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The independence numbers of fullerenes and benzenoids

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Abstract

We explore the structure of the maximum vertex independence sets in fullerenes: plane trivalent graphs with pentagonal and hexagonal faces. At the same time, we will consider benzenoids: plane graphs with hexagonal faces and one large outer face. In the case of fullerenes, a maximum vertex independence set may constructed as follows:

(i) Pair up the pentagonal faces.
(ii) Delete the edges of a shortest path in the dual joining the paired faces to get a bipartite subgraph of the fullerene.
(iii) Each of the deleted edges will join two vertices in the same cell of the bipartition; eliminating one endpoint of each of the deleted edges results in two independent subsets.

The main part of this paper is devoted to showing that for a properly chosen pairing, the larger of these two independent subsets will be a maximum independent set. We also prove that the construction of a maximum vertex independence set in a benzenoid is similar with the dual paths between pentagonal faces replaced by dual circuits through the outside face. At the end of the paper, we illustrate this method by computing the independence number for each of the icosahedral fullerenes.

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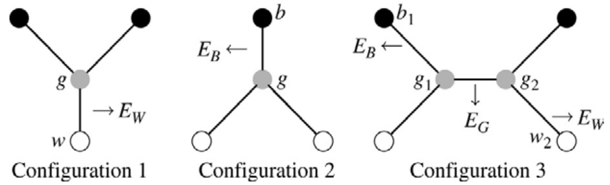

Fig. 1.

1. The independence number of a fullerene or benzenoid

Let $\Gamma = (V, E, F)$ be a fullerene,[1] that is, a trivalent plane graph with only pentagonal and hexagonal faces or a benzenoid,[2] that is, a plane graph with hexagonal faces and one large outer face such that all vertices have degree two or three with the vertices of degree two restricted to the boundary of the outside face. Let $\alpha(\Gamma)$ denote the (vertex) independence number of Γ. We wish to compute $\alpha(\Gamma)$.[3] To accomplish this we let W be a maximum vertex independent set of Γ, we let B be a maximum vertex independent set of Γ in $V - W$ and let $G = V - B - W$. We color the vertices in W white, the vertices in B black, and the vertices in G gray. A gray vertex with only black and gray neighbors could be recolored white, and a gray vertex with only white and gray neighbors could be recolored black. Hence, by the maximality of W and B:

Lemma 1. *In a fullerene or a benzenoid with the vertex coloring defined above, each gray vertex is adjacent to a black vertex and to a white vertex.*

Now if $g \in G$ is adjacent to two black vertices, let w be the white vertex adjacent to g and assign (g, w) to the edge set E_W; refer to Configuration 1 in Fig. 1. If $g \in G$ is adjacent to two white vertices, let b be the black vertex adjacent to g and assign (g, b) to E_B, Configuration 2, Fig. 1. Referring to Configuration 3, Fig. 1, given two adjacent gray vertices, arbitrarily label them, g_1 and g_2; then let b_1 be the black vertex adjacent to g_1 and let w_2 be the white vertex adjacent to g_2. Assign (g_1, b_1) to E_B, (g_2, w_2) to E_W and assign (g_1, g_2) to the edge set E_G. Finally, if Γ is a benzenoid and admits a gray degree 2 vertex, that vertex must be adjacent to one black and one white vertex. Hence we may interchange its color with that of either of its neighbors without altering $|W|$, $|B|$ and $|G|$. Repeating this operation as often as is necessary, we may "move" each degree 2, gray vertex into a degree 3, gray vertex. Hence, without loss of generality, we may assume that a benzenoid has no degree 2 gray vertices. This alteration is illustrated in the second part of Fig. 2.

Lemma 2. *Let $\Gamma = (V, E, F)$ be a fullerene or a benzenoid with the vertex coloring and edge partition defined above. Then $|G| = |E_B| + |E_W|$ and no two edges in $E_B \cup E_W$ have a common endpoint.*

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[1] For general information about fullerenes, consult [6,9,10] or [11].

[2] For general information about benzenoids, consult [1,2,5,12] or [13].

[3] For information about interpreting $\alpha(\Gamma)$ in the chemical context, see [7].

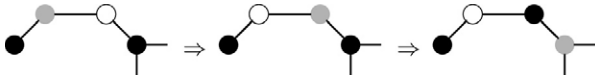

Fig. 2.

