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On the Diameter of Spherical Fullerene Graphs

Simone Dantas **Vinícius Linder** **Diego Nicodemos**
Thiago M. D. Silva

Abstract

Fullerene graphs are mathematical models for molecules composed exclusively of carbon atoms, discovered experimentally in the early 1980s. Formally, fullerene are 3-connected, cubic and planar graphs with pentagonal and hexagonal faces. Andova and Skrekovski (2012) conjectured a lower bound for the diameter of fullerene graphs. The relevance of this conjecture consists in the fact that it was conceived from perfectly spherical fullerene graphs, a property which gives these graphs symmetry and, theoretically, high stability. We know that the curvature of fullerene graphs is given by their pentagonal faces, in this way, icosahedral fullerene graphs preserve the same distance between their pentagonal faces, which is characterized by two non-negative parameters i and j, defined as $G_{i,j}$. It is known that the Andova-Skrekovski conjecture is valid for the cases when $0 = i < j$, $0 < i = j$ and $j \geq \frac{11i}{2}$. In order to contribute to the study of this problem, we verify the conjecture for the case $j = i+1$. Moreover, we present a lower bound for the diameter.

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1 Introduction

Simple substances are the ones formed by a unique chemical element. Simple substances and distinct structural forms, composed by the same chemical element, are called *allotropes*. As an example, we can cite *oxygen* O_2 and *ozone* O_3. Another kind of allotropy occurs by the atoms arrangement, as in the case of carbon atoms, that vary its geometric structure forming diamond and coal. In 1985, scientific community witnessed the birth of a new carbon allotrope, a high symmetric molecule, stable and composed exclusively by carbon atoms. They named it *buckminsterfullerene* – C_{60} – homaging the architect Richard B. Fuller. The structure of C_{60} is formed by 32 faces – 20 hexagonals and 12 pentagonals. In the end of the 1980s, many other carbon atoms with the same spacial structure of C_{60} were found, being named as *fullerene molecules*. Each fullerene molecule can be graph modelled: the atoms corresponds to the graph vertices and the chemical bonds to the edges. It is important to note that occasional double bonds between carbon atoms of the fullerene molecule origin only one edge.

To define a fullerene graph, we need some definitions. A graph $G = (V, E)$ is *planar* if it can be embedded in the plane, such that its edges intersect only at their endpoints. The *degree* $d(v)$ of a vertex $v \in V(G)$ is the number of edges incident to the vertex v. A graph G is *cubic* if $d(v) = 3$ for all $v \in V(G)$. A graph G is connected if there is a path between each pair of its vertices. A graph is 3-connected if it remains connected whenever fewer than 2 vertices are removed. If a graph G is connected, the *distance* $d(u, v)$ between two vertices u and v is the length of the shortest path between them. The *diameter* $diam(G)$ of a graph G is the greatest distance between any two vertices of G. In this way, we can define a *fullerene graph* as a planar, cubic, 3-connected graph with only pentagonal and hexagonal faces. An important result derived straightforward from the *Euler relation*, $V + F = A + 2$, where V is the number of vertices, F is the number of faces and A is the number of edges of G, says that every fullerene graph has exactly 12 pentagonal faces.

In 2013, Andova and Skrekovski [1] determined the diameter of fullerene graphs with complete icosahedral symmetry. This class, besides being highly symmetric, is perfectly spherical. These properties lead them to conjecture that the diameter of fullerene graphs with complete icosahedral symmetry is a lower bound for all fullerene graphs.

Conjecture 1. (Andova-Skrekovski [1]) *For every fullerene graph F with n vertices, $diam(F) \geq \left\lfloor \sqrt{\frac{5n}{3}} \right\rfloor - 1$.*

Later, this conjecture was disproved by Nicodemos and Stehlik [3] for an infinite family of nanodiscs.

In 1939, Goldberg [4] proposed the regular icosahedron planning in planar hexagonal lattices, which induced the definition of *solids with icosahedral symmetry.* Another motivation of this planning is the definition of *fullerene graphs with icosahedral symmetry.* This icosahedron planning depends on two integers and non-negative parameters i and j. They are the bi-dimensional componentes that generates all faces of the regular icosahedron. We consider $0 \leq i \leq j$. We denote by $G_{i,j}$ the *fullerene graph with icosahedral symmetry* generated by the vector $\vec{G} = (i, j)$. Andova and Skrekovski [1] detected the icosahedral symmetry of the fullerene graphs from the position of its pentagonal faces. That is, the centers of the 12 pentagonal faces of a fullerene graph, if connected, origin a regular icosahedron if, and only if, the graph is fullerene with icosahedral symmetry.

