Journal of Mathematical Chemistry Vol. 33, No. 2, February 2003 (© 2003)

Cyclical edge-connectivity of fullerene graphs and $(k, 6)$-cages

Tomislav Došlić

Department of Informatics and Mathematics, Faculty of Agriculture, University of Zagreb, Svetošimunska c. 25, 10000 Zagreb, Croatia
E-mail: doslic@faust.irb.hr

Received 12 August 2002; revised 12 December 2002

It is shown that every fullerene graph G is cyclically 5-edge-connected, i.e., that G cannot be separated into two components, each containing a cycle, by deletion of fewer than five edges. The result is then generalized to the case of $(k, 6)$-cages, i.e., polyhedral cubic graphs whose faces are only k-gons and hexagons. Certain linear and exponential lower bounds on the number of perfect matchings in such graphs are also established.

KEY WORDS: fullerene graphs, fullerenes, cyclical edge-connectivity, $(k, 6)$-cages, perfect matching

1. Introduction

In a recent series of articles [1–3] it has been shown that all fullerene graphs possess certain structural properties, such as bicriticality and 2-extendability, that further imply certain lower bounds on the number of perfect matchings in such graphs. To prove these properties, it was essential to establish certain lower bounds on the quantity called cyclical edge-connectivity. The main purpose of this paper is to establish the value of cyclical edge-connectivity of fullerene graphs exactly, and thus to solve the problem proposed by Zhang and Zhang in [3]. The same problem is then solved for more general graphs, known as $(k, 6)$-cages, and certain lower bounds on the number of perfect matchings in such graphs are established, following the approach of the paper [1].

For all graph-theoretical terms and concepts used, but not defined here, we refer the reader to any of classical textbooks, such as [4] or [5].

A *fullerene graph* is a planar, 3-regular and 3-connected graph, twelve of whose faces are pentagons, and any remaining faces are hexagons.

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. Obviously, if G is cyclically k-edge connected, it is also cyclically m-edge connected, for all $1 \leqslant m \leqslant k$. Let us denote by $\zeta(G)$ the greatest $k \in \mathbb{N}$ such that G is cyclically k-edge connected, and call this number the cyclical edge-connectivity of G.

0259-9791/03/0200-0103/0 © 2003 Plenum Publishing Corporation

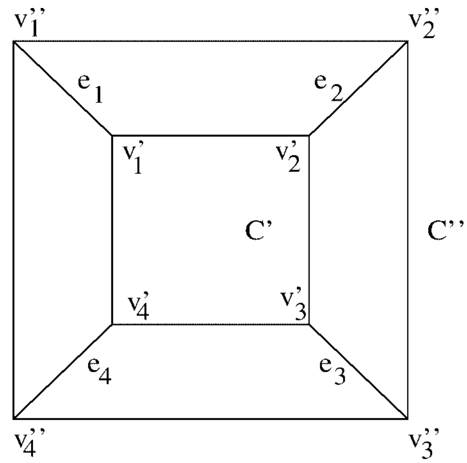

Figure 1. The cycles C' and C'' and the edges connecting them.

From 3-connectedness of fullerene graphs, it follows that $\zeta(G) \geqslant 3$, for every fullerene graph G. This trivial lower bound was improved in [1].

Theorem 1. Let G be a fullerene graph. Then $\zeta(G) \geqslant 4$.

We refer the reader to [1] for a detailed proof of this result.

2. The main result

Theorem 2. Let G be a fullerene graph. Then $\zeta(G) = 5$.

Proof. Obviously, $\zeta(G)$ cannot exceed 5, since by taking a pentagonal face of G, and by deleting 5 edges that connect this face with the rest of G, we obtain two components, and each of them contains a cycle. Combining this fact with theorem 1, it follows that either $\zeta(G) = 4$ or $\zeta(G) = 5$.

