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On lower bounds of number of perfect matchings in fullerene graphs

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Couting perfect matchings in graphs is a very difficult problem. Some recently developed decomposition techniques allowed us to estimate the lower bound of the number of perfect matchings in certain classes of graphs. By applying these techniques, it will be shown that every fullerene graph with p vertices contains at least $p/2 + 1$ perfect matchings. It is a significant improvement over a previously published estimate, which claimed at least three perfect matchings in every fullerene graph. As an interesting chemical consequence, it is noted that every bisubstituted derivative of a fullerene still permits a Kekulé structure.

The recently proposed [3] and subsequently verified truncated icosahedral structure of carbon species C_{60} has given birth to rise of scientific interest in theoretical research of the underlying graphs. Here it will be shown how some results, regarding numbers of perfect matchings in such graphs, can be obtained using elements of the structural theory of matchings, explained in [4]. All terminology and notations used in this article will be the same as in [4] if not stated otherwise.

Definition 1. 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 known under various names, such as *trivalent carbon cages* in chemical literature and $G_3(5, 6)$ in mathematical literature.

Definition 2. A *matching* M in graph G is a set of edges of G such that no two edges from M have a point in common. Point $v \in V(G)$ incident with some edge from M is *covered* by matching M. Matching M is *perfect* if it covers every point of G.

A perfect matching is in chemistry called a *Kekulé structure*.

The existence of a perfect matching in fullerene graph is an easy corollary of a classical result of Petersen [5]:

Theorem 1. Every connected 3-regular graph with no more than two cut-edges has a perfect matching.

It is obvious that every fullerene graph satisfies the conditions of theorem 1.

Motivated by the established correlation between the stability of benzenoid systems and the number of perfect matchings in underlying graphs, an interesting question arises: How many different perfect matchings does a given fullerene graph contain? Let us denote this number by $\Phi(G)$.

Unlike the problem of finding a perfect matching in a given graph which is, in algorithmical sense, an "easy" one, the problem of *counting* perfect matchings is very difficult. Hence, we are interested in establishing *bounds* and *estimates* of a number of perfect matchings in terms of various graph parameters (number of points, number of edges, connectedness, etc.).

Starting from the fact that every fullerene graph is 3-connected and using the methods of *Cathedral construction* (fully explained in [4, p. 166]), we can obtain the following lower bound for $\Phi(G)$:

Theorem 2. Every fullerene graph contains at least three different perfect matchings.

The bound from theorem 2 has been already published [2], but the result was established by using the Four-Color theorem. This assumption is not necessary in obtaining this result by Cathedral construction.

The bound just established is not very sharp. This is not surprising, because only 3-connectedness of fullerene graphs was used. Much better bounds can be obtained using other structural qualities of fullerene graphs.

Assuming the Four-Color theorem, it was noted in [2] that every edge in a fullerene graph G appears in some perfect matching of G. This fact can be established without resorting to the Four-Color theorem using the following result:

Theorem 3. If G is an r-regular, $(r-1)$-edge connected graph on an even number of points, then every edge of G is contained in a perfect matching of G.

Theorem 3 is a corollary of Plesník's result, the proof of which can be found in [4, p. 111].

Definition 3. Graph G is *1-extendable* if every edge of G appears in some perfect matching of G.

Using theorem 3 and this definition, we can conclude that every fullerene graph, being 3-regular and 3-edge connected, is 1-extendable.

1-extendable graphs deserve special attention because they permit *ear decomposition*. More details about ear decomposition can be found in [4, pp. 174–195].

Definition 4. Let G be a graph and G' subgraph of G. *An ear of G relative to G'* is any odd-length path in G having both endpoints – but no interior point – in G'. *An ear decomposition of G starting with G'* is a representation of G in the form

$G = G' + P_1 + \cdots + P_k$, where P_1 is an ear of $G' + P_1$ relative to G', and P_i is an ear of $G' + P_1 + \cdots + P_i$ relative to $G' + P_1 + \cdots + P_{i-1}$ for $2 \leqslant i \leqslant k$.

An ear decomposition of a given graph is not unique.

It can be shown that every 1-extendable graph permits an ear decomposition starting with any given edge of this graph. However, if we want that every intermediate graph in an ear decomposition of an 1-extendable graph be itself 1-extendable, we may have to add more than one ear at a time.

Definition 5. A subgraph G' of any graph G is *nice* if $G - V(G')$ has a perfect matching.

Definition 6. Let G be any graph and G' a subgraph of G. *An ear system of G relative to G'* is a set of point-disjoint paths in G of odd length each of which is openly disjoint from G', but has both endpoints in G'. A sequence of subgraphs of G, $(G_0, G_1, \ldots, G_m)$ is a *graded ear decomposition of G starting with G_0* if $G = G_m$, every G_i for $i = 0, \ldots, m$ is a nice 1-extendable subgraph of G and for each i, G_{i+1} is obtained from G_i by attaching an ear system relative to G_i. Integer $m + 1$ is a *length* of the decomposition.

