Mathematical Theory and Modeling www.iiste.org
ISSN 2224-5804 (Paper) ISSN 2225-0522 (Online)
Vol.3, No.6, 2013-Selected from International Conference on Recent Trends in Applied Sciences with Engineering Applications

Chiral Knots: An Application to Synthetic Chemistry

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Abstract

The purpose of this paper is to serve as an introduction to knot theory by mathematically defining a knotand equivalent knots in 3-space, specifically in terms of topology. Via the concepts of ambient isotopy and the Kauffman X polynomial refine definition of equivalent knots. The definition of equivalence interms of the Kauffman X Polynomial has a significant application to synthetic chemistry. All of this leads us to the study of chirality, determining whether a molecule can be deformed into its mirror image. Certain molecules, especially enzymes react differently if they are chiral, means they cannot be deformed into their mirror image.

Key words: Equivalent knots, ambient isotopy, Kauffman X polynomial, chirality.

1. Introduction

Originally, knot theory began as a result of a hypothesis made by Lord Kelvin that atoms were rings knotted in different ways to produce different elements. While this theory has long been disproved, mathematicians became interested in the study of knots. There are two main applications of knot theory. One is in the study of statistical and quantum mechanics. The other is the study of how to determine chirality, whether a molecule can be rigidly deformed to its mirror image, in molecules, which is what I studied. The study of chirality is important when looking at certain types of enzymes and how they interact, as well as in the study of DNA.

2. About Knot

A *knot* is a closed curve in space (a curve with no end points and which completely encloses an area) that doesn't intersect itself anywhere.

The *unknot*, or the *trivial knot* is the simplest knot because it can be deformed to a circle.

There is no non-trivial knot with either one or two crossings.

A *polygonal knot* is a knot that is the union of a finite number of straight-linesegments called edges.

A *tame knot*, or *finite knot* can be defined as a knot with a finite number of crossings.

A *wild knot*, on the other hand, is not tame; therefore, it cannot be represented by a polygonal knot.

Throughout this paper, we will be only working with tame knots to avoid running into wild knots.

3. Homeomorphism

A *homeomorphism* is a relation between two topological spaces. Let X and Y be topological spaces; let $f: X \rightarrow Y$ be a bijection. If both the function f and the inverse function $f^{-1}: Y \rightarrow X$ are continuous, then f is called a homeomorphism.

4. Equivalent Knots

Now we can begin developing a definition of equivalent knots: two knots *K1* and *K2*are equivalent if there is a homeomorphism $h: R^3 \rightarrow R^3$(3-space) such that *h(K1) = K2*.

We introduce the concept of homotopy to develop a better definition of knot equivalence.

5. Homotopy

Let$f, g: X \rightarrow Y$be continuous functions. Let I = [0,1]. We say that f and g are *homotopic* if there exists a continuous function $F: X \times I \rightarrow Y$such that F $(x,0) = f(x)$ and F$(x,1) = g(x)$for all x∈X. The function F is called a *homotopy* between f and g. The expression $f \simeq g$ denotes that f and g are *homotopic*.

5.1 Theorem. The relation $\simeq$ is an equivalence relation on the set of all continuous functions $f: X \rightarrow Y$.

Knot theory concerns itself with a particular type of homotopy, namely an ambient isotopy.

6. Isotopy

An *isotopy* is a special case of a homotopy restricted to R^3. A homotopy $F: X \times I \rightarrow Y$ is called an *isotopy* if $F \mid_{X \times \{t\}}$ is a homeomorphism for all t in I. In other words, an isotopy is a deformation of a space X over time that does not change the topology of X. This means that isotopy preserves shape and, unlike other homotopies, is a bijective function.

An *embedding* is the injection of a topological space Y into a topological space X.

