Bonded Knots,Graphs and Knotoids
Louis H Kauffman, UIC
(Joint work with Sofia Lambropoulou and
Ioannis Diamantis)

I. Recall Topological Invariants of Graphs

TRANSACTIONS OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 311, Number 2, February 1989

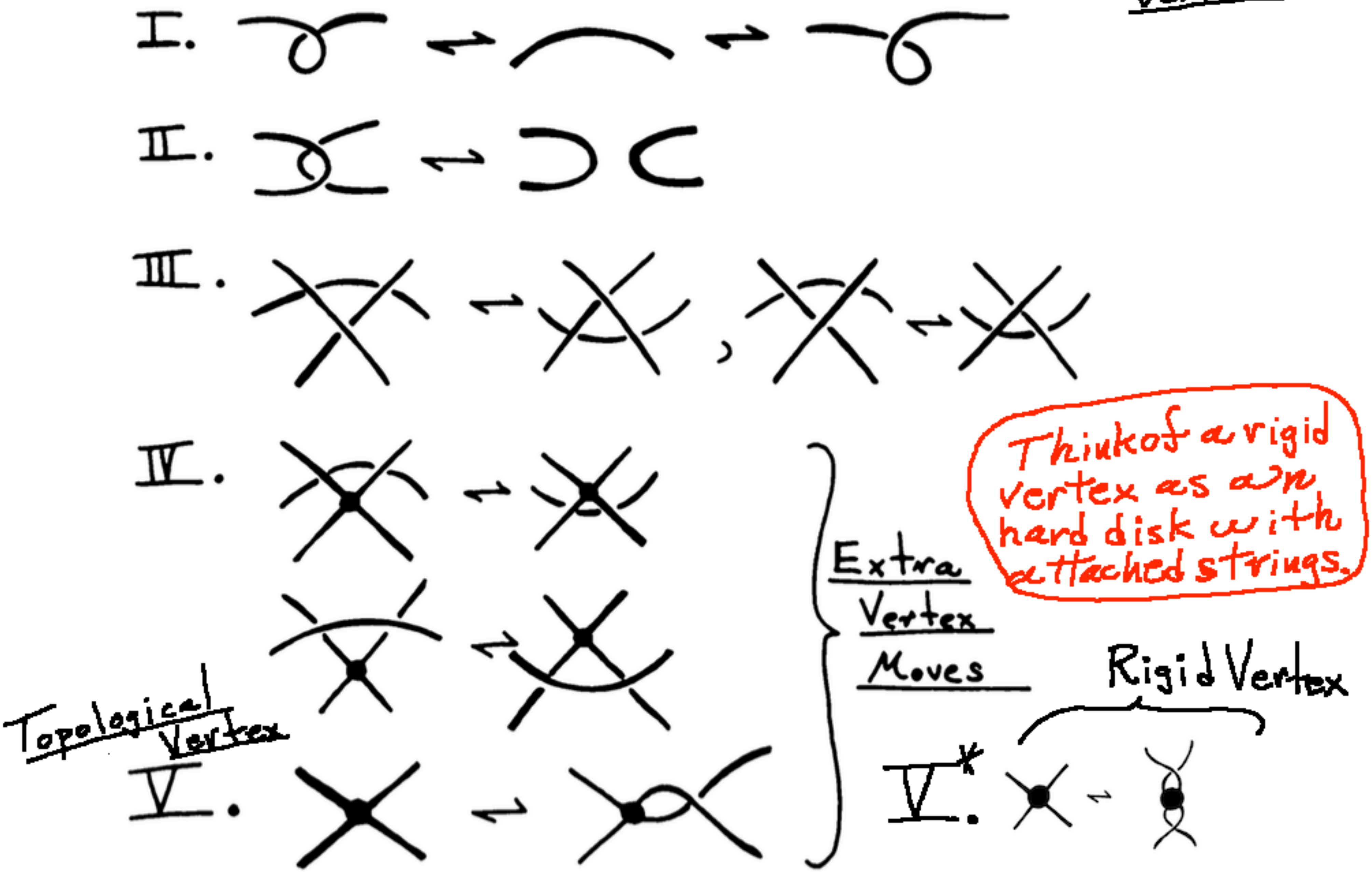
INVARIANTS OF GRAPHS IN THREE-SPACE

LOUIS H. KAUFFMAN

ABSTRACT. By associating a collection of knots and links to a graph in three-dimensional space, we obtain computable invariants of the embedding type of the graph. Two types of isotopy are considered: topological and rigid-vertex isotopy. Rigid-vertex graphs are a category mixing topological flexibility with mechanical rigidity. Both categories constitute steps toward models for chemical and biological networks. We discuss chirality in both rigid and topological contexts.

This talk is brought to you by the Banff Springs Hotel, its Celtic Knots and its hot chocolate.