Let us suppose that $\zeta(G) = 4$, and let us consider the Schlegel diagram of G. Then there are four edges in G, e_1, e_2, e_3 and e_4, whose deletion separates G into two components, G' and G'', each containing a cycle. Denote the endpoints of e_i in G' and G'' by v_i' and v_i'', respectively, for $i = 1, 2, 3, 4$. Because of 3-connectedness and 3-regularity of G, there are two cycles, C' and C'', such that every edge e_i has one endpoint, say v_i', on C', the other endpoint, v_i'', on C'', and no other edge connects C' with C'' (see figure 1). Namely, each of graphs G' and G'' is 2-connected, and in each of them there is only one face that is not a hexagon or a pentagon. The cycles C' and C'' are exactly the boundary cycles of these exceptional faces in G' and G'', respectively.

As both C' and C'' must be of length at least 5, there must be some additional vertices on each of them. Let us denote the number of these additional vertices on C' and C'' by k' and k'', respectively. Since G is 3-regular and 3-connected, k' (and k'') must

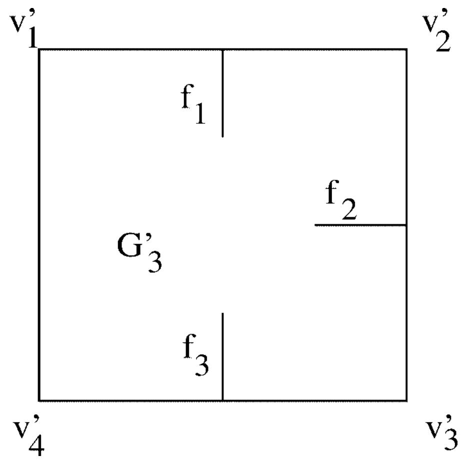

Figure 2. The case $k' = 3$.

be at least 3. (Let us suppose that $k' = 2$. Connecting these two additional vertices by an edge will result in forming either a triangle or a quadrangle, depending on their relative positions on C'. On the other hand, if these vertices are not connected by an edge, then there is a subgraph, denote it by G_2', that is fully contained in the interior of C'. But then, removing the two additional vertices from C' would disconnect G_2' from the rest of the graph, and this is in contradiction with 3-connectedness of G. Hence, the possibility $k' = 2$ must be dismissed.) Thus, $k' + k'' \geqslant 6$. On the other hand, $k' + k'' \leqslant 8$, because it is not possible to place more than 8 additional vertices on C' and C'', placing at least 3 on each of them, without forming a face of G with more than 6 sides.

Let us suppose that $k' = 3$. Consider the subgraph G_3' of G shown in figure 2. Denote by V', E' and F' the number of vertices, edges and faces of this subgraph, respectively.

We have $V' = 7 + r$, where r is the number of vertices of G that are in the interior of C'. Since all of them are of degree 3, we obtain $E' = (3r + 17)/2$. From the Euler formula, $V' - E' + F' = 2$, we then obtain that $F' = (r + 7)/2$, and hence, $F' \geqslant 4$. The only way to have $F' = 4$ is to have only one vertex of G in the interior of C'. Then this vertex must be the common endpoint of edges f_1, f_2 and f_3, and G must contain at least one quadrangle (or even worse, a triangle in the case when two of three additional vertices on C' are on the same side). Hence, r must be at least 3. But in this case, G_3' will have at least 5 faces, and at least one of them will contain only vertices of G that are in the interior of C'. Now, by deletion of edges f_1, f_2 and f_3, we obtain two components of G, and each of them contains a cycle, in contradiction with theorem 1. Since our reasoning does not depend on the way the additional $k' = 3$ vertices are distributed on C', we may conclude that the case $k' = 3$ is not possible. Hence, $k' \geqslant 4$.

Applying the same reasoning on C'', we obtain $k' = k'' = 4$.