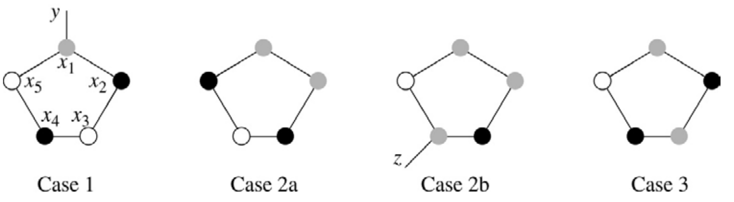

Fig. 3.

Proof. By definition, each gray vertex is the endpoint of exactly one edge in $E_B \cup E_W$ and each edge in $E_B \cup E_W$ has exactly one gray endpoint. Hence, $|G| = |E_B \cup E_W| = |E_B| + |E_W|$; the last equality holds since E_W and E_B are disjoint.

Now suppose $e, e' \in E_B \cup E_W$ have a common end point, x. Since each gray vertex is incident with exactly one edge in $E_B \cup E_W$, $x \notin G$. Suppose $x \in B$ and let y and y' be the other endpoints of e and e', respectively. Clearly, $y, y' \in G$. If y were adjacent to another black vertex, we would have Configuration 1 and (x, y) would not belong to E_B. Thus, neither y nor y' is adjacent to another black vertex. But, then we may recolor x gray and both y and y' black, contradicting the maximality of B. Similarly, $x \notin W$ and we conclude that no such x exists. $\square$

Lemma 3. *Let $\Gamma = (V, E, F)$ be a fullerene or a benzenoid with the vertex coloring and edge partition defined above.*

(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 $E_B \cup E_W$ or with no edges from $E_B \cup E_W$. Furthermore, if two edges from $E_B \cup E_W$ bound a hexagonal face and are opposite one another, they are both from E_B or both from E_W; if two edges from $E_B \cup E_W$ bound a hexagonal face and are not opposite one another, then one is from E_B and one from E_W.*

Proof. (i) Let $x_1, \ldots, x_5$ be the vertices of a pentagonal face listed in cyclic order. Clearly, at least one of these vertices must be gray, say x_1. There are three cases to consider and they are illustrated in Fig. 3.

Case 1: x_1 is the only gray vertex. Then, by symmetry, we may assume that x_2 and x_4 are black while x_3 and x_5 are white. Note first that (x_2, x_3), (x_3, x_4) and (x_4, x_5) are not in $E_B \cup E_W$. Let y be the third vertex adjacent to x_1. By the definitions of E_B and E_W: if y is colored white, $(x_1, x_2) \in E_B$ and $(x_1, x_5) \notin E_B \cup E_W$; if y is black, $(x_1, x_5) \in E_W$ and $(x_1, x_2) \notin E_B \cup E_W$; if y is gray, either $(x_1, x_2) \in E_B$ or $(x_1, x_5) \in E_W$ but not both.

Case 2: x_1 and x_2 are both colored gray. Then, $(x_1, x_2) \notin E_B \cup E_W$. Without loss of generality, we may assume that x_3 is black. Suppose x_5 is also black (Case 2a), then exactly one of (x_1, x_5) and (x_2, x_3) is in E_B. Furthermore, x_4 is either white or gray and

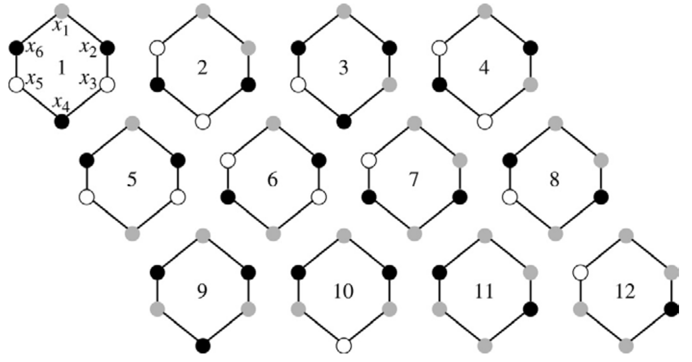

Fig. 4.

one easily checks that, in either case, neither of (x_3, x_4) and (x_4, x_5) belongs to $E_B \cup E_W$. Next suppose that x_5 is white (Case 2b). Then x_4 must be gray. Let z denote the third vertex adjacent to x_4. By symmetry, we may assume that z is black or gray. But then we may recolor x_1 and x_4 white and x_5 gray, contradicting our maximality condition. Hence this second option is not possible.