Reidemeister Moves + Topological Vertex OR Rigid Vertex



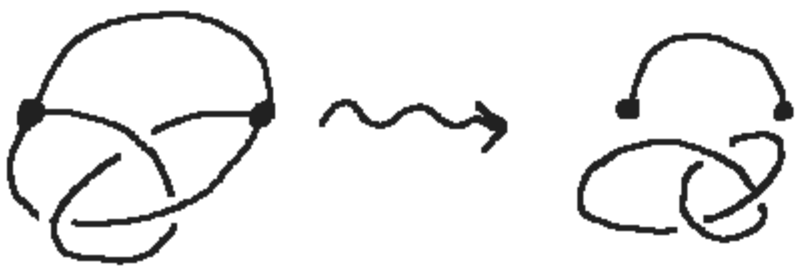
Topological vertex graphs (TV) are more flexible than rigid vertex graphs (RV).

A topological vertex absorbs braiding:

We'll see shortly that G is knotted as an RV graph.

Topological Method: • Unplug vertices.
• Examine knotting.

e.g.



The knot inside will not go away under topological moves.

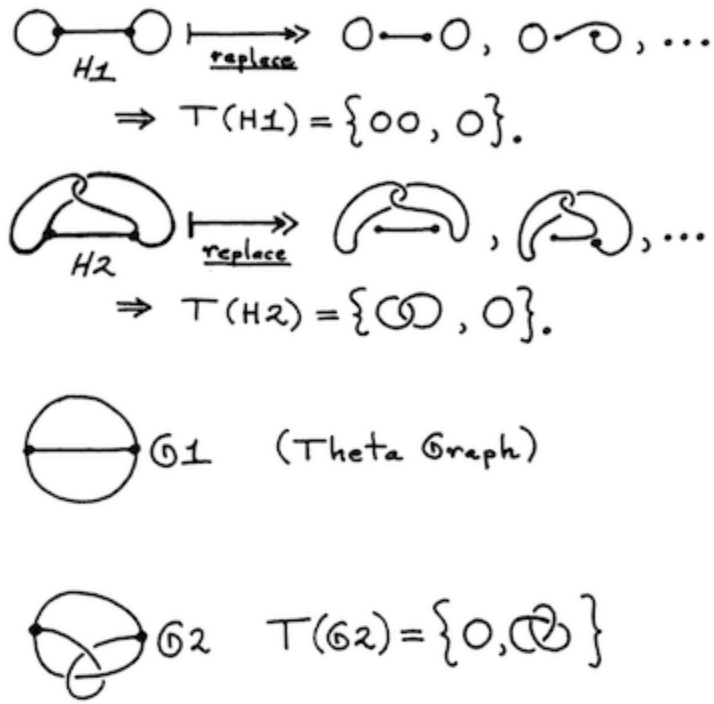
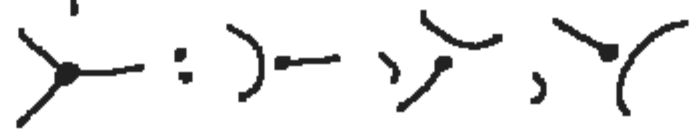


FIGURE 7. Braiding at a vertex permutes the replacements

Make all possible replacements.



The resulting collection of knots, links (throw away arcs) is a topological invariant of the graph with TV vertices.

In complex situations, you can apply topological invariants to the knots and links.

Rigid Vertex Graphs

This operation corresponds to a 180° rotation in 3-space and therefore it will perform an ambient isotopy on any tangle that you insert into the black box!

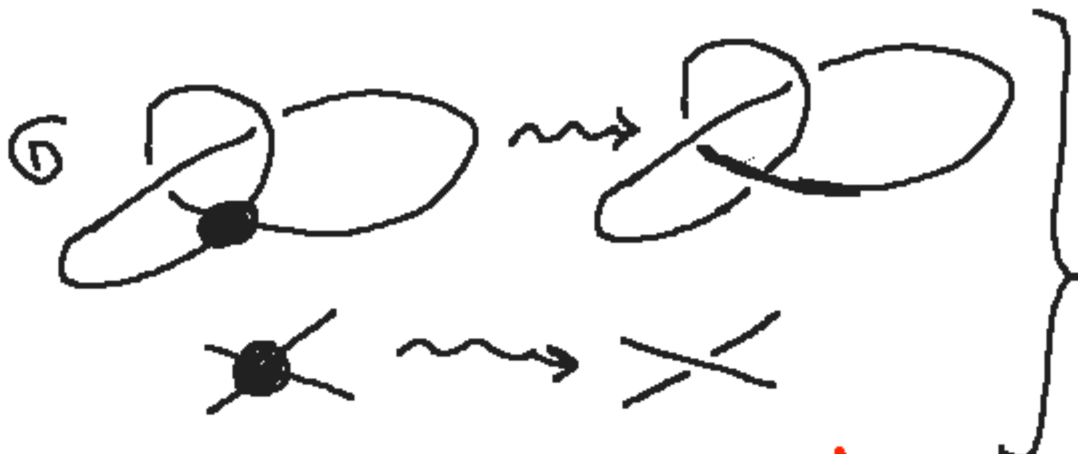
e.g.

