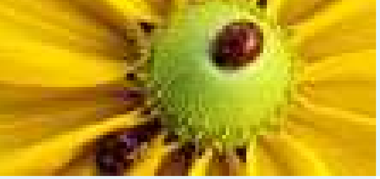
The Structure of Maximum Independent Sets in Fullerenes

Carly Vollet

Portland State University

carlyw@pdx.edu



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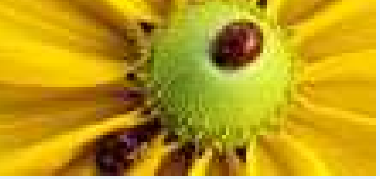

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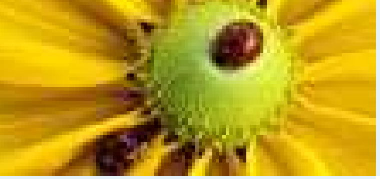

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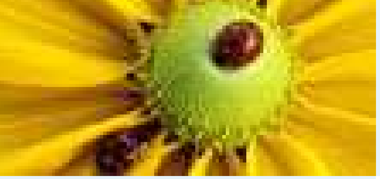

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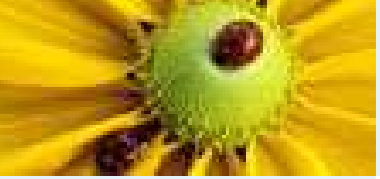

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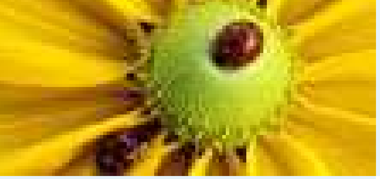

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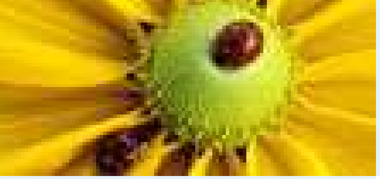

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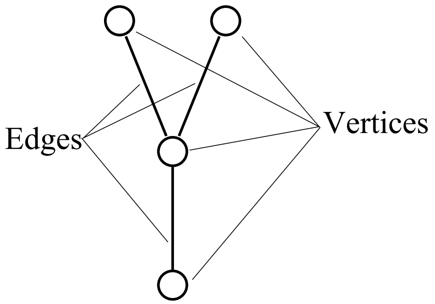
- In chemistry, a fullerene refers to a family of carbon allotropes that were discovered in 1985 by researchers at Rice University.
- Fullerenes are named after Buckminster Fuller, and are sometimes called buckyballs (the state molecule of Texas).
- The structure of a fullerene is very similar to that of graphite, which is composed of a sheet of hexagonal rings.
- However, fullerenes contain pentagonal rings that prevent the sheet from being planar.

General Graph Theory Terms

- A **graph** G is a triple consisting of a **vertex set** V, an **edge set** E, and a relation that associates with each edge, two vertices called **endpoints**.



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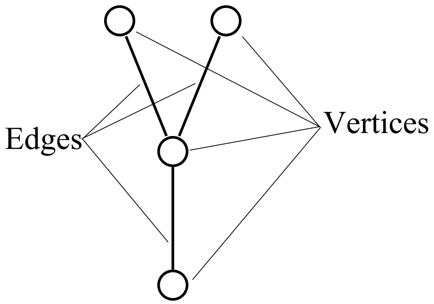
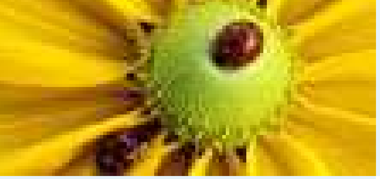


- A **simple** graph is a graph having no loops or multiple edges. A **loop** is an edge whose endpoints are equal. **Multiple edges** are edges having the same pair of endpoints.



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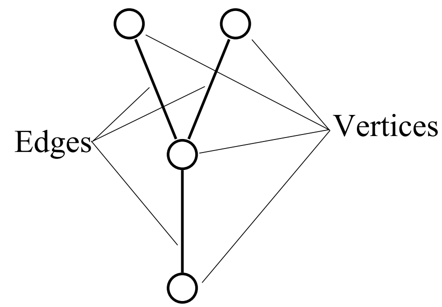
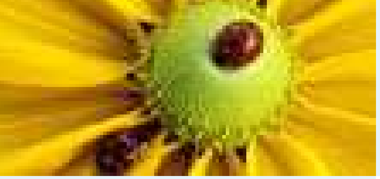


- A **simple** graph is a graph having no loops or multiple edges. A **loop** is an edge whose endpoints are equal. **Multiple edges** are edges having the same pair of endpoints.
- Two vertices u and v are said to be **adjacent** if they are joined by and edge. In this case, u and v are **neighbors**.



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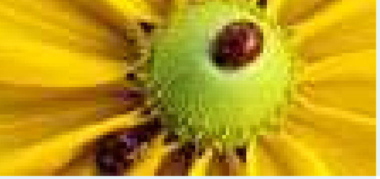

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- The **valency**, or **degree** of a vertex v is the number of edges the vertex is incident to, denoted $deg(v)$.
- A **planar graph** is a graph that can be drawn so that there are no edge crossings.

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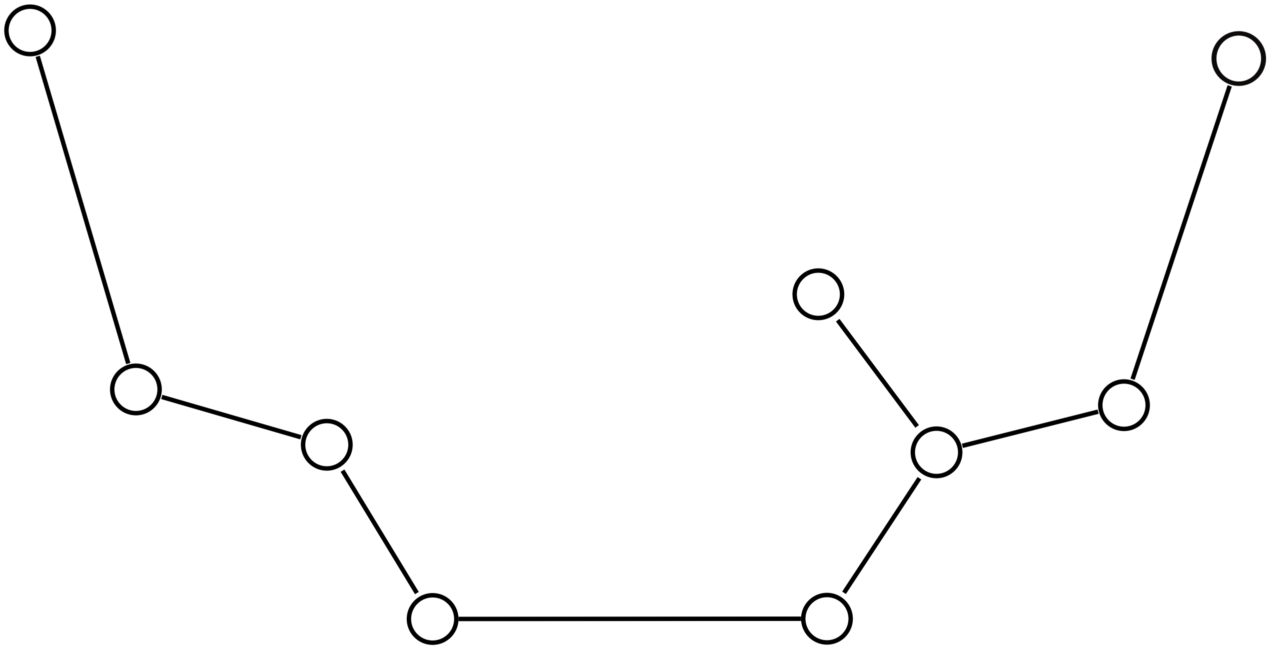

