THE STRUCTURE OF MAXIMUM INDEPENDENT SETS IN FULLERENES

CARLY VOLLET

Abstract. A fullerene is a trivalent (valency three), convex polyhedron with only convex pentagonal and convex hexagonal faces. The graph theoretic independence number of fullerenes may be a useful predictor for stability in chemistry. We explore the independence number of fullerenes by exploring the structure of two maximum independent sets and an independent edge set. We will see that certain pairings of pentagons result in maximum independent sets, and that these pairings can be used to compute the independence number of icosahedral fullerenes.

Contents

1. Acknowledgments

This paper is in partial fulfillment of the requirements for a Masters degree in Mathematics from Portland State University. This “Mathematics in Literature Problem” is based on Jack E. Gravers article “Independence Number of Fullerenes and Benzenoids” [3]. Special thanks to my adviser John Caughman, and my reader, Gerardo Lafferiere.

2. History

In chemistry, the term “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

Date: 08/15/07.

is composed of a sheet of hexagonal rings. However, fullerenes contain pentagonal rings that prevent the sheet from being planar. Around the same time of the discovery of fullerenes, Siemion Fajtlowicz, a mathematician at University of Houston developed a computer program called Graffiti [4]. Graffiti is a program that makes conjectures in various subfields of mathematics and chemistry. The first fullerene conjectures of Graffiti led to a new representation and characterization of the Buckminsterfullerene, which is defined later. Another conjecture inspired the paper "Graph-Theoretic Independence as a Predictor of Fullerene Stability" [5], written by Fajtlowicz and C.E. Larson. The independence number of a fullerene is a graph theoretic property, so it is from this perspective that we will explore the structure of maximum independent sets in fullerenes.

3. General graph theory definitions and lemmas

The following Graph Theory Definitions and Lemmas are adapted from Douglas B. West [6].

A **graph** G is a triple consisting of a **vertex set** V, an **edge set** E, and a relation that associates two vertices called **endpoints** to each edge.
A **loop** is an edge whose endpoints are equal. **Multiple edges** are edges having

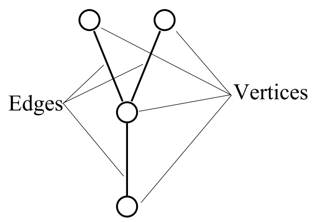


Figure 1. A simple graph

the same pair of endpoints. A **simple** graph is a graph having no loops or multiple edges. Two vertices u and v are said to be **adjacent** if they are joined by an edge. We will also say that u and v are **neighbors**.

If vertex v is the endpoint of an edge e, then we say that v and e are **incident**. The **valency**, or **degree** of a vertex v is the number of edges the vertex is incident to, denoted $deg(v)$.

A **walk** is a consecutive list of incident vertices and edges. A **path** is a walk with no repeated vertices. An **elementary path** is a path that is not crossed by any other path. A **cycle** is a closed walk.

Remark For the purposes of this paper, we will only deal with simple graphs. Therefore, a path can be described just by the ordered list of vertices, with the assumption that consecutive vertices in a walk are adjacent.

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.

A **planar graph** is a graph that *can be* drawn so that there are no edge crossings. A **plane graph** *is* a drawing of a plane graph o that there are no edge crossings. Any cycle on a planar graph that encloses a region and does not have any edges on the interior of the cycle is called a **face**.

Lemma 1 (The Degree Sum Formula)**.** *Let G be a graph with vertices $v_1, v_2 \dots, v_n$. The number $|E|$ of edges of a graph is related to the vertex valencies as follows:*

$$\sum_{i=1}^{n} deg(v_i) = 2|E| \tag{1}$$

Proof. Since $deg(v_i)$ denotes the valency of a vertex, we can use this to count the number of edges that originate from each vertex, v_i. However, since each edge has two endpoints, we are double counting each edge when we sum over all of the $v_i' s$. Therefore, $\sum_{i=1}^{n} deg(v_i) = 2e$. □

4. Graph theoretic properties of fullerenes

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

Every fullerene admits a planar embedding, with the outer face being either a pentagon or a hexagon. The smallest fullerene consists only of pentagons, the dodecahedron. The smallest fullerene in which no two pentagons share an edge is called the Buckminsterfullerene (C_{60} in chemistry), which looks exactly like a soccer ball. It consists of 12 pentagons and 20 hexagons. The figure below shows a planar embedding of the Buckminsterfullerene. Notice that the outside face is a pentagon, and all of the pentagons are shaded grey. The Buckminsterfullerene is also an icosahedral fullerene with Coxeter coordinates $(1, 1)$, as will be explained later.

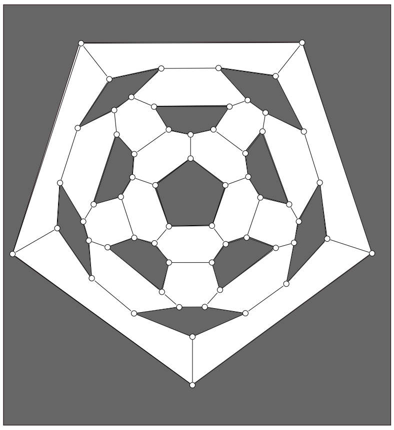


Figure 2. An planar embedding of the Buckminsterfullerene

Every fullerene has exactly 12 pentagons. Since fullerenes are planar, we can show this using Euler's formula.

Lemma 2 (Euler's Formula)**.** *If a finite, connected, planar graph is drawn in the plane without any edge intersections, and $|V|, |E|, |F|$ are the number of vertices, edges and faces respectively, then:*

$$|V| - |E| + |F| = 2$$

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

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

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

$$|E| = \frac{5|P| + 6|H|}{2}$$

Each vertex is adjacent to three polygons, so

$$|V| = \frac{5|P| + 6|H|}{3}$$

Substituting into Euler's formula:

$$\begin{aligned} 2 &= \frac{5|P| + 6|H|}{3} - \frac{5|P| + 6|H|}{2} + |P| + |H| \\ &= \frac{2(5|P| + 6|H|)}{6} - \frac{3(5|P| + 6|H|)}{6} + \frac{6|P| + 6|H|}{6} \\ &= \frac{|P|}{6} \end{aligned}$$

Hence $2 = \frac{|P|}{2}$, so $|P| = 12$

5. Vertex and edge colorings

Let $\Gamma = (V, E, F)$ be a fullerene with vertex set V, edge set E and face set F. As noted previously, a fullerene is a trivalent graph with only pentagonal and hexagonal faces. For our purposes, we will draw Γ as a planar graph with one large outer face that is a pentagon. Our goal is to calculate $\alpha(\Gamma)$, since it appears to be a useful selector in identifying stable fullerene isomers [5]. Let W be a maximum independent set in Γ and color the vertices in W white. Among the remaining vertices, $V - W$, let B be a maximum independent set, and color these vertices black. Let $G = V - B - W$, and color the vertices in G grey. This creates a vertex partition in which every vertex is colored either white, black or grey.

Remark We will use the *maximality* of W and B quite often in this paper. Since B and W are maximum independent sets, they are also *maximal*. That is, $|W|$ and $|B|$ cannot be extended subject to the constraints that B and W are independent ant B is contained in $V - W$.

Lemma 3. *In a fullerene with the vertex coloring defined above, each grey vertex is adjacent to a black vertex and to a white vertex.*

Proof. Let g be a grey vertex with only black and grey neighbors. Then g could be recolored white. Similarly, if g is a grey vertex with only white and grey neighbors, then g could be recolored black. By the maximality of W and B, such a g cannot exist. Therefore, every grey vertex is adjacent to a black vertex and to a white vertex.