Case 3: x_1 and x_3 are both colored gray; then, without loss of generality, we may assume that x_2 is black. If either of x_4 or x_5 are gray, we are in the previously considered case, 2b. Hence, by symmetry, we may assume that x_4 is black and x_5 is white. There is a Configuration 1 centered at x_3 and neither of (x_2, x_3) and (x_3, x_4) can belong to E_B. As we have argued before, no matter which configuration contains x_1, exactly one of (x_1, x_2) and (x_1, x_5) belongs to $E_B \cup E_W$.

(ii) Let $x_1, \ldots, x_6$ be the vertices of a hexagonal face listed in cyclic order. If none are gray, then none of the edges of this face belong to $E_B \cup E_W$. Hence, we assume that x_1 is gray. In each of the cases that we now consider, we can, without loss of generality, always assume that the non-gray vertex with smallest subscript is black. If there no other gray vertices on the face (Case 1, Fig. 4), then x_2, x_4 and x_6 are black and x_3 and x_5 are white. It follows at once and none of (x_2, x_3), (x_3, x_4), (x_4, x_5) and (x_5, x_6) belongs to $E_B \cup E_W$. Since both x_2 and x_6 are black, neither (x_1, x_2) nor (x_1, x_6) belongs to $E_B \cup E_W$.

Since the reasoning is much the same in all of these cases, we will only outline the remaining arguments. Now assume that there are exactly two gray vertices among the x_is. If x_2 is gray, we have Case 2. In this case, either $(x_1, x_6) \in E_W$ and $(x_2, x_3) \in E_B$ or neither (x_1, x_6) nor (x_2, x_3) belongs to $E_B \cup E_W$. If the second gray vertex is x_3, we have either Case 3 or Case 4. In Case 3, it is clear that none of the edges of the hexagon belongs to $E_B \cup E_W$. Consulting Case 4, either $(x_1, x_2) \in E_B$ or $(x_1, x_6) \in E_W$ and either $(x_2, x_3) \in E_B$ or $(x_3, x_4) \in E_W$. Of the four possible combinations only $(x_1, x_2) \in E_B$ and $(x_2, x_3) \in E_B$ is excluded (by Lemma 2). The only remaining possibilities for two gray vertices are pictures as Cases 5 and 6. By definition, none of the edges of Case 5 belongs to $E_B \cup E_W$. In Case 6, either $(x_1, x_2) \in E_B$ or $(x_1, x_6) \in E_W$ (but not both) and either $(x_4, x_5) \in E_B$ or $(x_3, x_4) \in E_W$ (but not both).

By Lemma 1, no gray vertex is incident with more than one other gray vertex. So there are no more than two consecutive gray vertices around this face. Thus, up to symmetry, there are just two possible patterns for three gray vertices and each yields two Cases, numbered 7 through 10.

Case 7: either $(x_1, x_6) \in E_W$ and $(x_2, x_3) \in E_B$ or neither (x_1, x_2) nor (x_1, x_6) belongs to $E_B \cup E_W$; furthermore, neither of (x_3, x_4) and (x_4, x_5) belongs to E_B.

Case 8: exactly one of (x_1, x_6) and (x_2, x_3) belongs to E_B and either $(x_3, x_4) \in E_B$ or $(x_4, x_5) \in E_W$ with the caveat that (x_2, x_3) and (x_3, x_4) cannot both belong to E_B.

Case 9: clearly none of the edges of the hexagon belongs to $E_B \cup E_W$.

Case 10: either $(x_2, x_3) \in E_B$ or $(x_3, x_4) \in E_W$ and either $(x_5, x_6) \in E_B$ or $(x_4, x_5) \in E_W$ with the caveat that (x_3, x_4) and (x_4, x_5) cannot both belong to E_W.

Finally, four gray vertices can be placed in only one way, up to symmetry, giving rise to two Cases.

Case 11: exactly one of (x_2, x_3) and (x_1, x_6) are in E_B and exactly one of (x_3, x_4) and (x_5, x_6) is in E_B. So by Lemma 2, either (x_2, x_3) and (x_5, x_6) are in E_B or (x_3, x_4) and (x_1, x_6) are in E_B.

Case 12: either $(x_2, x_3) \in E_B$ and $(x_1, x_6) \in E_W$ or $(x_3, x_4) \in E_B$ and $(x_5, x_6) \in E_W$; but Lemma 2 precludes the possibility that all four edges belong to $E_B \cup E_W$. □

If Γ is a benzenoid, let W_2 and B_2 denote the set of degree 2 white and black vertices, respectively; if Γ is a fullerene, let $W_2 = B_2 = \emptyset$. Recall that we may insist that no degree 2 vertex of a benzenoid is colored gray.

