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Importance and Redundancy in Fullerene Graphs

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The concept of importance of an edge in a fullerene graph has been defined and lower bounds have been established for this quantity. These lower bounds are then used to obtain an improved lower bound on the number of perfect matchings in fullerene graphs.

Key words: fullerene graphs, fullerenes, perfect matchings, enumeration.

INTRODUCTION

In recent years, polyhedral elemental carbon cages, also known as fullerenes, have become an area of intensive scientific research.[1] This development was followed by a rise of interest in the underlying graphs.[2–5] Apart from serving as mathematical models for fullerene molecules, these graphs also pose some mathematically interesting questions, the answers to which, in turn, may be relevant to the chemistry of the corresponding fullerene species. In this paper, we take further the line of research of our previous paper,[5] using some structural properties of fullerene graphs established there, and combining them with some elements of the structural theory of matchings in order to obtain an improved lower bound on the number of perfect matchings in fullerene graphs. We refer the reader to the cited monograph[6] for a detailed exposition of the structural theory of matchings, and also for all terms and concepts not explicitly defined here.

GRAPH – THEORETICAL PRELIMINARIES

All graphs considered here will be finite, simple and connected, with p vertices and q edges. For a given graph G, we denote by V(G) and E(G) the sets of its vertices and edges, respectively.

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

A matching M in a graph G is a set od 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 to some edge $e \in$ M, is covered by the matching M. Matching M is perfect if it covers every vertex of G.

Perfect matchings are known in chemistry as Kekulé structures. As the number of Kekulé structures of a chemical compound is often correlated with its stability, it may be of interest to find the number of different perfect matchings in the corresponding graph. However, the problem of counting matchings in graphs is a hard one, and exact results are only rarely at our disposal. Therefore, it makes sense to search for non-trivial upper and lower bounds on these quantities.

A remark is in order here on the exact meaning of the term »hard«. Fullerene graphs are planar, and for any particular fullerene graph G, Kasteleyn's method will yield the number of perfect matchings in G in polynomial time. However, this method provides only particular results; it enables us to make conjectures about the relationship between the size of a graph G and the number of different perfect matchings in G, but it does not help us to prove these conjectures. Thus, even for planar graphs, unless they have a very special structure, it remains hard to find exact results on the number of perfect matchings that are valid for all members of a given class.

We denote the number of different perfect matchings of a graph G by Φ(G).

Every fullerene graph has a perfect matching; this follows from the classical Petersen result that every connected cubic graph with no more than two cut-edges has a perfect matching. Also, it can be shown that every edge e of a fullerene graph G is contained in at least one perfect matching of G. This is a corollary of Theorem 3.4.2 from p. 111 of Ref. 6.

A graph G whose every edge e appears in some perfect matching of G is called 1-extendable, since every matching of size 1 can be extended to a perfect matching. If every matching of size 2 in G can be extended to a perfect matching of G, we say that G is 2-extendable.

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, since such graphs serve as basic building blocs in certain decomposition/construction procedures of the structural theory of matchings.

A subgraph H of a graph G is nice if G – V(H) has a perfect matching. In other words, a subgraph is nice if its removal from a graph leaves a graph with a perfect matching. It is obvious that all nice subgraphs of a graph with a perfect matching must have an even number of vertices.

The following structural properties have been established[5] for all fullerene graphs:

Theorem 1. Every fullerene graph G is 2-extendable.

Theorem 2. Every fullerene graphs G is a brick.

We shall also need the following result.

Theorem 3. Let G be a k-connected non-bicritical graph containing a perfect matching. Then, G contains at least $k!$ perfect matchings.

Theorem 3 here is Theorem 8.6.2 of monograph,[6] for a proof, the reader can consult pages 346–348 of this reference.

IMPORTANCE, REDUNDANCY AND LOWER BOUNDS

Let us consider a graph G with a perfect matching, and an edge e of G with the end-vertices u and v. If we want to count perfect matchings in G, and if e does not appear in any of them, we may rightly conclude that the edge e is not important for our purpose. Motivated by this observation, we define the importance $\iota(e)$ of e in G as the number of perfect matchings of G that contain e. Similarly, for an edge e of G we define its redundancy, $\rho(e)$, as the number of perfect matchings of G that do not contain e. More formally,

$$\iota(\mathrm{e}) = \Phi(\mathrm{G} - u - v), \qquad \rho(e) = \Phi(\mathrm{G} - e).$$

The non-important edges are usually called forbidden edges, and the edges with non-zero importance are called allowed. Thus, the concept of importance is a quantitative refinement of the concept of allowedness from the structural theory of matchings.