□

We will now begin to color the edges in E that are incident to vertices in G. Edges will be colored either white, black or grey, denoted by the sets E_W, E_B, and E_G respectively. In light of Lemma 3, there are three configurations to consider, shown below:

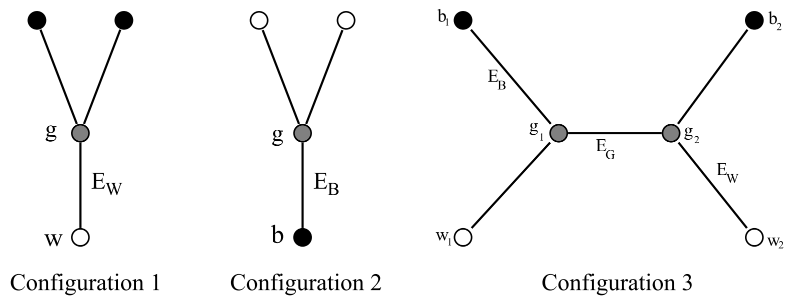


FIGURE 3

Edges will be colored as follows:

- If g is adjacent to two black vertices and one white vertex, w, color the edge (g, w) white (Configuration 1).

- If g is adjacent to two white vertices and one black vertex, b, color the edge (g, b) black (Configuration 2).

- Finally, if there are two adjacent grey vertices g_1 and g_2, each must have a single black and a single white neighbor. Color the edge (g_1, g_2) grey, and choose to color either (b_1, g_1) black and (g_2, w_2) white or (w_1, g_1) white and (b_2, g_2) black (Configuration 3). This configuration is the only configuration that offers a choice in the edge colorings. We will see later that this choice in colorings will largely be eliminated.

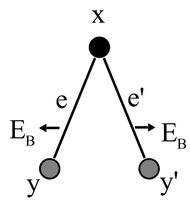
Remark We will only color edges that correspond to the configurations above, all other edges remain uncolored. Only colored edges will play a role in our results, so we will not bother giving the uncolored edges a special name.

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

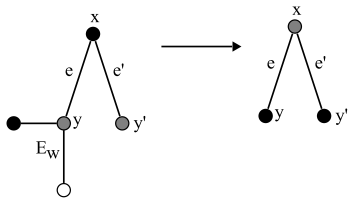
An **independent edge set** is an edge set where no two edges are incident to the same vertex. An independent edge set is also sometimes called a **matching**.

Lemma 4. *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.*

Proof. From the independence coloring ξ, every grey vertex is incident to exactly one edge in $E_B \cup E_W$, and each edge in $E_B \cup E_W$ has exactly one endpoint in G. Therefore, $|G| = |E_B \cup E_W|$ and since E_W and E_B are disjoint, $|E_B \cup E_W| = |E_B| + |E_W|$. Therefore $|G| = |E_B| + |E_W|$. Now suppose $e, e' \in E_B \cup E_W$ are incident to the same vertex, x. Since each grey vertex is incident with exactly one edge in $E_B \cup E_W$, $x \notin G$. WLOG, suppose $x \in$ B and let y, y' be the other endpoints of e, e' respectively. Now, $x \notin G$, so clearly $y, y' \in G$, since every edge in E_B has a grey endpoint. See the figure below:



Also, y cannot be adjacent to another black vertex, because this would lead to a Configuration 1, contradicting the assumption that $(x, y) \in E_B$. Similarly, y' is not adjacent to another black vertex. But now we may re-color x grey and both y and y' black–contradicting the maximality of B. Similarly, $x \notin W$, so we conclude



that no such x exists. Therefore, E_W and E_B are independent edge sets. □

Lemma 5. *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 from $E_W \cup E_B$ 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.*

Proof. (i) Let $x_1 \ldots, x_5$ be the vertices of a pentagonal face listed in cycle order. Clearly at least one of these vertices must be grey- say x_1. There are three cases to consider, illustrated below:

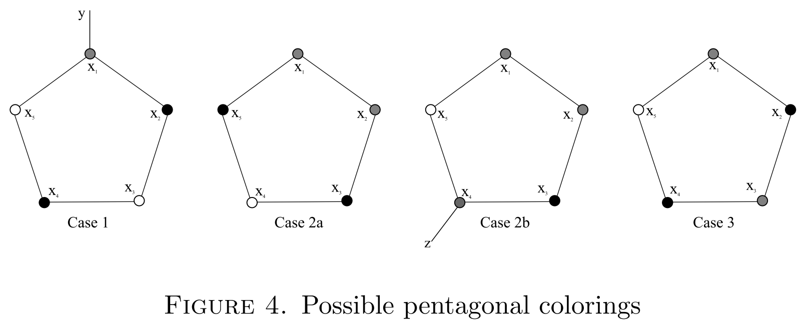
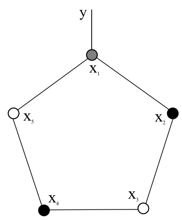


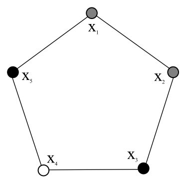
FIGURE 4. Possible pentagonal colorings

Case 1: There is only one grey vertex, x_1. By symmetry we can assume that the rest of the vertices alternate between black and white in cyclic order. So $x_2, x_4 \in B$ and $x_3, x_5 \in W$. The only edges on the pentagon that could be in $E_W \cup E_B$ are the edges that are incident to x_1. Let y be the third neighbor of x_1. The edges that could be colored are $(x_1, y), (x_1, x_2)$ and (x_1, x_5). By definition of the independence coloring ξ, if $y \in W$, then $(x_1, x_2) \in E_B$ and $(x_1, x_5) \notin E_B \cup E_W$; if $y \in B$, then $(x_1, x_5) \in E_W$ and $(x_1, x_2) \notin E_B \cup E_W$; if $y \in G$, either $(x_1, x_2) \in E_W$ or $(x_1, x_5) \in E_W$, but not both.



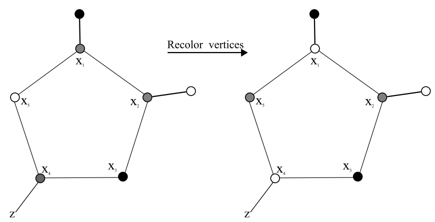
Case 1

Case 2: x_1 and x_2 are both colored grey. Then $(x_1, x_2) \notin E_B \cup E_W$. Without loss of generality, we may assume that x_3 is black. In Case 2a, we suppose that x_5 is also black. By Lemma 3, the neighbors of x_1 and x_2 must both be white, leading to a configuration 3. By the independence coloring ξ, we have that only one of (x_1, x_5) and (x_2, x_3) belong to E_B. Now, x_4 can be either white or grey, but in either case, neither of (x_3, x_4) and (x_4, x_5) belong to $E_W \cup E_B$.



Case 2a

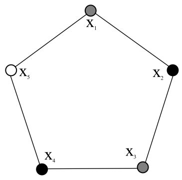
In case 2b, we suppose that x_5 is white. Then x_4 must be colored grey. Let z denote the third neighbor of x_4. By Lemma 3, the other neighbors of x_1 and x_2 are black and white respectively. Without loss of generality, we may assume that z is black or grey. However, we may then re-color x_1 and x_4 white and x_5 grey, contradicting the maximality conditions on W and B. See the figure below:



Case 2b

Hence, case 2b is not possible.