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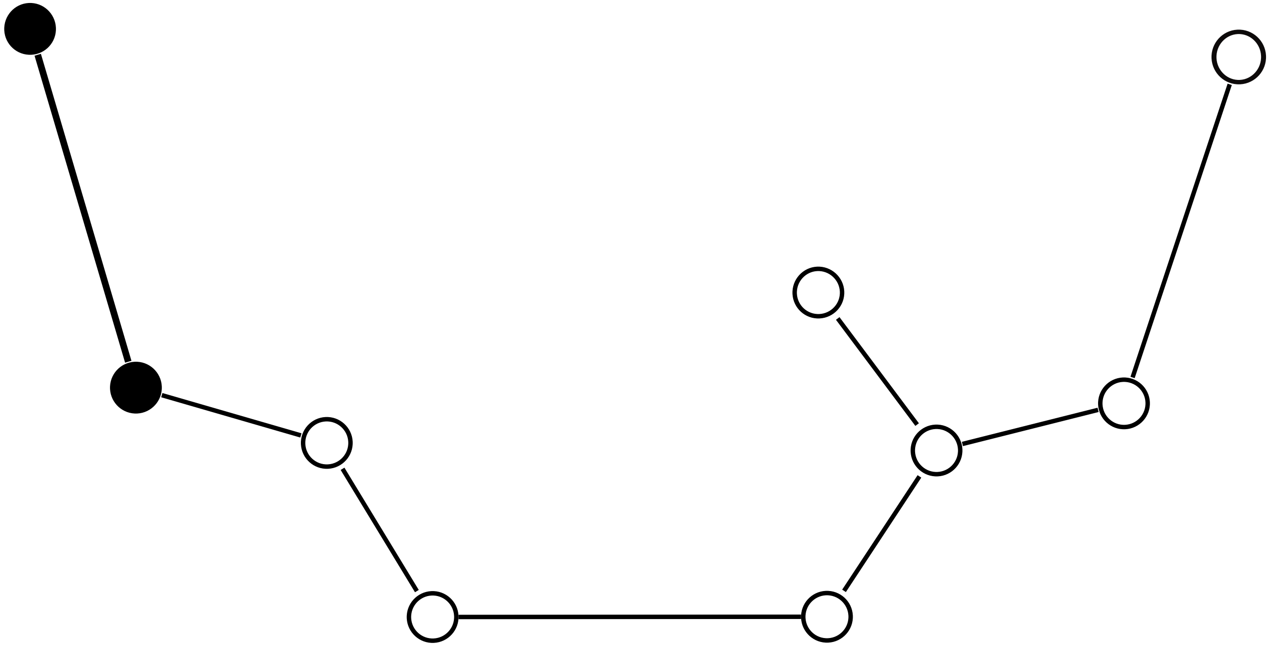

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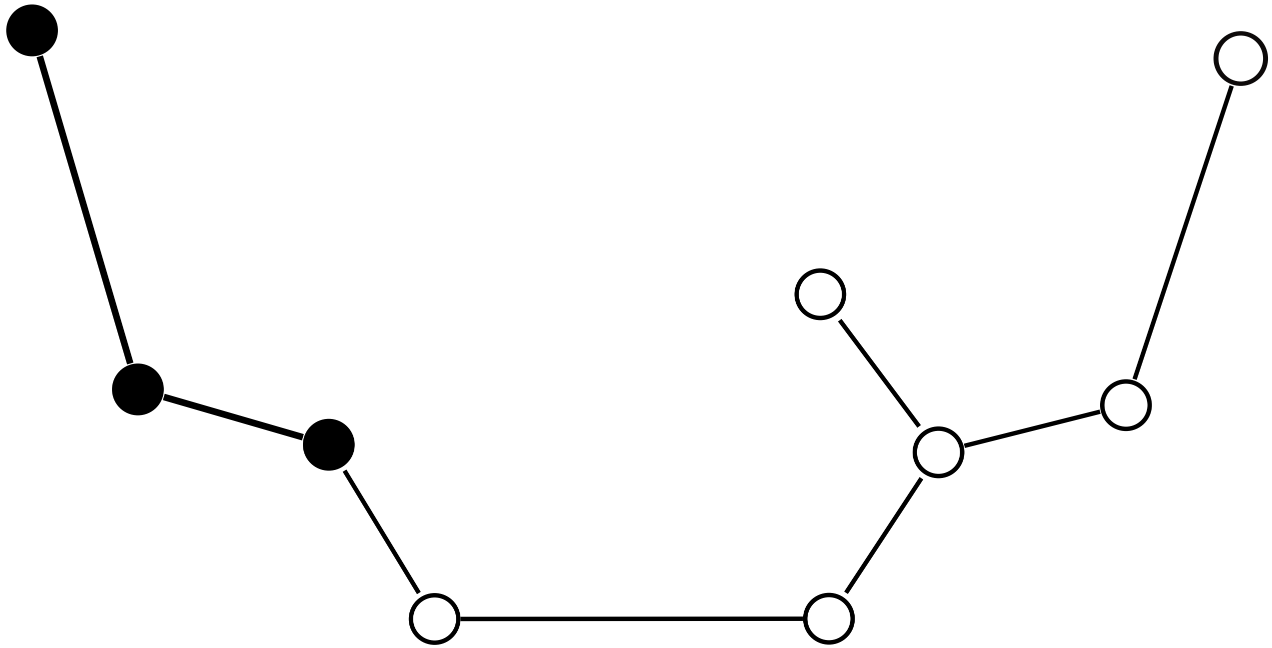

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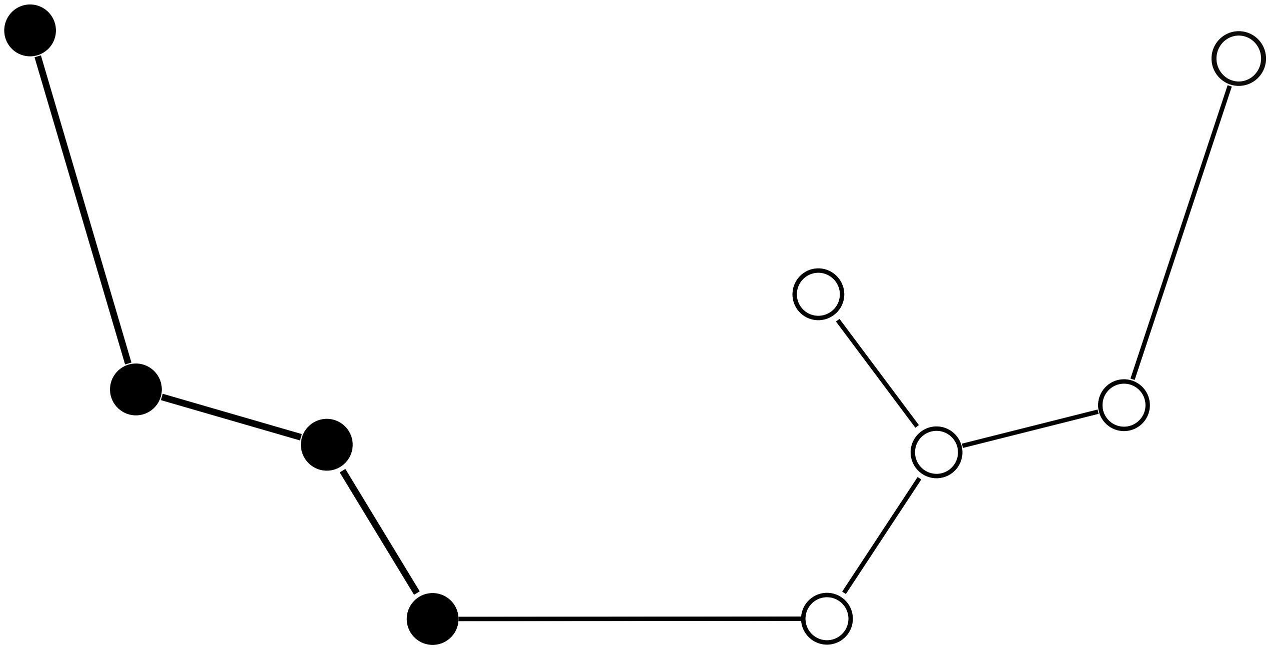

