Intrinsic chirality for spatial graphs

Fall Western Sectional Meeting of the AMS

University of California, Riverside

Hyoungjun Kim

Joint work with Howon Choi and Sungjong No

November 10, 2019

Ewha Womans University

Spatial Graph Theory

Spatial graph theory is the study of graphs embedded in $\mathbb{R}^3$.

- A *graph* $G = (V, E)$ is a set of vertices and edges.
- A *spatial graph* is an embedding of a graph in $\mathbb{R}^3$.
- A *knot* is an embedding of a circle in $\mathbb{R}^3$.
- A *link* is a collection of knots which do not intersect.

Chirality

Chirality is a geometric property of some molecules and ions.

A chiral molecule/ion is non-superposable on its mirror image.

Gal [2012]

The artificial sweetener aspartame has two enantiomers. L-aspartame tastes sweet whereas D-aspartame is tasteless.

Jaffe-Altman-Merryman [1964]

D-penicillamine is used in chelation therapy and for the treatment of rheumatoid arthritis whereas L-penicillamine is toxic as it inhibits the action of pyridoxine, an essential B vitamin.

Chirality

Chirality is a geometric property of some molecules and ions.

A chiral molecule/ion is non-superposable on its mirror image.

Gal [2012]

The artificial sweetener aspartame has two enantiomers.
L-aspartame tastes sweet whereas D-aspartame is tasteless.

Jaffe-Altman-Merryman [1964]

D-penicillamine is used in chelation therapy and for the treatment of rheumatoid arthritis whereas L-penicillamine is toxic as it inhibits the action of pyridoxine, an essential B vitamin.

Chirality

Chirality is a geometric property of some molecules and ions.

A chiral molecule/ion is non-superposable on its mirror image.

Gal [2012]

The artificial sweetener aspartame has two enantiomers.
L-aspartame tastes sweet whereas D-aspartame is tasteless.

Jaffe-Altman-Merryman [1964]

D-penicillamine is used in chelation therapy and for the treatment of rheumatoid arthritis whereas L-penicillamine is toxic as it inhibits the action of pyridoxine, an essential B vitamin.

A Molecular Structure and a Spatial Graph

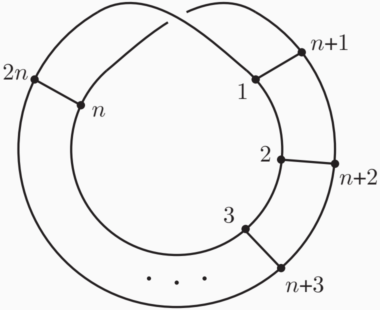
In spatial graph theory, molecular structures are interpreted as a graph embedded in S^3

- A molecule is *chemically achiral* if it can continuously change to its mirror image, otherwise it is *chemically chiral*.
- An embedding of a graph G in S^3 is *topologically achiral* if it is ambient isotopic to its mirror image, otherwise it is *topologically chiral*.
- A graph G is *intrinsically chiral* if every embedding of G in S^3 is topologically chiral, otherwise it is *achirally embeddable*.

Möbius Ladder M_n

A *Möbius ladder*, denoted by M_n, is the graph consisting of a $2n$-cycle K and n edges $\alpha_1, \ldots, \alpha_n$.

K is the *loop* of M_n and $\alpha_1, \ldots, \alpha_n$ are the *rungs* of M_n.

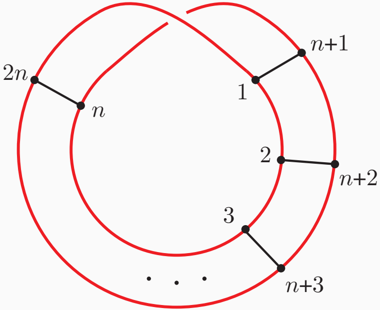


An standard embedding of M_n

Möbius Ladder M_n

A *Möbius ladder*, denoted by M_n, is the graph consisting of a $2n$-cycle K and n edges $\alpha_1, \ldots, \alpha_n$.

K is the *loop* of M_n and $\alpha_1, \ldots, \alpha_n$ are the *rungs* of M_n.

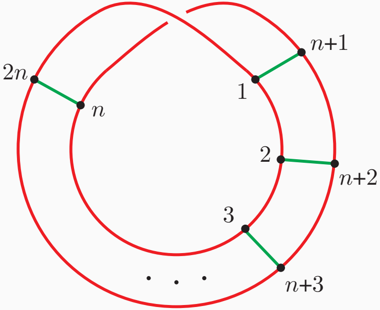


An standard embedding of M_n

Möbius Ladder M_n

A *Möbius ladder*, denoted by M_n, is the graph consisting of a $2n$-cycle K and n edges $\alpha_1, \ldots, \alpha_n$.

