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On some structural properties of fullerene graphs

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We show how some important structural properties of general fullerene graphs follow from the recently proved fact that all fullerene graphs are cyclically 4-edge connected. These properties, in turn, give us upper and lower bounds for various graph invariants. In particular, we establish the best currently known lower bound for the number of perfect matchings in fullerene graphs.

KEY WORDS: fullerene graphs, fullerenes, perfect matchings, enumeration

AMS subject classification: 05C75, 05C70, 05C40

1. Introduction

Soon after the establishment of the C_{60} structure [1] and the birth of fullerene chemistry, the underlying graphs became a subject of increasing scientific interest. As the main focus of the current chemical research is on buckminsterfullerene (the truncated icosahedron isomer of C_{60}) and its close relatives with isolated pentagons, there are many results concerning the structure and the graphical invariants of the corresponding graphs [2,3]. Much less is known about general fullerene graphs. We remind the reader here that all fullerene graphs are cyclically 4-edge connected [4], and we will show how many important structural properties follow from this fact. In doing this, we will use many elements of the structural theory of matchings. We refer the reader to the monograph [5] for more details on this topic. Also, all the terminology and notations used in this article will be the same as in [5], if not stated otherwise. In particular, all graphs considered here will be finite, simple and connected, with p vertices and q edges.

A *fullerene graph* is a planar, 3-regular and 3-connected graph, twelve of whose faces are pentagons, and any remaining faces are hexagons. These same objects are often referred to as fullerenes or by the more general term trivalent carbon cages in the chemical literature.

2. The main result

A graph G is *cyclically k-edge connected* if G cannot be separated into two components, each containing a cycle, by deletion of fewer than k edges.

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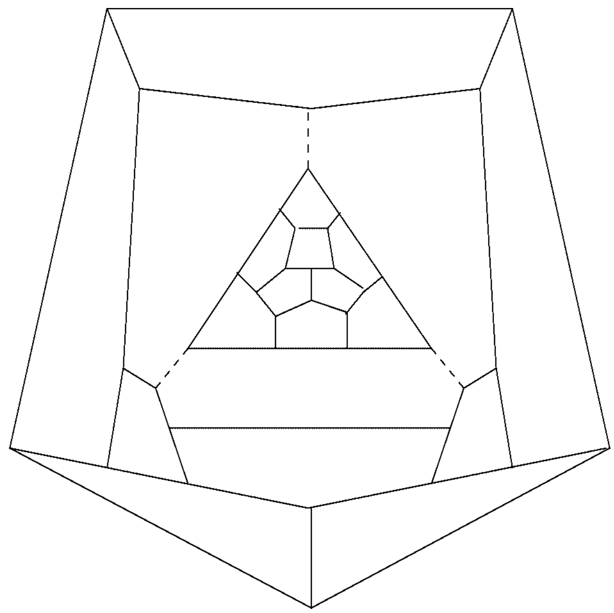

Figure 1. An example of a graph with girth 5 which is not cyclically 4-edge connected.

Theorem 1. Every fullerene graph is cyclically 4-edge connected.

The proof of this theorem is somewhat technical, and we refer the reader to [4], where it is given with full detail.

Let us mention that the non-existence of cycles of size 3 and 4 is not a sufficient condition for cyclical 4-edge connectivity. There are 3-connected, 3-regular planar graphs with girth at least five which are not cyclically 4-edge connected. An example is shown in figure 1.

3. Structural consequences and bounds

Let us now present some structural properties of fullerene graphs that follow from theorem 1. In the first part of this section we present these properties in such a way that they give successively better and better lower bounds for number of perfect matchings.

A *matching* M in a graph G is a set of edges of G such that no two edges from M have a vertex in common. The number of edges in a matching M is called the *size* of M. A vertex $v \in V(G)$ incident with some edge $e \in M$ is *covered* by the matching M. A matching M is *perfect* if it covers every vertex of G. Perfect matchings are in chemistry known as *Kekulé structures*. We denote the number of different perfect matchings of a graph G by $\Phi(G)$.