Lemma 4. *Let $\Gamma = (V, E, F)$ be a fullerene or a benzenoid with the vertex coloring and edge partition defined above. Then:*

$$|W| = \frac{|E| + |W_2|}{3} - \frac{2|E_W| + |E_B|}{3} \quad \textit{and} \quad |B| = \frac{|E| + |B_2|}{3} - \frac{2|E_B| + |E_W|}{3}.$$

Proof. Let c_i denote the number of type i configurations from Fig. 1 in Γ and let e_{bw}, e_{gw}, e_{gb} and e_{gg}, denote the number of black–white edges, gray–white edges, gray–black edges and gray–gray edges, respectively. These parameters are related by the following equations:

$$e_{gb} = 2c_1 + c_2 + 2c_3$$
$$e_{gw} = c_1 + 2c_2 + 2c_3$$
$$e_{gg} = c_3$$
$$e_{bw} = |E| - e_{gg} - e_{gb} - e_{gw}.$$

We also have:

$$|E_B| = c_2 + c_3$$
$$|E_W| = c_1 + c_3$$
$$|E_G| = c_3.$$

Eliminating the c_is, we get:

$$e_{gb} = 2|E_W| + |E_B| - |E_G|$$
$$e_{gw} = 2|E_B| + |E_W| - |E_G|$$

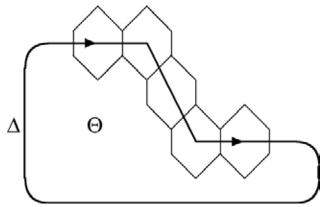

Fig. 5.

$$e_{gg} = |E_G|$$
$$e_{bw} = |E| - 3|E_B| - 3|E_W| + |E_G|.$$

Then:

$$3|W| - |W_2| = e_{bw} + e_{gw} = |E| - (2|E_W| + |E_B|).$$

Moving $|W_2|$ to the right-hand side and dividing by 3 gives the required formula for $|W|$; a similar derivation gives the formula for $|B|$. □

Let $\Gamma = (V, E, F)$ be a fullerene or a benzenoid and let $\Gamma^\perp = (F, E, V)$ be its dual; let Φ be subgraph of $\Gamma^\perp$ induced by the edge set $E_B \cup E_W$. Then, by Lemma 3, each vertex of Φ that has degree 6 in $\Gamma^\perp$ has degree 2 in Φ. If Γ is a fullerene, each vertex of Φ that has degree 5 in $\Gamma^\perp$ has degree 1 in Φ. Hence, if Γ is a fullerene, Φ is disconnected with six components, $\Pi_1, \ldots, \Pi_6$, each of which is an elementary path between a different pair of vertices of degree 5 and, possibly, additional components that are elementary circuits. If Γ is a benzenoid, the components of Φ consists of some elementary circuits meeting in the single vertex large degree and, possibly, other disjoint elementary circuits. In the next two lemmas, we explore the structure of Φ in more detail. Our aim is to show that Φ never includes additional disjoint elementary circuits.

Consider any portion of an elementary dual path or circuit in Φ. Lemma 3(ii) excludes the possibility of making sharp right or left turns. Hence, as we move along this path or circuit we have, at each hexagon, the possibility of moving straight across or across and branching right or left. Since sharp turns are excluded, we may use the terms *right turn* and *left turn* without ambiguity.

Lemma 5. *Let $\Gamma = (V, E, F)$ be a fullerene or a benzenoid with the vertex coloring and edge partition defined above. Let Δ be a circuit in Φ. If Γ is a benzenoid, we assume that the outside face is not a vertex of Δ. If $\Gamma = (V, E, F)$ is a fullerene 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 corresponding to Δ and its interior. Orient the circuit clockwise and let ℓ and r denote the number of left and right turns, respectively, and let p denote the number of interior pentagonal faces of Θ. Then $p = 6 + \ell - r$.*

Proof. Referring to Fig. 5, the number of degree 2 vertices in Θ is $n + r - \ell$, where n is the length of Δ. Hence, $3v - n - r + \ell = 2e$, where v and e are the numbers of vertices and edges of Θ. Next we note that the length of the boundary of the outside face of Θ is $2n + r - \ell$ and the number of hexagonal faces of θ is $f - p - 1$, where f is the total number