Let us now consider the subgraph G_4' of G, shown in figure 3. This subgraph has four vertices of degree 2, four additional vertices of degree 3, and an even number of

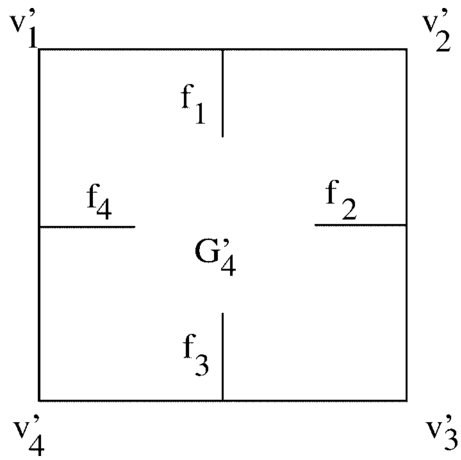

Figure 3. The case $k' = 4$.

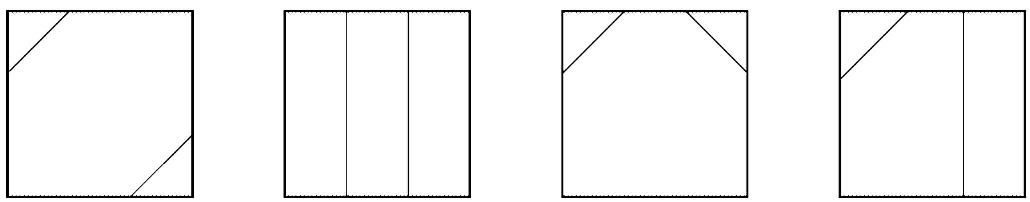

Figure 4. The case $r = 0$.

vertices of G that are in the interior of C', all of them of degree 3. Denoting again by V', E' and F' the number of vertices, edges and faces of G'_4, respectively, and applying the Euler formula, we obtain $8 + r - (3r + 20)/2 + F' = 2$, or $F' = (r + 8)/2$. If we take $r = 0$, there are four possible ways of connecting the four additional vertices on C' that respect the planarity, 3-regularity and 3-connectedness of G (see figure 4). (All notations in figures 4 and 5 have been suppressed for the sake of clarity. The cycle C' is represented by the sides of the outer square, and additional vertices, if any, by the points where two lines meet.) Obviously, each of those four ways generates at least one triangle or a quadrangle. Hence, r must be at least 2. Assuming $r = 2$, we get one of the seven possibilities shown in figure 5. Obviously, none of these graphs can be a subgraph of a fullerene graph, so the possibility $r = 2$ must be ruled out.

Hence, there must be at least four vertices of G in the interior of C'. But in this case $F' \geqslant 6$, and at least one of these faces is completely defined by the vertices of G in the interior of C'. Invoking again 3-connectedness and 3-regularity of G, we get that there must exist a cycle, say C'_1, that contains the endpoints of the edges f_1, f_2, f_3 and f_4. Now we have a situation similar to the one we started with, and we can apply the same reasoning to the cycle C'_1. Because of finiteness of G, after a finite number of steps, say n, we will obtain a cycle C'_n which will have no more that 2 vertices of G in its interior. Since we have just proved that a fullerene graph cannot contain such a subgraph, it follows that $\zeta(G)$ cannot be 4. Hence, $\zeta(G) = 5$. □