Every fullerene graph has a perfect matching; this is an easy consequence of the classical Petersen result that every connected cubic graph with no more than two cut-edges has a perfect matching.

A graph G is *n-extendable*, for $0 \leqslant n \leqslant p/2-1$, if it is connected, has a matching of size n, and every such matching can be extended to a perfect matching in G.

0-extendable graphs are simply the connected graphs with perfect matchings. A 1-extendable graph G is such that every edge appears in some perfect matching. 1-extendable graphs are interesting because there are some lower bounds of number of perfect matchings in such graphs.

It is known that n-extendability implies $(n-1)$-extendability [6]. We first establish 2-extendability of a general fullerene graph by combining theorem 1 with the following result [6].

Theorem 2. If G is a cubic, 3-connected planar graph which is cyclically 4-edge connected and has no face of size 4, then G is 2-extendable.

Theorem 3. Every fullerene graph is 2-extendable.

Proof. Follows directly from theorems 1 and 2 and from the definition of fullerene graphs. □

Corollary 4. Every fullerene graph is 1-extendable.

Using the fact that every 1-extendable graph with p vertices and q edges has at least $(q-p)/2+2$ perfect matchings [5], we obtain the following result.

Corollary 5. Every fullerene graph on p vertices contains at least $p/4+2$ perfect matchings.

Proof. As every fullerene graph is cubic, $q = 3p/2$, and the claim follows. □

Even better lower bounds for $\Phi(G)$ are possible. A graph G is *bicritical* if $G-u-v$ has a perfect matching for every pair of distinct vertices $u, v \in V(G)$. A 3-connected bicritical graph is called a *brick*.

For bicritical graphs, the following result holds.

Theorem 6. A bicritical graph G on p vertices contains at least $p/2+1$ different perfect matchings.

The proof of theorem 6 can be found on [5, p. 303]. In the same book, on page 206 we find a result which connects 2-extendable and bicritical graphs.

Theorem 7. Let G be a 2-extendable graph on $p \geqslant 6$ vertices. Then G is either bicritical or elementary bipartite.

(A bipartite graph G is *elementary* if every edge of G appears in some perfect matching of G.)

The bicriticality of fullerene graphs now follows easily.

Theorem 8. Every fullerene graph is a brick.

Proof. As no fullerene graph is bipartite, and all fullerene graphs have at least twenty vertices, we can see that all fullerene graphs satisfy the conditions of theorem 7, and hence are bicritical. The 3-connectedness then makes every fullerene graph a brick. □

Corollary 9. Every fullerene graph on p vertices contains at least $p/2+1$ perfect matchings.

The lower bound $\Phi(G) \geqslant p/2+1$ was established already in [4]. We see that only the bicriticality of a fullerene graph was required. A recently proved conjecture about bricks enabled us to exploit also the fact that every fullerene graph is also a brick. We do not need this result in its full generality, hence we cite the following weaker form.

Theorem 10. In every brick G different from K_4, $\overline{C_6}$ and the Petersen graph, there is an edge $e^\star$ such that $\Phi(G - e^\star) \geqslant q - p$.

Here K_4 denotes the complete graph on 4 vertices, and $\overline{C_6}$ is the complement of C_6, the cycle on 6 vertices.

Theorem 10 is a consequence of a more general result, proved in [7, theorem 3.2].

Now we can establish the best currently known lower bound for $\Phi(G)$.

Theorem 11. Every fullerene graph on p vertices contains at least $p/2 + 4$ perfect matchings.

Proof. Let G be a fullerene graph on p vertices. It obviously satisfies the conditions of theorem 10 (K_4 and $\overline{C_6}$ have 4 and 6 vertices, respectively, and the Petersen graph is nonplanar), so there is an edge $e^\star \in E(G)$ such that $\Phi(G - e^\star) \geqslant q - p = p/2$.

