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ORIGINAL PAPER

Finding more perfect matchings in leapfrog fullerenes

Tomislav Došlić

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Abstract We use some recent results on the existence of long cycles in leapfrog fullerenes to establish new exponential lower bounds on the number of perfect matchings in such graphs. The new bounds are expressed in terms of Fibonacci numbers.

Keywords Fullerene graph · Leapfrog fullerene · Perfect matching · Fibonacci numbers

1 Introduction

The central theme of research in fullerene graphs over the last two decades has been a search for a graph-theoretical invariant that could be used as a predictor of fullerene stability. A number of invariants has been proposed, examined, and tested, and none of them were found satisfactory. The number of perfect matchings was among the first candidates that were tried. It turned out that on its own it is not a very successful predictor [1]. However, there is some evidence that certain derived invariants that take into account the details of the local structure might be more relevant. Hence, the number of perfect matchings continued to attract the attention of researchers, and this resulted in a steady flow of results over the last couple of years. Most of those results have been concerned with the lower bound on this quantity, and one can follow a progress from constant [13] to linear [3,5,22] to exponential lower bounds [7,8,14,20]. The aim of the present paper is to further improve the lower bounds for the class of fullerene graphs known as the leapfrog fullerenes. This will be achieved by using some new results on the existence of long cycles in such graphs. Those results have been a part

T. Došlić (✉)
Department of Mathematics, Faculty of Civil Engineering, University of Zagreb,
Kačićeva 26, 10000 Zagreb, Croatia
e-mail: doslic@math.hr

of the recent progress toward establishing the conjectured hamiltonicity of fullerene graphs [17,14,15]. The lower bounds in question will follow by observing that such a long cycle corresponds to a catacondensed benzenoid of particular type whose number of perfect matchings can be bounded from below in terms of Fibonacci numbers.

2 Preliminaries

In this section we introduce the classes of graphs considered in the present paper and prove some auxiliary results. For graph-theoretic terms not defined here we refer the reader to any of standard monographs such as, e.g., [12], [21] or [16].

All graphs considered here are simple, finite, and connected. For a given graph G we denote its vertex set by $V(G)$ and its edge set by $E(G)$. A **matching** M in G is a collection of edges of G such that no two edges from M have a vertex in common. A matching M is **perfect** if every vertex from $V(G)$ is incident with some edge from M. The number of all different perfect matchings in G we denote by $\Phi(G)$.

A **fullerene graph** is a planar, 3-regular and 3-connected graph 12 of whose faces are pentagons and any remaining faces are hexagons. If no two pentagons in a fullerene graph G share an edge, we say that G is an **isolated pentagon** (IP) fullerene.

It is well known that fullerene graphs on p vertices exist for all even $p \geq 24$ and for $p = 20$ [11]. Similarly, IP fullerenes on p vertices exist for all even $p \geq 70$ and for $p = 60$ [13]. The smallest fullerene, $C_{20} : 1$, is the dodecahedron; the smallest IP fullerene is the buckminsterfullerene $C_{60} : 1812$. We refer the reader to Ref. [10] for more background information on fullerene graphs.

The buckminsterfullerene can be obtained from the dodecahedron via the so-called **leapfrog transformation**. The leapfrog transformation of a planar graph G is defined as the truncation of its dual [9]. We write it as $Le(G) = Tr(Du(G))$. Applied to dodecahedron it gives us the familiar truncated icosahedron structure of the buckminsterfullerene.

It is not difficult to see that $Le(G)$ has three time the number of vertices of G. Furthermore, if G is a fullerene, then $Le(G)$ is a fullerene. Finally, $Le(G)$ is always an IP fullerene.

It is obvious from the definition that the leapfrog transformation is invertible. Hence, for a given leapfrog fullerene G we can always find its parent fullerene $Le^{-1}(G)$.

The leapfrog fullerenes have many remarkable properties. We mention here two that are relevant for our aims.

