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Leapfrog fullerenes and Wiener index

Vesna Andova[a,*], Damir Orlić[b], Riste Škrekovski[c]

[a] Faculty of Electrical Engineering and Information Technologies, Ss Cyril and Methodius University, Ruger Boskovik 18, Skopje 1000, Macedonia

[b] Informatika d.d., Hajdrihova 2, 1000 Ljubljana, Slovenia

[c] Faculty of Mathematics and Physics & Ljubljana Faculty of Information Studies, Novo mesto & University of Primorska, FAMNIT, Koper, Slovenia

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ABSTRACT

Fullerene graphs are cubic, 3-connected planar graphs with only pentagonal and hexagonal faces. A fullerene is called a leapfrog fullerene, Le(F), if it can be constructed by a leapfrog transformation from other fullerene graph F. Here we determine the relation between the Wiener index of Le(F) and the Wiener index of the original graph F. We obtain lower and upper bounds of the Wiener index of Le^i(F) in terms of the Wiener index of the original graph. As a consequence, starting with any fullerene F, and iterating the leapfrog transformation we obtain fullerenes, Le^i(F), with Wiener index of order $O(n^{2.64})$ and $\Omega(n^{2.36})$, where n is the number of vertices of Le^i(F). These results disprove Hua et al. (2014) conjecture that the Wiener index of fullerene graphs on n vertices is of order $\Theta(n^3)$.

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1. Introduction

Fulleren es [16] are polyhedral molecules made of carbon atoms arranged in pentagonal and hexagonal faces, and their corresponding graphs, *fullerene graphs*, are 3-connected, cubic planar graphs with only pentagonal and hexagonal faces. The first discovered fullerene molecule C_{60}, is comprised only by 60 carbon atoms, and it resembles to Richard Buckminster Fuller's geodetic dome, therefore it was named buckminsterfullerene. The discovery of the buckminsterfullerene marked the birth of fullerene chemistry and nanotechnology. The leapfrog operation of a fullerene graph is a method that produces (bigger) fullerenes with the same symmetry group with the original fullerene graph. Even more the newly obtained fullerene graph satisfies the isolated pentagon rule (IPR), i.e., a fullerene graph with no two pentagons adjacent. For more results on fullerenes, and leapfrog fullerenes see [1–5,9,10,12].

Topological indices, or also known as *molecular descriptors* [19] are graph invariants that are calculated from the topological information contained in the structure of the graph of a molecule. They are numerical parameters of a graph which describe its structure or properties. Most of the topological indices are based on the degrees of the vertices, or on the distance between them [7]. The Wiener index is the first topological index introduced in [20] and defined as the sum of the lengths of the shortest paths between all pairs of vertices in a graph. In the same paper, the Wiener polarity index [17,18] of a graph G, denoted by $W_P(G)$, is defined as the number of unordered pairs of vertices $\{u, v\}$ of G at distance three in the graph G. These indices are representative of the distance based group of indices.

* Corresponding author.
E-mail addresses: vesna.andova@gmail.com, vesna_and@yahoo.com (V. Andova), damir@orlic.si (D. Orlić), skrekovski@gmail.com (R. Škrekovski).

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The Wiener index was studied in chemistry and pure mathematics under different names, and has found applications in sociometry and in the theory of social networks. Wiener index is closely related to the closeness centrality of a vertex in a graph, and hence to closeness and farness, important concepts in social networks [11]. The Wiener index initiated the boom of topological indices in QSPR/QSAR [8,19]. Based on the success of Wiener index, many new molecular descriptors have been developed afterwards. For more results on Wiener index see [14,15].

Let G be a connected graph. By $V(G)$ and $E(G)$ we denote the vertex and edge set of G, respectively. We set $n = |V(G)|$ and $m = |E(G)|$. For two vertices, $u, v \in V(G)$, by $d_G(u, v)$ we denote the distance from u to v in G. If u and v are adjacent vertices in the graph G, then we write $u \sim_G v$. The Wiener index of a graph G is defined by

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v).$$

In this paper, we determine the relation between the Wiener index of a leapfrog transformation of a fullerene graph F and the Wiener index of the original graph F. Let F be a fullerene graph obtained with a sequence of consecutive leapfrog transformations from a fullerene F_0. We determine the upper and lower bounds of the Wiener index of F depending on the starting graph F_0, i.e., we find lower and upper bound of $W(\mathrm{Le}^i(F_0))$ in terms of the Wiener index of the original graph. Hua et al. [13] conjectured that the Wiener index of a fullerene graph on n vertices is a cubic polynomial.