K is the *loop* of M_n and $\alpha_1, \ldots, \alpha_n$ are the *rungs* of M_n.



An standard embedding of M_n

Möbius Ladder

Simon [1986]

Every standard embedding of M_n, for $n \geq 4$,

there is no orientation reversing diffeomorphism h of S^3 with $h(M_n) = M_n$ and $h(K) = K$.

Flapan [1989]

Every embedding of M_n, for $n \geq 3$ be odd,

there is no orientation reversing homeomorphism h of S^3 with $h(M_n) = M_n$ and $h(K) = K$.

Möbius Ladder

Simon [1986]

Every standard embedding of M_n, for $n \geq 4$,

there is no orientation reversing diffeomorphism h of S^3 with $h(M_n) = M_n$ and $h(K) = K$.

Flapan [1989]

Every embedding of M_n, for $n \geq 3$ be odd,

there is no orientation reversing homeomorphism h of S^3 with $h(M_n) = M_n$ and $h(K) = K$.

Intrinsically Chiral Graphs

Flapan-Weaver [2013]

The complete graphs K_{4n+3} with $n \geq 1$ are intrinsically chiral, and all other complete graphs are achirally embeddable.

Minimum Condition of Vertices and Edges

Theorem 1

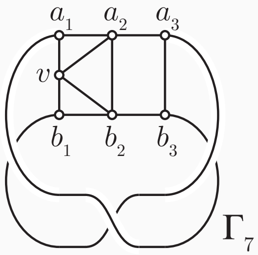
If a simple graph G is intrinsically chiral then G has at least seven vertices and at least eleven edges.

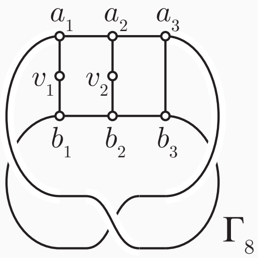
Theorem 2

If a graph G is intrinsically chiral which consists of vertices with degree 3 or more, then G has at least seven vertices and at least twelve edges.

Main theorem

$\mathit{\Gamma}_7$ and $\mathit{\Gamma}_8$ are minor minimal intrinsically chiral graphs.





Notations

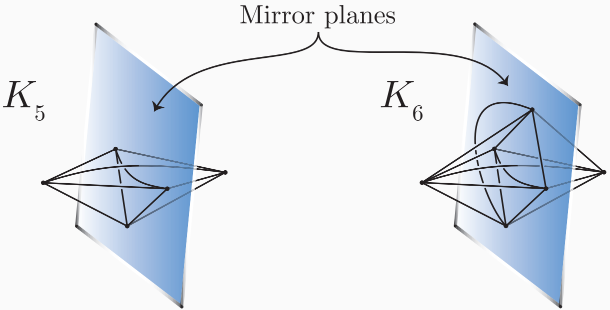
Let G be a simple connected graph.

- $|G|$: the number of vertices of G
- $\|G\|$: the number of edges of G
- $\deg(v)$: degree of a vertex v in G
- $\delta(G)$: the minimum degree among all vertices of G

The Mirror Symmetry Embedding

An embedding of a graph G is *mirror symmetry* when it is symmetrical on the left and right with respect to a plane $\mathcal{M}$.

The mirror symmetry embedding is topologically achiral.



Flapan [1989]

Let M_n be a Möbius ladder which is embedded in S^3 with loop K, where n is an odd number. Then there is no diffeomorphism $h : S^3 \to S^3$ which is orientation reversing with $h(M_n) = M_n$ and $h(K) = K$.

Definition

A *graph automorphism* of G is a permutation ϕ on the set of vertices V that satisfies the property that $\{u_i, u_j\} \in E$ if and only if $\{\phi(u_i), \phi(u_j)\} \in E$.

Proof of Theorem 1

Theorem 1

If a simple graph G is intrinsically chiral then $|G| \geq 7$ and $\|G\| \geq 11$.

Proof.

Let G be a simple graph.

It sufficient to show that if $|G| \leq 6$ or $\|G\| \leq 10$ then G is achirally embeddable.

First, we consider the case that $|G| \leq 6$.

If G has at most 5 vertices, then G is either a planar graph or K_5.

Proof of Theorem 1

Theorem 1

If a simple graph G is intrinsically chiral
then $|G| \geq 7$ and $\|G\| \geq 11$.

Proof.
Let G be a simple graph.