It is worthwhile to note that similar concepts have already made their appearance in chemistry. By dividing $\iota(e)$ by the total number of perfect matchings in G, we obtain a quantity that has been termed Pauling bond order of the edge e. A concept similar to our importance has been also considered[7] in the context of the moments of inertia of random matchings in honeycomb (or benzenoid) graphs. In the theory of benzenoid graphs, a graph without non-important edges is called normal. If a benzenoid graph with a perfect matching contains some non-important edges, such edges are called fixed single bonds, and the graph is called essentially disconnected, since removal of all non-important edges leaves a disconnected graph. In fact, this is valid for all connected bipartite graphs with perfect matchings:[6] either all edges of such a graph are important, or the removal of all non-important edges leaves a disconnected graph. Thus, importance is implicitly present at the basis of one benzenoid classification scheme, the so called *neo* classification.[8] An example of an essentially disconnected benzenoid graph with two non-important edges, *e* and *f*, is shown in Figure 1.

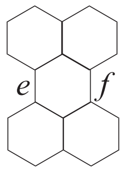


Figure 1. An essentially disconnected benzenoid graph.

As the exact values of numbers $\iota(e)$ and $\rho(e)$ may be difficult to establish, in what follows we shall use lower bounds for these quantities.

Obviously, fullerene graphs, being 1-extendable, do not contain non-important edges. From Theorem 3 it follows that $\iota(e) \geq 2$ for any edge e of a fullerene graph G, since $G - u - v$ has a perfect matching and is also 2-connected. It has been recently shown[5] that $\iota(e) \geq 4$. Here we follow the same line of reasoning and combine it with Theorem 3 in order to double this lower bound.

Lemma 4. $\iota(e) \geq 8$, for any edge e of a fullerene graph G.

Proof. Let us take an edge e of a fullerene graph G. Consider the situation shown in Figure 2. From 2-extendability of G it follows that each of the

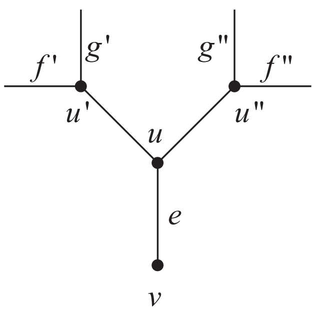


Figure 2. With the proof of Lemma 4.

four matchings, $\{f', f''\}$, $\{f', g''\}$, $\{g', f''\}$ and $\{g', g''\}$, extend to a perfect matching in G. Let us denote these perfect matchings by M_{ff}, M_{fg}, M_{gf} and M_{gg}, respectively. Obviously, no two of them can be equal, and the edge e must appear in all of them, since no other edge can cover the vertex u. We say that the edge e is forced in all these matchings. There may be some other forced edges besides e. We denote by F_{ij} the set of all edges that are forced in the matching M_{ij}, where $i,j \in \{f,g\}$. Obviously, F_{ij} is a nice subgraph of G for any $i,j \in \{f,g\}$.

The claim of the Lemma will follow if we prove that F_{ij} is reasonably small and that $G - V(F_{ij})$ is 2-connected for any choice of e and for any $i,j \in \{f,g\}$.

The edge e can appear in any of the six configurations shown in Figure 3.

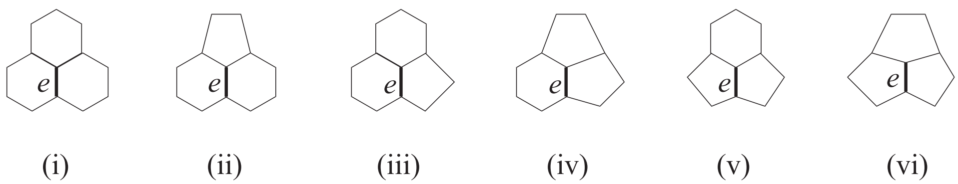


Figure 3. Possible configurations around the edge e.

We proceed by considering each of these configurations separately. The forced edges are shown in bold for these different configurations case by case:

(i) It is obvious from Figure 4 that $G - V(F_{ij})$ is 2-connected for any choice of edges $i,j \in \{f,g\}$.