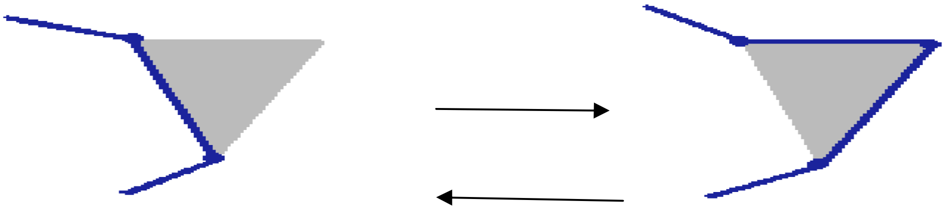
7. Ambient Isotopy

If f: $Y \rightarrow X$ and g: $Y \rightarrow X$ are embeddings of Y into X then we say that f and g are *ambient isotopic* if there is an isotopy F: f: $X \times I \rightarrow Y$ such that
(i) $F(x, 0) = x$ for all x∈X, and
(ii) $F(f(y), 1) = g(y)$ for all y∈ Y. X is called the "ambient space" and F is called the "ambient isotopy."
With this concept of ambient isotopy, a new definition of equivalent knots arises.

8. Equivalent Knots

Two knots $f, g: S^1 \rightarrow R^3$ are *equivalent* if they are ambient isotopic.
A collection of equivalent knots is called a knot type.To avoid the possibility of passing through a wild knot while deforming one knot to another, we introduce the concept of a Piecewise – Linear Ambient Isotopy.
A *piecewise-linear ambient isotopy* is defined by the operations Δ and Δ', also called " triangle moves" (note that these operations can only be applied to polygonal knots).

Δ: Replace an edge of the knot with two other edges, such that the three edges bound a triangle that intersects the original knot along just the first edge.
Δ': Replace two adjacent edges of the knot by one edge, such that the three edges bound a triangle that intersects the original knot in exactly the first two edges.



9. Projection (of a knot)

A *projection* is the planar curve that results when we project a polygonal knot in 3-space to a closed polygonal curve in a plane.
For a projection of a knot to be *regular*, the following three conditions must hold:
(i) No point in the projection corresponds to more than 2 points on the knot
(ii) Only finitely many points are double points ("crossings"), or projection points that correspond to two points on the knot.
(iii) No double point corresponds to a vertex of a knot.

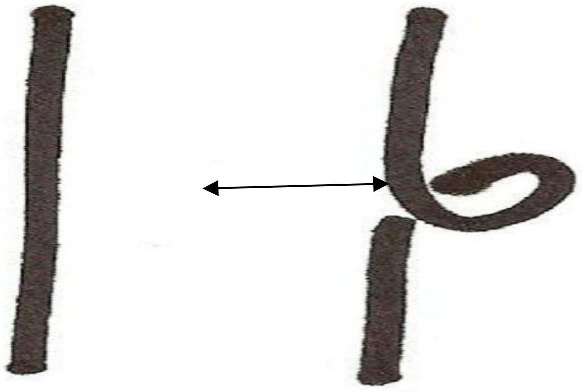
10. Knot Projection/ Diagrams

A *knot projection* is a regular projection that, at each double point, includes an indication of which strand is crossing over the other, relative to the projection plane.
Now, any two knots that we can construct from a given knot projection are equivalent. If two knots have the same knot projection, then they are isotopic.