It sufficient to show that if $|G| \leq 6$ or $\|G\| \leq 10$ then G is achirally embeddable.

First, we consider the case that $|G| \leq 6$.

If G has at most 5 vertices, then G is either a planar graph or K_5.

Proof of Theorem 1

Theorem 1

If a simple graph G is intrinsically chiral
then $|G| \geq 7$ and $\|G\| \geq 11$.

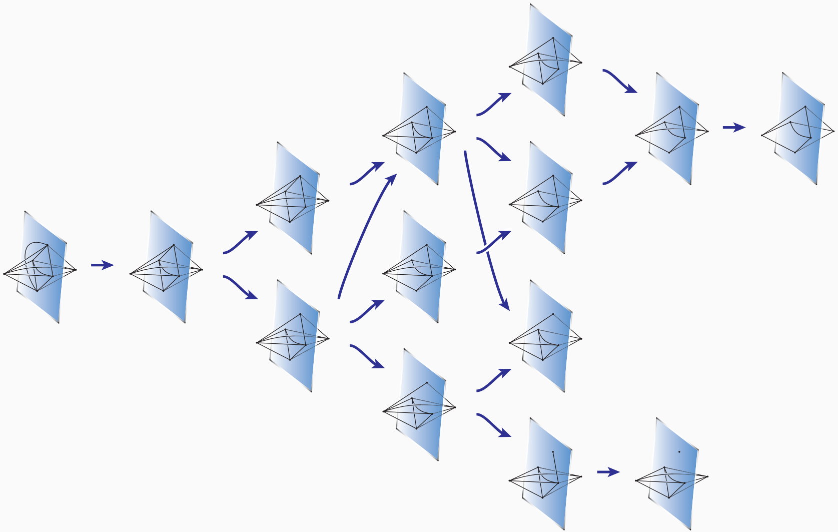
Proof.
Let G be a simple graph.

It sufficient to show that if $|G| \leq 6$ or $\|G\| \leq 10$ then G is achirally embeddable.

First, we consider the case that $|G| \leq 6$.

If G has at most 5 vertices, then G is either a planar graph or K_5.

Case of $|G| = 6$



Case of $\|G\| \leq 10$

Now consider the case that $|G| \leq 10$.

If G has at most 9 edges, then G is either a planar graph or $K_{3,3}$.

Lemma

Let G be a connected graph. If $\|G\| - |G| \leq 2$, then G is planar.

Proof.

If G is a non-planar graph, then G has $K_{3,3}$ or K_5 as minor.

Let e be an edge of G.

$\|G\| - |G| = \|G/e\| - |G/e| > \|G \setminus e\| - |G \setminus e|$

Since $\|K_{3,3}\| - |K_{3,3}| = 3$ and $\|K_5\| - |K_5| = 5$, $\|G\| - |G| \geq 3$. □

If G has at least 8 vertices then $\|G\| - |G| \leq 2$.

Thus G is planar.

Case of $\|G\| \leq 10$

Now consider the case that $|G| \leq 10$.

If G has at most 9 edges, then G is either a planar graph or $K_{3,3}$.

Lemma

Let G be a connected graph. If $\|G\| - |G| \leq 2$, then G is planar.

Proof.

If G is a non-planar graph, then G has $K_{3,3}$ or K_5 as minor.

Let e be an edge of G.

$\|G\| - |G| = \|G/e\| - |G/e| > \|G \setminus e\| - |G \setminus e|$

Since $\|K_{3,3}\| - |K_{3,3}| = 3$ and $\|K_5\| - |K_5| = 5$, $\|G\| - |G| \geq 3$. □

If G has at least 8 vertices then $\|G\| - |G| \leq 2$.

Thus G is planar.

Case of $\|G\| \leq 10$

Now consider the case that $|G| \leq 10$.

If G has at most 9 edges, then G is either a planar graph or $K_{3,3}$.

Lemma

Let G be a connected graph. If $\|G\| - |G| \leq 2$, then G is planar.

Proof.

If G is a non-planar graph, then G has $K_{3,3}$ or K_5 as minor.

Let e be an edge of G.

$\|G\| - |G| = \|G/e\| - |G/e| > \|G \setminus e\| - |G \setminus e|$

Since $\|K_{3,3}\| - |K_{3,3}| = 3$ and $\|K_5\| - |K_5| = 5$, $\|G\| - |G| \geq 3$. □

If G has at least 8 vertices then $\|G\| - |G| \leq 2$.

Thus G is planar.

Case of $\|G\| \leq 10$

Now consider the case that $|G| \leq 10$.

If G has at most 9 edges, then G is either a planar graph or $K_{3,3}$.