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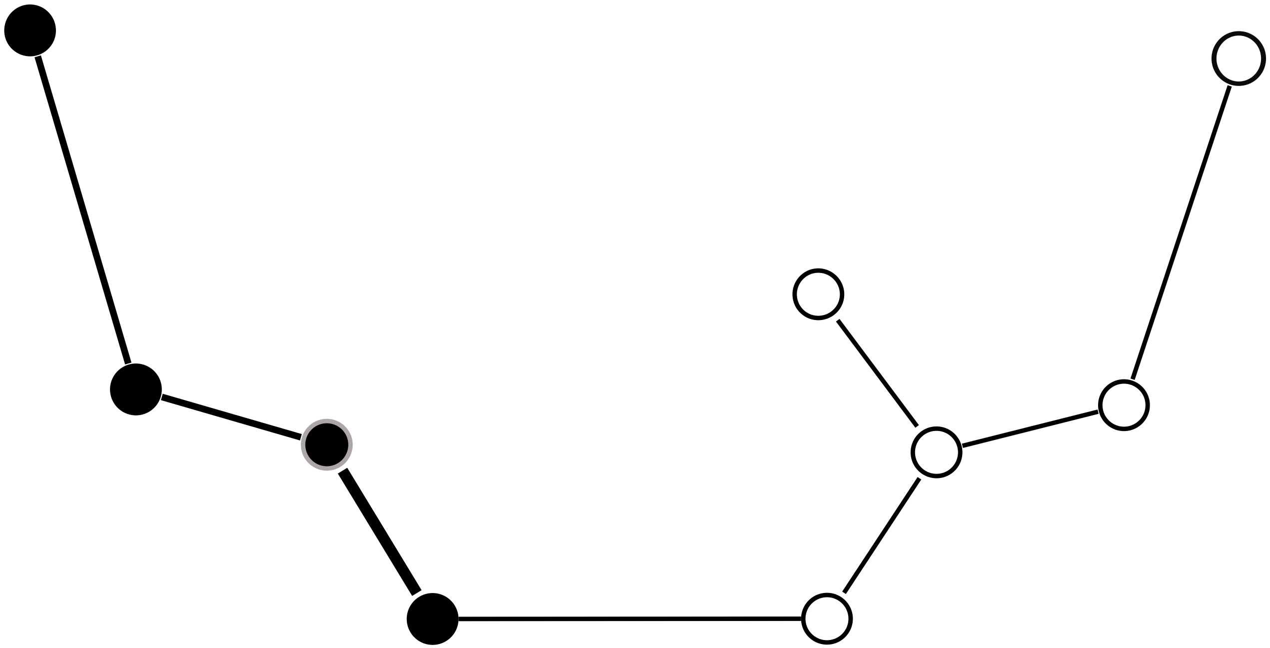
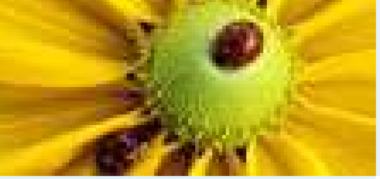
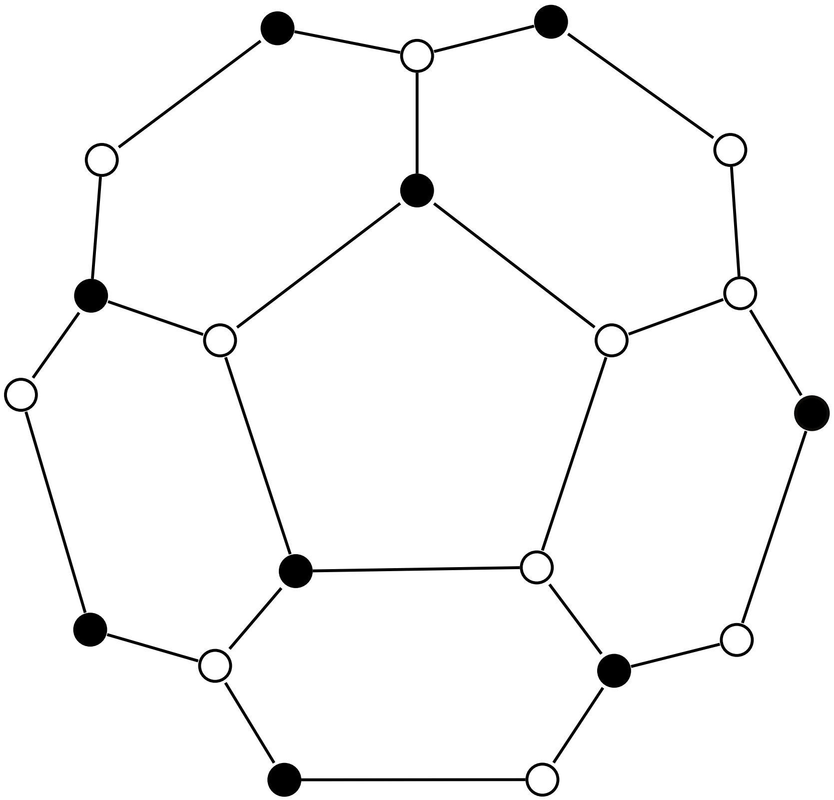




Independent Sets

An **independent set** in a graph G is a set pairwise nonadjacent vertices. The **independence** number of a graph G, $\alpha(G)$ is the size of a maximum independent set.



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- **Definition** A **fullerene** is a trivalent (valency three), convex polyhedron with only convex pentagonal and convex hexagonal faces.

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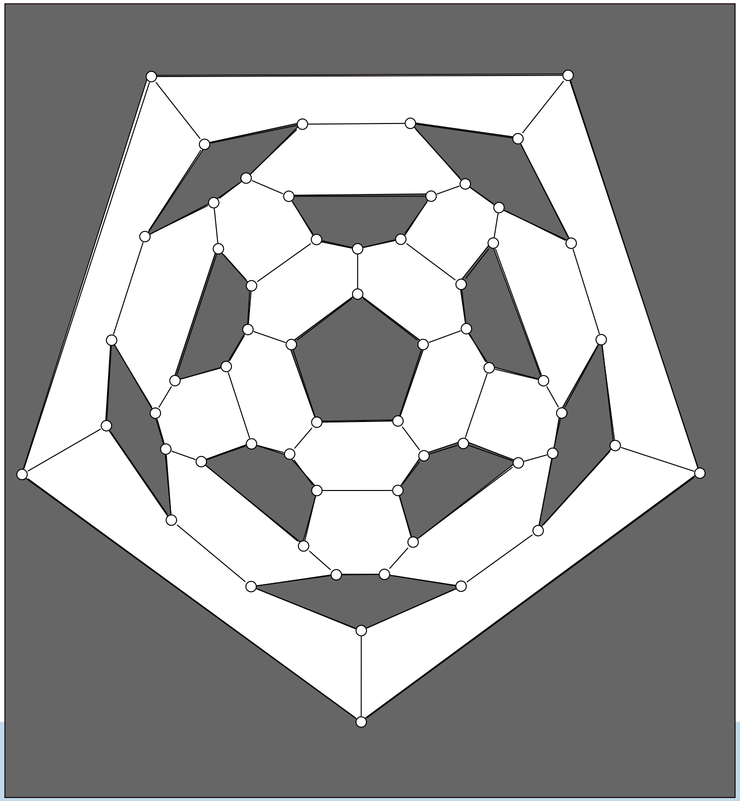

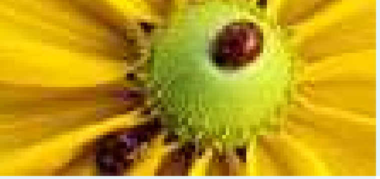

An Interesting Property of Fullerenes

Every fullerene has exactly 12 pentagons. We can show this using Euler's formula. If we have a planar graph and $|V|, |E|, |F|$ are the number of vertices, edges and faces respectively:

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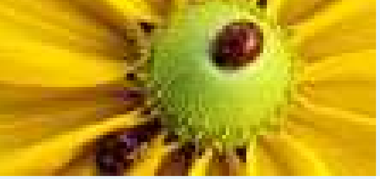
$$Euler's\,Formula \quad 2 = |V| - |E| + |F|$$



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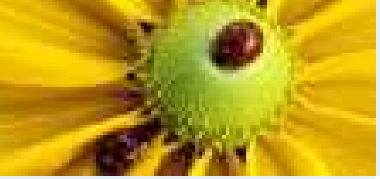
Since there are only pentagons and hexagons, let $|P|$ denote the number of pentagons, and $|H|$ denote the number of hexagons.



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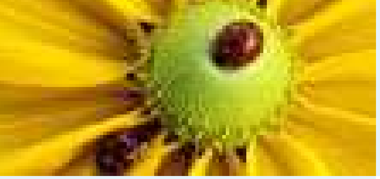
$$|F| = |P| + |H|$$

Interesting Property, Continued

Each edge is shared by at exactly two faces. Each pentagon has 5 edges, each hexagon has 6 edges, so:



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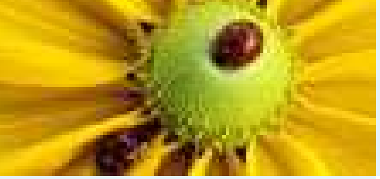

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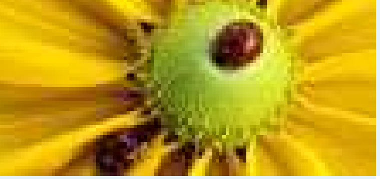
Substituting into Euler's formula:

$$2 = \frac{|P|}{6}$$

Vertex and Edge Colorings

- Let $\Gamma = (V, E, F)$ be a fullerene with vertex set V, edge set E, face set F.



