Leapfrog fullerenes have many perfect matchings

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Abstract   A leapfrog fullerene on p vertices contains at least $2^{p/8}$ different perfect matchings.

Over the course of last decade there has been a slow but steady improvement of the quality of lower bounds on the number of perfect matchings in fullerene graphs. The constant lower bound of 3 [19] was followed by a series of bounds linear in the number of vertices [1, 2, 4, 27]. Those bounds were established using the structural theory of matchings [22]. The best currently available lower bound valid for all fullerene graphs belongs to this class. It states that in a fullerene graph on p vertices there are at least $\left\lceil \frac{3(p+2)}{4} \right\rceil$ different perfect matchings [27]. However, the empirical results suggest that the average number of perfect matchings in all fullerene graphs on p vertices increases exponentially with p [5]. Indeed, exponential lower bounds on the number of perfect matchings were recently established for certain classes of nanotubes [20, 23, 24] and for highly symmetric fullerenes [5]. Furthermore, it has been shown that fullerene graphs on p vertices with exponentially many perfect matchings exist for all sufficiently large (even) values of p [5], but those graphs again have fairly high symmetries. The aim of the present paper is to break through the symmetry barrier and to show how some recent results on Clar numbers can be used to establish exponential lower bounds that will be valid for all leapfrog fullerenes, regardless of their symmetry. Although the leapfrog fullerenes represent only a tiny fraction of all possible fullerenes, the result is still interesting, since the density of leapfrog fullerenes is bounded away from zero by an absolute constant, while there is no known lower bound on the density of highly symmetric fullerenes.

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We start by defining the basic terms. For the general graph-theoretic terminology we refer the reader to any of standard monographs, such as, e.g., [15] or [25].

A *fullerene graph* is a planar, 3-regular and 3-connected graph that has only pentagonal and hexagonal faces. Such graphs on p vertices exist for all even $p \geq 24$ and for $p = 20$ [14].

A *matching M* in a graph G is a set of edges of G such that no two edges of M have a vertex in common. A matching M is *perfect* if every vertex of G is incident with an edge from M. A perfect matching is in the chemical literature often called a *Kekulé structure*. We denote the number of perfect matchings in a graph G by $\Phi(G)$.

Let G be a fullerene graph and M a perfect matching in G. A *benzenoid face* of G is any hexagonal face of G that contains three edges from M. A set of pairwise disjoint benzenoid faces of G is called a *resonant set* in G. The maximum cardinality of any largest resonant set over all perfect matchings of G is called *Clar number* of G and denoted by $\gamma(G)$.

By choosing one of the two possible perfect matchings in each benzenoid face in a resonant set, one can obtain the following lower bound on $\Phi(G)$.

Proposition 1 $\Phi(G) \geq 2^{\gamma(G)}$.

Hence, linear lower bounds on $\gamma(G)$ will yield exponential lower bounds on $\Phi(G)$. Such lower bounds were established in a recent paper by Graver, but only for leapfrog fullerenes.

Let G be a fullerene graph on p vertices. A *leapfrog transform G^l* of G is a graph on $3p$ vertices obtained by truncating the dual of G. Hence, $G^l = Tr(G^*)$, where G^* denotes the dual of G. It is easy to check that G^l itself is a fullerene graph. We say that G^l is a *leapfrog fullerene* obtained from G and write $G^l = Le(G)$. For a more thorough introduction and treatment of leapfrog fullerenes we refer the reader to [9] and [10].

The connection between leapfrog fullerenes and Clar-related concepts was noted quite early [10, 21]. However, the quantitative aspects of the relationship became elucidated only recently in a series of papers by Graver [11–13]. The most important for our purpose is the lower bound on the Clar number of a leapfrog fullerene in terms of the independence number of its parent graph.

A set I of vertices of G is *independent* if no two vertices from I are adjacent in G. The cardinality of any largest independent set in G is called the *independence number* of G and denoted by $\alpha(G)$.

The independence number of fullerene graphs has been subject of several papers [2, 8, 12]. It is known that it cannot exceed $p/2 - 2$, and it is conjectured that it is bounded from below by $p/2 - 8$ ([7], Conjecture 843), but we are not aware of any proven lower bound better than the one valid for all triangle-free planar cubic graphs, $\alpha(G) \geq \frac{3p}{8}$ [16]. Hence, we have

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

We quote the Graver's lower bound on $\gamma(G)$ without proof. For the proof, the reader might consult Theorem 2 of Ref. [12].

Theorem A Let G^l be a leapfrog fullerene obtained from the fullerene G. Then $\gamma(G^l) \geq \alpha(G)$.

Now we can establish our main result.

Theorem 2 Let G be a leapfrog fullerene on p vertices. Then

$$\Phi(G) \geq 2^{p/8}.$$

Proof Since G is a leapfrog fullerene, there must be a fullerene G' on $p' = p/3$ vertices such that $G = Le(G')$. For the independence number of G' we have $\alpha(G') \geq 3p'/8 = p/8$. Hence, $\gamma(G) \geq p/8$, and the result now follows from Proposition 1.

The result of Theorem 2 is important in two ways. First, it gives us an exponential lower bound on $\Phi(G)$ valid also for some fullerenes of low symmetry. Second, the fraction of leapfrog fullerenes among all fullerene graphs on $p = 6k$ vertices remains bounded from below by an absolute constant C. Namely, the number of fullerene graphs on p vertices scales polynomially with p, and the degree of the polynomial is at most 12. Moreover, using some heuristic arguments the degree can be lowered to nine, and it seems that such degree is in good agreement with empirical results [18]. Hence, the fraction of leapfrog fullerenes can be bounded from below by $C = 3^{-10}$, regardless of p.

We conclude by discussing the limitations of our approach. The most serious shortcoming is that it works only for the fullerene graphs whose number of vertices is divisible by six. (The fraction of leapfrog fullerenes remains, however, bounded away from zero even if one considers the cumulative number of all fullerenes with at most p vertices.) One possible way of working around this problem could be by considering another fullerene transforms, such as obtained by quadrupling (chamfering) and septupling (capra) transformations [17], and by establishing results analogous to Graver's Theorem A for those transforms. Another limitation is that there are linear upper bounds on the quantity $\gamma(G)$ valid for all fullerenes: Zhang and Ye proved recently that $\gamma(G) \leq \lfloor \frac{p-12}{6} \rfloor$ for all fullerene graphs on p vertices. Moreover, they proved that this upper bound is achieved for certain classes of nanotubes [26]. Their results imply that the exponential term in the lower bound $\Phi(G) \geq C(p)2^{p/6}$ cannot be further improved using the present approach. Any attempt to improve the lower bounds valid for all fullerenes will have to find a way to account for the perfect matchings that do not come from resonant sets.

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