Lemma

Let G be a connected graph. If $\|G\| - |G| \leq 2$, then G is planar.

Proof.

If G is a non-planar graph, then G has $K_{3,3}$ or K_5 as minor.

Let e be an edge of G.

$\|G\| - |G| = \|G/e\| - |G/e| > \|G \setminus e\| - |G \setminus e|$

Since $\|K_{3,3}\| - |K_{3,3}| = 3$ and $\|K_5\| - |K_5| = 5$, $\|G\| - |G| \geq 3$. □

If G has at least 8 vertices then $\|G\| - |G| \leq 2$.

Thus G is planar.

Case of $\|G\| \leq 10$

Now consider the case that $|G| \leq 10$.

If G has at most 9 edges, then G is either a planar graph or $K_{3,3}$.

Lemma

Let G be a connected graph. If $\|G\| - |G| \leq 2$, then G is planar.

Proof.

If G is a non-planar graph, then G has $K_{3,3}$ or K_5 as minor.

Let e be an edge of G.

$\|G\| - |G| = \|G/e\| - |G/e| > \|G \setminus e\| - |G \setminus e|$

Since $\|K_{3,3}\| - |K_{3,3}| = 3$ and $\|K_5\| - |K_5| = 5$, $\|G\| - |G| \geq 3$. □

If G has at least 8 vertices then $\|G\| - |G| \leq 2$.

Thus G is planar.

Case of $\|G\| \leq 10$

Now consider the case that $|G| \leq 10$.

If G has at most 9 edges, then G is either a planar graph or $K_{3,3}$.

Lemma

Let G be a connected graph. If $\|G\| - |G| \leq 2$, then G is planar.

Proof.

If G is a non-planar graph, then G has $K_{3,3}$ or K_5 as minor.

Let e be an edge of G.

$\|G\| - |G| = \|G/e\| - |G/e| > \|G \setminus e\| - |G \setminus e|$

Since $\|K_{3,3}\| - |K_{3,3}| = 3$ and $\|K_5\| - |K_5| = 5$, $\|G\| - |G| \geq 3$. □

If G has at least 8 vertices then $\|G\| - |G| \leq 2$.

Thus G is planar.

Case of $\|G\| \leq 10$

Now consider the case that $|G| \leq 10$.

If G has at most 9 edges, then G is either a planar graph or $K_{3,3}$.

Lemma

Let G be a connected graph. If $\|G\| - |G| \leq 2$, then G is planar.

Proof.

If G is a non-planar graph, then G has $K_{3,3}$ or K_5 as minor.

Let e be an edge of G.

$\|G\| - |G| = \|G/e\| - |G/e| > \|G \setminus e\| - |G \setminus e|$

Since $\|K_{3,3}\| - |K_{3,3}| = 3$ and $\|K_5\| - |K_5| = 5$, $\|G\| - |G| \geq 3$. □

If G has at least 8 vertices then $\|G\| - |G| \leq 2$.

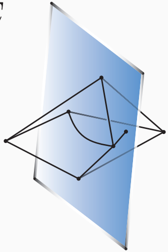
Thus G is planar.

Let G be a non-planar graph with 7 vertices and 10 edges.

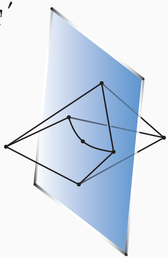
Since $\|G\| - |G| = 3$, G obtain $K_{3,3}$ by using one edge contraction.

Then G is either E or E'

E



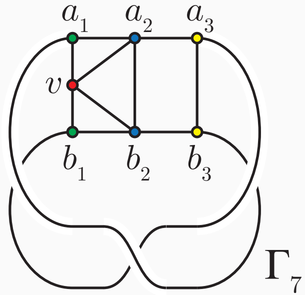
$E^{'}$



Γ_7 is an Intrinsically Chiral Graph

Let $h : S^3 \to S^3$ be a homeomorphism such that $h(\Gamma_7) = \Gamma_7$.

h induces an automorphism on the vertices of Γ_7.



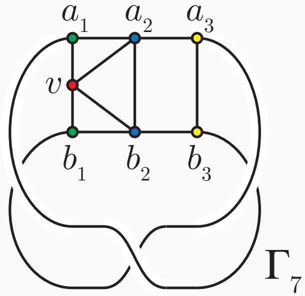
$$h(a_1a_2a_3b_1b_2b_3a_1) = \begin{cases} a_1a_2a_3b_1b_2b_3a_1 & \text{if } h(a_1) = a_1, \\ b_1b_2b_3a_1a_2a_3b_1 & \text{if } h(a_1) = b_1. \end{cases}$$

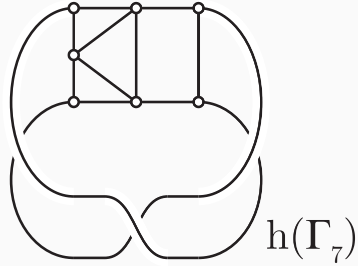
Since $h(K) = K$, h is not orientation reversing homeomorphism.

