$(3,4,6)$-Fullerene Graphs, Combinatorial Curvature Concept, Bipartite Edge Frustration and Maximum Independent Set

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Summary

$(3, 4, 6)$-*Fullerene Graphs*

- A $(3, 4, 6)$-**Fullerene Graph** is a 3-conected, cubic, planar graph with all faces of size 3, 4 or 6.
- Faces of size 3 = Triangular Faces.
- Faces of size 4 = Quadrangular Faces.
- Faces of size 6 = Hexagonal Faces.

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An Example of $(3, 4, 6)$-*Fullerene Graph*

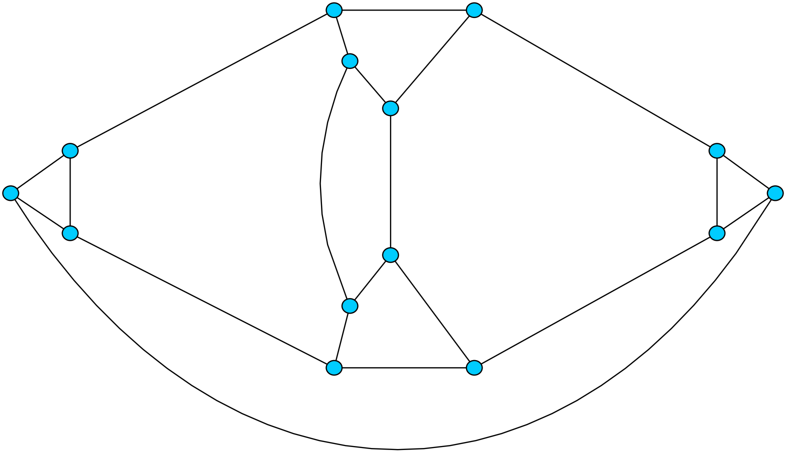

Figura: A $(3, 4, 6)$-fullerene.

Dual of a $(3, 4, 6)$-*Fullerene* Graph

$(3, 4, 6)$-**Fullerene Graph**	**Dual Graph**
Cubic	Triangulation
Planar	Planar
3-Conected	Without loops or multiple edges
All faces of size 3, 4 or 6	All vertices of degree 3, 4 or 6

Example of a $(3, 4, 6)$-*Fullerene* and its *Dual Graph*

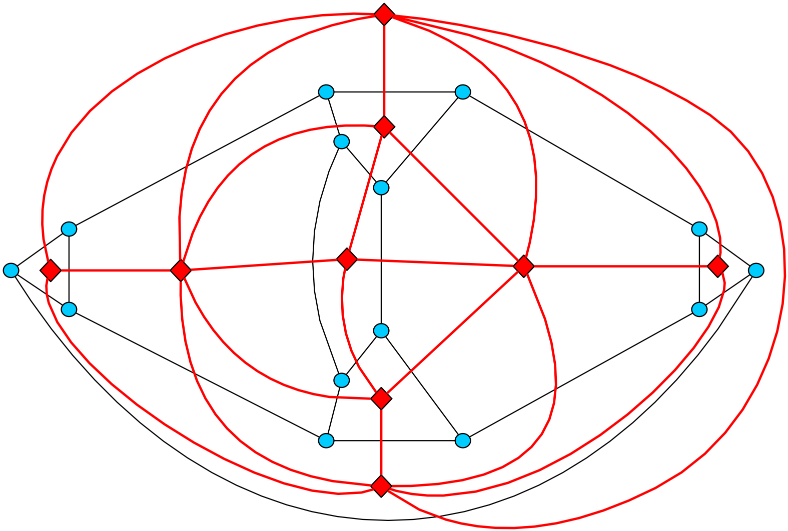

Figura: A $(3, 4, 6)$-fullerene and its dual graph.

Bipartite Edge Frustration

- Let $G = (V, E)$ be a graph. An edge $e \in E$ is frustrated with respect to a bipartition (X, Y) of V if both endpoints of e belong to the same class of the bipartition.
- Bipartite Edge Frustration Problem: determine the smallest number of edges that have to be deleted from the graph to obtain a bipartite spanning subgraph.
- $\tau_{odd}(G)$: bipartite edge frustration parameter.

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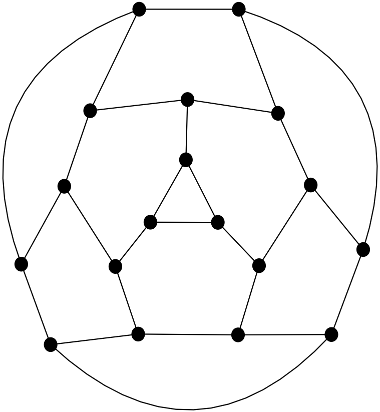

Figura: Graph G.