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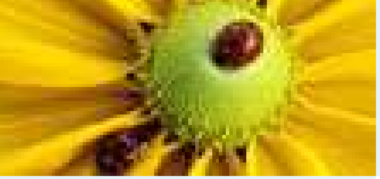

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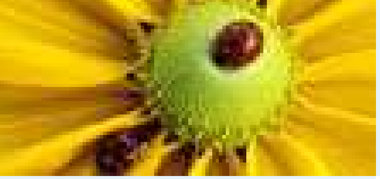

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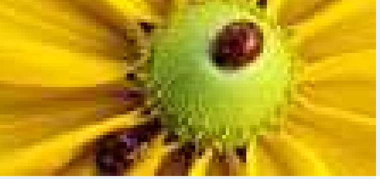

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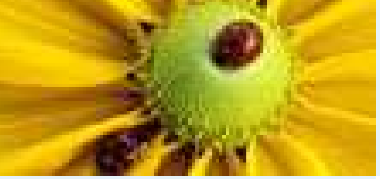

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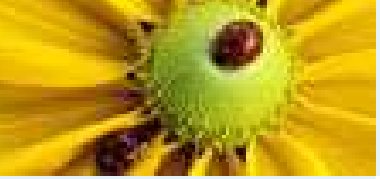
- Color the rest of the vertices grey.
- This creates a vertex partition in which every vertex is colored either white, black or grey.



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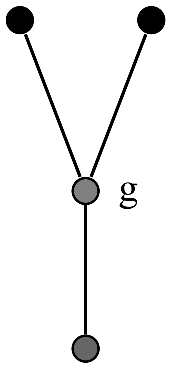

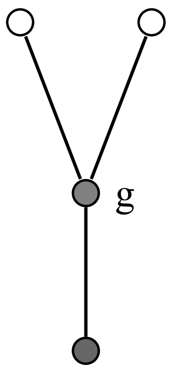

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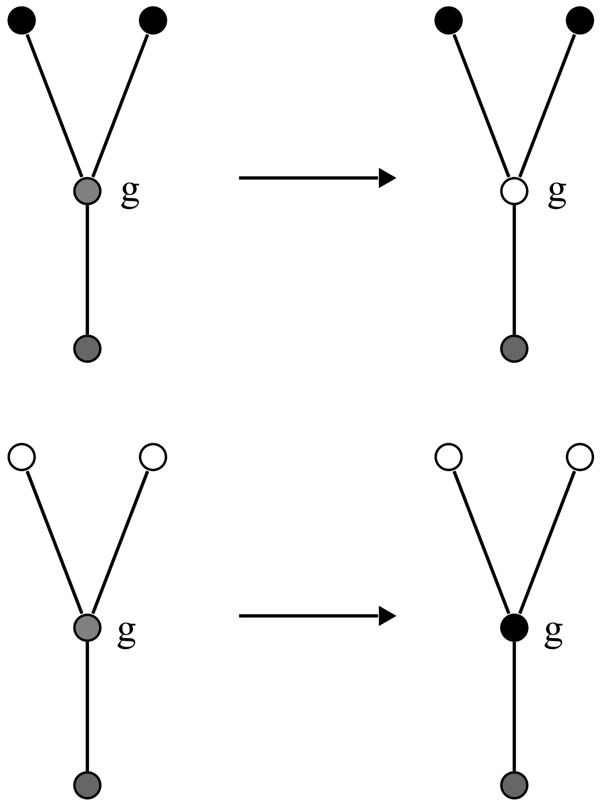

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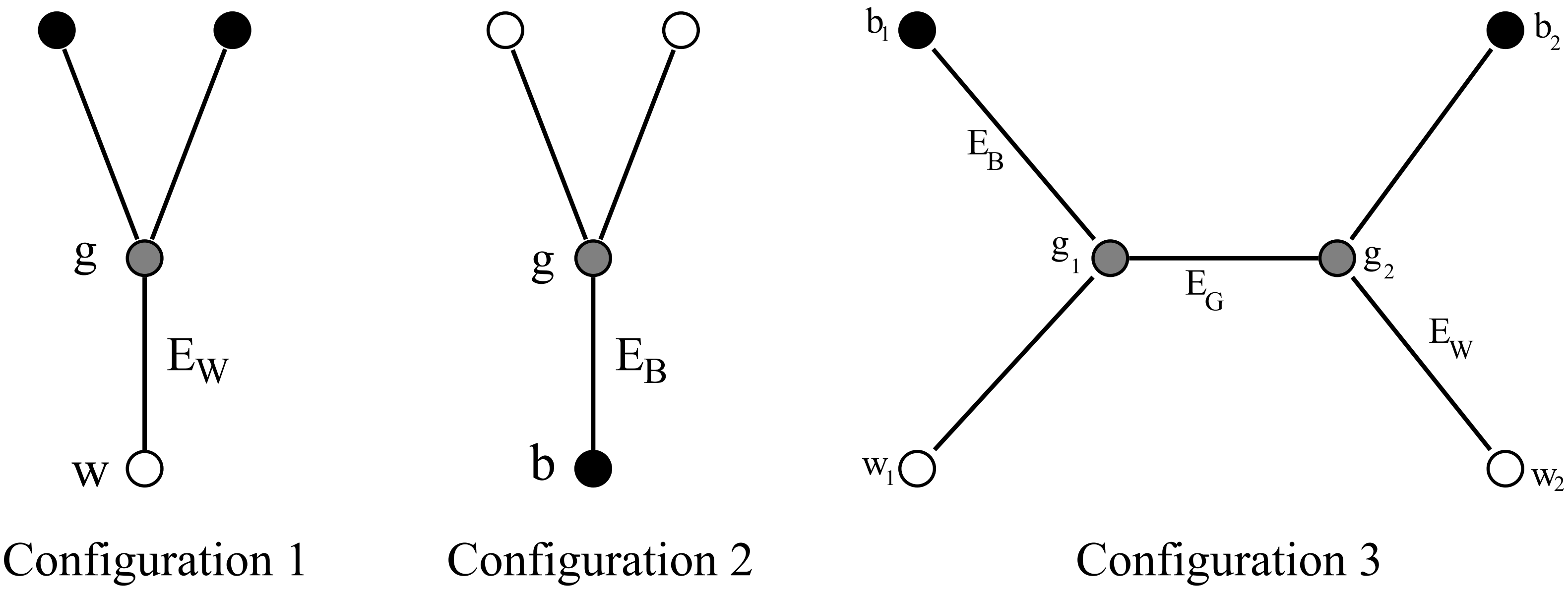
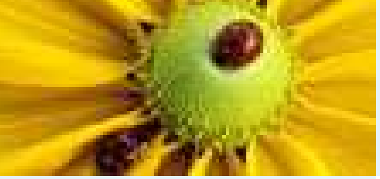
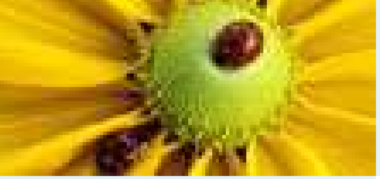




The IC and Lemmas

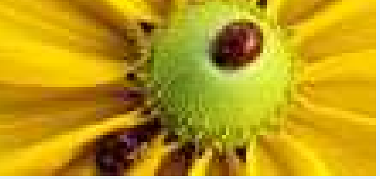
Definition A coloring of the vertices and edges in Γ as defined above will be called an **independence coloring**, denoted ξ.



The IC and Lemmas

Definition A coloring of the vertices and edges in Γ as defined above will be called an **independence coloring**, denoted ξ.