From the definition of Wiener index we have

$$W(G) = \sum_{u,v \in V(G)} d_G(u, v) \leq \binom{n}{2} \mathrm{diam}(G), \tag{1}$$

where $\mathrm{diam}(G)$ is the diameter of the graph G. In [6], the authors showed that icosahedral fullerene graphs have diameter of order $\Theta(\sqrt{n})$. This result and relation (1) imply that following observation.

Observation 1. Full icosahedral fullerenes on n vertices have Wiener index of order $O(n^2\sqrt{n}) = O(n^{2.5})$.

This observation shows that full icosahedral fullerenes disprove Hua et al. conjecture [13].

Here, applying our results we find that starting with any fullerene graph F_0, the fullerenes of the sequence $\{\mathrm{Le}^i(F_0)\}_i$ disprove this conjecture as well. Even more we show that these leapfrog fullerenes on n vertices, have Wiener index of order $O(n^{2.64})$ and $\Omega(n^{2.36})$.

2. Preliminaries

The leapfrog transformation is a composition of two operations. We first define the operations stellisation, dualisation and truncation for a given graph. The *stellisation*, $\mathrm{St}(G)$, adds a vertex in the center of each face of a planar graph G, and connects the new vertex with each boundary vertex of the corresponding face. Notice that this operation results with triangulation. The *dualization* of a graph G is the operation that produces the dual of G. Recall that the dual graph of a planar graph G, $\mathrm{Du}(G)$, is a graph with vertices corresponding to each face of G. Two vertices in $\mathrm{Du}(G)$ are adjacent if the corresponding faces in G share an edge. The *truncation*, $\mathrm{Tr}(G)$, of a plane graph G is an operation that adds two new vertices on each edge, and then removes the vertices of G. Two vertices are adjacent if they are added to the same edge of G or they belong to two consecutive edges incident to the same vertex of G. The truncation of a polyhedra cuts off one third of each edge at each of both ends. The leapfrog operation of a fullerene graph G, $\mathrm{Le}(G)$, is usually used for construction of bigger and isolated pentagon fullerenes. The *leapfrog* graph $\mathrm{Le}(G)$ is obtained by truncating the dual of a fullerene graph G, i.e.,

$$\mathrm{Le}(G) = \mathrm{Tr}(\mathrm{Du}(G)).$$

At the same time leapfrog operation can be viewed as a composition of stellisation $\mathrm{St}(G)$, and dualization $\mathrm{Du}(G)$,

$$\mathrm{Le}(G) = \mathrm{Du}(\mathrm{St}(G)).$$

Observe that $\mathrm{Le}(F)$ is an isolated pentagon fullerene graph. Fig. 1 shows the buckminsterfullerene as a leapfrog graph of the dodecahedron. It is easy to see that $\mathrm{Le}(F)$ is a fullerene graph on $2|E(F)|$ vertices, and therefore the following holds.

Proposition 2. *If F is a fullerene graph on n vertices, then $\mathrm{Le}(F)$ is a fullerene graph on $3n$ vertices.*

A graph G is called a *leapfrog fullerene* if there exists a fullerene F such that $\mathrm{Le}(F) = G$. We name *G-vertices* and *G-edges* the vertices and edges of the graph G, respectively. We usually embed the fullerene graph F and its leapfrog transformation $\mathrm{Le}(F)$ in a plane such that each F-vertex u is surrounded by six $\mathrm{Le}(F)$-vertices, incident to a hexagon H_u (see Fig. 2). If an $\mathrm{Le}(F)$-edge intersects with a F-edge in this planar representation, we say that the $\mathrm{Le}(F)$-edge is a *crossing* edge, all the other edges of $\mathrm{Le}(F)$ are called *non-crossing*. Let the edge $xy \in E(\mathrm{Le}(F))$ be a crossing edge over the edge $uv \in E(F)$, as shown on Fig. 2. We call the vertices $u, v \in V(F)$ the *parents* of x and y. The set of parents of x is denoted by $P(x)$. Thus $P(x) = P(y) = \{u, v\}$. Observe that each $\mathrm{Le}(F)$-vertex has precisely two parents.

We can assign to each $\mathrm{Le}(F)$-vertex a unique parent by introducing a map p. In order to do that we orient each face in the fullerene clockwise. We denote the intersection point of the edges uv and xy by w. As the edge uv is a crossing edge, the vertices u and v belong in two different faces of F in the corresponding planar embedment. Then the assigned parent of

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