Γ_7 is an Intrinsically Chiral Graph

Let $h : S^3 \to S^3$ be a homeomorphism such that $h(\Gamma_7) = \Gamma_7$.

h induces an automorphism on the vertices of Γ_7.





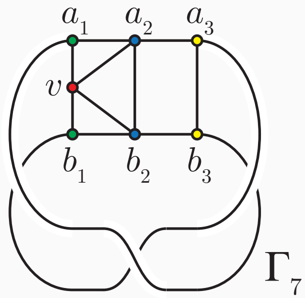
$$h(a_1 a_2 a_3 b_1 b_2 b_3 a_1) = \begin{cases} a_1 a_2 a_3 b_1 b_2 b_3 a_1 & \text{if } h(a_1) = a_1, \\ b_1 b_2 b_3 a_1 a_2 a_3 b_1 & \text{if } h(a_1) = b_1. \end{cases}$$

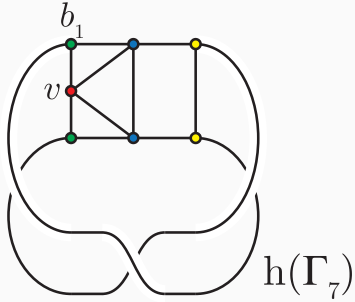
Since $h(K) = K$, h is not orientation reversing homeomorphism.

Γ_7 is an Intrinsically Chiral Graph

Let $h : S^3 \to S^3$ be a homeomorphism such that $h(\Gamma_7) = \Gamma_7$.

h induces an automorphism on the vertices of Γ_7.





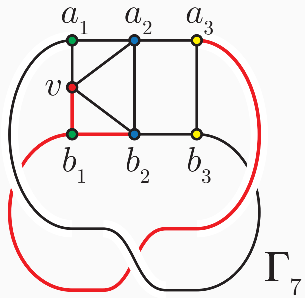
$$h(a_1 a_2 a_3 b_1 b_2 b_3 a_1) = \begin{cases} a_1 a_2 a_3 b_1 b_2 b_3 a_1 & \text{if } h(a_1) = a_1, \\ b_1 b_2 b_3 a_1 a_2 a_3 b_1 & \text{if } h(a_1) = b_1. \end{cases}$$

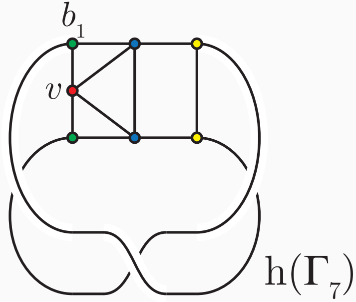
Since $h(K) = K$, h is not orientation reversing homeomorphism.

Γ_7 is an Intrinsically Chiral Graph

Let $h : S^3 \to S^3$ be a homeomorphism such that $h(\Gamma_7) = \Gamma_7$.

h induces an automorphism on the vertices of Γ_7.





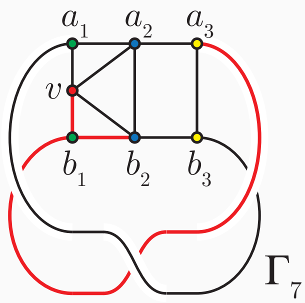
$$h(a_1a_2a_3b_1b_2b_3a_1) = \begin{cases} a_1a_2a_3b_1b_2b_3a_1 & \text{if } h(a_1) = a_1, \\ b_1b_2b_3a_1a_2a_3b_1 & \text{if } h(a_1) = b_1. \end{cases}$$

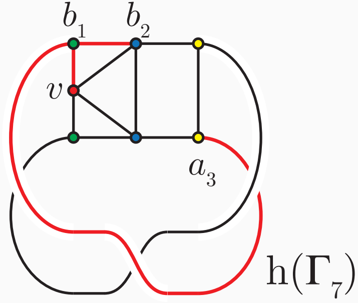
Since $h(K) = K$, h is not orientation reversing homeomorphism.

Γ_7 is an Intrinsically Chiral Graph

Let $h : S^3 \to S^3$ be a homeomorphism such that $h(\Gamma_7) = \Gamma_7$.

h induces an automorphism on the vertices of Γ_7.