Lemma 2. *Let $\Gamma = (V, E, F)$ be a fullerene with the independence coloring ξ defined above. Then $|G| = |E_B| + |E_W|$ and the collection $E_W \cup E_B$ is an independent edge set.*



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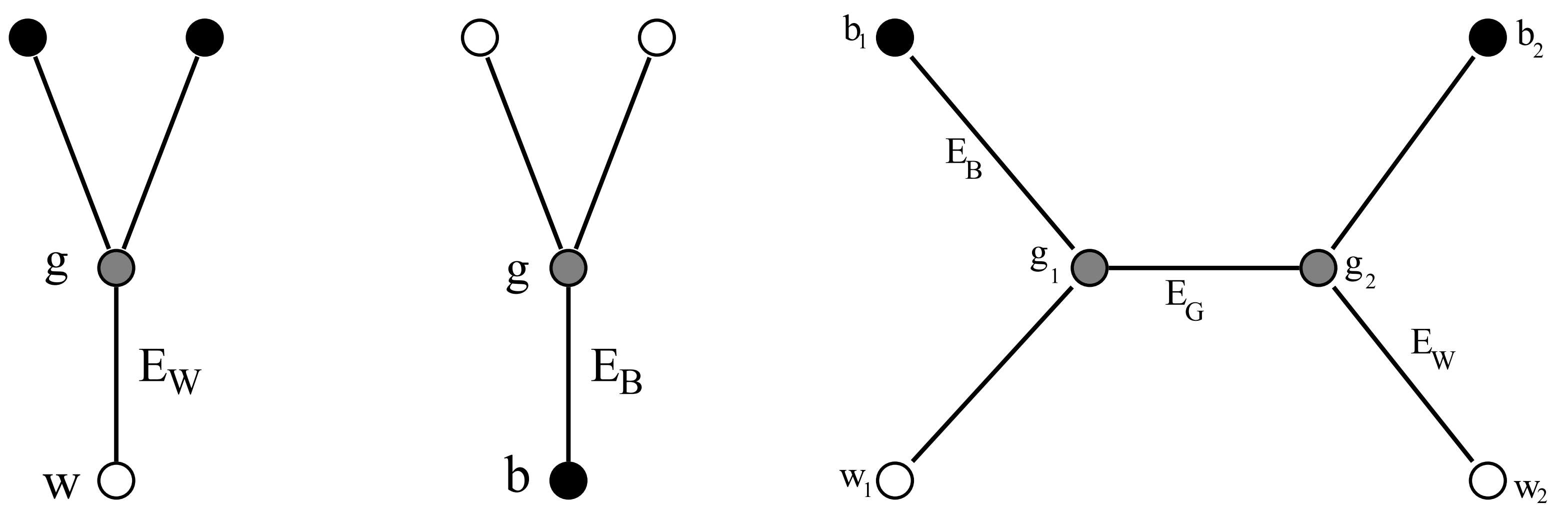
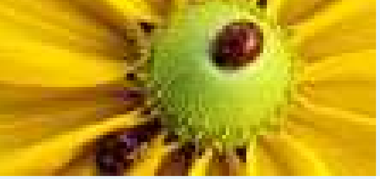


Configuration 1 Configuration 2 Configuration 3



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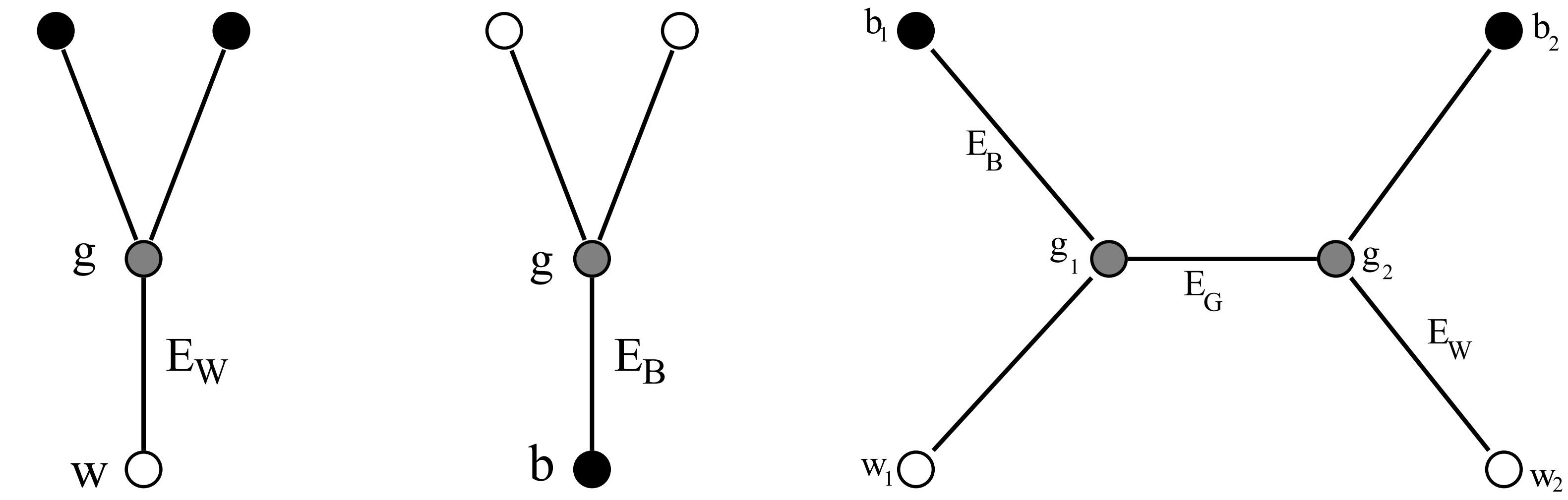

Configuration 1 Configuration 2 Configuration 3

The rest of the proof is lengthy . . .

More Lemmas

Lemma 3. *Let* $\Gamma = (V, E, F)$ *be a fullerene with independence coloring* ξ.

(i) Each pentagonal face is incident with exactly one edge from $E_B \cup E_W$.

(ii) Each hexagonal face is either incident with exactly two edges from $E_W \cup E_B$ *or with no edges from* $E_W \cup E_B$. *Furthermore, if two edges bound a hexagonal face and are opposite one another, they are both from* E_W *or both from* E_B. *If two edges from* $E_W \cup E_B$ *bound a hexagonal face and are not opposite one another, then one is from* E_W *and one is from* E_B.

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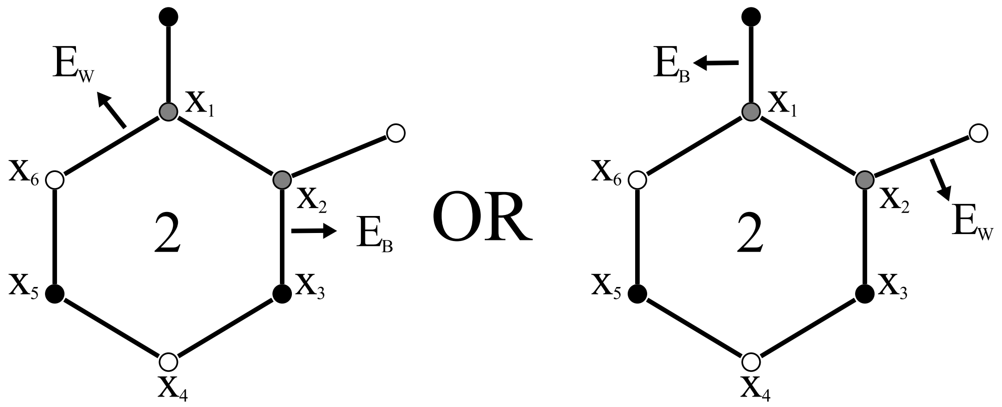
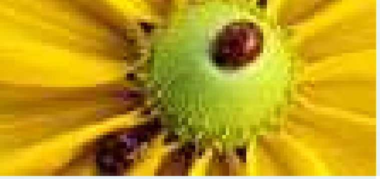


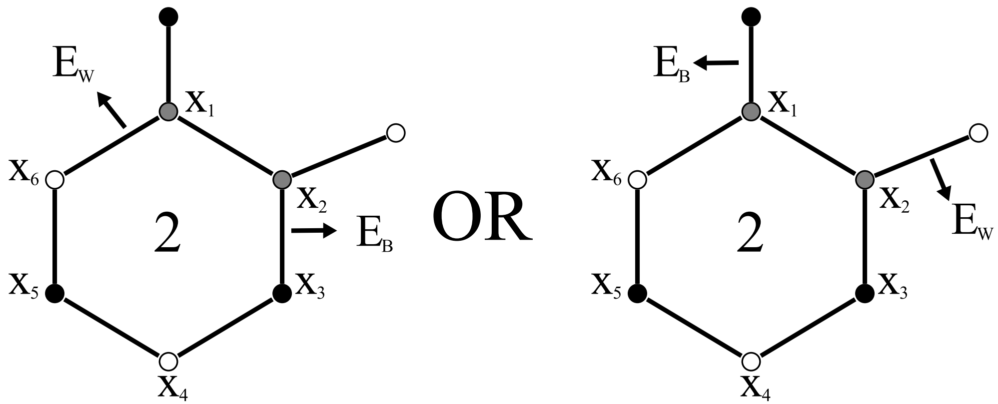


More Lemmas

Lemma 3. *Let $\Gamma = (V, E, F)$ be a fullerene with independence coloring ξ.*

(i) Each pentagonal face is incident with exactly one edge from $E_B \cup E_W$.