Case 3: If both x_1 and x_4 are grey; then, without loss of generality, we may assume that x_2 is black. x_4 and x_5 cannot be grey, because that would be the previously considered (impossible) Case 2b. Hence, by symmetry, we may assume that x_4 is black and x_5 is white (if we had assumed x_2 was white, it would be just the opposite). The other neighbor of x_3 must be white, which leads to a configuration 1 centered at x_3. However, neither (x_2, x_3) or (x_3, x_4) will be colored by the independence coloring ξ. As argued previously in Case 1, in any configuration that contains x_1, exactly one of (x_1, x_2) or(x_1, x_5) belongs to $E_W \cup E_B$.



Case 3

Therefore, each pentagonal face is incident with exactly one edge from $E_W \cup E_B$.

(ii) Let $x_1 \dots x_6$ be the vertices of a hexagonal face listed in cyclic order. If none of the vertices are grey, then none of the edges of this face belong to $E_W \cup E_B$. So, for the remainder of the proof, we shall assume that x_1 is grey. In each of the cases we now consider, we will always assume that the nongrey vertex of the smallest subscript will be black. There are a number of cases to consider. Because of symmetry, we will only consider 12 cases, pictured below.

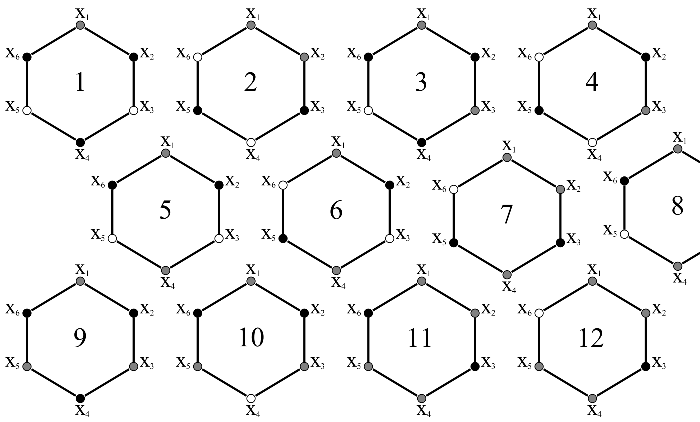
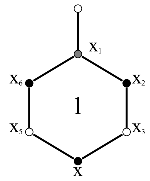


FIGURE 5. Possible hexagonal colorings–up to black/white symmetry

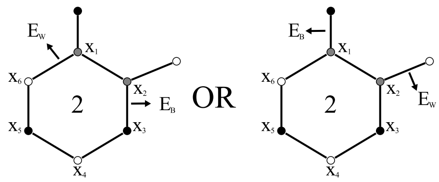
There is only one case if there is a single grey vertex. In Case 1, there are no other grey vertices, so the black and white vertices alternate in cyclic order. This means $x_2, x_4, x_6 \in B$ and $x_3, x_5 \in W$. If follows from the independence coloring ξ that none of the edges incident to x_1 are in $E_W \cup E_B$. Since both x_3 and x_5 are white, it is impossible to have a Configuration 3. Therefore, none of the edges incident to the hexagon are in $E_W \cup E_B$. See the figure.



Much of the reasoning is the same for all of the cases, so diagrams are presented in addition to outlines of the proofs.

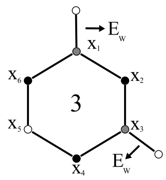
There are 5 cases where there are two grey vertices, Cases 2-6.

Case 2: In Case 2, x_1 and x_2 are both colored grey. Without loss of generality, we assume that x_3 is black. We must have a Configuration 3 that includes x_1 and x_2. Either $(x_1, x_6) \in E_B$ and $(x_2, x_3) \in E_W$, or neither of them are colored.

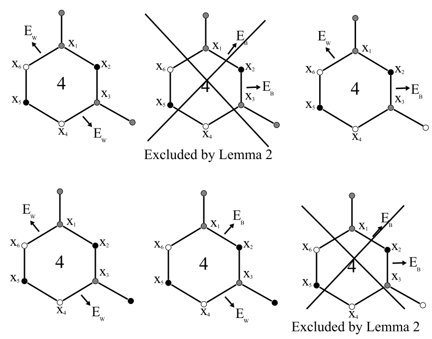


If the other grey vertex is x_3, this gives rise to cases 3 and 4.

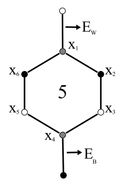
Case 3: In case 3 below, it is clear that none of the edges in the pentagon belong to $E_W \cup E_B$.



Case 4: If we consult the figure for case 4 we can see that it is possible to have any of the many possible configurations centered at $x_1$and x_3. The possible scenarios are outlined below (there are few cases due to symmetry):

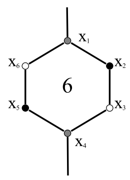


The other possibilities for two grey vertices are cases 5 and 6.



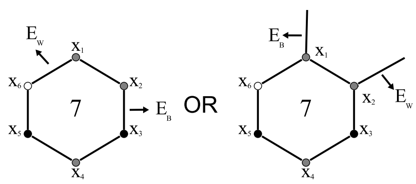
Case 5: By the independence coloring ξ, none of the edges in case five belong to $E_W \cup E_B$.

Case 6: In case 6, we could have $(x_1, x_6) \in E_W$ and $(x_3, x_4) \in E_W$ or $(x_1, x_2) \in E_B$ and $(x_4, x_5) \in E_B$ or $(x_1, x_6) \in E_W$ and $(x_4, x_5) \in E_B$ or $(x_1, x_2) \in E_B$ and $(x_3, x_4) \in E_W$.

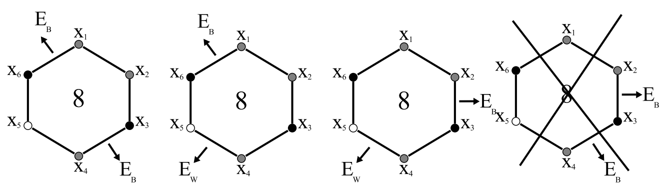


By Lemma 3, each grey vertex must have exactly one white and one black neighbor. This means that there can be no more than two consecutive grey vertices around the face of any hexagon. Thus, up to black/white symmetry, there are only three possible configurations of hexagons that contain three grey vertices; each of these cases has two sub cases.

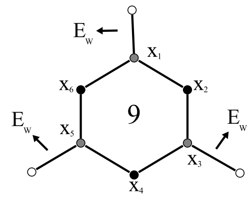
Case 7: Clearly none of the edges on the pentagon that are incident to $x_4$are in $E_W \cup E_B$. Since there is a Configuration 3 in this pentagon, there is a choice of which edges to color. We have either $(x_1, x_6) \in E_W$ and $(x_2, x_3) \in E_B$, or we have no edges that belong to $E_W \cup E_B$.