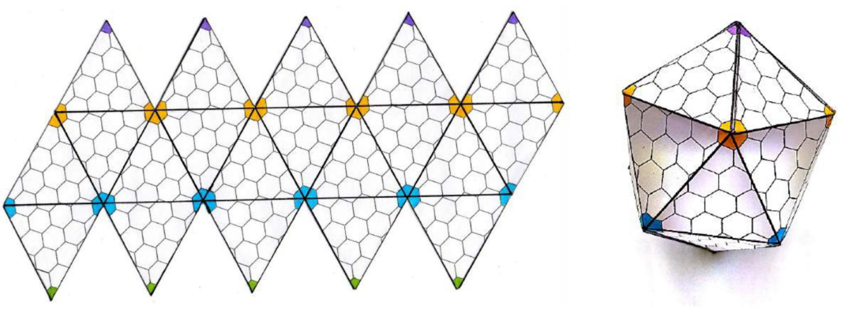
In this work, we study the problem of determining the diameter of spherical fullerene graphs with icosahedral symmetry $G_{i,j}$, $i, j \in \mathbb{N}$, $0 \leq i \leq j$ and we show properties about the diameter of $G_{i,j}$ where $j = i + 1$. The main result of this paper is the proposal of a new lower bound for $G_{i,i+1}$, contributing to the conjecture proposed by Andova and Skrekovski [1], that asks if $diam(G_{i,j})$, for some $i, j \in \mathbb{N}$, is a lower bound for $diam(F)$, F any fullerene graph.

2 Previous Works

In this section we show some known results referred to the study of the diameter of fullerene graphs with icosahedral symmetry. Goldberg [4] establishes the number of vertices and edges in a graph $G_{i,j}$. This result is shown in following corollary.

Corollary 2. (Goldberg [4]) *Let* $0 \leq i \leq j$ *be integers and* $G_{i,j}$ *be a fullerene graph with icosahedral symmetry. The number of vertices and edges are given, respectively, by* $n = 20(i^2+ij+j^2)$ *and* $m = 30(i^2+ij+j^2)$.

Graph $G_{1,4}$ depicted in Figure 1 is an example of this result. By Corollary 2, $|V(G_{1,4})| = 20\times(1+4+16) = 420$ and $|E(G_{1,4})| = 30\times(1+4+16) = 630$. Applying *Euler relation*, the number of faces of $G_{1,4}$ is 212, being 200 hexagonal and 12 pentagonal faces. Figure 1 shows $G_{1,4}$ as a construction of its planning in a hexagonal lattice. The vertices of the triangles in the planning of $G_{1,4}$ (Fig. 1(a)) are the centers of its 12 pentagonal faces.



(a) Planning of $G_{1,4}$ (b) $G_{1,4}$

Figure 1: Fullerene graph with icosahedral symmetry $G_{1,4}$.

The problem of proving or disproving Conjecture 1 has been studied for more than 5 years. However, another important research is related to precisely determining the diameter of fullerene graphs with icosahedral symmetry $G_{i,j}$. In the following two results, Theorem 3 presents a lower and an upper bound for the diameter of every fullerene graphs, and Theorem 4 gives the diameter of spherical graphs $G_{i,j}$ for all cases where $i = 0$ and $j > 0$.

Theorem 3. (Andova-Skrekovski [1]) *Let G be a fullerene graph with n vertices. Then,*

$$\frac{\sqrt{24n-15}-3}{6} \leq diam(G) \leq \frac{n}{5}+1$$

Theorem 4. (Andova-Skrekovski [1]) *The diameter of a fullerene graphs with icosahedral symmetry $G_{0,j}$, with $j > 0$, is $diam(G_{0,j}) = 6j-1$.*

By Corollary 2, the number of vertices of $G_{0,j}$ is $|V(G_{0,j})| = 20(i^2+ij+j^2) = 20(0^2+0j+j^2) = 20j^2$. Thus Conjecture 1 is valid, $\left\lfloor \sqrt{\frac{5}{3} \times 20j^2} \right\rfloor = \left\lfloor \sqrt{\frac{100}{3}} \right\rfloor j = 5j$. Thus, $diam(G_{0,j}) = 6j-1 > 5j-1$. It means that the conjecture is true for $G_{0,j}$ for all $j > 0$. Andova and Skrekovski [1] also studied the diameter for fullerene graphs $G_{j,j}$ for $j > 0$. This result is presented in Theorem 5.