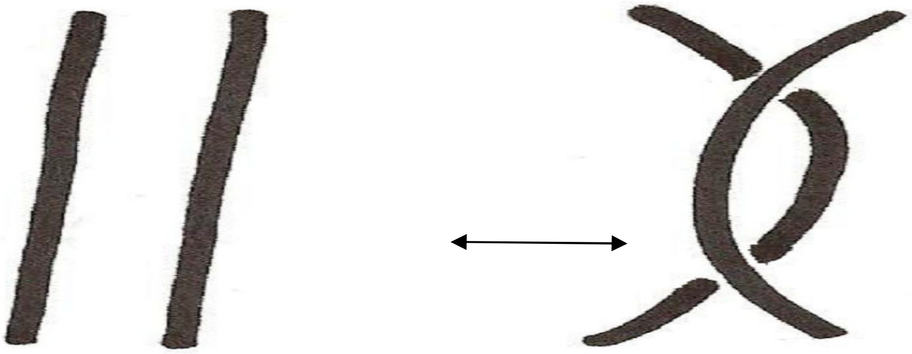
11. Planar Isotopy

A *planar isotopy* is a piecewise-linear isotopy of the plane which deforms a polygonal knot projection to another without changing the structure of the associated topological graph in the plane.
Note that an ambient isotopy between two knots does not necessarily project to a planar isotopy. Thus, we cannot define equivalent knots in terms of planar isotopy (alone).
Reidemeister (1893 – 1971) showed that the existence of an ambient isotopy is equivalent to the existence of a sequence of Reidemeister moves.
There are three types of Reidemeister moves, defined as follows:

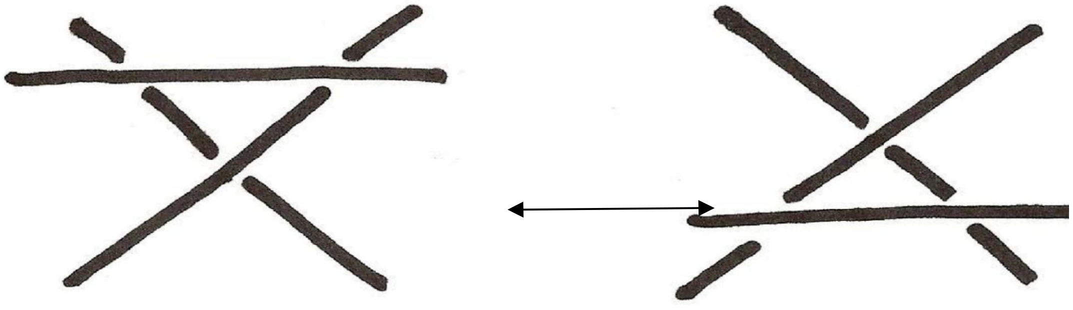
TYPE I – Put in or take out a kink in the projection



TYPE II – Slide one of two adjacent strands under the other OR slide one strand out from under another, resulting in adjacent strands.



TYPE III – A strand is slid past a crossing (over or under)



11.1 Reidemeister's Theorem. Two knots are equivalent if and only if there is a finite sequence of planar isotopies and Reidemeister moves taking a knot projection of one to a knot projection of the other.

Proof. Suppose two knot projections correspond to equivalent knots.We want to show that there exists a sequence of planar isotopies and Reidemeister moves from one to another.

Assume that both knots are polygonal (then the topological graph is composed of line segments attached at vertices)

Since the two knots represented are equivalent, there exists a piecewise linear ambient isotopy from R^3 to R^3 that deforms one knot to the other.

Because isotopy is piecewise-linear, by definition we can realize its impact on the knot by a sequence of triangle moves.

But what happens when a stage of the ambient isotopy does NOT yield aregular projection? Then we have a Reidemeister move.

Thus, when triangle moves project in a diagram, they result in a sequence of planar isotopies and Reidemeister moves.

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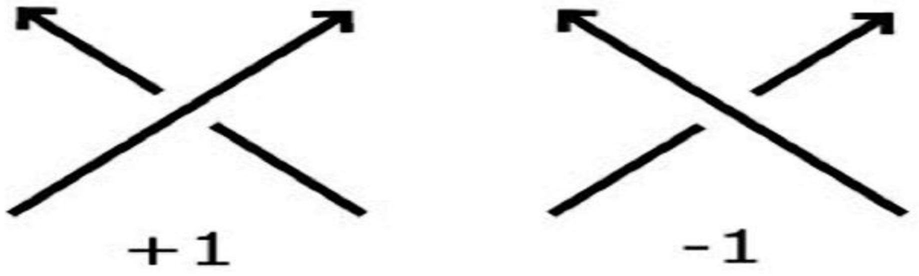
Note: Knot equivalence is an equivalence relation.