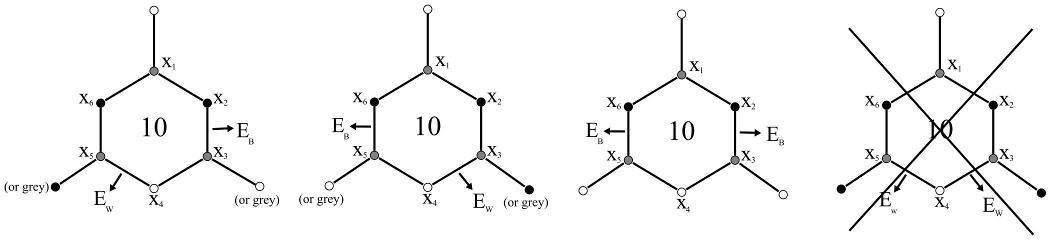
Case 8: There is a Configuration 3 centered at $x_1$and x_2. There is either a Configuration 1 or 2 centered at x_4. So, we have one of $(x_1, x_6), (x_2, x_3) \in E_B$, but not both. We also have that one of $(x_3, x_4), (x_4, x_5) \in E_W$, but not both. Also, Lemma 2 excludes the possibility of both $(x_2, x_3), (x_3, x_4) \in E_B$.



Case 9: By Lemma 3, x_1, x_3, $x_4$must be incident to vertices from E_W. This gives rise to three Configuration 1's, which leaves all of the edges incident to the pentagon uncolored by the independence coloring ξ.



Case 10: Clearly none of the edges incident to $x_1$belong to $E_W \cup E_B$. We will have at least one of $(x_5, x_6), (x_4, x_5) \in E_W \cup E_B$, and at least one of $(x_2, x_3), (x_3, x_4) \in E_W \cup E_B$, except that only one of $(x_3, x_4), (x_4, x_5)$ can belong to E_W (by Lemma 4).



Finally, there is only one way to place four grey vertices, and up to black/white symmetry, this gives rise to two cases.

Case 11: There are type 3 configurations centered at (x_1, x_2) and (x_4, x_5). By the independence coloring ξ , only one of $(x_1, x_6), (x_2, x_3) \in E_B$, and only one of $(x_3, x_4), (x_5, x_6) \in E_B$. But Lemma 4, we cannot have both $(x_2, x_3), (x_3, x_4) \in E_B$ or both $(x_1, x_6), (x_5, x_6) \in E_B$. So we must have $(x_1, x_6), (x_3, x_4) \in E_B$.

Case 12: There are type 3 configurations centered at (x_1, x_2) and (x_4, x_5). By the independence coloring ξ , we could have $(x_1, x_6) \in E_W$ and $(x_2, x_3) \in E_B$ as well as $(x_3, x_4) \in E_B$ and $(x_5, x_6) \in E_W$. Lemma 4 makes it impossible for all four edges to belong to $E_W \cup E_B$.

□

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

Lemma 6. *Let* $\Gamma = (V, E, F)$ *be a fullerene with the independence coloring* ξ *defined previously. Then:*

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

Proof. Let c_i denote the number of type i configurations from Figure 3 in Γ and let e_{bw}, e_{gw}, e_{gb} and e_{gg} denote the number of black-white, grey-white, grey-black and grey-grey edges respectively. Since each of these types of edges arise from the three different configurations, these parameters are related by the following equations:

$$\begin{aligned} e_{gb} &= 2c_1 + c_2 + 2c_3 \\ e_{gw} &= c_1 + 2c_2 + 2c_3 \\ e_{gg} &= c_3 \\ e_{bw} &= E - e_{gb} - e_{gw} - e_{gg} \end{aligned}$$

We also have from the independence coloring ξ :

$$\begin{aligned} |E_B| &= c_2 + c_3 \\ |E_W| &= c_1 + c_3 \\ |E_G| &= c_3 \end{aligned}$$

Solving for the $c_i s$ we get:

$$\begin{aligned} c_3 &= |E_G| \\ c_1 &= |E_W| - |E_G| \\ c_2 &= |E_B| - |E_G| \end{aligned}$$

Substituting the $c_i s$, we have:

$$\begin{aligned} e_{gb} &= 2|E_W| + |E_B| - |E_G| \\ e_{gw} &= 2|E_B| + |E_W| - |E_G| \\ e_{gg} &= |E_G| \\ e_{bw} &= |E| - 3|E_B| - 3|E_W| + |E_G| \end{aligned}$$

Since a fullerene is trivalent, each white vertex is incident to three edges, so:

$$\begin{aligned} 3|W| &= e_{bw} + e_{gw} \\ &= |E| - (2|E_W| + |E_B|) \end{aligned}$$

Dividing both sides by 3 gives the result: $|W| = \frac{|E|}{3} - \frac{2|E_W|+|E_B|}{3}$
Similarly:

$$\begin{aligned} 3|B| &= e_{bw} + e_{gb} \\ &= |E| - (2|E_B| + |E_W|) \end{aligned}$$

So, $|B| = \frac{|E|}{3} - \frac{2|E_B|+|E_W|}{3}$

$\square$

7. Paths and circuits through edges in Γ

We will begin to construct paths through the fullerene Γ. Our paths will not be through vertices and edges in Γ, rather they will originate in the centers of the faces of Γ, and exit the face through an edge of the face. If we look at the planar dual of Γ, we will have a more natural and graph theoretic description of these paths.

Definition A **planar dual** of the graph $X = (V, E, F)$ is denoted $X^{\perp}$. The vertex set of $X^{\perp}$ is in one-to-one correspondence with the faces of X. Adjacency of a vertex in $X^{\perp}$ is determined by adjacency of faces in X. For example, if $f_1 \sim f_2$, and x_1, x_2 are the corresponding vertices in $X^{\perp}$, then $x_1 \sim x_2$.

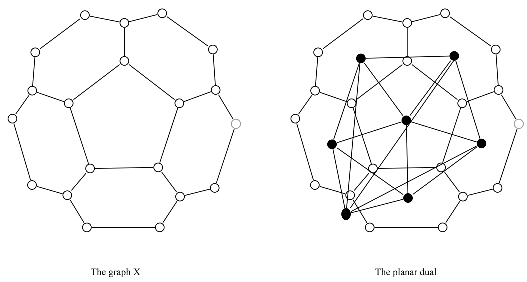
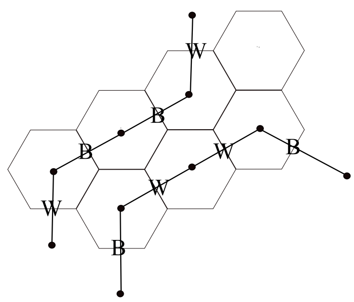


Figure 6. Construction of the Planar Dual

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 (meaning they share an edge) in Γ, make the two corresponding vertices adjacent in $\Gamma^{\perp}$. A simple example of the planar dual is shown above.

It can be easily seen that in the case that X is a fullerene, $X^{\perp}$ is a solid with only triangular faces. The vertices that correspond to hexagons will have valency 6, while the vertices that correspond to pentagons will have valency 5. This structure resembles a geodesic sphere, which once again reminds us of Buckminster Fuller. This structure is also useful for one construction of Coxeter coordinates, which will be discussed later.

Let $\Gamma^{\perp} = (F, E, V)$ be the planar dual of the fullerene $\Gamma = (V, E, F)$ and let Φ be the sub graph of $\Gamma^{\perp}$ induced by the edge set $E_W \cup E_B$. That is, Φ consists only of those edges in $\Gamma^{\perp}$ that corresponded to colored edges in Γ. In the figure below, only the darkest segments belong to Φ.



By Lemma 5, each vertex of Φ that has degree six in $\Gamma^{\perp}$ will have degree 2 in Φ.

Remark Note that hexagons that have no colored edges will not contribute to Φ; only the hexagons that have exactly two colored edges will contribute to Φ.

Also, each vertex in Φ that has degree 5 in $\Gamma^{\perp}$ has degree 1 in Φ. Thus, there are exactly 12 degree 1 vertices in Φ, so there are exactly 6 elementary paths (Lemma 5 excludes the possibility of paths crossing). There also may be circuits in Φ.