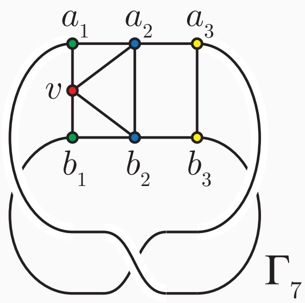


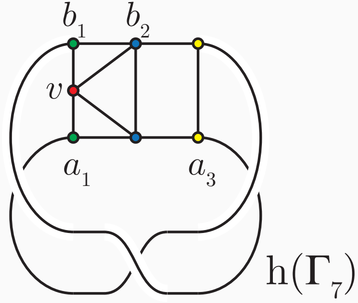
$$h(a_1a_2a_3b_1b_2b_3a_1) = \begin{cases} a_1a_2a_3b_1b_2b_3a_1 & \text{if } h(a_1) = a_1, \\ b_1b_2b_3a_1a_2a_3b_1 & \text{if } h(a_1) = b_1. \end{cases}$$

Since $h(K) = K$, h is not orientation reversing homeomorphism.

Let $h : S^3 \to S^3$ be a homeomorphism such that $h(\Gamma_7) = \Gamma_7$.

h induces an automorphism on the vertices of Γ_7.



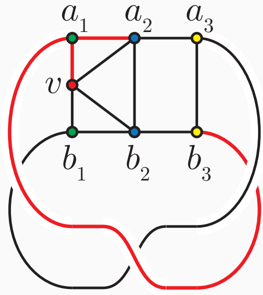


$$h(a_1a_2a_3b_1b_2b_3a_1) = \begin{cases} a_1a_2a_3b_1b_2b_3a_1 & \text{if } h(a_1) = a_1, \\ b_1b_2b_3a_1a_2a_3b_1 & \text{if } h(a_1) = b_1. \end{cases}$$

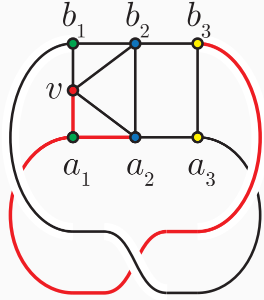
Since $h(K) = K$, h is not orientation reversing homeomorphism.

Let $h : S^3 \to S^3$ be a homeomorphism such that $h(\Gamma_7) = \Gamma_7$.

h induces an automorphism on the vertices of Γ_7.



Γ_7



$h(\Gamma_7)$

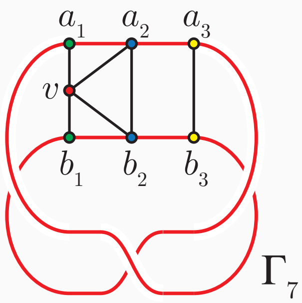
$$h(a_1a_2a_3b_1b_2b_3a_1) = \begin{cases} a_1a_2a_3b_1b_2b_3a_1 & \text{if } h(a_1) = a_1, \\ b_1b_2b_3a_1a_2a_3b_1 & \text{if } h(a_1) = b_1. \end{cases}$$

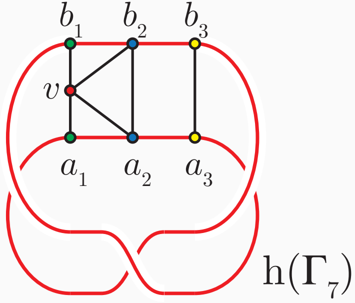
Since $h(K) = K$, h is not orientation reversing homeomorphism.

Γ_7 is an Intrinsically Chiral Graph

Let $h : S^3 \to S^3$ be a homeomorphism such that $h(\Gamma_7) = \Gamma_7$.

h induces an automorphism on the vertices of Γ_7.





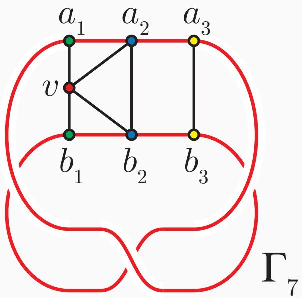
$$h(a_1 a_2 a_3 b_1 b_2 b_3 a_1) = \begin{cases} a_1 a_2 a_3 b_1 b_2 b_3 a_1 & \text{if } h(a_1) = a_1, \\ b_1 b_2 b_3 a_1 a_2 a_3 b_1 & \text{if } h(a_1) = b_1. \end{cases}$$

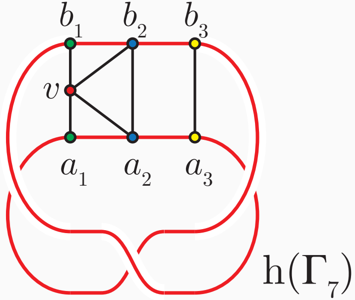
Since $h(K) = K$, h is not orientation reversing homeomorphism.