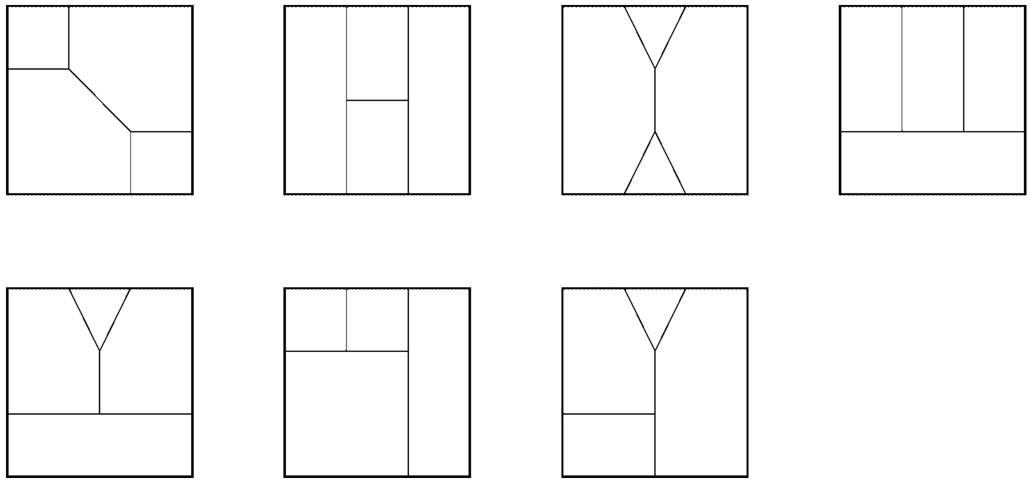

Figure 5. The case $r = 2$.

3. $(k, 6)$-cages

Fullerene graphs form a subclass of a more general class of graphs, called $(k, 6)$-cages.

Let $k \geqslant 3$ be an integer. A $(k, 6)$-*cage* is a 3-regular, 3-connected planar graph whose faces are only k-gons and hexagons.

Obviously, fullerenes are (5, 6)-cages. An example of a (3, 6)-cage is the Schlegel diagram of a truncated tetrahedron. Similarly, the Schlegel diagram of a truncated octahedron serves as a canonic example of a (4, 6)-cage. The values $k = 3, 4$ and 5 are the only values of k for which $(k, 6)$-cages exist.

Proposition 3. If a $(k, 6)$-cage exists, then $k = 3, 4$ or 5.

Proof. If a $(k, 6)$-cage exists, it must have an integer number, say $m(k)$, of k-gonal faces. If we denote the number of hexagonal faces by $n(k)$, the total number of faces is $m(k) + n(k)$, the number of vertices is $(km(k) + 6n(k))/3$, and the number of edges is given by $(km(k) + 6n(k))/2$. Substituting these values into the Euler formula, we obtain $m(k) = 12/(6 - k)$. The only values of $k \geqslant 3$ that yield integer $m(k)$ are 3, 4 and 5, and the corresponding values of $m(k)$ are 4, 6 and 12, respectively. □

Remark. We may extend our definition of a $(k, 6)$-cage to the case $k = 2$, if we are willing to consider non-simple graphs, but in this case we have to drop the condition of 3-connectedness. An example of a so defined (2, 6)-cage is shown in figure 6.

Let us consider a tubular structure whose Schlegel diagram is shown in figure 7. (For the sake of symmetry, it is shown as seen from one of its vertices.) It con-

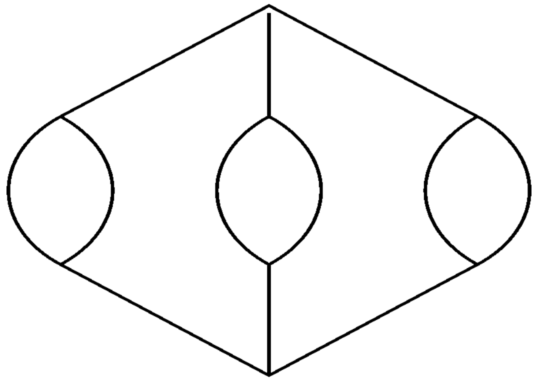

Figure 6. A $(2, 6)$-cage.