Corollary 7. *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.*

Proof. Note first that turns correspond to edges that were on the faces of hexagons in Γ. By Lemma 4, the edges in $E_W \cup E_B$ are an independent edge set. So, paths in Φ can only go straight, veer right, or veer left. See the figure below:

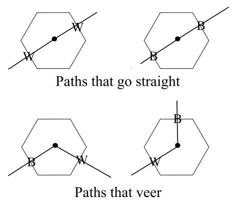


FIGURE 7. Possible path directions (Without loss of generality)

□

Remark We will now use the terms *right* and *left* without ambiguity, since we have excluded the possibility of sharp turns.

Lemma 8. *Let $\Gamma = (V, E, F)$ be a fullerene with the independence coloring ξ. Let Δ be a circuit in Φ. Arbitrarily choose some face not among the hexagons that correspond to vertices of Δ to be the "outside" face. Let Θ denote the subgraph of Γ consisting of the hexagons that correspond to Δ and its interior. Orient the circuit clockwise and let l and r denote the number of right and left turns respectively, and let p denote the number of interior pentagonal faces of Θ. Then $p = 6 + l - r$.*

Proof. By construction, Θ consists only of degree two and degree three vertices. Referring to the figure below, you can see that every straight portion contributes one degree two vertex, every right turn contributes two, and every left turn contributes zero. If n is the total length of Δ, and s is the number of straight portions of Δ, $n = s + r + l$. So, the number of degree two vertices in Θ is $s + 2r$, which simplifies to $s + r + l + r - l = n + r - l$. Hence, by Lemma 1, the degree sum formula,

$$3(v - (n + r - l)) + 2(n + r - l) = 3v - n - r + l = 2e$$

where v and e are the number of vertices and edges of Θ. Next, we note that the length of the boundary of the outside face of θ is

$$\begin{aligned} 2s + 3r + l &= 2s + 2r + 2l + r - l \\ &= 2n + r - l \end{aligned}$$

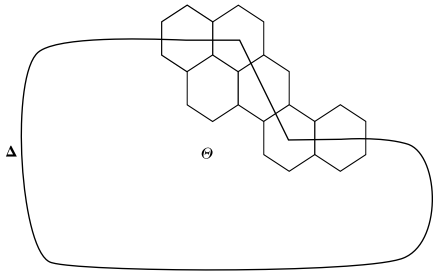


FIGURE 8

The number of hexagonal faces of Θ is $f-p-1$, where f is the total number of faces of Θ (including the outer face). If we wish to count the edges of Λ, note that edges that are completely on the interior of Λ can be counted using the hexagons and pentagons, and edges on the boundary of Λ can be counted using the formula $2n+r-l$. However, this results in a double counting of all of the edges so,

$$6(f-p-1)+5p+(2n+r-1)=2e$$

We solve equation for $6v$ and $6f$ to obtain:

$$\begin{aligned} 6v &= 4e+2n+2r-2l \\ 6f &= 2e+6f+6-5p-2n-r+l \end{aligned}$$

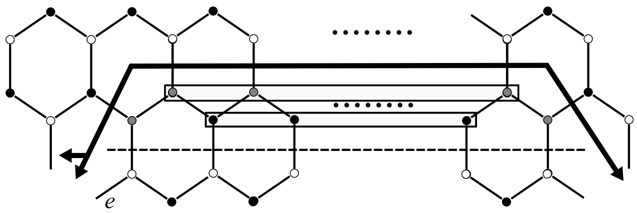
Substituting into Euler's Formula gives us:

$$\begin{aligned} 6v-6e+6f &= 4e+2n+2r-2l-6e+2e+6f+6-5p-2n-r+l \\ &= r-l+p+6 \\ &= 12 \end{aligned}$$

Solving for p, we get $p=6+l-r$. □

Lemma 9. *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 hexagons 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 the left before it makes another turn.*

Proof. By way of contradiction. Assume that our path or circuit makes two consecutive turns in the same direction, or takes a turn followed by a pentagonal face abutting two hexagons on the same side of the direction of the turn. Assume further that among all such configurations, we have selected the one with the shortest distance between the turns or the turn and the pentagonal face. Without loss of generality, we may orient the segment so that the first turn is a right turn as we move along the segment clockwise. We may assume that none of the hexagons on the right of the above mentioned segment belong to another circuit or path; we know paths cannot cross, so the second circuit would also have to make two right turns with a shorter distance between them (a contradiction since we have chosen the smallest configuration), or a turn with a pentagonal face closer together (again a contradiction). There are only three configurations that we need to investigate: two right turns, and a right turn followed by a pentagon on the right (two sub-configurations). Our goal is to show that such configurations do not result in maximal sets for B and W. We will begin with two consecutive right turns, as pictured below:

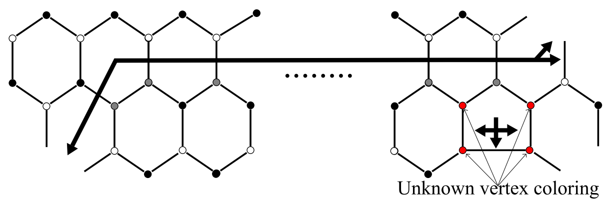


The dual path or circuit Π is indicated by the heavy line. A vertex coloring that will result in two consecutive turns has been selected.

Remark If an edge belongs to E_W (E_B) the its endpoints are colored grey and white (black), but which endpoint is colored white (black) is completely optional.

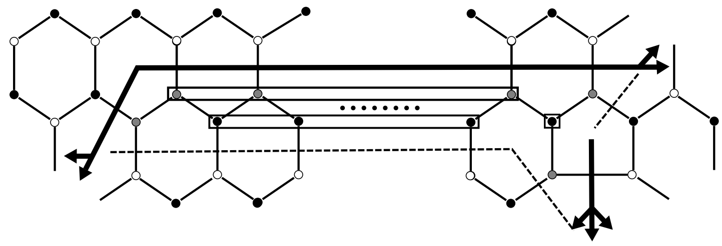
This portion of the circuit or path starts on the left in a hexagonal or pentagonal face. If it is a hexagonal face, the arrows indicated the possible directions in which this portion could continue to the left. The possibility of crossing the edge labeled e is excluded since, if e did belong to E_W, its white and grey endpoints could be swapped, resulting in three consecutive grey vertices (see remark above). Now, we see that by relocating the segment of Π along the dashed line, they grey vertices in the upper box will be recolored black and the black vertices in the lower box may be recolored grey. This new coloring has the same number of white vertices, but an additional black vertex, a contradiction.

We assume next that we have a right turn followed by a pentagonal face on the right. This pentagonal face is the terminal vertex of a second dual path in Φ and this path could exit the face to the left, right or down.



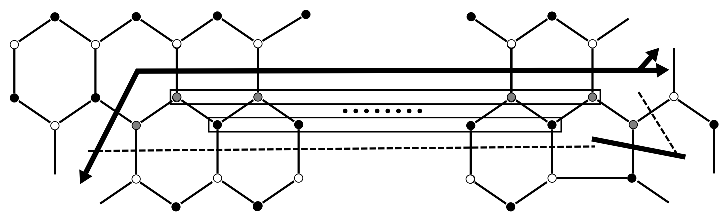
One can easily see that the path cannot exit to the top of the pentagon, since that would violate Lemma 4. Also, it is clear that the path can not exit the pentagon to the left, since this would violate Lemma 4 in the adjacent hexagon. There are just two cases to left: paths that exit the pentagon to the right, and paths that exit down.