These are topologically equivalent keeping endpoints fixed.

Simplest example:

Rigid Vertex Graphs

You can insert <u>any tangle</u> in the blackbox. The resulting knot or link is a topological invariant of the RV graph.



$\Rightarrow$ G is a non-trivial RG graph.

Note: This a good insertion.
If insert $\supset\subset$ or $\times$, get an unknot.

But 

and this also shows G is non-trivial.

By using insertion we can create many invariants of RG graphs.

e.g. 

Then any graph goes to a sum of knots and links $\Sigma(G)$ and you can apply any invariant $\mathcal{I}$ to $\Sigma(G)$ + get $\mathcal{I}(\Sigma(G))$ an invariant of G.

We will come back to this.

---

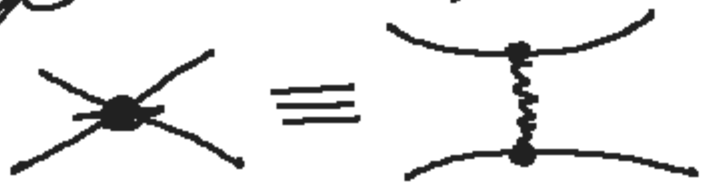
e.g. Bracket Poly 

$$\langle OK \rangle = \delta \langle K \rangle, \quad \delta = -A^{2} - A^{-2}$$

$$f_K = (-A^3)^{-wr(K)} \langle K \rangle \rightsquigarrow$$ models the Jones polynomial

Bonds

We want to think of a vertex as a *bond*.



Then our graphs will have trivalent nodes  each with one *bond-edge*.

 local bonds

 *long bonds*

 *even knotted bonds*

Again we can have
topological nodes
where  $\underset{Top}{\sim}$ 

and we can have RV bonds
where the vertices are rigid
and  ~ 
is required.

In this talk we'll concentrate
on RV bonds and include this
restriction at long distance. Thus

with this restriction on rigidity insertion of tangles continues to hold for RV-long bond graphs.

In fact

Theorem. Every RV long bond graph is $\widetilde{RV}$ a graph with only local bonds.

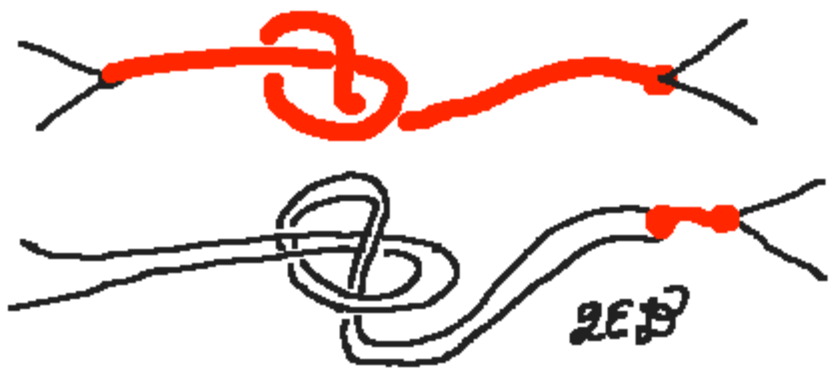
Proof.

$\widetilde{RV}$

QED

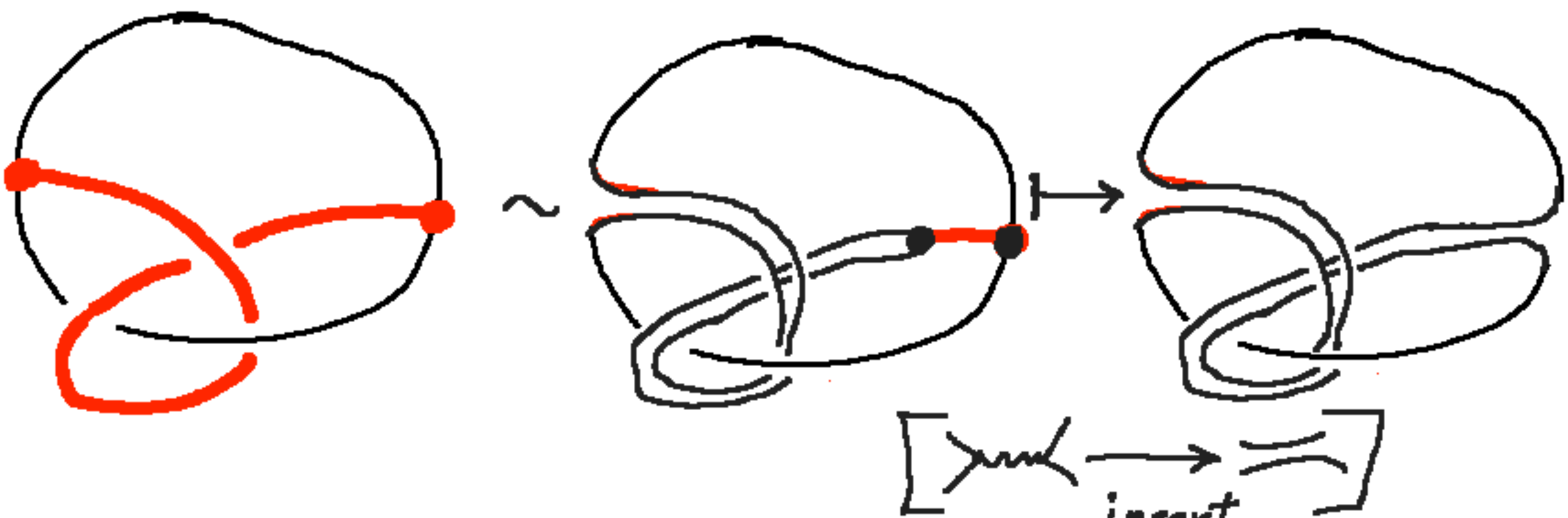
Theorem. Every RV long bond graph is $\widetilde{RV}$ a graph with only local bonds.