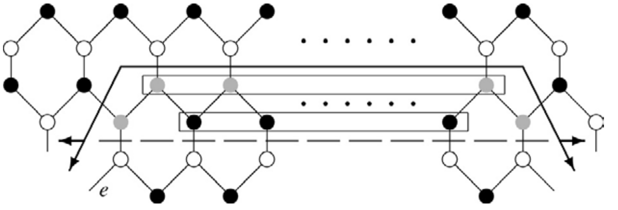

Fig. 6.

of faces of Θ. Hence, $6(f-p-1)+5p+(2n+r-\ell)=2e$. Solving these two equations for $6v$ and $6f$, respectively, and substituting them into Euler's formula $6v-6e+6f=12$ yields the required formula. □

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

Proof. Assume that our path or circuit takes two consecutive turns in the same direction or takes a turn followed by a pentagonal face same side and assume 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 left to right.

We may assume that none of the hexagons on the right of the path between the two turns or between the turn and the pentagonal face belongs to another circuit or another path: since paths and circuits cannot cross, the second circuit would have to have two turns or a turn and pentagonal face closer together. There are just three configurations that we need to investigate.

Consider two consecutive right turns as pictured in Fig. 6. The dual path or circuit Π is indicated by the heavy line. A vertex coloring has been selected. Note that if an edge belongs to E_W (E_B) then its endpoints are colored gray and white (black) but which endpoint is colored gray and which is colored white (black) is completely optional. In the figures illustrating this proof, we have moved all of the gray vertices below the path or circuit. The portion of the circuit or path in Fig. 6 starts on the left in a hexagonal or pentagonal face or in the outer face (for a benzenoid). If it is a hexagonal face, the arrows indicate the possible directions in which it could continue to the left. The possibility of crossing the edge labeled e is excluded since, if it were to belong to E_W, its white endpoint could be recolored gray, giving three consecutive gray vertices. By relocating this segment of Φ along the thinner dashed line, the gray vertices in the upper box will be recolored black and the black vertices in the lower box may be recolored gray. This new coloring has the same number of white vertices and one more black vertex for a contradiction. Note that this argument is valid if we have a benzenoid and one or more of the faces on the right between the two turns are the outer face.

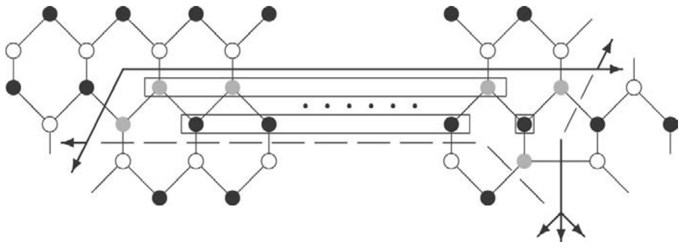

Fig. 7.

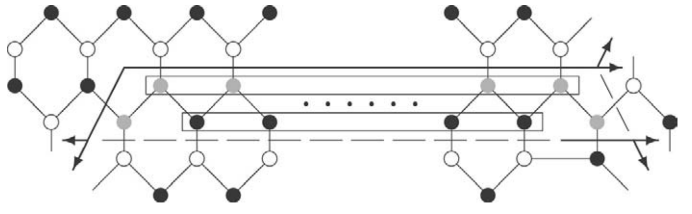

Fig. 8.

We assume next that we have a right turn followed by a pentagonal face abutting the path on the right. That pentagonal face is the terminal vertex of a second dual path in Φ and that path could exit the face to the left, the right or down. However, one easily sees that exiting the pentagon to the left would contradict the coloring rules. So just two cases are left; these are pictured in Figs. 7 and 8.

In the case that the path exits the pentagonal face downward, pictured in Fig. 7, we relocate the segment of Φ coming in from the left and connect it to the path leaving the pentagon and diverting the right end of our segment into the pentagon where it now terminates. The gray vertices in the upper box will be recolored black, the black vertices in the lower long box are recolored gray and the black vertex in the small box is recolored white for the same number of black vertices, an increase of one white vertex and a contradiction.

In the case pictured in Fig. 8, we relocate the segment of Φ coming in from the left and connect it to pentagon where it terminates. We then divert the right end of our segment to the remainder of the path that started at the pentagon. Again the gray vertices in the upper box will be recolored black and the black vertices in the lower box are recolored gray for the same number of white vertices, an increase of one black vertex and a contradiction. □

We now have the tools to eliminate the possibility of circuits in Φ when Γ is a fullerene and circuits that do not pass through the outside face when Γ is a benzenoid. We dispose of the case of benzenoids first. Since a benzenoid has no pentagonal faces, Lemma 5 tells us that a circuit not through the outside face must have six more right turns than left turns. But then it must make two consecutive right turns, which is impossible by Lemma 6. The case of fullerenes is a bit more complicated.