Bipartite Edge Frustration Problem

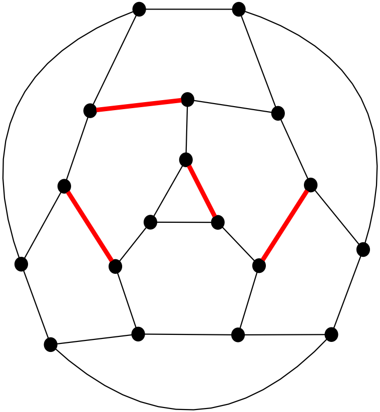

Figura: Removing the red edges we solve bipartite edge frustration for G.

Bipartite Edge Frustration Problem

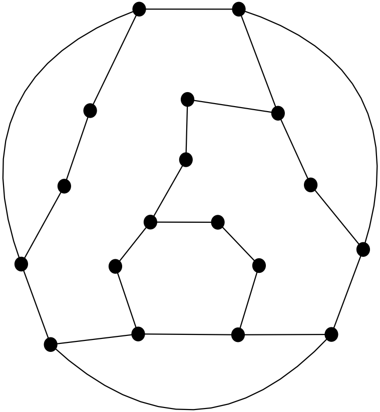

Figura: Bipartite Graph.

Bipartite Edge Frustration Problem

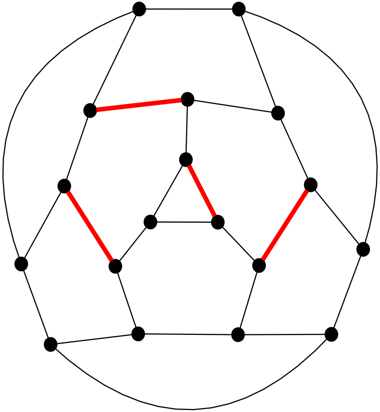

Figura: $\tau_{odd}(G) = 4$.

Combinatorial Curvature Concept

- Combinatorial Curvature measures the degree of difficulty of tiling the plane by faces of a graph.
- Let G be a planar graph. The function $\phi(\cdot) : F(G) \to \mathbb{R}$,

$$\phi_G(f) = 6 - d(f)$$

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Combinatorial Curvature for $(3, 4, 6)$-Fullerenes

- The Hexagonal Faces have zero curvature.
- The Quadrangular Faces have curvature equal to 2.
- The Triangular Faces have curvature equal to 3.
- $(3, 4, 6)$-Fullerene Graphs have total curvature equal to 12.

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Main Objective

- Determine an upper bound to the BIPARTITE EDGE FRUSTRATION PROBLEM on $(3, 4, 6)$-*Fullerene Graphs*.

Dual Problem of Bipartite Edge Frustration

- Bipartite Edge Frustration Problem: determine the smallest number of edges that have to be deleted from the graph to obtain a bipartite spanning subgraph.

- G is a Bipartite Graph $\Leftrightarrow$ G has no odd cycles.

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Dual Problem of Bipartite Edge Frustration

- Dual Problem to Bipartite Edge Frustration: determine the smallest number of edge that have to be deleted from the graph to obtain all vertices of even degree.

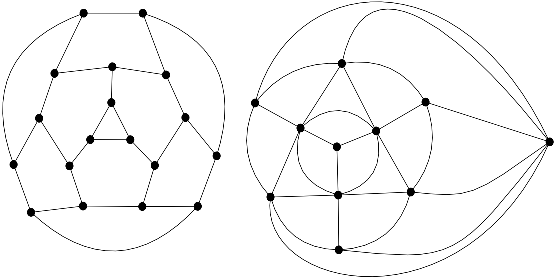

Figura: Graph G and its dual G^*.

Dual Problem of Bipartite Edge Frustration

- In the dual the goal is find a smaller set of edges such that its removal leave all vertices with even degree.

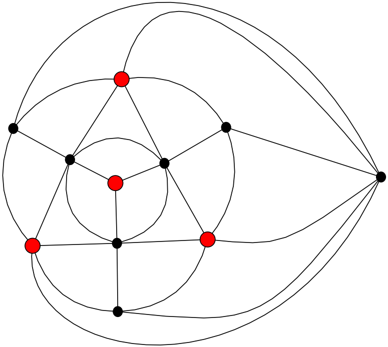

Figura: Dual Graph G^*.