Proof.

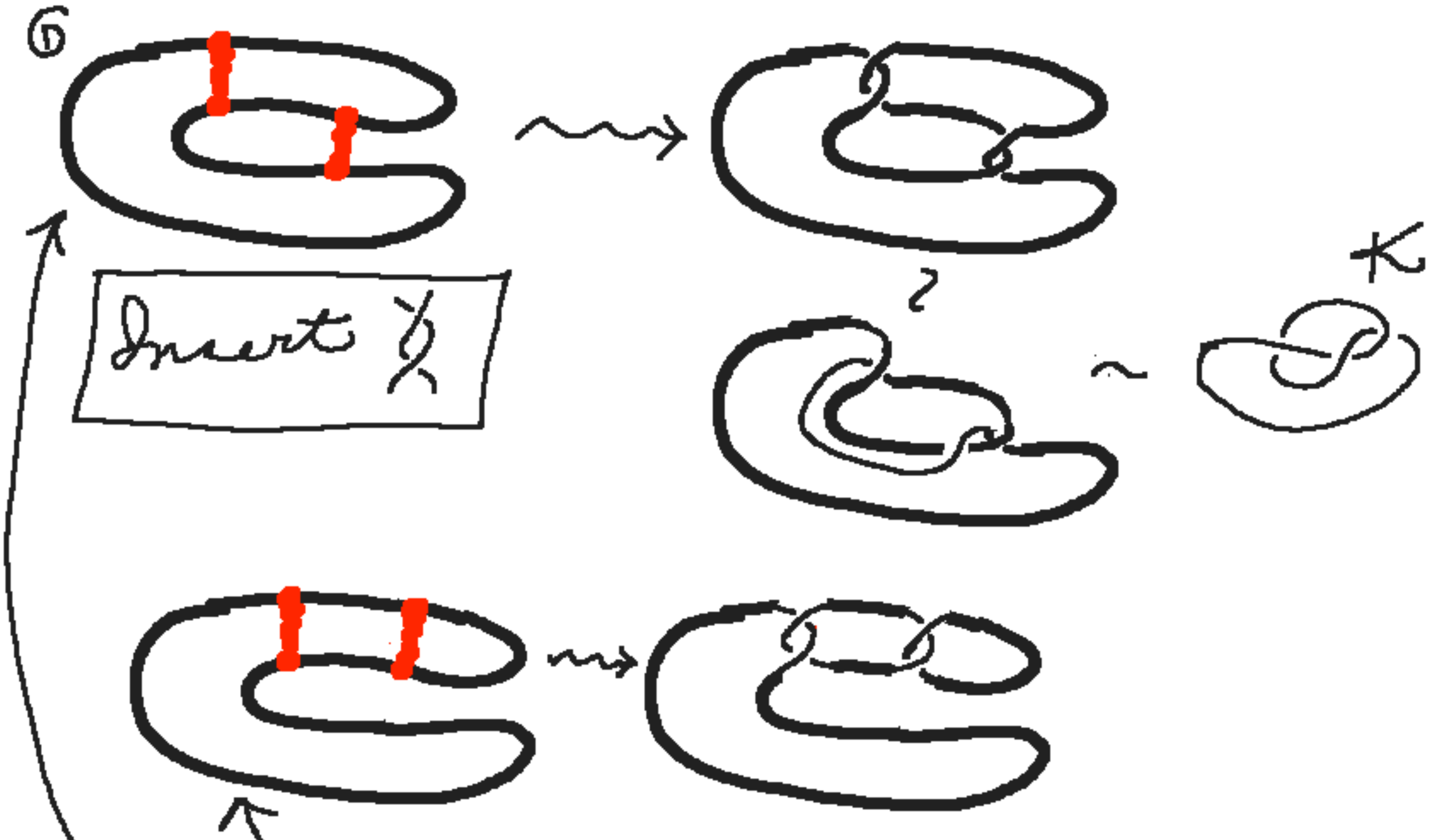


$\widetilde{RV}$

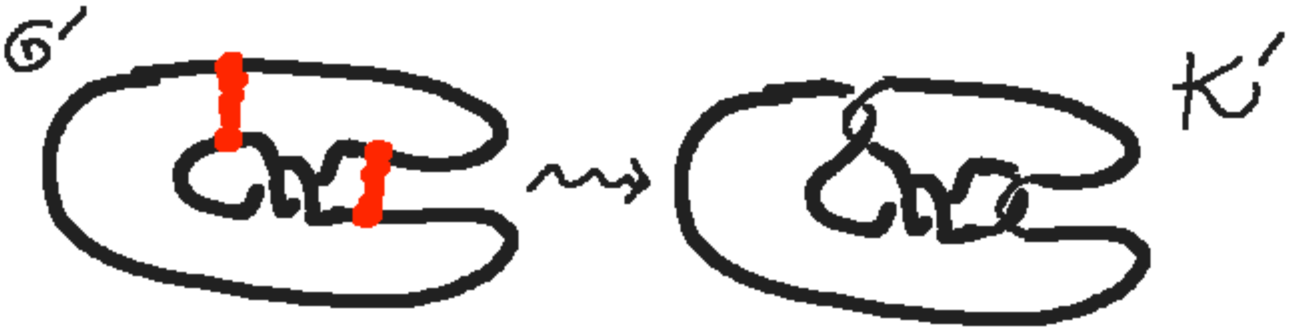
A link of an unknotted circle and a trefoil knot.



Some Examples (RV)



So these foldings are RV distinct.



Insert 

On previous page $G \to K \simeq$ 
Here K' is a twist knot distinct from the trefoil. You can calculate an invar to check this e.g. Alex poly or bracket or ...

Large Question

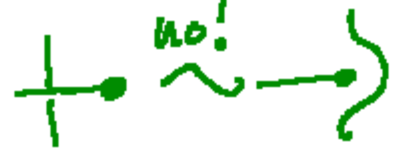
Bonded RV Graphs + Chosen Tangles (CT) $\xrightarrow{CT}$ Knots & Links

Given RV bonded graphs G, G' such that $G \not\approx G'$, does there exist a choice of tangle insertions such that $CT(G)$ and $CT(G')$ are topologically distinct links? Can this be done using only <u>one</u> tangle?

<u>Note</u>:

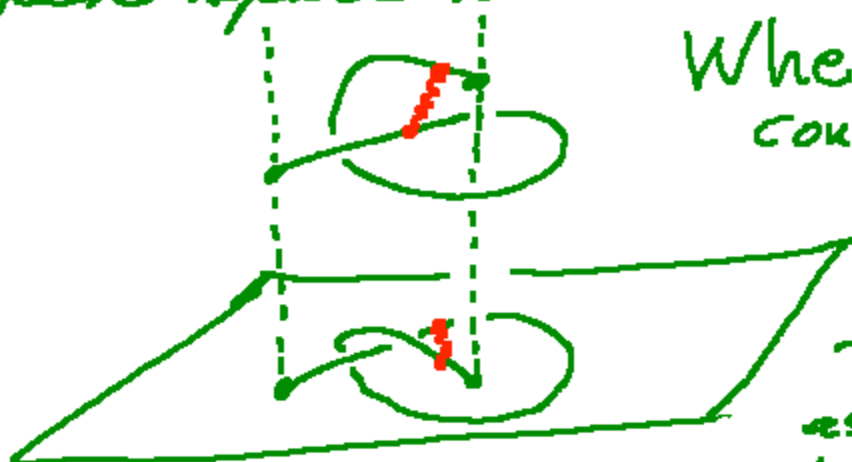
We generalize to <u>bonded knotoids</u>.

A knotoid is open-ended, with endpoints in (possibly) different regions.

(Forbidden to move like this: 

).

Knotoids can be projections of open space curves.



When the open curve is confined to keep its end points on the "rails", then the projection moves as a knotoid, or bonded knotoid.

Article

Topological models for open knotted protein chains using the concepts of knotoids and bonded knotoids

