Properties of fullerene graphs with icosahedral symmetry

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Abstract

Fullerene graphs are based on a famous carbon allotrope and have become a popular class of graphs (see references in [2]). They are characterized as 3-regular and 3-connected planar graphs, with only pentagonal or hexagonal faces. The fullerene graph with icosahedral symmetry is a particular class of fullerene graphs with precisely 12 pentagonal faces. Moreover, the midpoints of its pentagonal faces form the planning of an icosahedron. They can be described by a vector (i, j), where $j \geq i \geq 0$ and $j > 0$, determining the graph $G_{i,j}$. In 2013, Andova and Skrekovski presented and proved formulas to compute the diameter of the graphs $G_{0,j}$ and $G_{j,j}$. Moreover, they presented a conjecture stating a lower bound for the diameter of all fullerene graphs. Therefore, in this study, we investigate properties of fullerene graphs with icosahedral symmetry. We show that, for $i, j \in \mathbb{N}^*$, $j \geq i$, every graph $G_{i,j}$ contains a reduced $G_{0,j-i}$ and that every graph $G_{i,j}$ is contained in an augmented $G_{j,j}$.

Introduction

An (undirected) graph G is a geometric object composed of a set of vertices and edges. Figure 1 shows a simple graph, i.e., a graph that does not have more than one edge between the same pair of vertices, and has no edges intersecting a vertex to itself. Before investigating the fullerene graphs, we require some graph theory definitions and concepts. A graph G is k-regular if all of its vertices have degree k. A graph G is k-connected if it remains connected whenever fewer than k edges are removed.

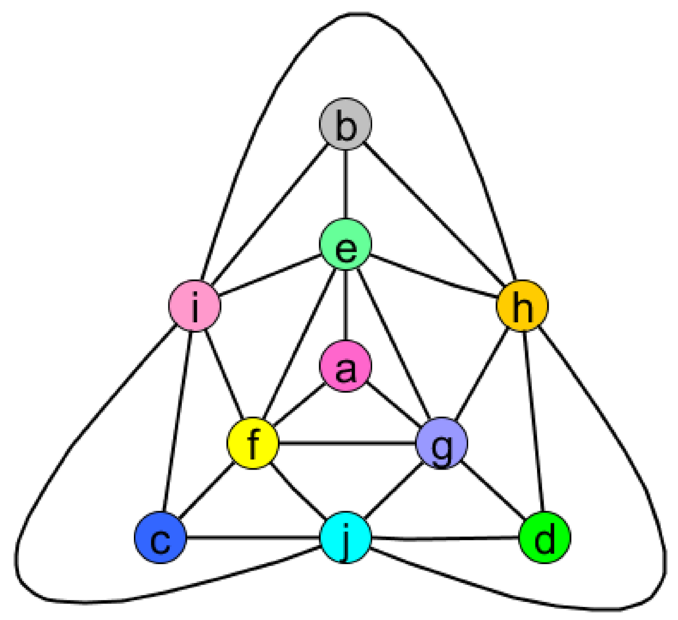

Figure 1: A simple Graph G.

A graph G is planar if it has an immersion in the plane so that its edges intersect only at their endpoints. The diameter of a graph is the maximum distance between any pair of vertices of G.

As an example, Figure 2 displays the Fullerene graph C_{60}: it is planar (no two edges intersect each other); it is 3-regular (all vertices have degree 3); and it is 3-connected (it remains connected if we remove one or two edges). Fullerene graphs are 3-regular and 3-connected planar graphs with only pentagonal and hexagonal faces. Figure 2 shows the Fullerene graph C_{60}.