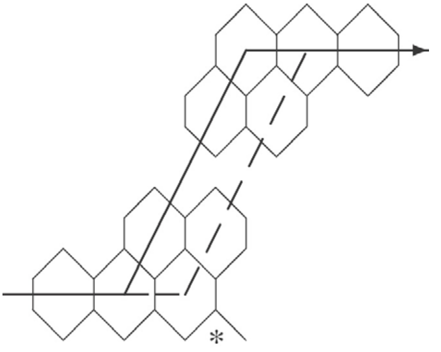

Fig. 9.

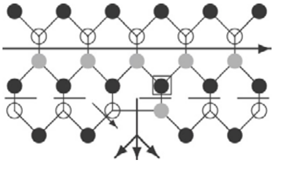

Fig. 10.

Let Γ be a fullerene and Δ a circuit in Φ. We first note that, since the 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. Then it follows from Lemma 5 that, unless there are six pentagonal faces on each side of Δ, Δ must take two consecutive right turns or two consecutive left turns, in direct conflict with Lemma 6. We conclude that Δ has the same number (perhaps zero) of left and right turns and that they must alternate around Δ.

In Fig. 9, we consider the case of at least one pair of turns. Applying the shift alteration pictured in that figure we decrease the number of faces on the right side of the circuit and one easily checks that the shift does not alter the numbers $|W|$ and $|B|$. Repeated shifts must eventually bring the circuit in contact with a pentagonal face. If that pentagon meets two of the hexagons in the circuit, we are in conflict with Lemma 6. However, if the pentagon in the position indicated by the asterisk in the figure, the first contact does not satisfy the hypothesis of Lemma 6. But then, one more shift and this case is also eliminated.

Finally, suppose that the circuit makes no turns. If it does not meet a pentagonal face on the right, we may shift the entire circuit to the circuit of hexagons on its right without altering $|W|$ and $|B|$. Again, we continue this shift until we meet a pentagonal face as illustrated in Fig. 10. Here we shift down once more amalgamating the circuit and the path leaving the pentagonal face into a single path exiting the pentagon to the right as indicated. The vertices in the row of gray vertices are recolored black and the black vertices in the next row are recolored gray, except for the one in the box which is recolored white for a net increase of one white vertex.

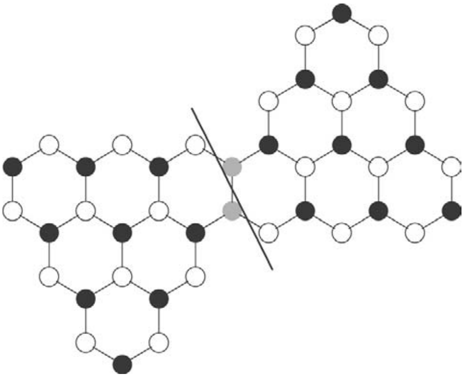

Fig. 11.

We conclude that "stand alone" circuits of hexagonal faces cannot occur, completing the proof of our main result.

Theorem 1. *Let $\Gamma = (V, E, F)$ be a fullerene or a benzenoid with the vertex coloring and edge partition defined above and let $\Gamma^{\perp} = (F, E, V)$ be its dual; let Φ be subgraph of $\Gamma^{\perp}$ induced by the edge set $E_B \cup E_W$. Then, if Γ is a fullerene, Φ is disconnected with six components, $\Pi_1, \ldots, \Pi_6$, each of which is an elementary path between a different pair of vertices of degree 5; if Γ is a benzenoid, then Φ is empty or consist of elementary circuits all meeting in the single vertex corresponding to the outer face.*

Before moving on to fullerenes, we illustrate this result for benzenoids by drawing, in Fig. 11, a smallest benzenoid that has a nonempty Φ. In the figure, the two cells of the bipartition of Γ are symmetric, each consisting of 21 atoms. However, $\alpha(\Gamma) = 22$ as is illustrated in the figure. The dual elementary circuit through the outside face that makes up Φ is indicated by the heavy line. The reader should now see how one can construct a benzenoid with independence number arbitrarily larger than the largest cell of the bipartition and requiring arbitrarily many circuits in Φ.