Every 1-extendable graph has a graded ear decomposition starting with any given edge of this graph [4, p. 176]. 1-extendability of intermediate graphs $G_1, \ldots, G_{m-1}$ is important because it implies that upon attaching an ear system to the graph G_i we obtain graph G_{i+1} with $\Phi(G_{i+1}) > \Phi(G_i)$. (Every perfect matching of G_i can be extended to the perfect matching of G_{i+1} by taking every second, fourth and so on edge on every ear attached to the G_i. But 1-extendability of G_{i+1} implies that there has to be at least one perfect matching of G_{i+1} which contains odd-numbered edges on ears attached to the G_i. Such a matching, restricted to the graph G_i, leaves endpoints of the ears uncovered, so it cannot be a perfect matching of G_i.)

Since each ear is a path with one more point than edge, one can conclude that the number of ears (but not the number of ear systems) in an ear decomposition of a given 1-extendable graph is always equal to $q - p + 2$, where the starting edge is counted as the first ear, and p and q are numbers of points and edges in this graph, respectively. As each ear system adds one more perfect matching to the already constructed graph, it is possible to obtain a lower bound for $\Phi(G_i)$ by finding the longest ear decomposition of G. An important result, called the Two-Ear theorem [4, p. 182] states that it is always possible to find a graded ear decomposition of a 1-extendable graph in which each ear system, except the first two, contains at most two ears. The first two ear systems are guaranteed to consist of single ears.

In the worst case, all ear systems except the first two will require two ears, and all possible ears will be spent in $(q - p)/2$ steps. This leads to the following result:

Theorem 4. Every 1-extendable graph contains at least $(q-p)/2+2$ different perfect matchings.

For fullerene graphs, satisfying $q = (3/2)p$, this result reads as follows:

Theorem 5. Every fullerene graph on p points contains at least $(p/4) + 2$ different perfect matchings.

Even better bounds can be obtained using the fact that fullerene graphs belong to the class of bicritical graphs.

Definition 7. A graph G is *bicritical* if G contains an edge and $G - u - v$ contains a perfect matching, for every pair of distinct points $u, v \in V(G)$.

For bicritical graphs, we have the following lower bound for $\Phi(G)$ [4, p. 303]:

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

We will show that every fullerene graph is bicritical using the following characterization of bicritical graphs [4]:

Definition 8. 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.

Theorem 7. If, for some $k \geqslant 3$, G is a non-bipartite, k-regular, cyclically $(k + 1)$-edge-connected graph on an even number of points, then G is bicritical.

Let us show that every fullerene graph satisfies conditions required in this characterization.

Theorem 8. Every fullerene graph is cyclically 4-edge-connected.

Proof. Suppose, to the contrary, that G is not cyclically 4-edge-connected. This means that G can be separated into two components, each containing a cycle, by deleting exactly three edges. (Less than three edges would not suffice because of the 3-connectedness of G.) Let us denote these 3 edges by e_i, $i = 1, 2, 3$, and their endpoints by v_i', v_i'', $i = 1, 2, 3$, respectively. Let us consider the Schlegel diagram of G. 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''. If there were no additional points on C', then C' would be a triangle, contrary to the fact that G is a fullerene graph. The same is valid for C''. Let us denote the number of additional points on C' and C'' by k' and k'', respectively. Because of 3-regularity and 3-connectedness of G, k' (and k'') must be at least 3. (It is possible to retain these properties even with $k' = 2$, but in this case the two additional points must be connected by an edge, forming a triangle in G. So the case $k' = 2$ must be dismissed.) Thus, $k' + k'' \geqslant 6$. On the other hand, $k' + k'' \leqslant 6$, because it is not possible to place more than 6 additional points on C' and C'' placing at least 3 on each of them, without forming a face of G with more than 6 sides. So, $k' = k'' = 3$, i.e., each one of the cycles C', C'' is a hexagon. Let C' be the inner one. Then each one of 3 additional points on C' is an endpoint of an edge pointing toward the interior of C'. Let us denote these edges by e_i', $i = 1, 2, 3$. If any two of them have a common endpoint, v', then the 3-connectedness and the 3-regularity of G imply that the third edge has to have v' as its endpoint, too. In this case, G would contain at least one triangular or quadrangular face (depending on the placement of additional points on C'), contrary to our assumptions about G. Then the same reasoning as above implies that endpoints of e_i' must be on a cycle, C_1', with exactly 3 additional points on C_1'. We can proceed further in applying the above reasoning on C_1'. Because of the finiteness of G, after a finite number of steps, say n, we will obtain a cycle C_n' which will be either a triangle, or a hexagon with exactly one point inside. Both of these outcomes are in contradiction with our initial assumptions about G. □

As fullerene graphs are 3-regular, the main result in this article follows directly from theorems 6, 7 and 8.

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

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.

Although presented bounds do not look very impressive when compared with actual numbers of perfect matchings in fullerene graphs (e.g., 12500 in the case of truncated icosahedron isomer of C_{60} [1]), it should be noted that they were obtained relying on remarkably simple concepts and ideas, and that they are fully independent of the particular isomer. Also, they are the first ones which reflect relations between the size of a fullerene graph and the number of its perfect matchings.

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References

[1] D.J. Klein et al., J. Am. Chem. Soc. 108 (1986) 1301.
[2] D.J. Klein and X. Liu, J. Math. Chem. 11 (1992) 199.
[3] H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl and R.E. Smalley, Nature 318 (1985) 162.

[4] L. Lovasz and M.D. Plummer, *Matching Theory*, Ann. Discrete Math., Vol. 29 (North-Holland, Amsterdam, 1986).
[5] J. Petersen, Acta Math. 15 (1891) 193.