Dimos Goundaroulis [1,2], Neslihan Gügümcü [3], Sofia Lambropoulou [3], Julien Dorier [1,4], Andrzej Stasiak [1,2] and Louis Kauffman [5]*

1. Center for Integrative Genomics, University of Lausanne, 1015 Lausanne, Switzerland
2. SIB Swiss Institute of Bioinformatics, 1015 Lausanne, Switzerland
3. Department of Mathematics, National Technical University of Athens, Zografou Campus 15780, Athens, Greece
4. Vital-IT, SIB Swiss Institute of Bioinformatics, 1015 Lausanne, Switzerland
5. Department of Mathematics, Statistics and Computer Science, University of Illinois at Chicago, Chicago IL 60607-7045, USA

* Correspondence: kauffman@uic.edu

Academic Editor: name
Version September 8, 2017 submitted to Polymers

Abstract: In this paper we introduce a method that offers a detailed overview of the entanglement of an open protein chain. Further, we present a purely topological model for classifying open protein chains by taking also into account any bridge involving the backbone. For these results we implemented the concepts of planar knotoids and bonded knotoids. We show that the planar knotoids technique provides more refined information regarding the knottedness of a protein when compared to established methods in the literature. Moreover, we demonstrate that our topological model for bonded proteins is robust enough to distinguish all types of lassos in proteins.