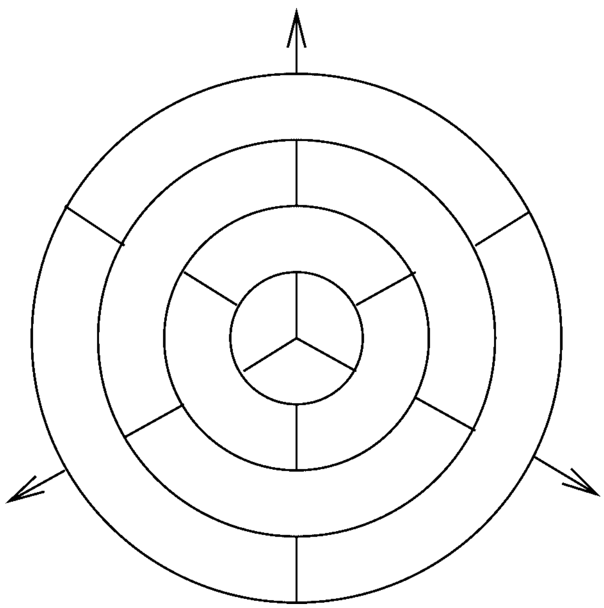

Figure 7. A tubular $(4, 6)$-cage with two caps.

sists of three concentric layers of hexagons, capped on each end by a cap formed by three quadrangles. Obviously, this structure is a $(4, 6)$-cage. Let us denote such tubular $(4, 6)$-cage with n layers of hexagons by T_n, and the family of all such tubes by $\mathcal{T} = \bigcup_{n \geqslant 1} T_n$. (In the degenerate case $n = 0$, we get the ordinary cube.) Obviously, the cyclical edge-connectivity of a member of $\mathcal{T}$ does not depend on n, and equals 3. (It is enough to remove any three radial edges in the same hexagonal layer.) So, it is possible for a $(4, 6)$-cage G to have the cyclical edge-connectivity strictly less than 4. It turns out that only such $(4, 6)$-cages are exactly the members of $\mathcal{T}$.

Lemma 4. Let G be a (4, 6)-cage with $\zeta(G) = 3$. Then $G \in \mathcal{T}$.

Proof. We proceed along the same lines as in the proof of theorem 2. Let us denote by e_1, e_2 and e_3 any three edges whose removal separates G into two cycle-containing components. Then there must be two cycles, C' and C'' in G such that each e_i has one endpoint on C', the other endpoint on C'', and no other edge connects C' and C''. Since G is a (4, 6)-cage, there must be additional vertices on each C' and C'', and by the same reasoning as in theorem 2, we conclude that there must be exactly three additional vertices on each of them. Consider the inner cycle, say C'. We have three edges, e'_1, e'_2 and e'_3, emanating from C' toward its interior. These three edges either have a common endpoint, or their endpoints are on another cycle, C'_1. The second possibility means that the whole situation is repeated in the interior of C', and this can happen only finitely many times. So, after finitely many steps we will get a cycle, C'_m, such that there is only one vertex of G in its interior, and this vertex will serve as the top of a cap characteristic for the family $\mathcal{T}$. Applying the same reasoning to the exterior of C'', after finitely many steps we will arrive at a cycle, say C''_l, with only one vertex of G in its exterior. From there we can conclude that $G = T_{m+l+1}$, hence, $G \in \mathcal{T}$. □

Now we may state the complete solution to the problem of cyclical edge-connectivity of $(k, 6)$-cages.

Theorem 5. Let G_k be a $(k, 6)$-cage, $G_k \notin \mathcal{T}$. Then $\zeta(G_k) = k$.

Proof. The case $k = 5$ follows from theorem 2. Since all $(k, 6)$-cages are 3-connected, they are also 3-edge-connected, so $\zeta(G_k)$ is at least 3. On the other hand, $\zeta(G_k) \leqslant k$, since it suffices to remove any k edges connecting a k-gonal face of G_k to the rest of the graph. This settles the case $k = 3$. The case $k = 4$ follows from $\zeta(G_k) \leqslant k$ and from lemma 4. □

We may observe that the results of theorem 5 remain valid also for the degenerate case $k = 2$.