No sequence of Reidemeister moves and planar isotopies exist between a trivial and non-trivial knot. We have a way to classify knots, but there is also a way to distinguish a knot from its mirror image.

12. Links and Linking Number

A *link* is an embedding of a set of circles into R^3. Two links are equivalent if one canbe deformed into another via ambient isotopy. A link that has n-components is called an *n-component link.*

The orientation is the direction chosen to travel around the components. Each crossing appears as one of the following:



Crossing labels

We label each crossing with +1 or –1, depending on which of the images in above figure the crossing relates to. The *orientation* is the direction chosen to travel around the components. We denote a crossing number of *c* by *l(c).*
The linking number of a diagram of an oriented two-component link L is given by $lk(L) = ½ \sum l(c)$, where the sum is taken over all of the crossings c involving both of the components of the link (Linking number is defined for a link projection associated to a given oriented link).

12.1 Theorem. If two oriented links are equivalent, then all of their diagrams have the same linking number.
Proof. We want to show that given two link projections of equivalent oriented links, the linking numbers are the same.
If two links are equivalent, then the link projections are related through a sequence of planar isotopies and Reidemeister moves. Recall that planar isotopies do not change crossings, so therefore they do not change linking number.
Now we will prove that Reidemeister moves do not change linking number either.
TYPE I – This move eliminates or creates a crossing between a component and itself. Since this crossing is not labeled in either case, the linking number does not change.
TYPE II – This move could result in one of the following cases
(i) Create a crossing with one component
(ii) Create or remove a +1 and –1 crossing
Case (i) does not change linking number because the crossing is not labeled. Case (ii) does not change the linking number because the pair of crossing cancel out to zero regardless.
TYPE III – This move only changes the positions of crossings, not the numberof crossings, so the linking number is unchanged.
We have proven that Reidemeister moves leave the linking number unchanged.
Therefore, all diagrams of equivalent oriented links have the same linking number.
The linking number is an invariant of oriented links.

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If two links have different linking numbers, then they are different links. However, if two links have the same linking number, they are not necessarily the same link.
We will reduce the polynomial to a polynomial with one variable A, called a *bracket polynomial.* Denote the bracket polynomial of a projection L by <L>. The bracket polynomial is not a polynomial invariant.
Thus, we introduce the concept of *writhe.*
Given a projection *P* of an oriented link, the *writhe* of *P*, denoted *w(P),* is the sum of the labels, +1 or–1, at all of the crossings in *P.*

13. Kauffman *X* Polynomial

The Kauffman *X* polynomial of an oriented link is defined to be the polynomial

$$X(P) = (-A^3)^{-w(P)} < P >.$$

13.1 Theorem. The Kauffman *X* polynomial is an invariant for knots and for oriented links.

Note: This theorem indicates that the X polynomial is an invariant for knots, whether oriented or not, and for links that are oriented. Why this difference? Because the writhe of a projection does not change for a knot with changed orientation, but the writhe of an oriented link can change if the orientation of one of the link components is changed.

13.2 Theorem. The trefoil knot is not equivalent to the trivial knot.

Two knots are equivalent if they have the same Kauffman *X* polynomial.

14. Amphichiral Knot

An *amphichiral knot* is a knot that is equivalent to its mirror image in terms of the Kauffman *X* Polynomial. The mirror image of a knot is obtained by changing all thecrossings of the given knot.