Γ_7 is an Intrinsically Chiral Graph

Let $h : S^3 \to S^3$ be a homeomorphism such that $h(\Gamma_7) = \Gamma_7$.

h induces an automorphism on the vertices of Γ_7.





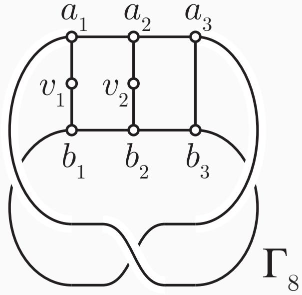
$$h(a_1a_2a_3b_1b_2b_3a_1) = \begin{cases} a_1a_2a_3b_1b_2b_3a_1 & \text{if } h(a_1) = a_1, \\ b_1b_2b_3a_1a_2a_3b_1 & \text{if } h(a_1) = b_1. \end{cases}$$

Since $h(K) = K$, h is not orientation reversing homeomorphism.

Γ_8 is an Intrinsically Chiral Graph

Let $h : S^3 \to S^3$ be a homeomorphism such that $h(\Gamma_8) = \Gamma_8$.

h induces an automorphism on the vertices of Γ_7.



$$h(a_1 a_2 a_3 b_1 b_2 b_3 a_1) =$$

$$\begin{cases} a_1 a_2 a_3 b_1 b_2 b_3 a_1 & \text{if } h(a_1) = a_1, \\ a_2 a_1 b_3 b_2 b_1 a_3 a_2 & \text{if } h(a_1) = a_2, \\ b_1 b_2 b_3 a_1 a_2 a_3 b_1 & \text{if } h(a_1) = b_1, \\ b_2 b_1 a_3 a_2 a_1 b_3 b_2 & \text{if } h(a_1) = b_2. \end{cases}$$

Since $h(K) = K$, h is not orientation reversing homeomorphism.

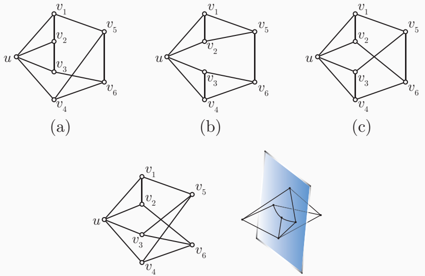
Proof of Theorem 2

Theorem 2

If a graph G is intrinsically chiral with $\delta(G) \geq 3$, then $|G| \geq 7$ and $\|G\| \geq 12$.

Proof.

We only need to consider the case that $|G| = 7$ and $\|G\| = 11$.



(d)

Intrinsically Chiral Graphs with at most 11 Edges

Let G be an intrinsically chiral graph with at most 11 edges, and w be a vertex with minimal degree of G.

By Theorem 1, $|G| \geq 7$ and $\|G\| = 11$.

By the lemma, $|G| \leq 8$. (If $|G| \geq 9$ then $\|G\| - |G| \leq 2$.)

By Theorem 2, w is degree 1 or 2 vertex.

Intrinsically Chiral Graphs with at most 11 Edges

Let G be an intrinsically chiral graph with at most 11 edges, and w be a vertex with minimal degree of G.

By Theorem 1, $|G| \geq 7$ and $\|G\| = 11$.

By the lemma, $|G| \leq 8$. (If $|G| \geq 9$ then $\|G\| - |G| \leq 2$.)

By Theorem 2, w is degree 1 or 2 vertex.

Intrinsically Chiral Graphs with at most 11 Edges

Let G be an intrinsically chiral graph with at most 11 edges,

and w be a vertex with minimal degree of G.

By Theorem 1, $|G| \geq 7$ and $\|G\| = 11$.

By the lemma, $|G| \leq 8$. (If $|G| \geq 9$ then $\|G\| - |G| \leq 2$.)

By Theorem 2, w is degree 1 or 2 vertex.

Intrinsically Chiral Graphs with at most 11 Edges

Let G be an intrinsically chiral graph with at most 11 edges, and w be a vertex with minimal degree of G.

By Theorem 1, $|G| \geq 7$ and $\|G\| = 11$.

By the lemma, $|G| \leq 8$. (If $|G| \geq 9$ then $\|G\| - |G| \leq 2$.)

By Theorem 2, w is degree 1 or 2 vertex.