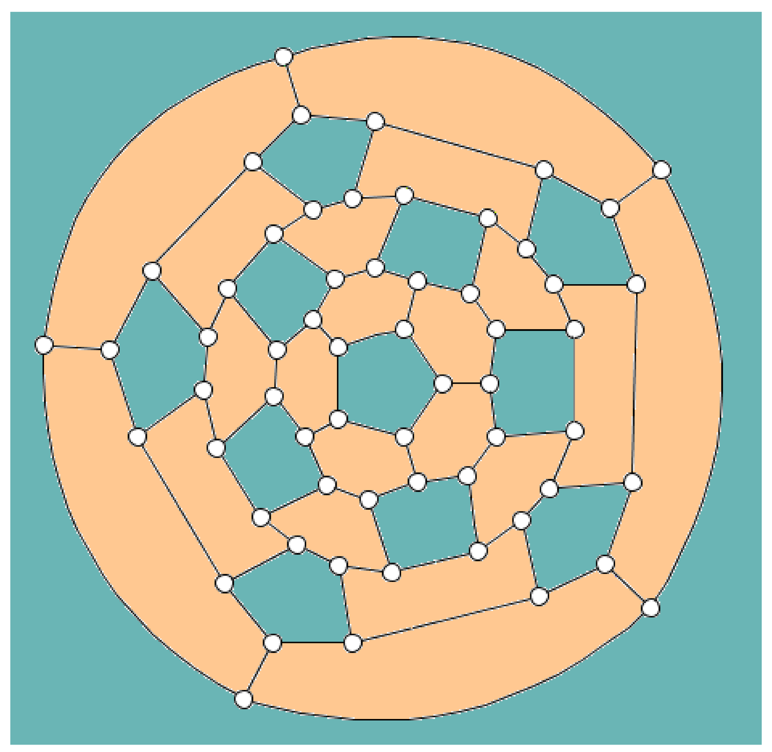

Figure 2: Fullerene graph C_{60}.

Icosahedral Symmetry

Fullerene graphs with icosahedral symmetry have exactly 12 pentagonal faces. All other faces are hexagons. Moreover, their pentagonal faces shape the planning of an icosahedron. They are described by $G_{i,j}$, $i, j \in \mathbb{N}^*$, $j \geq i$, where i and j determine the distance between the vertices, with i as the number of hexagons in direction $\overrightarrow{x}$ and j as the number of hexagons in direction $\overrightarrow{y}$ (see Figure 3). Figure 3 displays the planning of the graph Fullerene graph with icosahedral symmetry $G_{1,4}$.