Keywords: Protein knots; Knot theory; Topology; Knotoids.

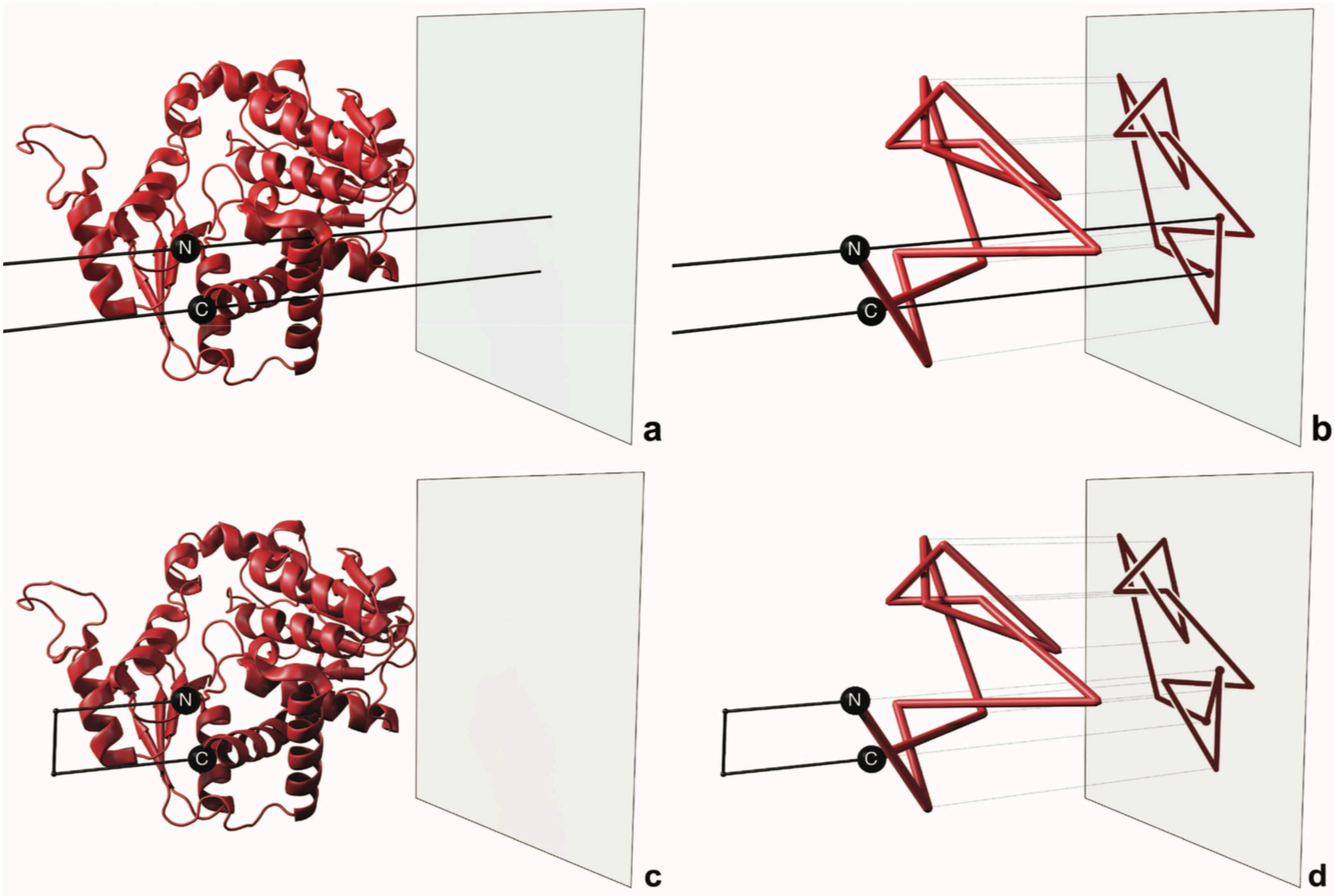
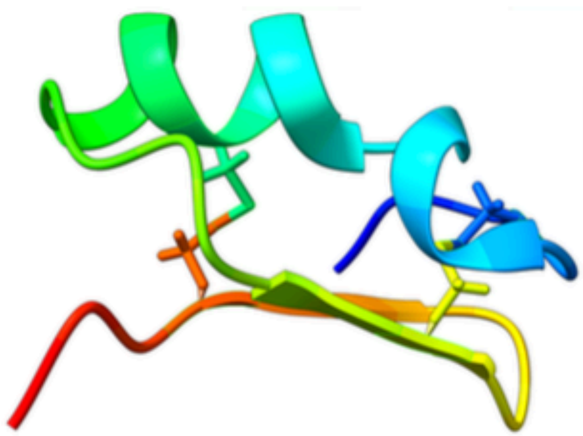


FIG. 5: Projection of a protein chain using two different techniques. Top Row: Knotoids technique. (a) The two black infinite lines pass through the N and C termini of the protein chain and are perpendicular to a chosen plane. (b) The two infinite lines pass through the N and C termini of the reduced protein backbone are perpendicular to a chosen plane. Bottom Row: Stochastic closure technique. (c) A choice of closing direction and the two rays extending from the termini towards that direction. The ends of the two rays are connected when they exit the sphere that contains the protein chain. (d) The resulting knot diagram.