(ii) Each hexagonal face is either incident with exactly two edges from $E_W \cup E_B$ or with no edges from $E_W \cup E_B$. Furthermore, if two edges bound a hexagonal face and are opposite one another, they are both from E_W or both from E_B. If two edges from $E_W \cup E_B$ bound a hexagonal face and are not opposite one another, then one is from E_W and one is from E_B.



I will not present this proof because it is rather lengthy.

Lemma 4. *Let $\Gamma = (V, E, F)$ be a fullerene with the independence coloring ξ defined previously. Then:*

$$
\begin{aligned}
|W| &= \frac{|E|}{3} - \frac{2|E_W| + |E_B|}{3} \\
|B| &= \frac{|E|}{3} - \frac{2|E_B| + |E_W|}{3}
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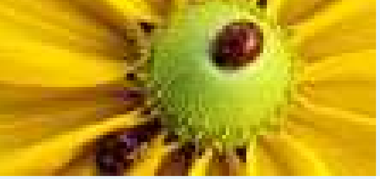

Some counting results for $|B|$ and $|W|$

Lemma 4. *Let $\Gamma = (V, E, F)$ be a fullerene with the independence coloring ξ defined previously. Then:*

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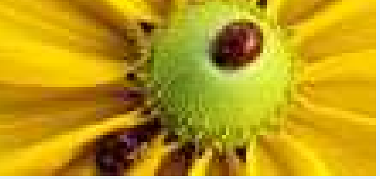
. . . An interesting counting proof that requires lots of algebra

Paths and Circuits

Our paths will pass through the centers of the faces of Γ, and exit through an edge of face. The planar dual is suitable for these purposes.



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To construct the planar dual $\Gamma^{\perp}$, for each face in Γ (including the outer face), assign a vertex in $\Gamma^{\perp}$. When two faces are adjacent in Γ, make the two corresponding vertices adjacent in $\Gamma^{\perp}$.

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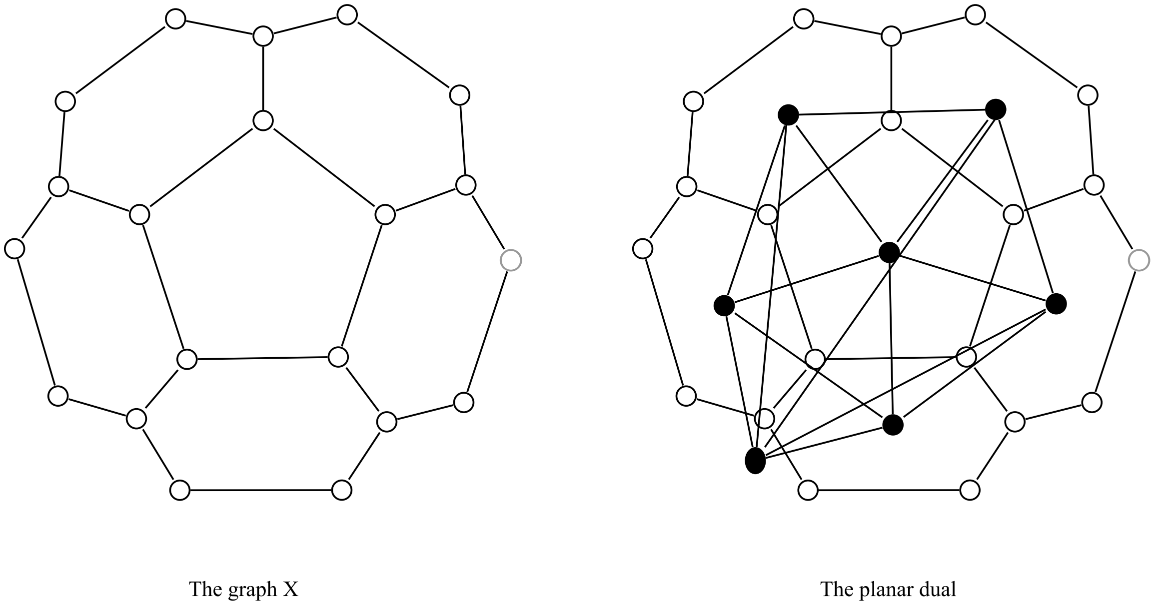
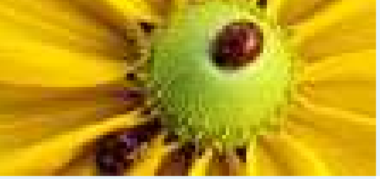


Figure 1: Construction of the Planar Dual



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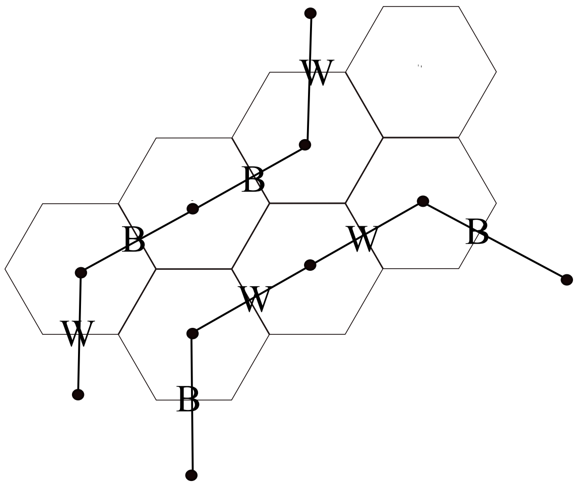

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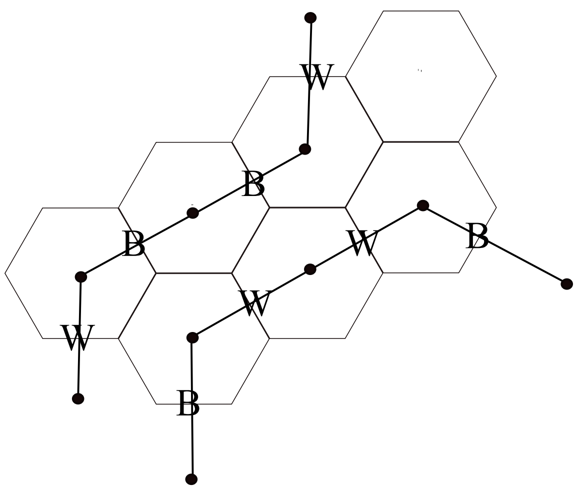

- By Lemma 3, each vertex of Φ that has degree six in $\Gamma^{\perp}$will have degree 2 in Φ.

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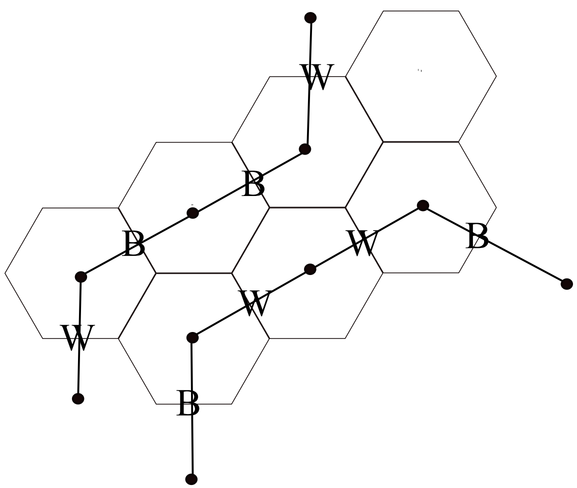

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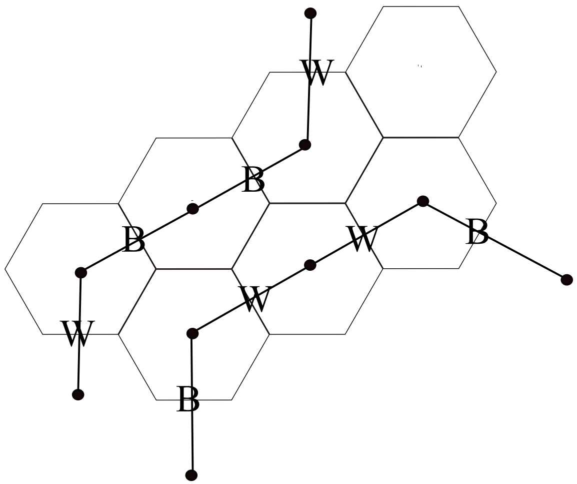
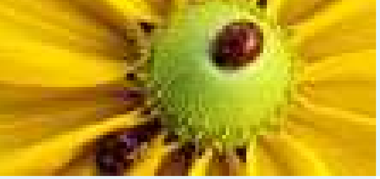
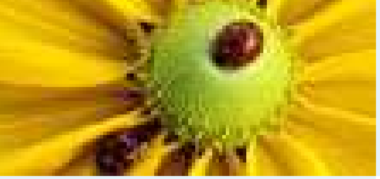


- By Lemma 3, each vertex of Φ that has degree six in $\Gamma^{\perp}$will have degree 2 in Φ.
- Each vertex in Φ that has degree 5 in $\Gamma^{\perp}$has degree 1 in Φ.
- There are exactly 6 elementary paths in Φ.