Thus, the fullerene graphs have the greatest cyclical edge-connectivity of all $(k, 6)$-cages. It would be interesting to determine the exact values of cyclical edge-connectivity for $(k, 5)$-cages; it is known that there are such cages, such as the (8, 5)-cage shown in figure 1 of [2], that have the minimal possible cyclical edge-connectivity of 3.

We may now take our reasoning one step further, and consider all *simple polyhedra*, i.e., all 3-regular, 3-connected planar graphs. Such graphs have been also called trivalent carbon cages in [6].

Theorem 6. Let H be a simple polyhedron. Then $\zeta(H) \leqslant 5$.

Proof. Let H be a simple polyhedron with $m(k)$ k-gonal faces. Then H has $(\sum_{k\geqslant 3} km(k))/3$ vertices, and from the Euler formula we obtain $\sum_{k\geqslant 3}(6-k)m(k) = 12$.

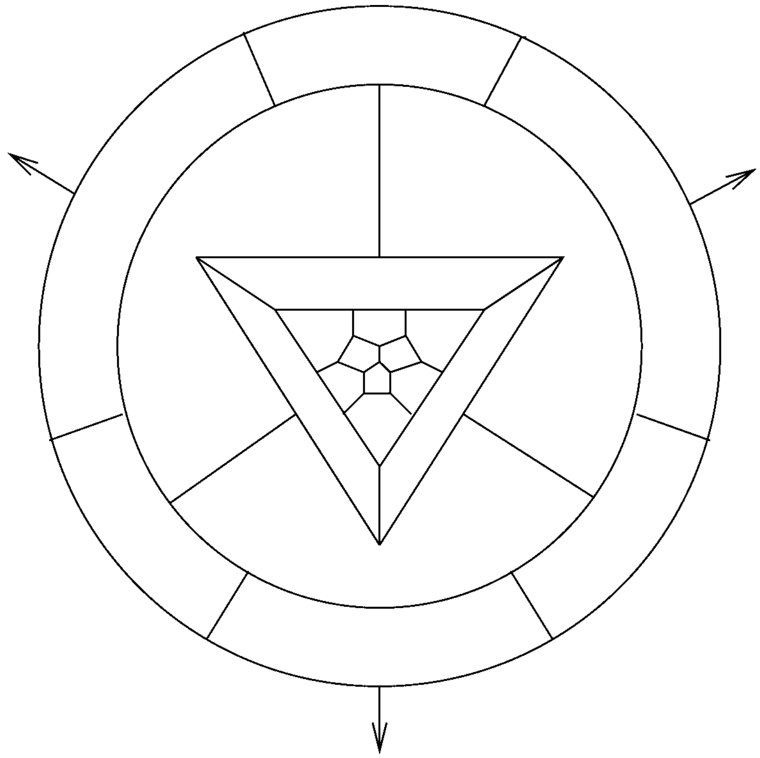

Figure 8. A generalized fullerene with $\zeta(G) = 3$.

Supposing $m(k) = 0$ for $3 \leqslant k \leqslant 5$, the left-hand side of this equality becomes non-positive, and this is a contradiction. Hence, H must contain at least one face that is connected with the rest of H by $l \leqslant 5$ edges. Removing these l edges, we obtain two components, each containing a cycle. Thus, $\zeta(H) \leqslant l \leqslant 5$. □

So, a fullerene is at least as difficult to tear apart into two cycle-containing components as any other simple polyhedron. For non-simple polyhedra this is not true. (A polyhedron is non-simple if it contains a vertex where more than three edges meet.) For example, $\zeta(I) = 9$, and $\zeta(A_n) = 6$, where I is the icosahedron, and A_n is the n-sided anti-prism.