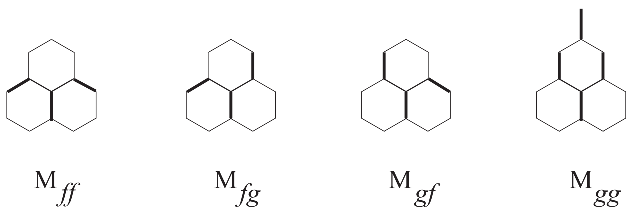


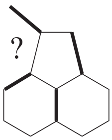
Figure 4. With case (i).

(ii) There are no problems with M_{ff} and M_{gg}. As can be seen in Figure 5, the graphs $G - V(F_{ff})$ and $G - V(F_{gg})$ are both 2-connected.

M_{ff} M_{gg}

Figure 5. With case (ii).

Let us consider the choice M_{fg}. The situation is shown in Figure 6. If the face denoted by ? is a hexagon, we have the situation from Figure 7 (a). There are 4 forced edges in F_{fg} and $G - V(F_{fg})$ is 2-connected. If the face ? from Figure 6 is a pentagon, we get the situation shown in Figure 7 (b).



M_{fg}

Figure 6. Possible problems with the face ?.

a) b)

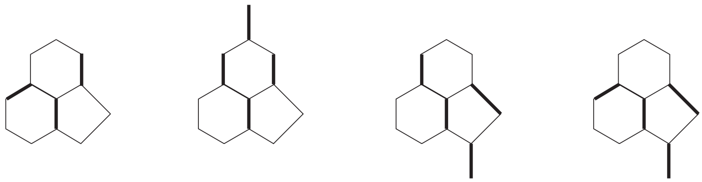
Figure 7. Possible configurations with regard to face ?.

One more edge is forced, $|F_{fg}| = 5$, and $G - V(F_{fg})$ is 2-connected. The choice M_{gf} now follows by symmetry.

(iii) It is obvious from Figure 8 that $G - V(F_{ij})$ is 2-connected for all choices.

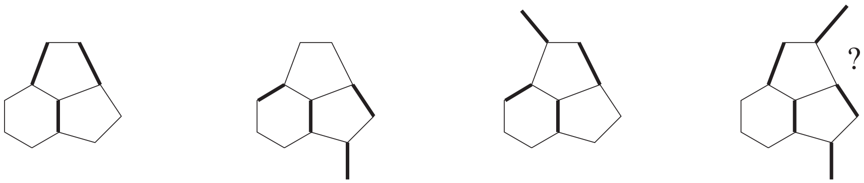
(iv) Choices M_{gg} and M_{ff} are obvious from Figure 9, and for choice M_{fg} we apply the same reasoning as for choice M_{fg} of configuration (ii).

Choice M_{gf} is the most complicated one in the whole analysis. If the face denoted by ? is a hexagon, we have the situation shown in Figure 10 (a).



M_{fg} M_{gg} M_{gf} M_{ff}

Figure 8. With case (iii).



M_{gg} M_{ff} M_{fg} M_{gf}

Figure 9. With case (iv).

$|F_{gf}| = 5$, no further forcing of edges occurs, and $G - V(F_{gf})$ is 2-connected. However, if the face ? is a pentagon, a futher edge is forced and we get the situation from Figure 10 (b). Now the face denoted by ?? becomes relevant. If this face is a pentagon, no further forcing of edges occurs, and $G - V(F_{gf})$

a) b)

Figure 10. Possible situations with the face ?.

is 2- connected, as it can be seen from Figure 11 (a). If the face ?? is a hexagon, one more edge, denoted by h in Figure 11 (b), is forced. Now, $|F_{gf}| = 7$ and $G - V(F_{gf})$ is again 2-connected.

Figure 11. Possible situations with the face ??.

(v) We can see from Figure 12 that the only problematic choice is M_{ff}. If the face denoted by ? is a pentagon, there are no more forced edges, and if the face ? is a hexagon, one more edge is forced. In both cases, $G - V(F_{ff})$ is 2- connected, as it can be seen from Figures 13(a) and (b), respectively.