Theorem A [8]
Let G be a leapfrog fullerene on p vertices. Then $\Phi(G) \geq 2^{p/8}$. □

Theorem B [17]
Let G be a fullerene on p vertices. Then the leapfrog fullerene $Le(G)$ has a Hamilton cycle if $p \equiv 2 (\mathrm{mod} 4)$, and contains a long cycle missing out only two adjacent vertices if $p \equiv 0 (\mathrm{mod} 4)$. □

The long cycles of Theorem B are worth looking at in more detail. It turns out that they arise via the leapfrog transformation from induced trees in the parent fullerene G. The existence of such trees of a given size follows from the fact that all fullerenes are cyclically 5-edge connected [6,19] via an old result of Payan and Sakarovich [18]. Moreover, the area enclosed by those cycles in a Schlegel diagram of $Le(G)$ is a topological disk made of hexagons that are either disjoint or share a whole edge; hence, it is a benzenoid graph. A benzenoid graph is **catacondensed** if no vertex is shared by more than two hexagons. We refer the reader to [2] for more information on benzenoid graphs.

Lemma 1 *Let T be an induced tree in a fullerene G. Then the hexagons in $Le(G)$ corresponding to the vertices of T form a catacondensed benzenoid.*

Proof A leapfrog fullerene $Le(G)$ on p vertices contains $p/2-10$ hexagons. Exactly $p/3$ of them arise from the vertices of the parent fullerene G via the dualization/ truncation procedure, while the remaining ones correspond to the hexagons in the parent fullerene. Moreover, the "new" hexagons share an edge in $Le(G)$ if and only if the corresponding vertices are adjacent in G. (Hexagons corresponding to the old hexagons are isolated in $Le(G)$; that is also the reason that makes $Le(G)$ an IP fullerene.) Let T be an induced tree in G and $Le(T)$ the hexagons in $Le(G)$ corresponding to the vertices of T. Then the inner dual of $Le(T)$ is isomorphic to T, hence it is a tree, and then $Le(T)$ must be a catacondensed benzenoid. □

The set $Le(T)$ has an additional important property: it is **nowhere straight**, i.e., it does not contain a straight chain of three hexagons as a subgraph. (An alternative term for such benzenoids could be **anthracene-free**.) In a nowhere straight catacondensed benzenoid in every non-terminal hexagon we have either a branching or a kink.

Lemma 2 *Let T be an induced tree in a fullerene G. Then the catacondensed benzenoid $Le(T)$ is nowhere straight.*

Proof A vertex $v \in V(T)$ can be of degree 1, 2, or 3 in T. It is clear from the construction that a vertex of degree 1 in T gives rise to a terminal hexagon in $Le(T)$. Similarly, a vertex of degree 3 in T gives a branching hexagon in $Le(T)$. It remains to show that a vertex of degree 2 gives a kink hexagon. But this is again obvious from the construction, as shown in Fig. 1. Hence, $Le(T)$ cannot contain a straight chain of three hexagons, and the claim follows. □

It is well known that an unbranched catacondensed benzenoid (i.e., a hexagonal chain) has the largest possible number of perfect matchings exactly when it is nowhere straight. Moreover, a nowhere straight hexagon chain with h hexagons has exactly F_{h+2}, where F_{h+2} denotes the $h+2$-nd Fibonacci number. We will show that any

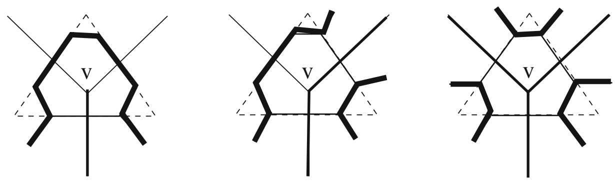

Fig. 1 With the proof of Lemma 2

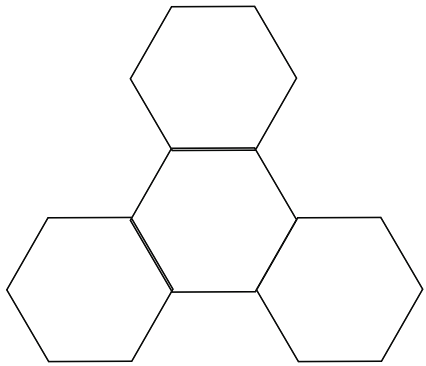

Fig. 2 The smallest branched nowhere straight catacondensed benzenoid

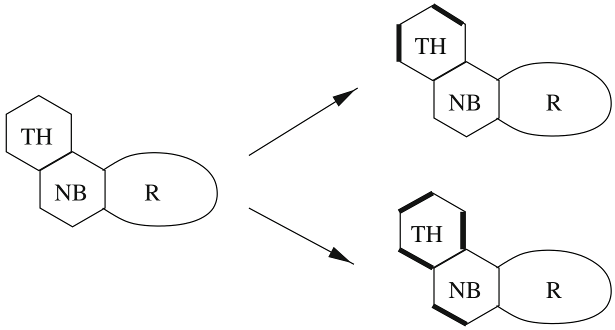

Fig. 3 A terminal hexagon is adjacent to a non-branching hexagon

nowhere straight catacondensed benzenoid on h hexagons contains at least that many perfect matchings.