We will begin with paths that exit down:



In the case that the path exits the pentagon downward, we relocate the segment of Π coming in from the left and connect it to the path leaving the pentagon. We divert the right end of the segment into the pentagon where it will now terminate. To do so, we will re-color the grey vertices in the upper box black, the black vertices in the lower box grey, and the single black vertex in the small box will be recolored white. We now have no change in the number of black vertices, but an increase in white vertices, a contradiction.

For paths that exit to the right:

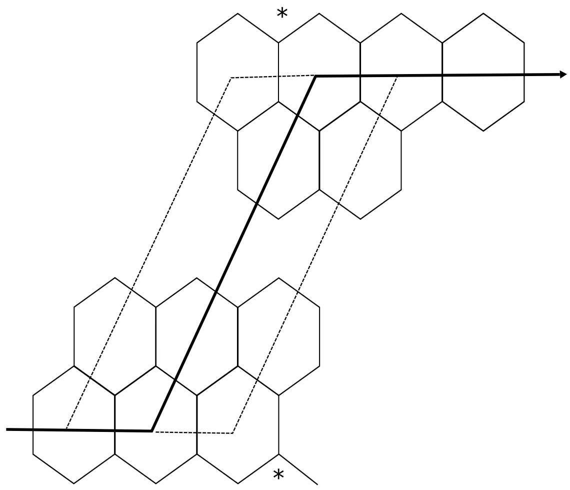


In the case pictured above, we relocate the segment of Π coming in from the left and connect it to the pentagon where it terminates. We divert the right end of the segment to the remainder of the path that started in the pentagon. Again, the grey vertices in the upper box will be recolored black, and the black vertices in the lower box will be recolored gray. This results in a net increase of a single black vertex, leaving $|W|$ unchanged, a contradiction. $\square$

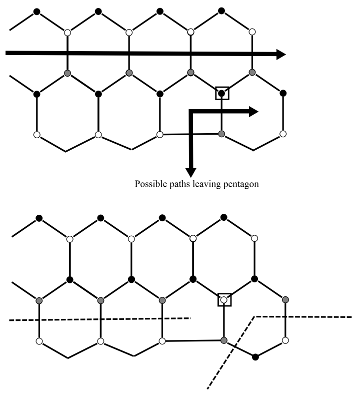
Lemma 10. *If $\Gamma = (V, E, F)$ is a fullerene, and Φ is the induced subgraph of $\Gamma^\perp$ constructed as described previously, there are no circuits in Φ.*

Proof. Let Γ be a fullerene and Δ a circuit in Φ. We first note that since pentagonal faces must be joined in pairs by paths that cannot cross Δ, there must be an even number of pentagonal faces on each side of Δ. It follows from Lemma 8 ($p = 6 + l - r$) that, unless there are 6 pentagonal faces on each side of Δ, Δ must take two consecutive right turns or two consecutive left turns in direct conflict of Lemma 9. So we must have 6 pentagons on each side of Δ. We conclude that Δ has the same number (perhaps zero) of left and right turns, and that they must alternate around Δ. In the figure below, we consider at least one pair of turns.

Applying the shift alterations shown (either right or left) we decrease the number of faces on the right side of the circuit without altering $|W|$ and $|B|$. Repeated shifts will eventually bring the circuit in contact with a pentagonal face. If that pentagon meets two of the hexagons in Δ, we are in conflict of Lemma 9. However, if the pentagon is in the position indicated by the asterisk (depending on whether we have shifted left or right), the first contact does not satisfy the hypothesis of Lemma 9. But in one more shift, this case will also be eliminated.



Finally, suppose that the circuit makes no turns. If it does not meet a pentagonal face on the right, we may shift to the circuit of hexagons on the right without altering $|W|$ and $|B|$. Again, we continue this shift until we meet a pentagonal face as illustrated in the figure below. Here we shift down once more, amalgamating the circuit and the path leaving the pentagonal face into a single path, as indicated. The vertices in the row of grey vertices are recolored black and the black vertices in the next row are recolored grey, except for a single black vertex which is recolored white, a contradiction.



Therefore, we conclude that circuits cannot occur in Φ □

We are now ready to state the main result:

Theorem 11. *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.*

8. Going towards the independence number of the icosahedral fullerenes

We will use some of the same techniques of the proof of Theorem 11 to say a little bit more about the structure of the maximum independent sets (recall that there are two, B and W) of an icosahedral fullerene.

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 "nearby" pentagons.

The soccer ball is an example of an icosahedral fullerene.

Let $\Gamma = (V, E, F)$ be fullerene and let $\Gamma^\perp = (F, E, V)$ be its planar dual; let Φ be the subgraph of $\Gamma^\perp$ induced by the edge set $E_W \cup E_B$ and let Π be a path in Φ connecting two pentagonal faces. Suppose that Π takes at least two turns. By Lemma 9, these turns must alternate in direction. Assume that the path makes a left turn and then a right turn as illustrated below.

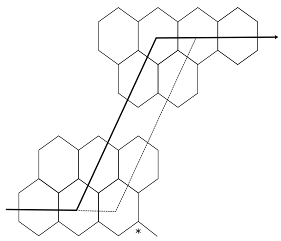


Figure 9

Now relocate the path by shifting to the right, as indicated in the figure. If we were to encounter another pentagonal face along the "wave" front, i.e. anywhere along the new portion of the path except the position indicated by the asterisk, we would be in conflict with Lemma 9. Hence, we must be able to continue this alteration until we have a path with exactly one left turn. We may then shift in the opposite direction until we have a path with exactly one right turn, sweeping out a parallelogram of hexagonal faces between the two pentagonal faces. We call such a parallelogram *clear field*. We have shown:

Lemma 12. *Let $\Gamma = (V, E, F)$ be a fullerene with the independence coloring ξ defined previously and let Φ be the subgraph of $\Gamma^\perp$ induced by the edge set $E_W \cup E_B$. Then, if two pentagonal faces of Γ are joined by a path in Φ, they are separated by a clear field.*

In order to provide further results, we must introduce a system or coordinates for icosahedral fullerenes.

9. Coxeter coordinates

According to Graver [1], there are two ways to construct Coxeter coordinates. The first way is to consider the regular triangular tessellation of the plane, and the other is to consider the regular hexagonal tessellation of the plane. Both methods apply to fullerenes, so we will start with triangles.

Consider Λ, the regular triangular tessellation of the plane. If Λ is considered to be a graph, it is an infinite plane graph with vertex valency 6. By a *segment* in Λ, we mean the straight line that joins the two vertices. We assign Coxeter coordinates to each segment that does not coincide with a"line" of the tessellation as follows: select one endpoint to be the origin, take the edge of the graph to the right of the segment as the unit vector in the p direction, take the edge of the graph to the left of the segment as the unit vector in the q direction, finally, use these unit vectors to assign coordinates to the other endpoint of the segment.