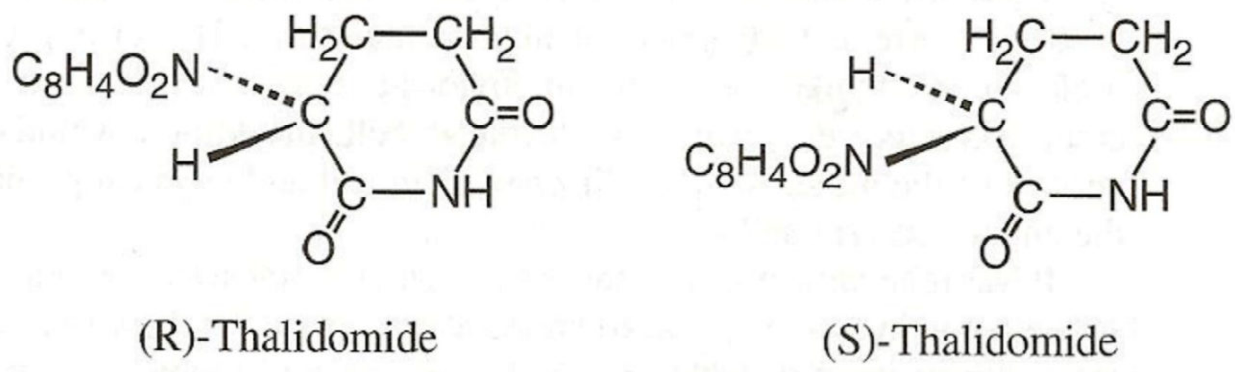
14.1 Theorem. Let *K* be a knot with Kauffman *X* polynomial *P*. If K^* is the mirror image of *K*, then the Kauffman *X* polynomial of K^* is obtained by substituting A^{-1} for *A* in *P*.

From this theorem, it follows that if *X(K) ≠ X(K*)* under the substitution, then the knot and its mirror image are NOT equivalent and therefore, the knot is chiral. Polynomials that don’t change under this substitution are *palindromic*.

A polynomial $a_{-n}A^{-n} + a_{-n+1}A^{-n+1} + \ldots + a_{n-1}A^{n-1} + a_nA^n$ is called *palindromic,*
if $a_{-j} = a_j \; \forall j = 1, 2, \ldots, n$.

14.1.1 Corollary. If the Kauffman *X* polynomial of a knot *K* is not palindromic, then *K* is chiral.

This concept of chirality has a significant application in synthetic chemistry. *Achiral molecule* is a molecule that cannot be superimposed on its mirror image.Thalidomide, for example, is a chiral molecule. As drug was prescribed to pregnant women to alleviate morning sickness. Unfortunately, the drug was also linked to a wave of birth defects. It was later discovered that while (R)-Thalidomide is effective, (S)-Thalidomide - the *mirror image* molecule of (R)-Thalidomide - was responsible for the unfortunate side effects.



(R)-Thalidomide and its mirror image molecule, (S)-Thalidomide.

Thus, chemists could not assume that a molecule had the same properties as its mirror image molecule. A chiral molecule and its mirror image have similar physical properties and similar interactions with achiral molecules, but dramatically different reactions with other *chiral* molecules.

If a molecule is represented by an amphichiral knot, then the molecule is automatically chiral, which means its mirror image will have different chemical properties, as exemplified by the Thalidomide molecule. Knot theorists investigate which knots are equivalent to their mirror image. This study of chiral knots can be a time and cost-effective method for scientists to study the property of chemicals, as synthesizing the chemicals may no longer be necessary to identify study its physical and chemical properties.

15. Summary and Conclusion

To prove the equivalence of two knots, we utilized the concept of ambient isotopy, planar isotopy and Reidemeister moves: two knots are equivalent if there exists a sequence of Reidemeister moves and planar isotopies between them. It follows that a knot is a member of an equivalence class, specifically an isotopy class. If two knots are equivalent, then they are members of the same isotopy class and therefore of the same knot type.

The Kauffman *X* polynomial is a knot invariant that distinguishes one knot not only from all others, but also from its mirror image. This latter distinction is essential in determining whether or not a knot is chiral, that is, equivalent in terms of the Kauffman X Polynomial to its mirror image. This concept of chirality has an important application to the field of synthetic chemistry, and is just one of the several ways in which knot theory can be applied to the physical sciences.

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