Dual Problem of BIPARTITE EDGE FRUSTRATION

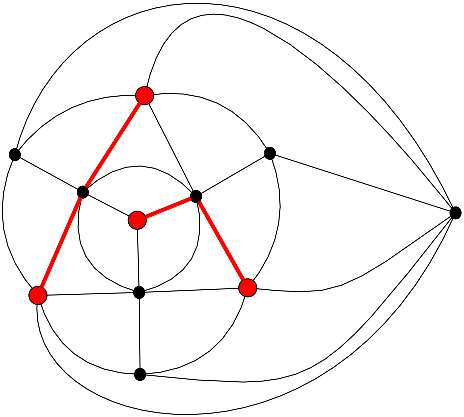

Figura: $\tau(G^*) = 4$, because 4 edges will be deleted to solve the dual problem.

Dual Problem of Bipartite Edge Frustration

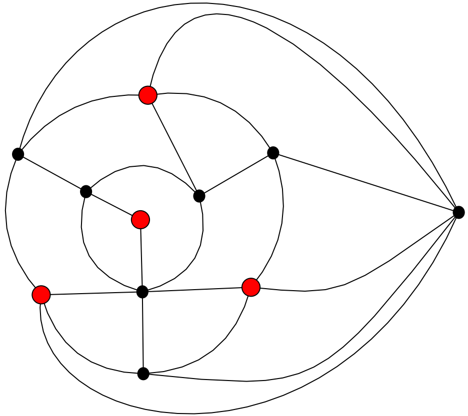

Figura: Graph with all vertices of even degree.

Tools to the BIPARTITE EDGE FRUSTRATION

- D is the set of vertices of degree 3 in the dual graph of $(3, 4, 6)$-fullerene. The set D is called the set of defective vertices.

- Inner Product $\langle \cdot, \cdot \rangle$ in $\mathbb{R}^{|D|}$, given by

$$\langle a, b \rangle = \sum_{u \in D} a_u b_u.$$

- Euclidean norm $\| \cdot \|$, given by $\|a\|^2 = \langle a, a \rangle$.

- Cauchy-Schwarz inequality: if $u, v \in \mathbb{R}^{|D|}$, then

$$\langle u, v \rangle^2 \leq \|u\|^2 \|v\|^2.$$

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Bipartite Edge Frustration on (3, 4, 6)-Fullerenes

- Sketch of the proof

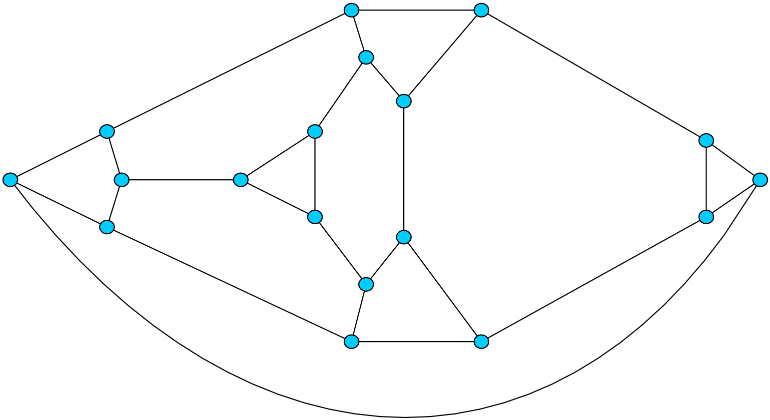

Figura: $(3, 4, 6)$-fullerene G.

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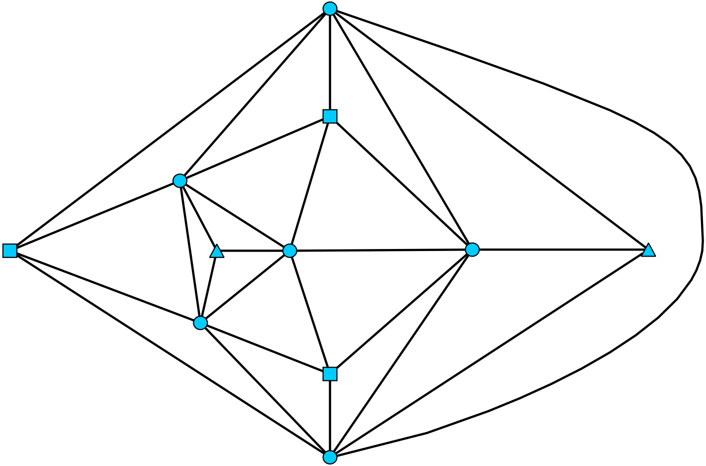

Figura: Dual Graph G^* of $(3, 4, 6)$-fullerene G.

