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New lower bound on the number of perfect matchings in fullerene graphs *

Heping Zhang [a,**] and Fuji Zhang [b]

[a] *Department of Mathematics, Lanzhou University, Lanzhou, Gansu 730000, P.R. China*
E-mail: zhanghp@lzu.edu.cn
[b] *Department of Mathematics, Xiamen University, Xiamen, Fujian 361005, P.R. China*
E-mail: fjzhang@jingxian.xmu.edu.cn

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A fullerene graph is a cubic and 3-connected plane graph (or spherical map) that has exactly 12 faces of size 5 and other faces of size 6, which can be regarded as the molecular graph of a fullerene. T. Došlić [3] obtained that a fullerene graph with p vertices has at least $(p+2)/2$ perfect matchings by applying the recently developed decomposition techniques in matching theory of graphs. This note gets a better lower bound $\lceil 3(p+2)/4 \rceil$ of the number of perfect matchings of a fullerene graph by finding its 2-extendability. This property further implies a chemical consequence that every derivative of a fullerene by substituting any two pairs of adjacent carbon atoms permits a Kekulé structure.

KEY WORDS: fullerene, Kekulé structure, perfect matching, bicritical graph, 2-extendable graph

The discovery of the carbon species C_{60} [7] has been giving significant scientific interest in theoretical research of the underlying graphs. A fullerene, F_n, is a carbon molecule which can be seen a trivalent 3-polyhedron of 12 pentagons and other hexagons. For all even $n \geqslant 20$ vertices or carbons, fullerene F_n can be constructed except for $n = 22$. The enumeration of isomers of fullerenes is given in a constructive way [2]. Among these isomers, a fullerene of n carbon atoms whose pentagons are isolated (i.e., any pentagons does not share an edge (bond)) is denoted by C_n. It is known that the unique C_{60}, buckminsterfullerene, is the truncated icosahedron.

A *fullerene graph* is a 3-regular (cubic) and 3-connected plane graph (or spherical map) that has exactly 12 faces of size 5 and other faces of size 6. A *matching* of a graph G is a set M of edges of G such that no two edges of M share an end-vertex; further a matching M of G is *perfect* if any vertex of G is incident with an edge of M. A fullerene

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graph is the molecular graph of a fullerene and perfect matching in graphs coincides with Kekulé structure in organic chemistry. As early as in 1891 Petersen [10] obtained that every 3-regular graph with no more than two cut-edges has a perfect matching, which implies that a fullerene graph has a perfect matching. This also gives a chemical explanation that fullerenes are a class of stable carbon clusters. A natural and interesting problem is to count perfect matchings of any given fullerene graph. For example, the numbers of perfect matchings of C_{60} and C_{70} were computed to be 12500 and 52168 [1], respectively, in computer programme. It should be mentioned that for all plane graphs, a physicist Kasteleyn developed a Pfaffian method to compute the number of perfect matchings in polynomial times (cf. [9]).

But to give an explicit expression of perfect matchings of a family of graphs (such as fullerenes) is still a difficult problem. Hence it is an interesting topic to give some simple bounds or estimations of perfect matchings. The famous Four-Color theorem has an equivalent proposition: the edge-set of a 2-edge connected 3-regular graph can be decomposed into the union of three edge-disjoint perfect matchings. Thus a fullerene graph has at least three perfect matchings [6] and each edge lies in a perfect matching.

T. Došlić [3] gave a better lower bound $p/2+1$ of the number of perfect matchings of fullerene graphs with p vertices by applying some decomposition techniques, such as the Cathedral Construction and Two-Ear theorem (cf. [9]), recently developed in matching theory. The bounds are fully independent of the particular isomer and the first ones which reflect relations between the size of a fullerene graph and the number of perfect matchings. In this note we first obtain a stronger structural property that every fullerene graph is 2-extendable, then show that every fullerene graph has at least $\lceil 3(p+2)/4 \rceil$ perfect matchings, accordingly improving the Došlić's bound. Here $\lceil a \rceil$ denotes the minimum integer that is not less than the given real number a.

We now introduce some further concepts appeared in matching theory, which will play significant role in some structural properties of fullerenes. A connected graph G with at least $2k+2$ points is said to be k-extendable if it contains a matching of size k and every such matching is contained in a perfect matching. A graph G is said to be *bicritical* if $G-u-v$ has a perfect matching for every choice of a pair of points u and v. 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. The terminology and notations in graph theory used but not unexplained in this article are standard and can be found in many textbooks.

Holton and Plummer [8] established the following relation between the cyclic edge-connection and extendability of a fullerene graph.

Theorem 1. If G is a cubic 3-connected planar graph which is cyclically 4-edge-connected and has no faces of size 4, then G is 2-extendable.

Došlić in [3] showed the following result.