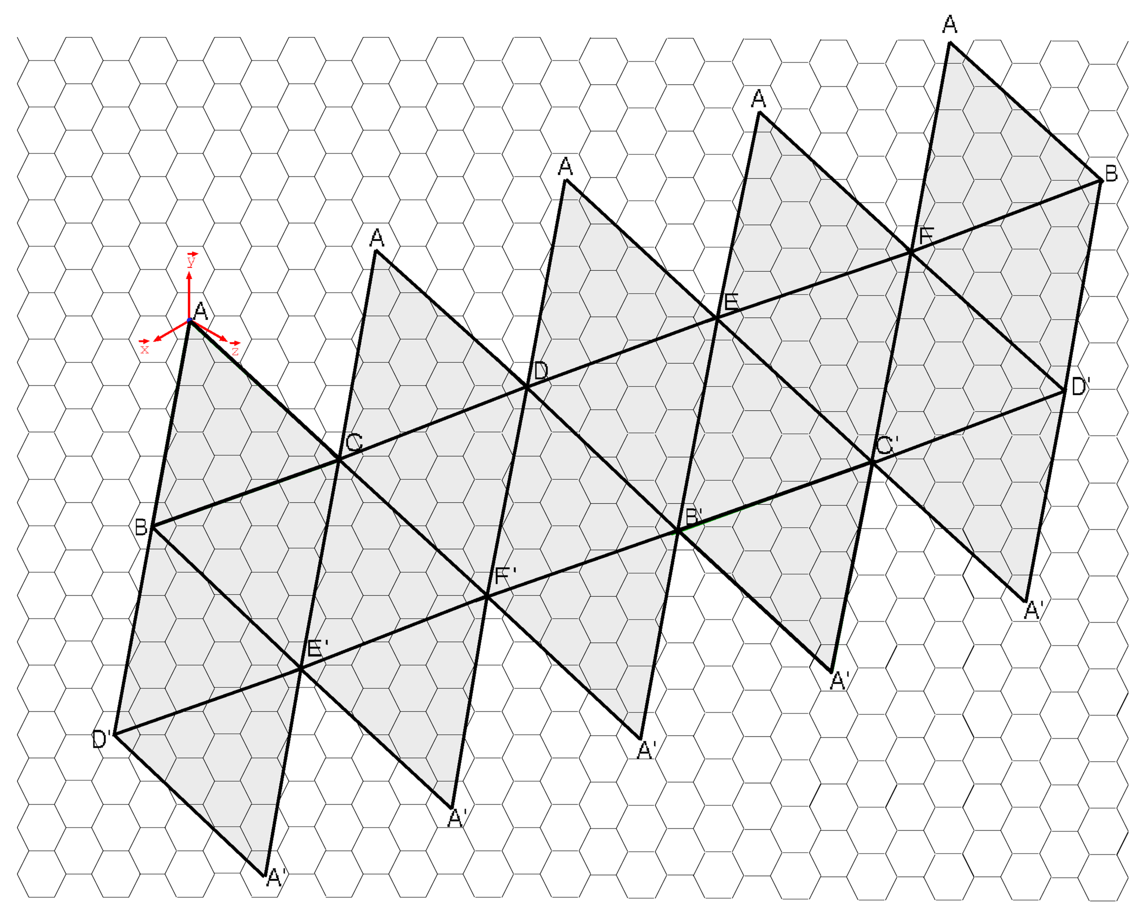

Figure 3: Planning of the graph $G_{1,4}$.

Results

Theorem 1

Every fullerene graph with icosahedral symmetry $G_{i,j}$, $i, j \in \mathbb{N}^*$, $j \geq i$, contains a reduced graph $G_{0,j-i}$.

Theorem 2

Every fullerene graph with icosahedral symmetry $G_{i,j}$, $i, j \in \mathbb{N}^*$, $j \geq i$, is contained in an augmented graph $G_{j,j}$.

The proofs of both theorems are based on vectorial operations of the vector $\overrightarrow{x}$ and $\overrightarrow{y}$ and the hexagonal lattice's symmetry characteristics. Figure 4 displays the results of Theorems 1 and 2 for the graph $G_{1,4}$. The black triangle corresponds to a section of $G_{1,4}$. As a visual proof of Theorem 1, note that the blue triangle corresponds to the graph $G_{0,3}$, entirely included in $G_{1,4}$. Similarly for Theorem 2, the red triangle corresponds to the $G_{4,4}$, which wholly contains the graph $G_{1,4}$.

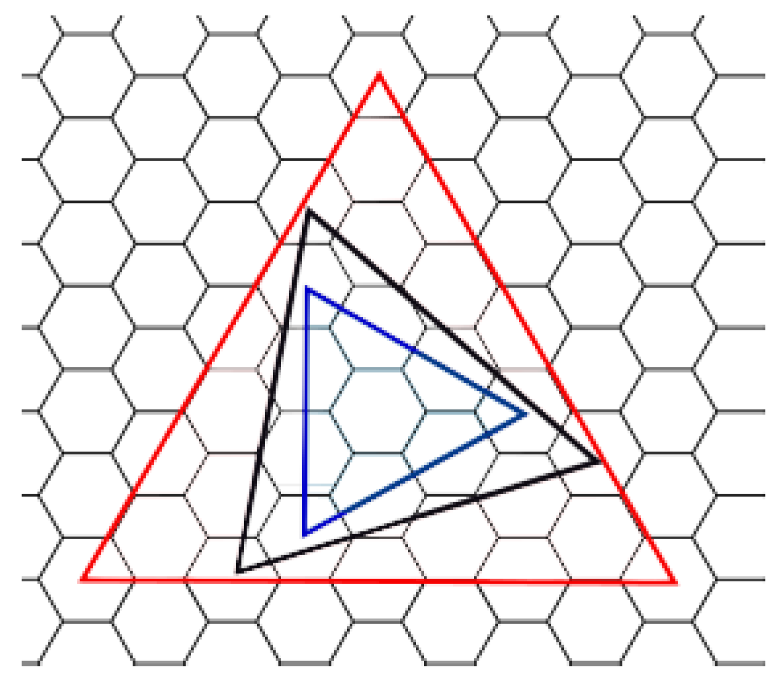

Figure 4: Example of Theorems 1 and 2 for $G_{1,4}$.

References

[1] Andova, V; Skrekovski, R. Diameter of Fullerenes Graphs with Full Icosahedral Symmetry. *MATCH*, 2013.

[2] Nicodemos, D; Stehlik, M. Fullerene graphs of small diameters. *MATCH*, 2017.