Lemma 3 *Let T_h be a nowhere straight catacondensed benzenoid on h hexagons. Then $\Phi(T_h) \geq F_{h+2}$.*

Proof If T_h is unbranched, then $\Phi(T_h) = F_{h+2}$ and we are done. Suppose, then, that T_h has at least one branching hexagon. The smallest such benzenoid is T_4, shown in Fig. 2. It is easy to see that $\Phi(T_4) = 9 \geq 8 = F_6$. Now we proceed by induction on h, and suppose that the claim of Lemma is valid for all nowhere straight catacondensed benzenoids with at most h hexagons. Let T_{h+1} be an arbitrary nowhere straight catacondensed benzenoid with $h+1$ hexagons. Then it must contain at least two terminal hexagons. If one terminal hexagon is adjacent to a non-branching hexagon NB, we have a situation shown in Fig. 3. It follows that

$$\Phi(T_{h+1}) = \Phi(R \cup NB) + \Phi(R).$$

Since both R and $R \cup NB$ are nowhere straight catacondensed benzenoids with at most h hexagons, we have $\Phi(T_{h+1}) \geq F_{h+2} + F_{h+1} = F_{h+3}$, and the claim of Lemma follows.

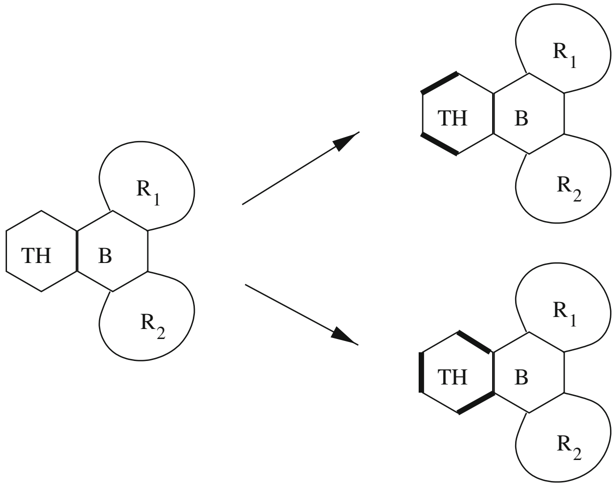

Fig. 4 A terminal hexagon is adjacent to a branching hexagon

It remains to consider the case when all terminal hexagons are adjacent to branching hexagons. The situation is shown in Fig. 4. We have

$$\Phi(T_{h+1}) = \Phi(R_1 B R_2) + \Phi(R_1) \cdot \Phi(R_2).$$

The first term on the right-hand side is at least F_{h+2}, by the inductive hypothesis. Let us consider the second term. By the inductive hypothesis, $\Phi(R_i) \geq F_{|R_i|+2}$, where $|R_i|$ denotes the number of hexagons in R_i, $i = 1, 2$. Since R_1 and R_2 together have exactly $h - 1$ hexagons, and neither of them is empty, the claim will follow if we prove that $F_k F_{n-k} \geq F_{n-2}$ for all $k \geq 2$, $n \geq k + 2$. The cases $n = 4$ and $n = 5$ are easily verified. Now suppose that $F_k F_{m-k} \geq F_{m-2}$ is valid for all $m \leq n$ and consider $F_k F_{n+1-k}$:

$$F_k F_{n+1-k} = F_k(F_{n-k} + F_{n-1-k}) = F_k F_{n-k} + F_k F_{n-1-k}.$$

By the inductive hypothesis, the first term in the right-hand side is at least F_{n-2}, the second one is at least F_{n-3}, and hence their sum is at least F_{n-1}. This completes the step of induction and verifies that $\Phi(R_1) \cdot \Phi(R_2) \geq F_{h+1}$. But then $\Phi(T_{h+1}) \geq F_{h+3}$, and the Lemma is proved. $\square$

3 Main results

Now we can formulate and prove our main result.