For segments that coincide with a"line" of the tessellation, that segment is assigned the single Coxeter coordinate (p), where p is the number of edges in the segment. An example is shown below:

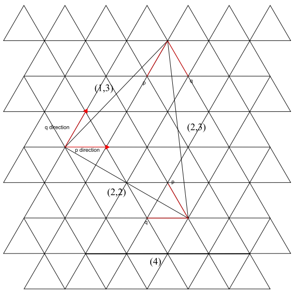


FIGURE 10. Coxeter Coordinates on a Triangular Tessellation

Coxeter coordinates can be determined in a similar way using a hexagonal tessellation of the plane. Consider $\Lambda^{\perp}$, the regular hexagonal tesselation (which is the planar dual of the regular triangular tessellation). Instead of graph theoretic distances, we will count the number of full hexagons that we pass through in the p and q directions. See the diagram below:

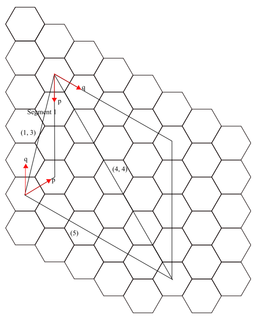


FIGURE 11. Coxeter Coordinates on a Hexagonal Tessellation

In the figure above, segment 1 has Coxeter Coordinates $(1, 3)$ because its component vectors pass through the centers of two hexagons in the p direction, each contributing $\frac{1}{2}$ to the coordinate. In the q direction, the component vectors pass through 2 full hexagons, and through 2 centers, resulting in a coordinate of 3 in the q direction. Note: Coxeter coordinates are the same when using either a triangular tessellation, or a hexagonal tessellation, as illustrated below:

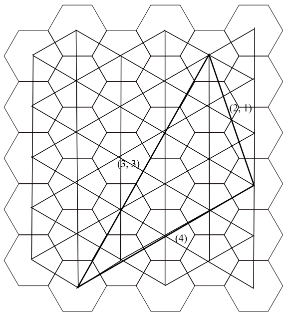


FIGURE 12. Equivalence of Triangular and Hexagonal Coxeter Coordinates

10. The independence number of icosahedral fullerenes

In the figure below, we have drawn a portion of the icosahedral fullerene with Coxeter coordinates $(4, 7)$.

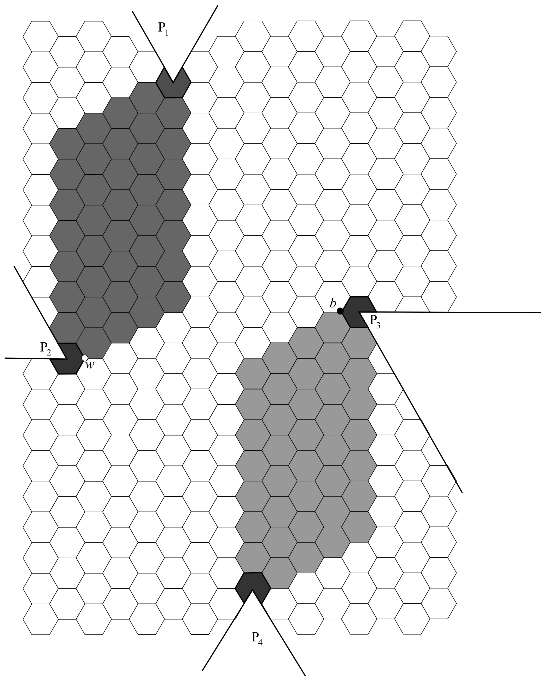


FIGURE 13. Part of an icosahedral fullerene with Coxeter Coordinates $(4, 7)$

These Coxeter coordinates only refer to segments that could be drawn between two “nearby” pentagons. By nearby pentagons, we mean only the pentagons that are closest to a given pentagon. You can see that the Coxeter coordinates are related to the dimension of the clear field separating the pentagons; there is a 4 by 7 clear field separating the pentagons. Recall that icosahedral fullerenes are highly symmetric, so we will see the same type of clear field between any two pentagons that are nearby.

Two of the 4 by 7 clear fields are shaded in. There is also a 4 by 7 clear field separating P_1 and P_3, as well as P_2 and P_4. Notice that there is a 15 by 3 clear field separating P_1 from P_4, but P_1 and P_4 are not nearby. In general, in an icosahedral fullerene with Coxeter coordinates $(p, p+r)$, two nearby pentagonal faces are separated by a p by $p+r$ clear field and any two non nearby but not antipodal pentagonal faces are separated by an r by $3p+r$ clear field. Recall that in a fullerene $\Gamma = (V, E, F)$, $2|E| = 3|V|$ (a simple application of Lemma 1). So the formula for the independence number of a fullerene $\alpha(\Gamma) = |W|$ from Lemma 6 can be written in the form $|W| = \frac{|V|}{2} - \frac{2|E_W|+|E_B|}{3}$. Hence we must select the pairings of pentagons in order to minimize $2|E_W| + |E_B|$.

We first note that any alternating paths in the clear field between paired pentagons have the same contribution to $2|E_W| + |E_B|$; hence that contribution is a property of the pairing. Referring to figure 14, if the vertex labeled w on the boundary of P_1 is colored white, the pair P_1, P_2 will contribute 4 to E_W and 7 to E_B for a total contribution of $2 \times 4 + 7 = 15$ to $2|E_W| + |E_B|$. If the pair P_3, P_4 is also selected, coloring w white will force the vertex labeled b on the boundary of P_3 to be colored black. So that pairing will contribute $2 \times 7 + 4 = 18$ to $2|E_W| + |E_B|$. We also note that the pair P_1, P_4 would contribute $2 \times 3 + 15 = 21$ or $2 \times 15 + 3 = 33$ to $2|E_W| + |E_B|$. Hence, we would like to find a set of pairings that minimizes contributions to $2|E_W| + |E_B|$. Since 15 was the smallest contribution, we wish to find pairings so that each pairing contributes exactly 15 to $2|E_W| + |E_B|$. We will now show that such a pairing exists.

Refer again to figure 14. We first note that in the full fullerene, P_3 has 5 neighboring pentagons; label the remaining two P_5 and P_6 so that P_1, P_2, P_4, P_5, P_6 appear counterclockwise around P_3. One easily checks that if P_1, P_2 are paired, they contribute 15 to $2|E_W| + |E_B|$ (w is white, since that will give us a smaller contribution). The pairs P_3, P_4 and P_3, P_6 would each contribute 18, while the pair P_3, P_5 would only contribute 15. Hence, to minimize $2|E_W| + |E_B|$, we must select the pair P_3, P_5. Once we have selected the pair P_1, P_2, and the coloring that makes its contribution 15, then the selection of the remaining pairs are forced. The pattern of pairs is pictured in figure 15. Pentagons that are near each other are connected with a line, pentagons that are paired are connected with a thick line.

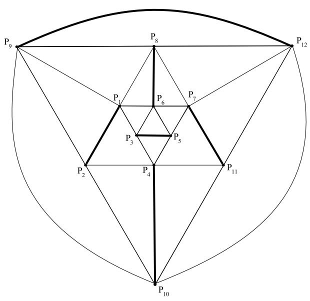


FIGURE 14. Pentagonal pairings to minimize $2|E_W| + |E_B|$

With the exception of the case $r = 0$, this is true for general icosahedral fullerenes with Coxeter coordinates $(p, p+r)$. Let $\Gamma = (V, E, F)$ be the icosahedral fullerene with Coxeter coordinates $(p, p+r)$ where $p, r \geq 0$ and at least one is positive. A pairing of nearby pentagons will contribute $2\times p+(p+r) = 3p+r$ or $2\times(p+r)+p = 2p+2r$ to $2|E_W|+|E_B|$, depending on the orientation of the pair. As noted above, any two nonadjacent, non-antipodal pentagonal faces are separated by a $3p+r$ clear field. Such a pair contributes $2\times r+(3p+r) = 3p+3r$ or $2\times(3p+r)+r = 6p+3r$ to $2|E_W|+|E_B|$, again depending on the orientation. As noted above, each of the six sets illustrated in figure 15 can be oriented so that each pair contributes $2\times p+(p+r) = 3p+r$ to $2|E_W|+|E_B|$. Hence:

$$\frac{|E|-6(3p+r)}{3} = \frac{|V|}{2} - (6p+2r)$$

Referring to Graver [2] we can see that a fullerene with Coxeter coordinates $(p, p+r)$ has $|V| = 60p^2+60pr+20r^2$. So this simplifies to:

$$\begin{aligned} \frac{|E|-6(3p+r)}{3} &= \frac{|V|}{2} - (6p+2r) \\ &= 30p^2+30pr+10r^2-6p-2r \end{aligned}$$

We have proved the following corollary.