2. The independence numbers of the icosahedral fullerenes

We can use the techniques of the proof of Theorem 1 to say a bit about the structure of the maximum independent sets in a fullerene. Let $\Gamma = (V, E, F)$ be a fullerene and let $\Gamma^{\perp} = (F, E, V)$ be its dual; let Φ be subgraph of $\Gamma^{\perp}$ induced by the edge set $E_B \cup E_W$ and let Π be a path in Φ connecting two pentagonal faces. Suppose that Π takes at least two turns. By Lemma 6, these turns must alternate in direction. Assume the path makes a left then a right turn as pictured in Fig. 9. Now relocate the path by shifting the "wave front" to the right as indicated in the figure. If we were to encounter another pentagonal face along this 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 6. Hence we must be able to continue this alteration until we have a path with exactly one left turn. We may then

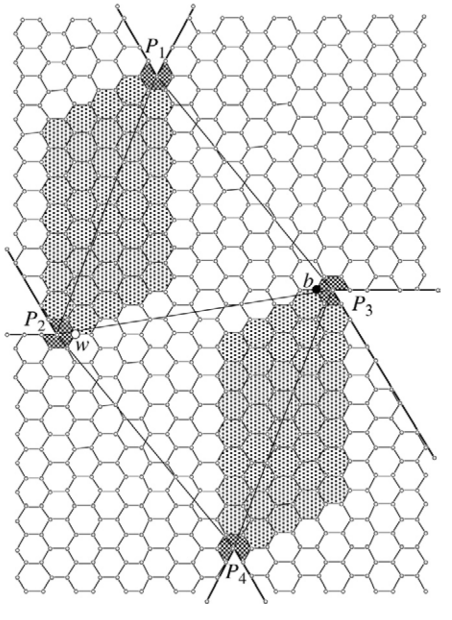

Fig. 12.

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 a *clear field*. Clear fields between pairs of pentagonal faces have been shaded in Fig. 12. We have proved:

Lemma 7. *Let $\Gamma = (V, E, F)$ be a fullerene with the vertex coloring and edge partition defined above and let Φ be subgraph of $\Gamma^\perp$ induced by the edge set $E_B \cup E_W$. Then, if two pentagonal faces of Γ are joined by a path in Φ, they are separated by a clear field in Γ.*

The icosahedral fullerenes are the duals of the planar triangulations introduced by Goldberg [8], Caspar and Klug [3] and Coxeter [4]. These fullerenes are constructed by cutting an equilateral triangle out of the hexagonal tessellation of the plane (with vertices at the centers of faces of the tessellation) and pasting 20 copies of it on the faces of an icosahedron. Since the relative position of two faces is uniquely determined by two non-negative numbers, the triangle and the entire fullerene is uniquely determined by this pair of numbers which we call the Coxeter coordinates of the fullerene.

In Fig. 12, we have drawn a portion of the icosahedral fullerene with Coxeter coordinates (4, 7). Two of the 4 by 7 clear field parallelograms are shaded in. Of course, pentagons P_2 and P_3 are also separated by a 4 by 7 clear field that is not shaded. In addition, pentagons P_1 and P_4 are separated by a 15 by 3 clear field that is not shaded. In the icosahedral fullerene with Coxeter coordinates $(p, p + r)$, two adjacent pentagonal faces are separated by a p by $p + r$ clear field and any two nonadjacent but nonantipodal pentagonal faces are separated by an r by $3p + r$ clear field.

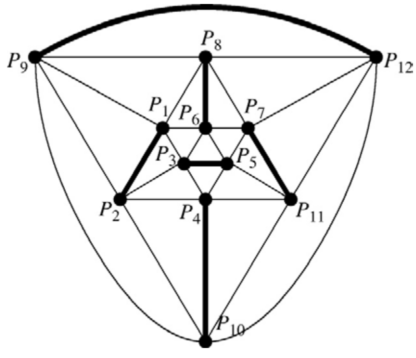

Fig. 13.

Recall that in a fullerene $\Gamma = (V, E, F)$, $2|E| = 3|V|$. So the formula for the independence number of a fullerene (from Lemma 4) 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 such a way as to minimize $2|E_W| + |E_B|$. We first note that any two alternating paths in the clear field between paired pentagons will have the same contribution to $2|E_W| + |E_B|$; hence that contribution is a property of the pairing. Referring to the figure, if the vertex labeled w on the boundary of P_2 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 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 so that each pair contributes the minimum of 15 to $2|E_W| + |E_B|$. We now show that such a pairing exists.