Let us now find out in how many perfect matchings of G the edge $e^\star$ itself appears. Consider the situation shown in figure 2. From 2-extendability of G it follows that each of the four matchings, $\{e', f'\}$, $\{e', f''\}$, $\{e'', f'\}$, $\{e'', f''\}$ extends to a perfect matching in G. Let us denote these perfect matchings by M_1, M_2, M_3 and M_4, respectively. Obviously, no two of them can be equal, and the edge $e^\star$ must appear in all of them, since no other edge can cover the vertex $u^\star$. So, $e^\star$ appears in at least four different perfect matchings of G. The claim now follows from the fact that every perfect matching of G containing the edge $e^\star$ is a perfect matching of $G - u^\star - v^\star$, and the obvious relation $\Phi(G) = \Phi(G - e^\star) + \Phi(G - u^\star - v^\star)$. □

The bicriticality of fullerene graphs has, besides purely mathematical, interesting chemical consequences, too. It means that every bisubstituted derivative of a fullerene still permits a Kekulé structure. It may be of some chemical relevance to investigate

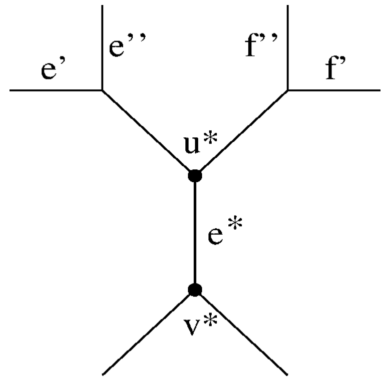

Figure 2. With the proof of theorem 11.

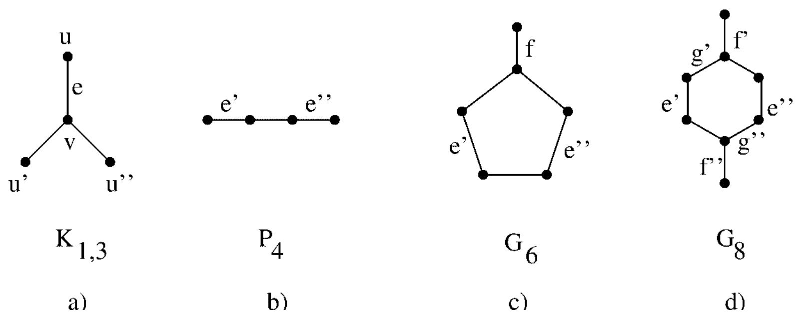

Figure 3. Some nice subgraphs of a fullerene graph.

how far one can carry the substitution process and still retain a Kekulé structure. In other words, we would like to find a broader class of induced subgraphs whose removal from a fullerene graph leaves a graph with a perfect matching. Such subgraphs are said to be *nice*. It is clear that all nice subgraphs must have an even number of vertices.

Theorem 12. The following graphs are nice subgraphs of any fullerene graph:

(a) the graph consisting of two isolated vertices;

(b) K_2, the complete graph on two vertices;

(c) the graph consisting of two disjoint copies of K_2;

(d) $K_{1,3}$ (figure 3(a));

(e) P_4, a path on 4 vertices (figure 3(b));

(f) the "fulvene" graph G_6 (figure 3(c));

(g) the "quinoid" graph G_8 (figure 3(d)).

Proof. The claim (a) follows from bicriticality, the claim (b) from 1-extendability and the claim (c) from 2-extendability of fullerene graphs.

To prove (d), take a vertex $v \in V(G)$ and remove two of its neighbors, say u' and u''. Any perfect matching M in the remaining graph (there is one, since G is bicritical!) must cover the vertex v by the edge e, and it is obvious that $M - e$ is a perfect matching in the graph $G - v - u - u' - u''$.