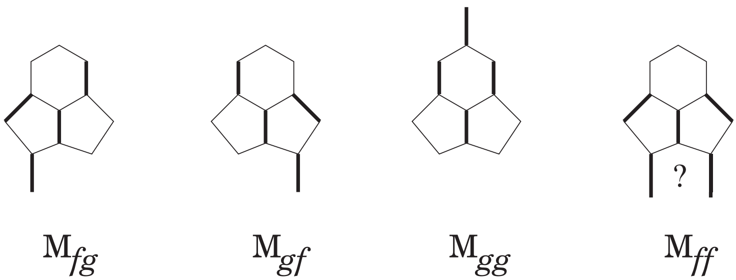


Figure 12. With case (v).

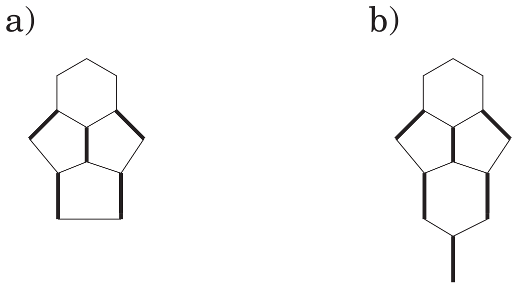


Figure 13. Possible situations with the face ?.

(vi) This case is shown in Figure 14. The choice M_{gg} is obvious. the choice M_{ff} is essentially the same as the choice M_{ff} of (v). For the choice M_{gf} the

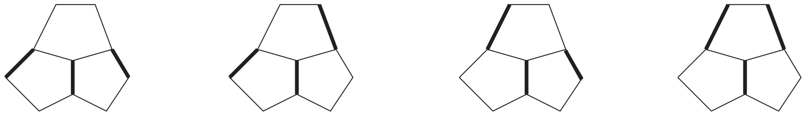


Figure 14. With the case (vi).

same discussion is valid as for the choice M_{gf} of (iv), and the choice M_{fg} then follows by the symmetry of configuration (vi). So, $G - V(F_{ij})$ is 2-connected for all choices.

Hence, regardless of the configuration in which the edge e appears, it is always possible to extend any of the matchings $\{f',f'',e\}$, $\{f',g'',e\}$, $\{g',f'',e\}$ and $\{g',g'',e\}$ to a perfect matching of G in at least two different ways. Consequently, the edge e appears in at least 8 different perfect matchings of G and hence the claim.

The case-by-case analysis of Lemma 4 can be made simpler if we restrict our attention to certain subsets of fullerenes. For instance, for the subset of isolated-pentagon fullerenes, only cases (i) – (iii) are possible. However, the results remain essentially the same.

Let us now turn our attention to redundancy. The following result on redundancy of an edge in a fullerene graph is a corollary of a much stronger result[5,9] concerning general bricks.

Lemma 5. In every fullerene graph G on p vertices there is an edge e* such that $\Phi(G - e^*) \geq p/2$.

Our main result follows now easily by combining the preceding two Lemmas.

Theorem 6. Every fullerene graph G on p vertices contains at least $p/2$ + 8 different perfect matchings.

Proof. For any edge e of G we have $\Phi(G) = \iota(e) + \rho(e)$. From Lemma 5, there is an edge e^* with $\rho(e^*) \geq p/2$, and from Lemma 4, we know that $\iota(e^*) \geq 8$.

We conclude by noting that for some edges of G it is possible to prove better the lower bound of their importance.

Corollary 7. In every fullerene graph G on p vertices there are at least two edges with importance at least $\lceil p/4 \rceil$.

Proof. Let e^* be an edge of G such that $\rho(e^*) \geq p/2$. Consider the situation from Figure 15. Since there are only two edges, f' and g', available to cover the vertex u', at least one of them must appear in at least half of the perfect matchings of $G - e^*$. The same reasoning is valid for the edges f'' and g'', and the claim follows.

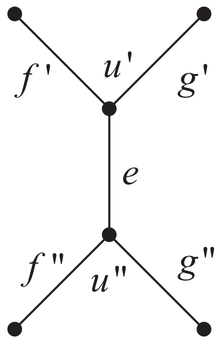


Figure 15. With the proof of Corollary 7.

As a final remark, we add that the recent result[10] $\Phi(G) \geq [3(p + 2)/4]$ can be also easily obtained using the concept of edge-importance.

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SAŽETAK

O važnosti i zalihosti u fullerenskim grafovima

Tomislav Došlić

Definiran je pojam važnosti brida u fullerenskom grafu i ustanovljene su donje ograde za tu veličinu. Te su ograde zatim iskorištene za dobivanje poboljšane donje ograde broja savršenih sparivanja u fullerenskim grafovima.