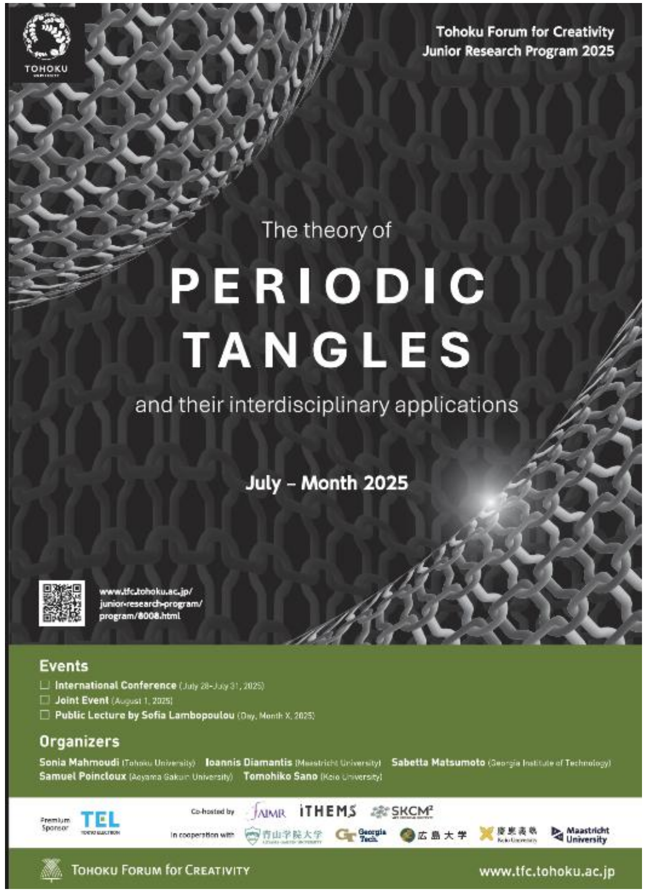


Figure: Carbon Nanotube Woven Fabricb(DOI: 10.1007/978-3-319-26893-4)



DP Tangles: Motivations - Polymers

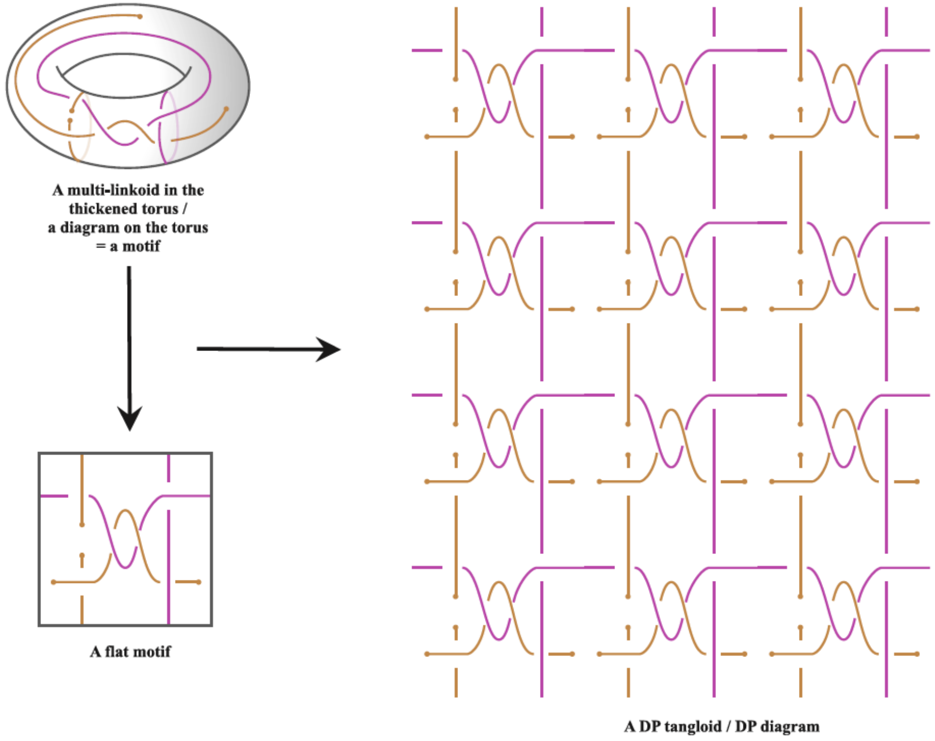
- The entanglement of filaments arises in many physical systems: in micro-scale, e.g. polymers; middle-scale, e.g. fabrics, fluid flows; and macro-scale, e.g. cosmic filaments.
- Polymer chains are long flexible molecules that impose topological constraints to each other, which are proved to affect the physical properties of the polymer.
- For the modeling of a bulk system Periodic Boundary Conditions (PBC) are used.

DP Tangloids

We shall say *linkoids* for knotoids, linkoids or multi-knotoids.

Definition

Let τ be a linkoid in $T^2 \times I$. A *doubly periodic tangloid*, or *DP tangloid*, is the lift of τ under the covering map ρ, and is denoted by τ_∞. Moreover, the projection of τ onto $T^2 \times \{0\}$ is called a *linkoid diagram* of τ, denoted by d, and the lift of d under ρ is called a *doubly periodic diagram*, or *DP diagram*, denoted by d_∞. In this context, d (resp. τ) is called a *motif* for d_∞ (resp. for τ_∞).



- The topological classification of DP tangles is at least as hard a problem as the full classification of knots and links in the three-space.
- Such problems are approached by constructing topological invariants.
- The equivalence relation that these invariants respect is based on assumptions of **minimal motifs**, that is motifs that are minimal for reproducing the DP tangles under 2-periodic boundary conditions.
- Note however that obtaining a minimal motif of a DP tangle is known to be a non trivial problem.

Thank you for your attention!