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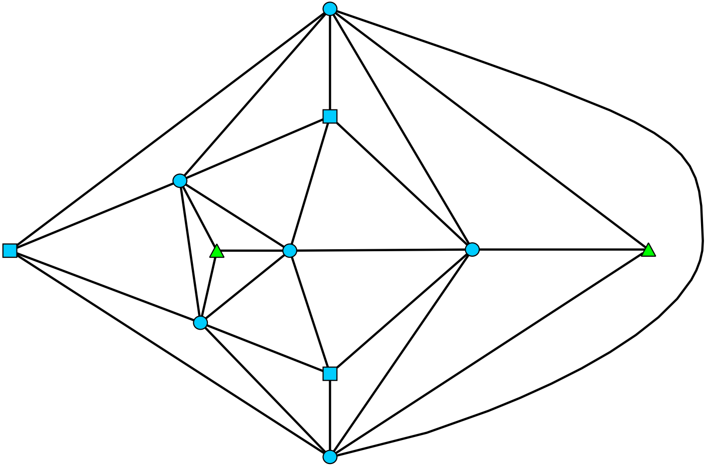

Figura: Green defective vertices with odd degree.

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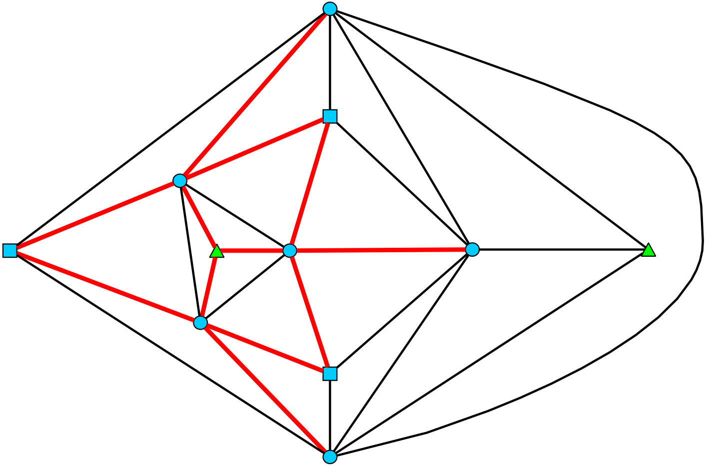

Figura: Building disks surrounding each defective vertex.

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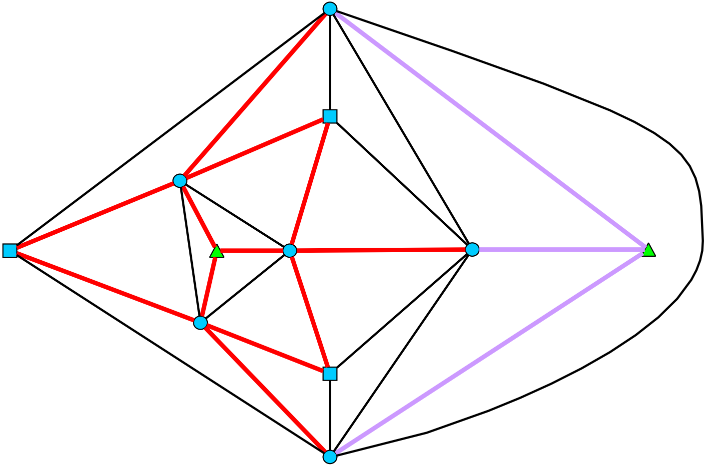

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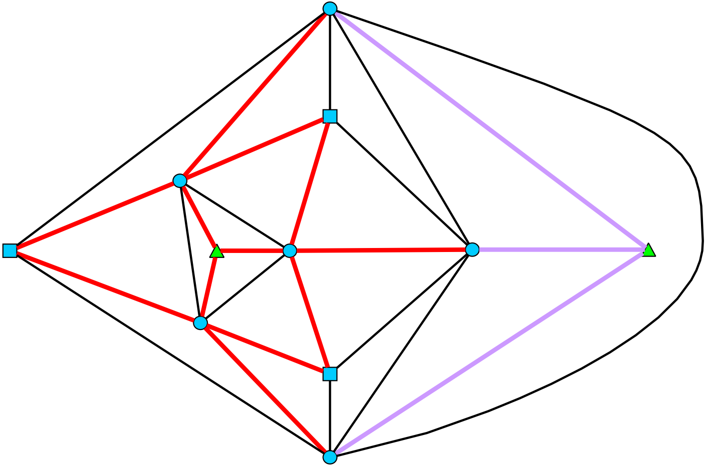

Figura: The vector $\vec{u} = (2, 1)$ holds the radius of each disk.