Corollary 13. *Let* $\Gamma = (V, E, F)$ *be the icosahedral fullerene with Coxeter coordinates* $(p, p+r)$ *where* $p, r \geq 0$ *and at least one is positive. Then* $\alpha(\Gamma) = 30p^2+30pr+10r^2-6p-2r$

For a concrete example, see the next page.

Here is a particular example of the icosahedral fullerene with $p = 1$ and $r = 0$.

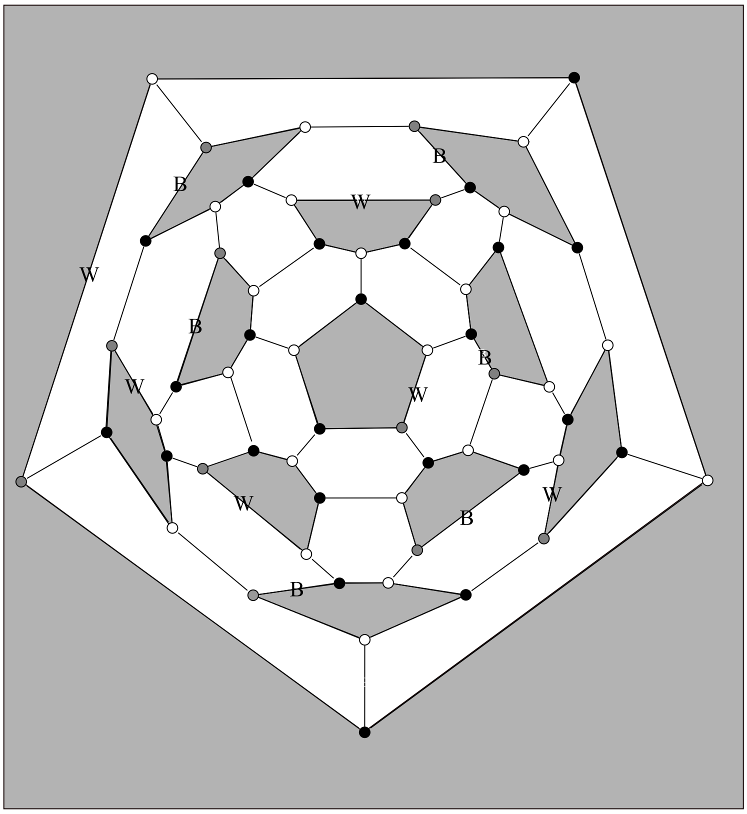


FIGURE 15. An icosahedral fullerene with Coxeter Coordinates (1,1)

Using Corollary 13, we see that $\alpha(\Gamma) = 30 - 6 = 24$. As you can see in the figure above, the independence coloring ξ has been respected. Lemma 4 and Lemma 5 are also satisfied. We have $|E_W| = 6$ and $|E_B| = 6$. Comparing this to Lemma 5 we see that

$$\begin{aligned}\frac{|E|}{3} - \frac{2|E_W| + |E_B|}{3} &= \frac{90}{3} - \frac{2(6) + 6}{3} \\ &= 30 - 6 \\ &= 24 \\ &= |W|\end{aligned}$$

And:

$$\begin{aligned}\frac{|E|}{3} - \frac{2|E_B| + |E_W|}{3} &= \frac{90}{3} - \frac{2(6) + 6}{3} \\ &= 30 - 6 \\ &= 24 \\ &= |B|\end{aligned}$$

We can see the construction of Φ below:

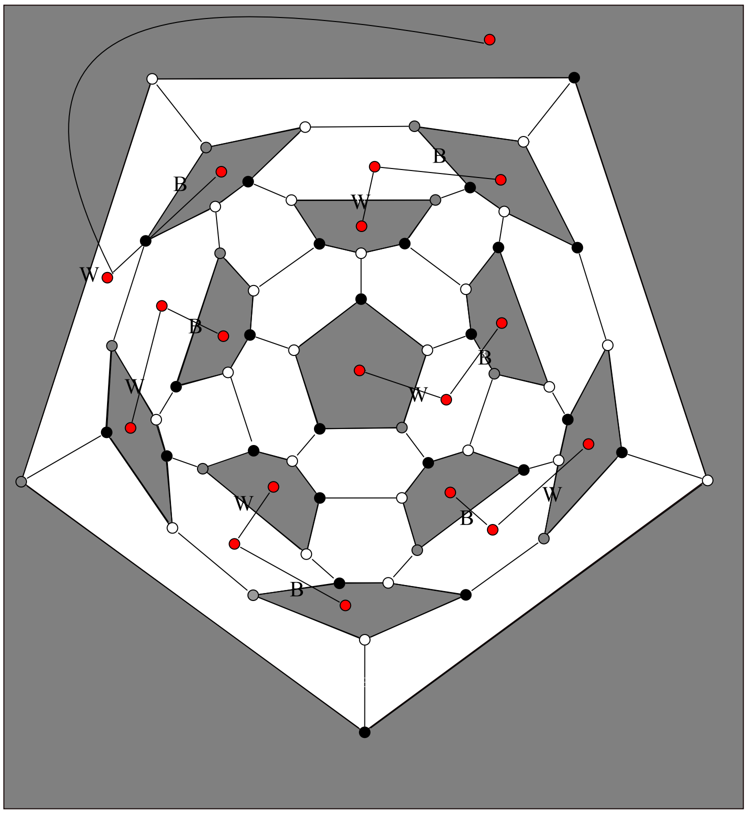


FIGURE 16

It is interesting to note that, in the case of the icosahedral fullerene with Coxeter coordinates (p, p), any pairing of pentagons separated by (p, p) clear fields yield maximum independent sets. Hence, these icosahedral fullerenes admit far more maximal independent sets, relative to their size than do other icosahedral fullerenes. Further extensions of this paper could include calculations of the independence number of other symmetric fullerenes. For example, it may be possible to calculate the independence number of fullerenes with two Coxeter coordinates. For further information on such fullerenes see Jack E. Gravers "Catalog of All Fullerenes with Ten or More Symmetries" [2].

REFERENCES

[1] Jack E. Graver. Encoding fullerenes and geodesic domes. *SIAM Journal of Discrete Mathematics*, 17(4):596–614, 2004.

[2] 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.

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

[4] Craig Larson. Graffiti and automated conjecture-making. Web. http://math.uh.edu/ clarson/graffiti.html.

[5] C. E. Larson S. Fajtlowicz. Graph-theoretic independence as a predictor of fullerene stability. *Preprint submitted to Elsevier Science*, 2003.

[6] Douglas B. West. *Introduction to Graph Theory*. Pearson Education, Saddle River, NJ, 2001.