Path Lemmas and Corollaries

Corollary 5. *Let* $\Gamma = (V, E, F)$ *be a fullerene with the independence coloring* ξ *defined previously. Let* Φ *be the induced subgraph of* $\Gamma^{\perp}$*, also defined previously. Then, any portion of an elementary path or circuit in* Φ *cannot make any sharp left, or sharp right turns.*



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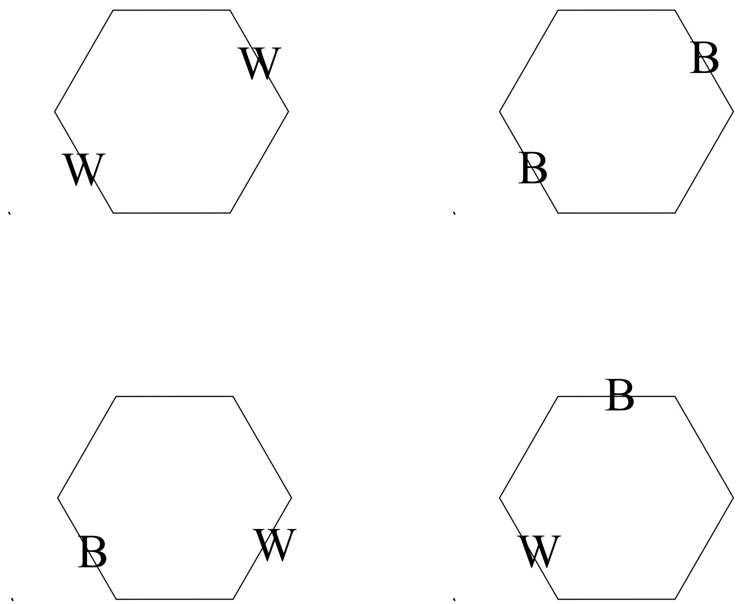
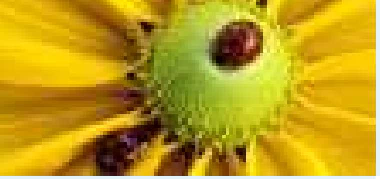
This is clear from Lemmas 2 and 3





More Lemmas . . .

Lemma 6. *Let* $\Gamma = (V, E, F)$ *be a fullerene with the independence coloring* ξ *defined above. Let* Π *be a path or circuit in* Φ*, the subgraph of* $\Gamma^{\perp}$ *induced by the edge set* $E_W \cup E_B$*. Then* Π *cannot make two consecutive right turns or two consecutive left turns. Furthermore, if a path or circuit makes a right turn, then no pentagonal face can abut two of its adjacent pentagons on the right before it makes another turn. Similarly, if a path or circuit makes a left turn, then no pentagonal face can abut two of its adjacent hexagons on left before it makes another turn.*

More Lemmas . . .

- Outline of the talk

Introduction/History

What is a fullerene?

Counting and Coloring Lemmas

Path Lemmas
- Paths and Circuits
- The induced subgraph Φ
- Path Lemmas and Corollaries
- More Lemmas . . .

Main Result

A tangible result

Acknowledgments

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Actually, the above lemma helps show that:

More Lemmas . . .

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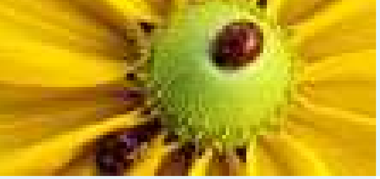
Actually, the above lemma helps show that:

Lemma 7. *If $\Gamma = (V, E, F)$ is a fullerene, and Φ is the induced subgraph of $\Gamma^\perp$ constructed as described previously, there are no circuits in Φ.*

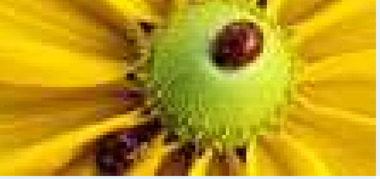


The Main Result

Theorem 8. *Let $\Gamma = (V, E, F)$ be a fullerene with the independence coloring ξ defined previously and let $\Gamma^{\perp} = (F, E, V)$ be its planar dual; let Φ be the subgraph of $\Gamma^{\perp}$ induced by the edge set $E_W \cup E_B$. Then Φ is disconnected with six components $\Pi_1, \Pi_2, \ldots, \Pi_6$, each of which is an elementary path between different pairs of vertices of degree 5 in $\Gamma^{\perp}$. These paths correspond exactly to the 12 pentagons of Γ.*

Icosahedral Fullerenes

We can extend these results further by using the same proof techniques as in previous lemmas. In particular, we can say more about $\alpha(\Gamma)$, when Γ is a highly symmetric icosahedral fullerene.



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Definition An **icosahedral fullerene** is a fullerene that shares its symmetries with the icosahedron. It can be considered to be a truncated icosahedron, with an equal number and configuration of hexagons between each pentagon.

Characterization of icosahedral fullerenes

We will characterize icosahedral fullerenes by the number of hexagons that separate “nearby” pentagons.

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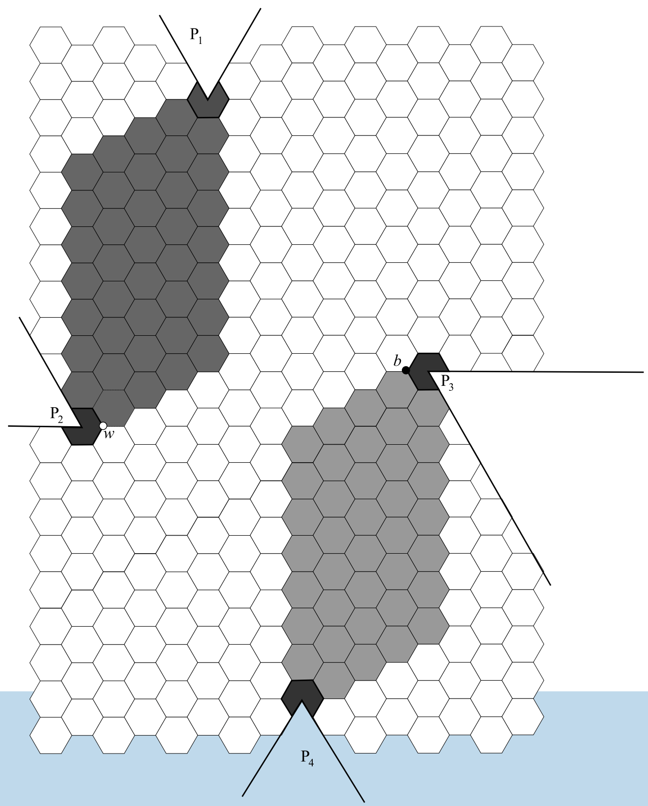
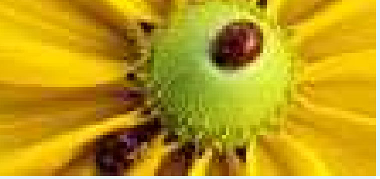
This icosahedral fullerene has a 4 by 7 parallelogram of hexagons between "nearby" pentagons. A more technical characterization would give this fullerene $(p, p+r)$ coordinates with $p = 4$ and $r = 3$.