The claims (e)–(g) follow from the 2-extendability of fullerene graphs. Any perfect matching containing the edges e' and e'' of a path P_4 will also contain a perfect matching of the graph $G - P_4$. Similarly, any perfect matching containing the edges e' and e'' of the graph G_6 must also contain the edge f, and the remaining edges form a perfect matching of $G - G_6$. The same argument proves the claim (g). □

Cyclical connectivity can be defined in terms of vertices, too. A graph G is *cyclically k-connected* if it cannot be separated into two components, each containing a cycle, by removing fewer than k vertices. The following property of fullerene graphs is a consequence of their 3-regularity and cyclical 4-edge connectivity.

Corollary 13. Every fullerene graph G is cyclically 4-connected.

Proof. Take a fullerene graph G and a cut-set $C = \{v_1, v_2, v_3\}$ such that both components, G' and G'' of $G - C$, contain a cycle. There are nine edges emanating from C toward the rest of G. At least three of them must connect C and G'. If there are exactly 3 such edges, we get a contradiction, since G is cyclically 4-edge connected. From the same reason, no component of $G-C$ can be connected with C by more than 5 edges. So, the only remaining possibility is 4 edges from C to one component, say G', and 5 edges to the other component. From there it follows that two vertices of C, say v_1 and v_2, issue one edge each toward G', and the third vertex, v_3, issues two edges toward G'. But now, the two edges between $\{v_1, v_2\}$ and G' and the edge between v_3 and G'' form a set of three edges, whose removal leaves two components, each containing a cycle. we have arrived at a contradiction again, hence G must be at least cyclically 4-connected. □

As a consequence, we get the existence of a Hamilton cycle in all fullerenes with less than 42 vertices. It follows from a result, proved in [8], that every cyclically 4-connected cubic planar graph on at most 40 vertices is Hamiltonian. In the same article it is verified that every 3-connected cubic planar graph with face size at most 6 on at most 176 vertices is Hamiltonian. As the existence of a Hamilton cycle in a general fullerene graph is still an open problem, we find it worthwhile to state this result explicitly.

Corollary 14. Every fullerene graph on at most 176 vertices is Hamiltonian.

For the proof, see [8].

In a planar graph, the existence of a Hamilton cycle is equivalent to the existence of a tree-partition in its dual [9].

A *tree-partition* of a graph G is a partition (V_1, V_2) of $V(G)$ such that both graphs induced by V_1 and V_2 are trees. The tree-partition is *balanced* if $|V_1| = |V_2|$. Not every graph has a tree-partition (for example, K_n for $n \geqslant 5$). The example of two copies of K_4, connected by an edge, shows that the existence or a tree-partition is not guaranteed even in planar graphs.

Theorem 15. Every fullerene graph has a balanced tree-partition.

Proof. The existence of a tree-partition follows via the fact that the dual of a 3-regular cyclically 4-edge connected planar graph is a 4-connected maximal planar graph, and hence has a Hamilton cycle [10]. It remains to prove that this tree-partition is balanced. It follows from [9, proposition 6]. We reproduce here the proof for the convenience of the reader.

Let $G = (V, E)$ be a fullerene graph with a tree-partition (V_1, V_2). Then the graphs $G[V_i]$ induced by V_i are trees, so $G[V_i]$ is connected $(i = 1, 2)$. Define $n := |V|$, $T_i := G[V_i]$, $n_i := |V_i|$. Denote by x_i, y_i and z_i the numbers of vertices in T_i with degree 1, 2 and 3, respectively $(i = 1, 2)$. Then $n_1 + n_2 = n$, $|E| = 3n/2$, $|E(T_i)| = n_i - 1$, for $i = 1, 2$. Because $G[V_i]$ is a tree for $i = 1, 2$, all edges of G not in T_1 or T_2 are between V_1 and V_2, and there are $|E| - (n_1 - 1) - (n_2 - 1) = n/2 + 2$ of them. It is easily seen that the number of edges between T_1 and T_2 is equal to $2x_1 + y_1 = 2x_2 + y_2$. Furthermore, since $n_i \geqslant 2$, $x_i = 2 + z_i$ for $i = 1, 2$, hence,

$$\begin{aligned} n_1 &= x_1 + y_1 + z_1 = x_1 + y_1 + x_1 - 2 = 2x_1 + y_1 - 2 \\ &= 2x_2 + y_2 - 2 = x_2 + y_2 + x_2 - 2 = x_2 + y_2 + z_2 = n_2. \end{aligned}$$

□

Let us now turn our attention to some other graphical invariants of fullerene graphs.