Before we leave the topic of cyclical edge-connectivity, let us add a short remark about generalized fullerenes that contain heptagonal faces. A *generalized fullerene* is, hence, a 3-regular, 3-connected planar graph whose faces are pentagons, hexagons and heptagons. If we denote by $m(k)$ the number of k-gonal sides, from the Euler formula it follows that $m(5) - m(7) = 12$. Unlike the ordinary fullerenes, generalized fullerenes are not, in general, cyclically 5-edge-connected. An example of a generalized fullerene with 18 pentagons, 3 hexagons and 6 heptagons that is only cyclically 3-edge-connected is shown in figure 8. Hence, cyclical edge-connectivity cannot be used to establish lower bounds on the number of perfect matchings in generalized fullerenes analogous to those from [1] and [3]. At the moment, no better lower bounds are known for generalized fullerenes than for any other simple polyhedra (see theorem 10).

We conclude by few remarks concerning enumeration of perfect matchings in $(k, 6)$-cages and simple polyhedra. As we have already mentioned in the introduction, cyclical edge-connectivity played an essential role in establishing [1] and improving [3] linear (in terms of number of vertices) lower bounds on the number of perfect matchings in fullerenes. We are not aware of any such results for general $(k, 6)$-cages. Although the approach of [1] and [3] cannot be fully extended to the case of $(k, 6)$-cages, it may be worthwhile to follow it as far as it is possible. Let us denote the number of different perfect matchings in a graph G by $\Phi(G)$.

A graph G is 1-*extendable* if every edge of G is contained in some perfect matching of G. For a 1-extendable graph G on p vertices and q edges, we have $\Phi(G) \geqslant (q - p)/2 + 2$ (cf. [1, theorem 4]). If G is also 3-regular, then $q = 3p/2$, and hence, $\Phi(G) \geqslant p/4 + 2$.

Theorem 7. Let G be a $(k, 6)$-cage. Then G is 1-extendable.

Proof. As G is a 3-regular and 2-edge-connected graph on an even number of vertices, the claim follows by applying [1, theorem 3]. □

Corollary 8. Let G be a $(k, 6)$-cage on p vertices. Then $\Phi(G) \geqslant p/4 + 2$.

We are not aware of any better lower bounds valid for $k = 3$. However, for the case $k = 4$, we may observe that $(4, 6)$-cages are bipartite, and then apply [5, theorem 8.1.7] to prove the following lower bound.

Theorem 9. Let G be a $(4, 6)$-cage on p vertices. Then $\Phi(G) \geqslant (4/3)^{p/2}$.

Note that the lower bound of theorem 9 is *exponential* in number of vertices. Although exponential lower bounds for $\Phi(G)$ can be also proved for some classes of fullerene graphs, no such lower bound is known in the general case.

The reasoning from the proof of theorem 7 applies also to the case of simple polyhedra.

Theorem 10. Let G be a simple polyhedron on p vertices. Then $\Phi(G) \geqslant p/4 + 2$.

Thus, theorem 10 improves the lower bound of $\Phi(G) \geqslant 3$ from [6, theorem A]. We are not aware of similar lower bounds for non-simple polyhedra.

References

[1] T. Došlić, On lower bounds of number of perfect matchings in fullerene graphs, J. Math. Chem. 24 (1998) 359–364.

[2] T. Došlić, On some structural properties of fullerene graphs, J. Math. Chem. 31 (2002) 187–195.

[3] H. Zhang and F. Zhang, New lower bound on the number of perfect matchings in fullerene graphs, J. Math. Chem. 30 (2001) 343–347.
[4] D.B. West, *Introduction to Graph Theory* (Prentice Hall, Upper Saddle River, NJ, 1996).
[5] L. Lovász and M.D. Plummer, *Matching Theory*, Ann. Discr. Math., Vol. 29 (North-Holland, Amsterdam, The Netherlands, 1986).
[6] D.J. Klein and X. Liu, Theorems for carbon cages, J. Math. Chem. 11 (1992) 199–205.