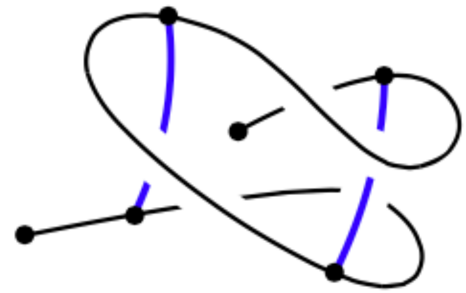
INVARIANTS OF BONDED KNOTOIDS AND APPLICATIONS TO PROTEIN FOLDING

NESLIHAN GÜGÜMCÜ, BOSTJAN GABROVSEK, AND LOUIS H.KAUFFMAN

ABSTRACT. In this paper, we study knotoids with extra graphical structure (bonded knotoids) in the settings of rigid vertex and topological vertex graphs. We construct bonded knotoid invariants by applying tangle insertion and unplugging at bonding sites of a bonded knotoid. We demonstrate that our invariants can be used for the analysis of the topological structure of proteins.



(A) A Ribbon diagram.



(B) Simplified presentation as a bonded knotoid.

FIGURE 1. The PiTX-Kβ Emperor scorpion toxin with two disulphide bonds (pdb 1c49).

In Figure 1a, we view the ribbon diagram of the protein PiTX-Kβ with two disulphide bonds and the corresponding bonded knotoid diagram. We denote the corresponding bonded knotoid diagram by K, shown also in Figure 24..

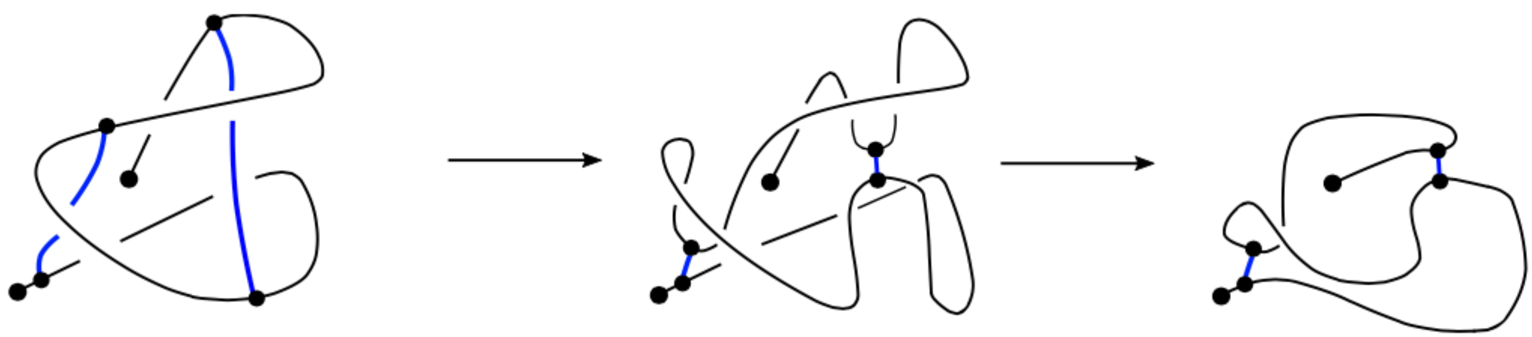


FIGURE 24. An equivalence transformation between bonded knotoid diagrams $K, K^{'}, K^{''}$.