The connection between paths and $\alpha(\Gamma)$

- Recall the formula for $|W|$ from Lemma 4:

$$|W| = \frac{|E|}{3} - \frac{2|E_W| + |E_B|}{3}$$

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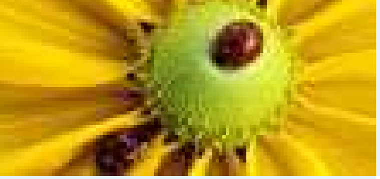

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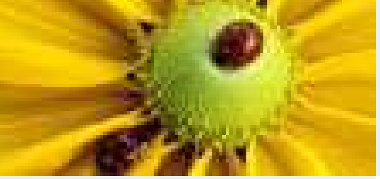

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- So the formula for the independence number of a fullerene can be written in the form $|W| = \frac{|V|}{2} - \frac{2|E_W|+|E_B|}{3}$.
- So $|E_W|$ and $|E_B|$ play a central role in calculating $\alpha(\Gamma)$.

Minimizing $2|E_W| + |E_B|$

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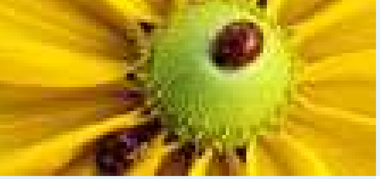
$$
\begin{aligned}
|W| &= \frac{|E| - 6(3p+r)}{3} \\
&= \frac{|V|}{2} - (6p + 2r)
\end{aligned}
$$

A tangible result

- Referring to Graver [1] we can see that such a fullerene has $|V| = 60p^2 + 60pr + 20r^2$. So:



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Corollary 9. *Let* $\Gamma = (V, E, F)$ *be the icosahedral fullerene with coordinates* $(p, p+r)$ *where* $p, r \geq 0$ *and at least one is positive. Then* $\alpha(\Gamma) = 30p^2 + 30pr + 10r^2 - 6p - 2r$

Illustration of tangible results

Illustration of tangible results

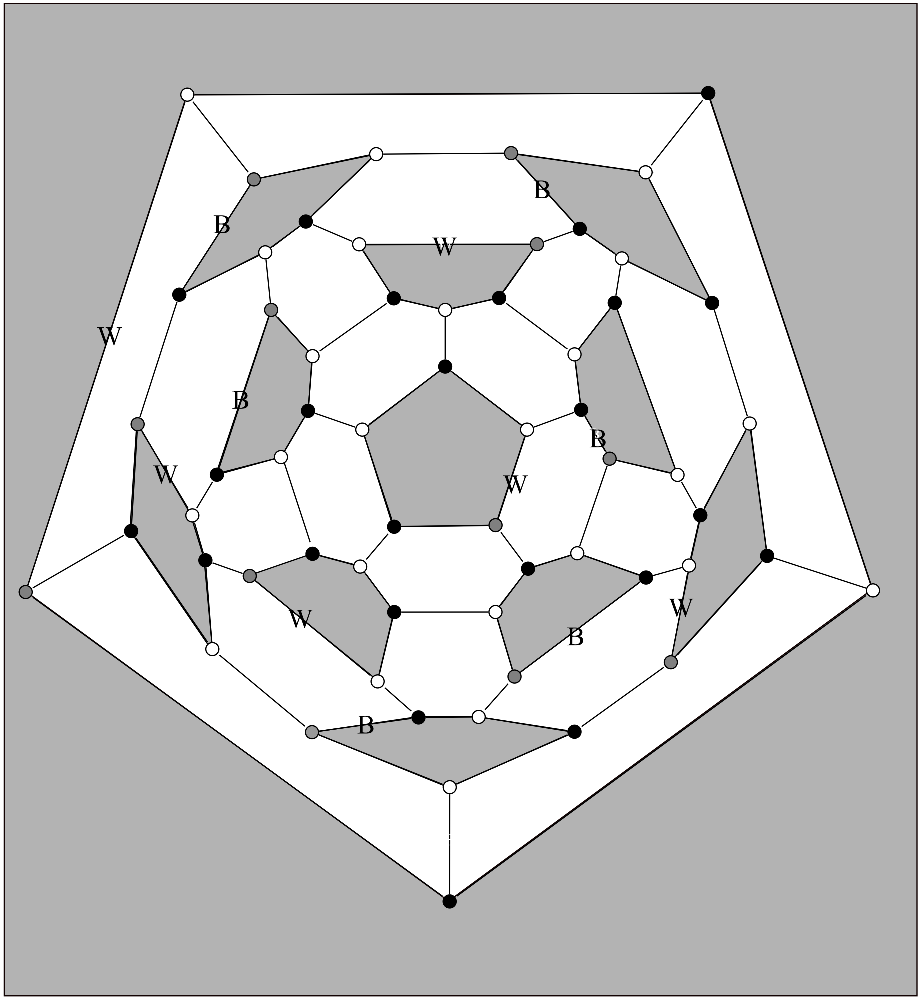


Figure 3: An icosahedral fullerene with Coxeter Coordinates (1,1)

Illustration of tangible results

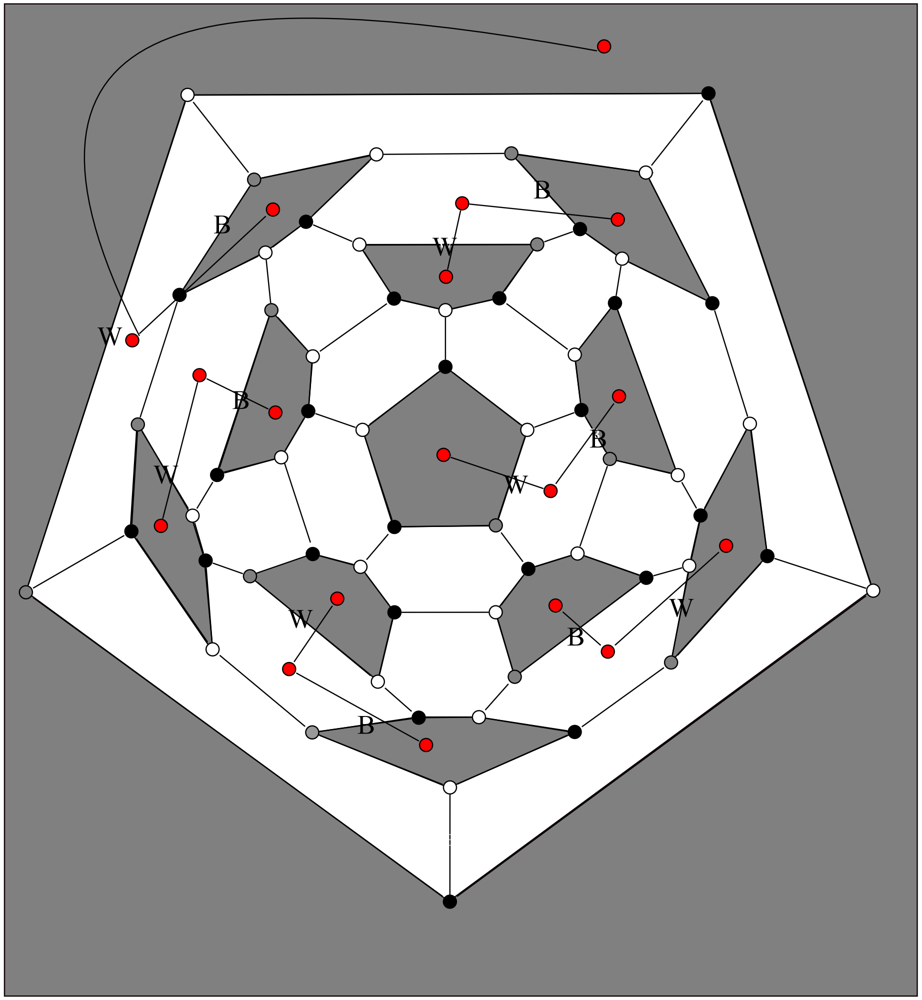
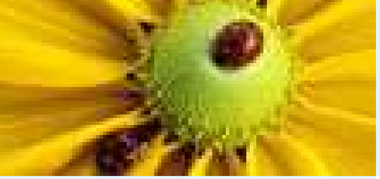


Figure 3:



Acknowledgments

This paper is in partial fulfillment for a Masters of Science degree in Mathematics from Portland State University. This “Mathematics in Literature Problem” is based on Jack E. Gravers *Independence Number of Fullerenes and Benzenoids*" [2]. Special Thanks to my adviser John Caughman, and my reader, Gerardo Lafferiere.

[1] Jack E. Graver. Catalog of all fullerenes with ten or more symmetries. *DIMACS Series in Discrete Mathematics and Theoretical Computer Science*, 69:167–188, 2005.

[2] Jack E. Graver. The independence number of fullerenes and benzenoids. *European Journal of Combinatorics*, 27(6):850–863, 2006.