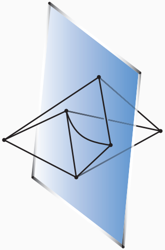
Case of $|G| = 7$, $\|G\| = 11$

If $\deg(w) = 1$ then $|G \setminus w| = 6$ and $\|G \setminus w\| = 10$.

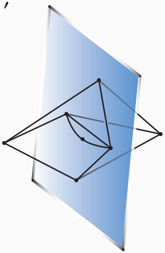
Since G is non-planar, $G \setminus w$ is the graph F.

If $\deg(w) = 2$ then G is either the graph obtained from F by a subdivision of an edge, say e_1, or the graph F'.

F



$F^{'}$



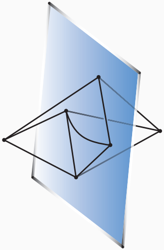
Case of $|G| = 7$, $\|G\| = 11$

If $\deg(w) = 1$ then $|G \setminus w| = 6$ and $\|G \setminus w\| = 10$.

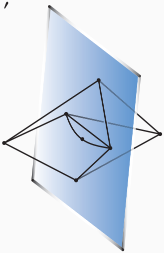
Since G is non-planar, $G \setminus w$ is the graph F.

If $\deg(w) = 2$ then G is either the graph obtained from F by a subdivision of an edge, say e_1, or the graph F'.

F



$F^{'}$



Case of $|G| = 8$, $\|G\| = 11$

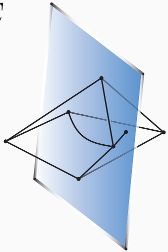
Since $\|G\| - |G| = 3$, we may obtain $K_{3,3}$ from G by using edge contractions twice.

If $\deg(w) = 1$ then $G \setminus w$ is either E or E'.

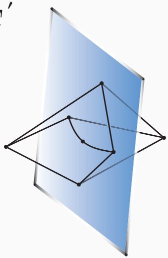
If $\deg(w) = 2$ then G is obtained from $K_{3,3}$ by twice of subdivisions of edges.

If G is not Γ_8, we can obtain an achiral embedding of G.

E



E'



Case of $|G| = 8$, $\|G\| = 11$

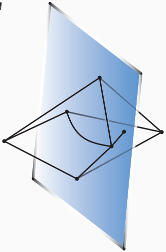
Since $\|G\| - |G| = 3$, we may obtain $K_{3,3}$ from G by using edge contractions twice.

If $\deg(w) = 1$ then $G \setminus w$ is either E or E'.

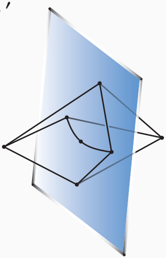
If $\deg(w) = 2$ then G is obtained from $K_{3,3}$ by twice of subdivisions of edges.

If G is not Γ_8, we can obtain an achiral embedding of G.

E



$E^{'}$



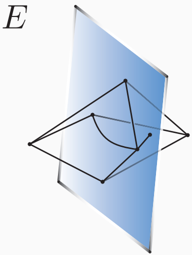
Case of $|G| = 8$, $\|G\| = 11$

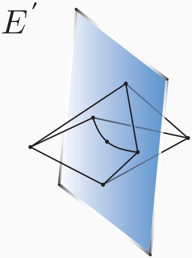
Since $\|G\| - |G| = 3$, we may obtain $K_{3,3}$ from G by using edge contractions twice.

If $\deg(w) = 1$ then $G \setminus w$ is either E or E'.

If $\deg(w) = 2$ then G is obtained from $K_{3,3}$ by twice of subdivisions of edges.

If G is not Γ_8, we can obtain an achiral embedding of G.





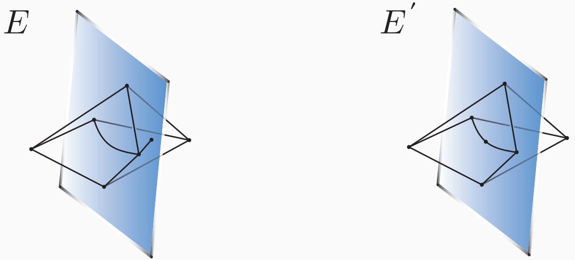
Case of $|G| = 8$, $\|G\| = 11$

Since $\|G\| - |G| = 3$, we may obtain $K_{3,3}$ from G by using edge contractions twice.

If $\deg(w) = 1$ then $G \setminus w$ is either E or E'.

If $\deg(w) = 2$ then G is obtained from $K_{3,3}$ by twice of subdivisions of edges.

If G is not Γ_8, we can obtain an achiral embedding of G.



Thanks for listening