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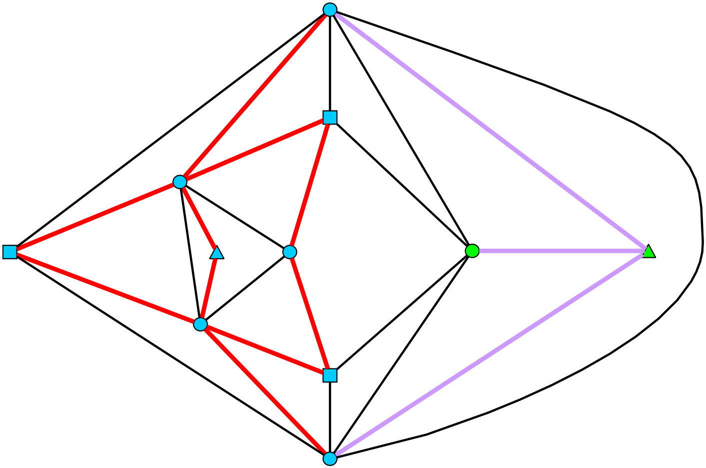

Figura: Removing exactly one radius of the left disk...

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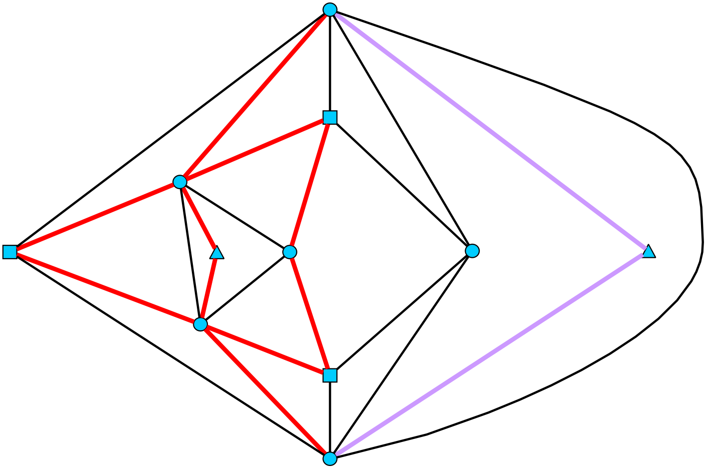

Figura: Removing exactly one radius of the right disk...

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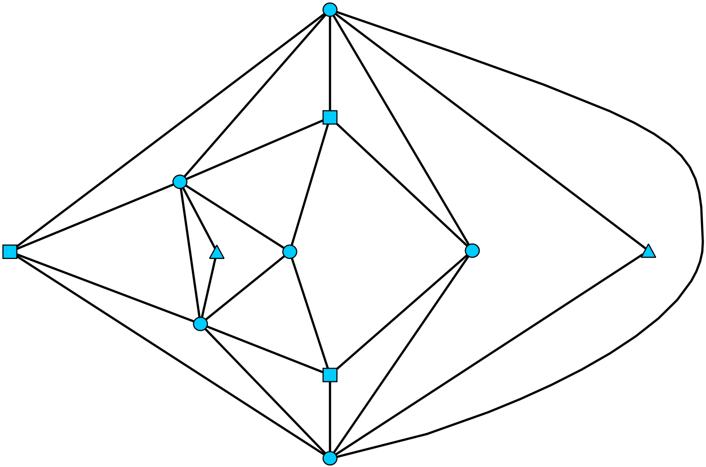

Figura: A graph with all vertices of even degree.