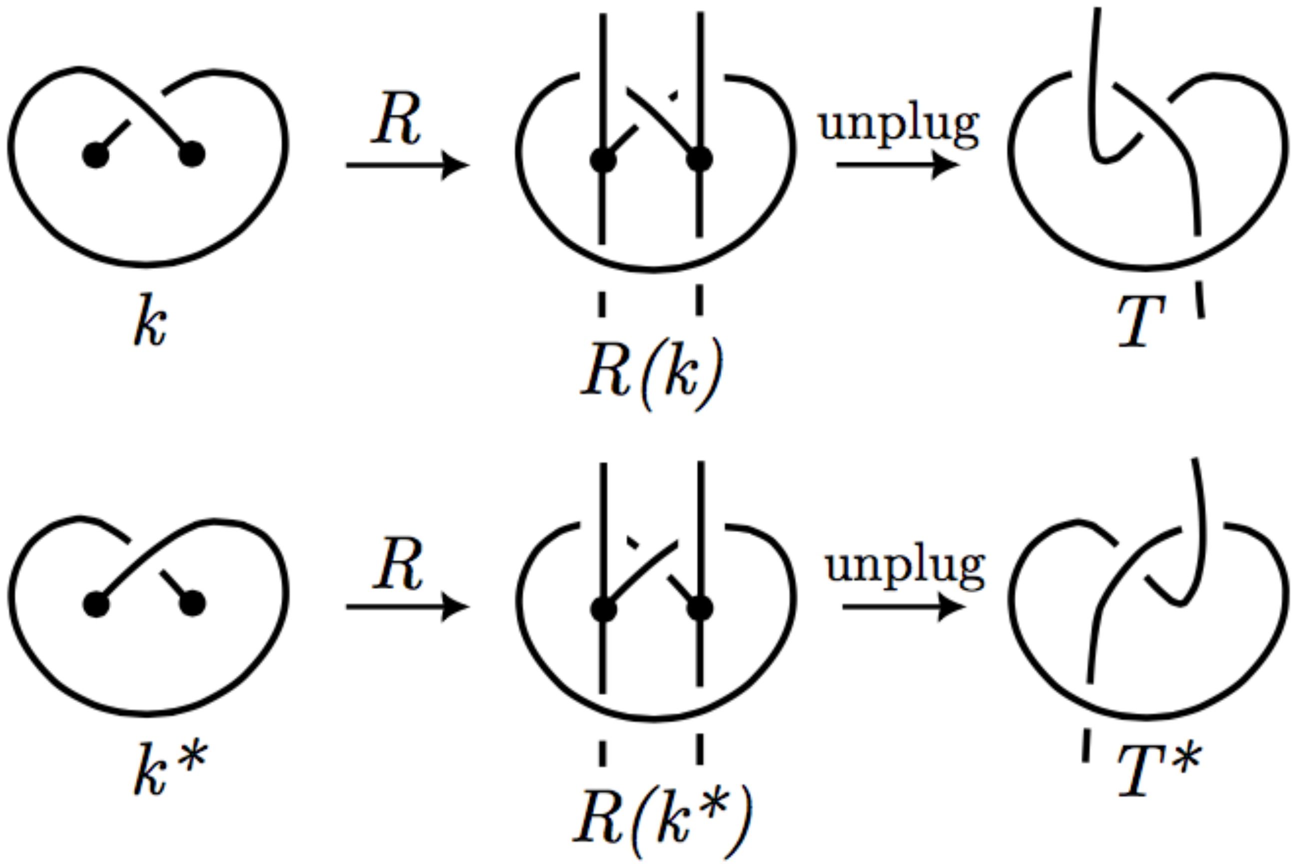


FIGURE 20. Two knotoids (left), their rail closure (middle) and their local replacements (right). Since $T \ncong T^*$ it follows $k \ncong k^*$

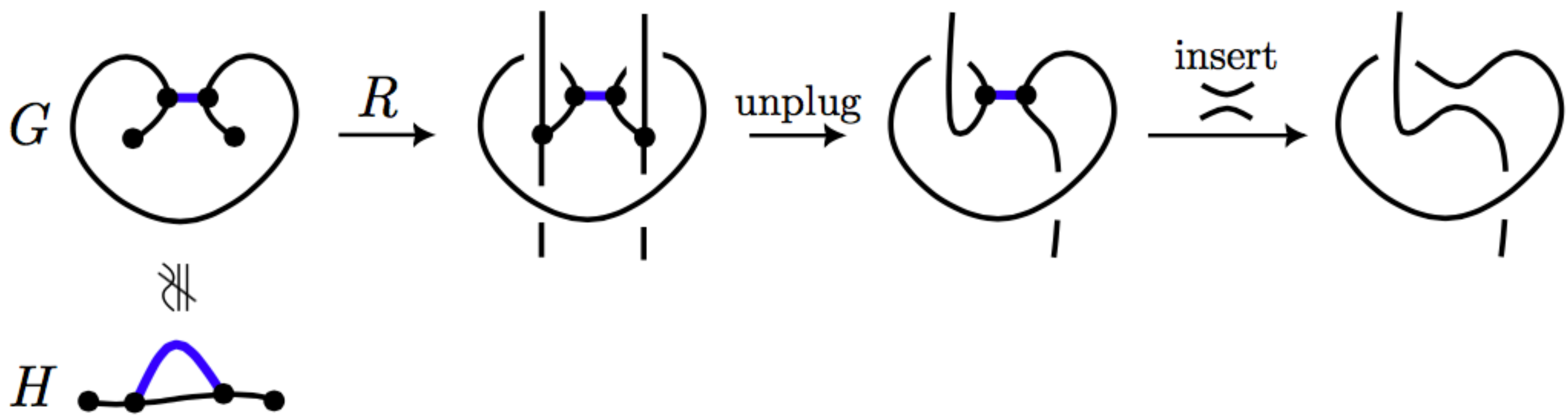


FIGURE 21. The bonded knotoid G is not equivalent to the trivial bonded knotoid H.

Thank you for your attention!