A set $I \subseteq V(G)$ is *independent* if no two vertices from I are adjacent. The cardinality of any biggest independent set in $V(G)$ is called the *independence number* of G and denoted by $\alpha(G)$. A set $S \subseteq V(G)$ is a *point cover* of G if every edge of G has at least one end in S. The *cover number* of G is the cardinality of any smallest vertex cover of G. We denote the cover number of G by $\tau(G)$.

A well known property of bipartite graphs is that the biggest matching and the smallest vertex cover have the same size. This property is called the *König property*. Some nonbipartite graphs also have the König property (e.g., the "fulvene" graph G_6), but the fullerenes are not among them.

Theorem 16. No fullerene graph has the König property.

Proof. Every fullerene graph is a brick, and every brick contains an even subdivision of K_4 or $\overline{C_6}$ in its ear decomposition. But [5, theorem 6.3.7] states that a graph G has the König property if and only if it does not contain a nice subgraph that is an even subdivision of K_4 or an even subdivision of a certain graph on 6 vertices which is a subgraph of $\overline{C_6}$. The claim now follows by combining these results. □

The following bounds are direct consequences of theorem 16.

Corollary 17. For any fullerene graph G on p vertices we have $\tau(G) > p/2$ and $\alpha(G) < p/2$.

The upper bound for $\alpha(G)$ follows from the fact that G has a perfect matching, i.e., is 0-extendable. A better upper bound will follow if the 2-extendability of G is used.

Corollary 18. For any fullerene graph G on p vertices we have

$$\frac{3}{8}p \leqslant \alpha(G) \leqslant \frac{p}{2} - 2.$$

Proof. The right inequality follows from the fact that the independence number of an n-extendable graph cannot exceed $p/2 - n$ [11]. The left inequality was proved in [12] for triangle-free cubic planar graphs, and is hence valid for fullerenes too. □

The upper bound, $\alpha(G) \leqslant p/2 - 2$, cannot be improved for general fullerenes, as the example of C_{20}, the dodecahedral fullerene graph, shows. Regarding the lower bound, there are some results for the fullerenes with isolated pentagons, but we are not aware of any better results valid for all fullerenes.

The following property of independent sets in fullerene graphs is also a consequence of their bicriticality.

Corollary 19. Every nonempty independent set in a fullerene graph has more neighbors than elements.

We conclude our review of fullerene properties by presenting bounds for their saturation number.

A *saturation number*, $s(G)$, of a graph G is the minimum size of a maximal matching in G. (A matching in G is *maximal* if it is not contained in any matching of G of greater cardinality. A perfect matching of $G - u - v$ in a bicritical graph G is an example of a maximal matching in G which is not perfect, assuming the vertices u and v are not adjacent.)

Theorem 20. For every fullerene graph on p vertices,

$$\left\lceil \frac{p}{4} + 1 \right\rceil \leqslant s(G) \leqslant \frac{p}{2} - 2.$$

Proof. The lower bound follows from the 2-extendability of G, using the result, proved in [11], that in an n-extendable graph its saturation number must be at least $\lceil p/4 + n/2 \rceil$.

To prove the upper bound, we construct a maximal matching in G with $p/2 - 2$ edges. Let us refer once more to figure 3(d), and take a perfect matching M containing the edges e', e'', f' and f'' of the graph G_8. Such a matching exists, since G_8 is a nice subgraph of G (theorem 12). By replacing the edges e', e'', f' and f'' in M by the edges g' and g'', we get a matching M' of G which is obviously maximal and its size is $p/2 - 2$. $\square$

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