Referring again to Fig. 12, we note that, in the complete fullerene, P_3 has five neighboring pentagonal faces; label the remaining two P_5 and P_6 so that P_1, P_2, P_4, P_5 and P_6 occur in counterclockwise order around P_3. One easily checks that, given P_1, P_2 contributes 15 to $2|E_W| + |E_B|$ (w is white), then the pairs P_3, P_4 and P_3, P_6 would each contribute 18 while the pair P_3, P_5 would contribute only 15. Hence to minimize $2|E_W|+|E_B|$, we must select the pair P_3, P_5. In fact 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 that contribute 15 is forced. The pattern of pairs is pictured in Fig. 13. Since there are just five choices for a pair containing P_1, there are just five sets of pairings that yield maximum independent sets. With the exception of the case $r = 0$, this is true for general icosahedral fullerenes.

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 two nearby pentagons will contribute $2 \times p + (p + r) = 3p + r$ or $2 \times (p + r) + p = 3p + 2r$ to $2|E_W| + |E_B|$, depending on the orientation of the pair. As we noted above, any two nonadjacent but nonantipodal pentagonal faces are separated by an r by $3p + r$ 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 of the pair. As we noted above, each the five sets of pairing illustrated in Fig. 13 is oriented so that each pair contributes $2 \times p + (p + r) = 3p + r$ to

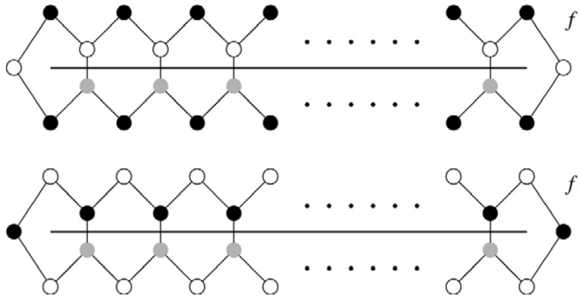

Fig. 14.

$2|E_W| + |E_B|$. Hence:

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

We have proved:

Corollary 2.1. *Let $\Gamma = (V, E, F)$ be the icosahedral fullerene with Coxeter coordinates $(p, p + r)$ where $p, r \geq 0$ and at least one of p and r is positive. Then $\alpha(\Gamma) = \frac{|V|}{2} - (6p + 2r)$.*

It is interesting to note that, in the case of icosahedral fullerene with Coxeter coordinates (p, p) $(r = 0)$, any pairing of pentagons separated by (p, p) clear fields yields maximum independent sets and some pairings including pairs separated by $(3p)$ clear fields also yield maximum independent sets. Hence these icosahedral fullerene admit far more maximum independent sets, relative to the their size, than do other icosahedral fullerenes.

3. Comments

For an arbitrary fullerene, one could compute the size of the maximum independent set given by each of the 10 395 possible pairings of its pentagonal faces and select the largest. There should be some way to quickly eliminate many pairings from consideration, leading to a reasonable algorithm for computing the independence number of an arbitrary fullerene. One suspects that, for fullerenes with few symmetries, the number of pairings that yield maximum independent sets will be quite small, perhaps just 1.

Once a pairing that gives the independence number has been determined, one could construct all maximum independent sets associated with that pairing by coloring the vertices in each clear field in all possible ways. The number of ways of coloring the clear field will depend only on the Coxeter coordinates of the path and the “color” of the path. Referring to Fig. 12, we will say that the upper left-hand path (clear field) has color *white* while the lower right-hand path has color *black*. The number of ways that one may extend the “outside” black and white coloring of the vertices to a black, white and gray coloring of the vertices of the clear field that yield distinct maximum white independent sets will be denoted by $f(w, p, q)$ for a white path with Coxeter coordinates (p, q) and $(f(b, p, q))$ for a black path with those coordinates. We illustrate these definitions in Fig. 14 with the simplest of paths.

In the case of a black path with Coxeter coordinates $(0, q)$ we see that each of the 2^q possible ways to interchange adjacent white and gray vertices correspond to different (white) maximum independent sets. On the other hand, interchanging adjacent black and gray vertices in the black path does not alter the (white) maximum independent set. If we let $\Pi_1 \ldots \Pi_6$ denote the paths in Φ that lead to a maximum independent (white) set, then there will be $f(c_1, p_1, q_1) \times \cdots \times f(c_6, p_6, q_6)$ maximum independent sets associated with this collection of paths, where c_i is the color of Π_i and (p_i, q_i) are its Coxeter coordinates. Finally the total number of maximum independent sets will be obtained by summing this product over all choices of collection of six paths in Φ that give maximum independent sets.

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