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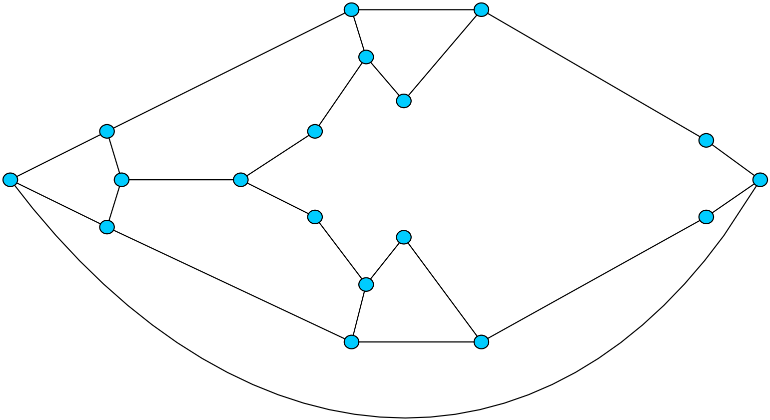

Figura: A bipartite graph.

Bipartite Edge Frustration on $(3, 4, 6)$-Fullerenes

- Note that, $\tau(G^*) \leq \sum_{u \in D} r_u$.
- The area of each disk of radius $r > 0$, centered in a defective vertice, is equal to $3r^2$.
- $\sum_{u \in D} 3r_u^2 \leq f$.

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Bipartite Edge Frustration on $(3, 4, 6)$-Fullerenes

- If $\vec{u} = \left(r_1, r_2, ..., r_{|D|}\right)$ holds the radii of the disks surrounding each defective vertice,
- Then $\|\vec{u}\|^2 = \sum_{u \in D} r_u^2$.
- If $\vec{v} = (1, 1, ..., 1)$,
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- By Cauchy-Schwarz, $\left(\sum_{u\in D} r_u\right)^2 \leq |D| \cdot \sum_{u\in D} r_u^2$.

- $\frac{3}{|D|}\left(\sum_{u\in D} r_u\right)^2 \leq 3\sum_{u\in D} r_u^2 \leq f$.

- Therefore, $\tau(G^*) \leq \sum_{u\in D} r_u \leq \sqrt{\frac{|D|f}{3}}$.

- Finally, $\tau_{odd}(G) \leq \sqrt{\frac{|D|n}{3}}$.

- The worst case is when $|D| = 4$. So, $\tau_{odd}(G) \leq \sqrt{\frac{4n}{3}}$.

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Bipartite Edge Frustration on $(3, 4, 6)$-Fullerenes

Theorem (Nicodemos, Klein e Faria)

- *If G is a* $(3, 4, 6)$*-fullerene graph on n vertices, then* $\tau_{odd}(G, T) \leq \sqrt{4n/3}$. *Equality holds if and only if* $n = 12k^2$, *for some* $k \in \mathbb{N}$, *and* $Aut(G) \cong T_d$.

Maximum Independent Set Problem

- A set of vertices $X \subseteq V(G)$ is *independent* if the graph $G[X]$ has no edges.

- Maximum Independent Set Problem: determine a independent set of vertices of maximum cardinality in a graph.

- The maximum size of an independent set in G is the independence number $\alpha(G)$.

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Maximum Independent Set Problem on $(3, 4, 6)$-Fullerenes

Corollary (Nicodemos, Klein e Faria)

- *If G is a $(3, 4, 6)$-fullerene graph on n vertices, then $\alpha(G) \geq n/2 - \sqrt{n/3}$. Equality holds if and only if $n = 12k^2$, for some $k \in \mathbb{N}$, and $Aut(G) \cong T_d$.*

Bipartite Edge Frustration and maximum Independent Set on (3, 4, 6)-Fullerene Graphs

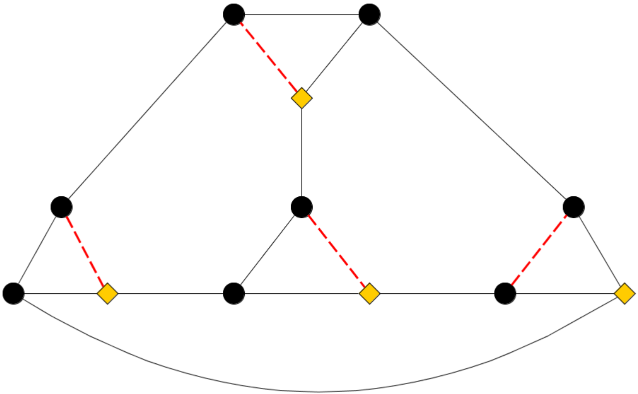

Figura: (3, 4, 6)-Fullerene: $\tau_{odd}(G) = \sqrt{\frac{4 \cdot 12}{3}} = 4$, $\alpha(G) = \frac{12}{2} - \sqrt{\frac{12}{3}} = 4$.

Gracias!

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