Theorem 4 *Let G_p be a leapfrog fullerene on p vertices. Then*

$$\Phi(G_p) \geq F_{\lceil p/4 \rceil + 1} + 1.$$

If p is divisible by 4, then

$$\Phi(G_p) \geq F_{p/4+1} + p/2.$$

Proof Let us first consider the case $p \equiv 2 \pmod 4$. It follows from Theorem B that G_p contains a Hamiltonian cycle C. In Ref. [17] it was shown that C is the border of a tree of hexagons $Le(T)$ that correspond to the vertices of some induced tree T in $Le^{-1}(G_p)$ under the leapfrog transformation. By Lemma 2, $Le(T)$ is a nowhere straight catacondensed benzenoid on $(p-2)/4$ hexagons. Now, by Lemma 3, $Le(T)$ contains at least $F_{(p-2)/4+2} = F_{\lfloor p/4 \rfloor+2} = F_{\lceil p/4 \rceil+1}$ different perfect matchings, and each of them is also a perfect matching of G_p. An additional perfect matching is formed by the edges of $E(G_p) - C$, and the claim follows.

Suppose now that $p \equiv 0 \pmod 4$. Then, by Theorem B, G_p contains a cycle C of length $p-2$ that misses out exactly two adjacent vertices. Denote those two vertices by u and v, and the edge connecting them by e. Again, the cycle C is the boundary cycle of a nowhere straight catacondensed benzenoid $Le(T)$ generated by the leapfrog transformation from an induced tree T in $Le^{-1}(G_p)$. Since $|C| = p-2$, $Le(T)$ contains $(p-4)/4 = p/4 - 1$ hexagons; hence it has at least $F_{p/4+1} = F_{\lceil p/4 \rceil+1}$ different perfect matchings. We note that all of those perfect matchings must contain the edge e. On the other hand, it is known that for any edge e in a fullerene graph on p vertices there are at least $p/2$ perfect matchings that do not contain e [5]. The claim now follows by observing that a perfect matching of G_p either contains e and is counted by $F_{\lceil p/4 \rceil+1}$, or does not, and in that case is counted by $p/2$. □

The lower bound we have just established compares favorably with the one from Theorem A. It is well known that the asymptotic behavior of Fibonacci numbers is given by $F_n \sim \phi^n$, where $\phi = \frac{1+\sqrt{5}}{2}$ is the golden section. Hence $\Phi(G_p)$ is bounded from below by a quantity proportional to $\sqrt[4]{\phi}^p$. Since $\sqrt[4]{\phi} \approx 1.12784 > \sqrt[8]{2} \approx 1.09051$, it follows that the bound of Theorem 4 is better.

The lower bound from Theorem 4 can be slightly improved for those leapfrog fullerenes on $p \equiv 0 \pmod 4$ vertices whose parent fullerenes have isolated pentagons. For this we need a recent result by Kutnar, Marušič and Vukičević:

Theorem C [15]
Let G_p be a leapfrog fullerene on $p \equiv 0 \pmod 4$ vertices such that $Le^{-1}(G_p)$ has isolated pentagons. Then the vertex set of G_p can be partitioned into two sets, S and S', such that S induces a cycle of length 6, and S' are vertices of a cycle of length $p-6$. □

The above result is slightly weakened Theorem 3.5 from reference [15].

Theorem 5 *Let G_p be a leapfrog fullerene on $p \equiv 0 \pmod 4$ vertices such that $Le^{-1}(G_p)$ has isolated pentagons. Then G_p contains at least $2F_{p/4} + 1$ different perfect matchings.*

Proof It follows by the same arguments as in the previous cases that S' are vertices of the boundary cycle of a nowhere straight catacondensed benzenoid on $p/4 - 2$

hexagons. By Lemma 3, such a benzenoid contains at least $F_{p/4}$ different perfect matchings. As each of them can be combined with either of 2 perfect matchings of the cycle C_6 induced by S, we have at least $2F_{p/4}$ perfect matchings in G_p. The claim now follows by observing that the $p/2$ edges not contained in the cycles defined by the partition form a perfect matching different from all $2F_{p/4}$ already constructed ones. □

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