Theorem 2. Every fullerene graph is cyclically 4-edge-connected.

Fowler et al. [4,5] revealed some properties of the dual of a fullerene, which are actually equivalent to theorem 2, in showing a generlized ring spiral algorithm for coding fullerenes.

Theorem 3. The following statements are equivalent.

(i) Every fullerene graph is cyclically 4-edge-connected;

(ii) No dual of a fullerene has a separating triangle;

(iii) The dual of a fullerene is 4-connected.

Proof. We give only a sketch. It suffices to prove only that the negative propositions of three statements in the theorem are equivalent. Let F denote a fullerene graph and F^* its dual. Since F^* is also a 3-polytope graph, F^* is 3-connected. A separating triangle of F^* means a cycle of 3-length the removal of which results in a disconnected graph. Suppose that the minimum edge-cuts of F and vertex-cuts of F^* contain exactly three elements. It is easily known that a cyclic 3-edge-cut of F corresponds to a separating triangle of F^* and the latter further corresponds to a 3-vertex-cut of F^*; conversely, a 3-vertex-cut of F^* corresponds to a separating triangle of F^* and to a cyclic 3-edge-cut of F. Here a cyclic 3-edge-cut of F means a set of three edges such that F would be separated into at least two components, each containing a cycle, by the deletion of these three edges. So the theorem follows. □

Combining theorems 1 and 2, we have immediately the following 2-extendability of fullerene graphs.

Theorem 4. Every fullerene graph is 2-extendable.

Since a 2-extendable graphs with non-bipartite is bicritical (cf. [11]) and a bicritical graph must be 1-extendable, we thus have the following two consequences, which have been shown in [3].

Corollary 5. Every fullerene graph is bicritical.

Corollary 6. Every fullerene graph is 1-extendable.

We now turn to the estimation for the number of perfect matchings of fullerene graphs by applying the above structural properties obtained. By the Two-Ear decomposition of 1-extendable graphs (cf. [9]), Došlić observed the following result.

Theorem 7. A 1-extendable graph with p vertices and q edges contains at least $(q - p)/2 + 2$ perfect matchings.

For bicritical graphs, we have the following result [9, p. 303].

Theorem 8. A bicritical graph with p vertices contains at least $p/2+1$ perfect matchings.

Since a fullerene graph is bicritical (corollary 6), by the above theorem the following result is obvious.

Theorem 9 [3]. Every fullerene graph has at least $p/2+1$ perfect matchings.

We now have a better result than the above theorem by using 2-extendability of a fullerene graph.

Theorem 10. Every fullerene graph with p vertices has at least $\lceil 3(p+2)/4 \rceil$ perfect matchings.

Proof. Let F_p denote a fullerene graph with p vertices. For any given vertex u of F_p, the three neighbors of u are denoted v_1, v_2 and v_3. Let $\mathcal{M}_i$ denote the set of perfect matchings of F_p containing the edge $uv_i (i = 1, 2, 3)$. Thus the perfect matchings of F_p can be decomposed into three disjoint classes $\mathcal{M}_i$, $i = 1, 2, 3$. Let $F' = F_p - u - v_i$. Then the number of perfect matchings of F' is equal to the size of $\mathcal{M}_i$. Since F_p is 2-extendable, then F' is 1-extendable. It is obvious that F' has exactly $p-2$ vertices and $3p/2-5$ edges. By theorem 7 it follows that F' has at least $(p/4+1/2)$ perfect matchings; that is, $|\mathcal{M}_i| \geqslant p/4+1/2$. Thus F_p has at least $3(p/4+1/2)$ perfect matchings. Since the number of perfect matchings is an integer, the theorem follows. □

From the basic structural properties that every fullerene graph is cyclically 4-edge connected and 2-extendable, theorem 10 establishes a new lower bound of the number of perfect matchings of a fullerene, which is only relied on the number of vertices but independent of the concrete polyhedral structures. This lower bound further improves greatly various lower bounds [3,6] previously obtained.

The *cyclic edge-connectivity*, $c\lambda$, of a graph G is the maximum integer k such that G is cyclically k-edge-connected. Combining Sachs' result that for 2-edge connected cubic graph $c\lambda \leqslant 5$ (cf. [11]) and theorem 2, we know that for fullerene graphs $4 \leqslant c\lambda \leqslant 5$. Here we propose a problem: to determine the cyclic edge-connectivity of fullerene graphs.

The *extendability* of a graph G is a maximum integer k such that G is k-extendable. It is known that no planar graphs are 3-extendable (cf. [11]). From theorem 4 we know that the extendability of every fullerene graph is 2. The 2-extendability of a fullerene graph implies a chemical consequence that every derivative of a fullerene by substituting any two pairs of adjacent carbon atoms permits a Kekulé structure.

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