Theorem 5. (Andova-Skrekovski [1]) *The diameter of a fullerene graphs with icosahedral symmetry $G_{j,j}$, with $j > 0$, is $diam(G_{j,j}) = 10j-1$.*

Making the same analysis as before, we verify that the Conjecture 1 is valid for $G_{j,j}$. By Corollary 2, $n = 20(j^2+j^2+j^2) = 60j^2$. So, $\left\lfloor \sqrt{\frac{5}{3} \times 60j^2} \right\rfloor = \left\lfloor \sqrt{\frac{300}{3}} \right\rfloor j = 10j$. Thus $diam(G_{0,j}) = 10j-1$ and we conclude that Conjecture 1 is still valid for $G_{j,j}$ with $j > 0$. Nicodemos [2] studied the diameter for another two classes of graphs $G_{i,j}$. Theorem 6 shows that Conjecture 1 is valid for $G_{i,j}$, $j \geq \frac{11}{2}i$ and Theorem 7 provides a sharp value for $diam(G_{1,j})$.

Theorem 6. (Nicodemos [2]) *Let $G = G_{i,j}$ be a fullerene graph with icosahedral symmetry. If $j \geq \frac{11i}{2}$, than $diam(G_{i,j}) \geq \left\lfloor \sqrt{\frac{5n}{3}} \right\rfloor - 1$.*

Theorem 7. (Nicodemos [2]) *The diameter of a fullerene graphs with icosahedral symmetry $G_{1,j}$, with $j \geq 3$, is $diam(G_{1,j}) = 6j + 1$.*

Suppose $j = 3$. By Corollary 2, $n = 260$. Thus, $\left\lfloor \sqrt{\frac{5n}{3}} \right\rfloor - 1 = 19$, which is the sharp value given by Theorem 7. By induction on j we get that Conjecture 1 is valid for $G_{1,j}$ $\forall j > 0$.

3 Results

Now, we show the results obtained from studying the diameter and the structure of $G_{i,i+1}$ fullerene graphs. Consider the planning of $G_{1,4}$, depicted in Figure 2. Define the *antipodal pentagons* as the pentagonal faces with center in $P1$ and $P12$.

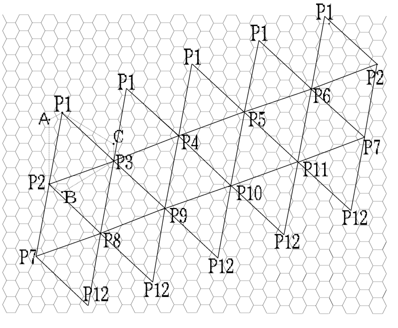


Figure 2: Planning of $G_{1,4}$.

Lemma 8 establishes a lower bound for $diam(G_{i,i+1})$. The proof of this lower bound follows by induction on $i \geq 0$. Figure 3 shows an example of Lemma 8 for $G_{2,3}$.

Lemma 8. *The distance between antipodal pentagons in a fullerene graph with icosahedral symmetry $G_{i,i+1}$ is $10i + 3$.*

Next result states a condition on spherical fullerene graphs $G_{i,j}$ describing whether the center of the triangles defined by its pentagonal faces is a hexagonal face or a vertex.

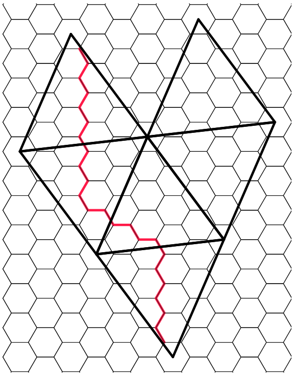


Figure 3: A shortest path between two antipodal pentagons in $G_{2,3}$ depicted in red with length $10 \times 2 + 3 = 23$.

Property 9. *Let $G = G_{i,j}$ be a fullerene graph with icosahedral symmetry. The center of a triangle in its planning is:*

i) a vertex, if $j - i \equiv 1$ or $j - i \equiv 2 (\mod 3)$;

ii) a hexagonal face, if $j - i \equiv 0 (\mod 3)$.

For all graphs $G_{i,i+1}$, with $j - i \equiv 1 (\mod 3)$, the center of each triangle formed by its pentagonal faces is a vertex. We say that a vertex is *pentagonal* if it is in a pentagonal face. For instance, the vertex $P1$ in Figure 2 represents a pentagonal face, hence all vertices of the face represented by $P1$ are pentagonal vertices. Lemma 10 determines the distance between a pentagonal vertex and the central vertex of the triangle in which they are positioned for $G = G_{i,i+1}$.

Lemma 10. *Let $G = G_{i,j}$ be a fullerene graph with icosahedral symmetry such that $j = i + 1$. The distance between a pentagonal vertex and the center vertex of the triangle they belong is $d = 2i$.*

In order to verify the validity of Lemma 10, we note that there are i hexagonal faces between the central vertex O and a pentagonal vertex p. To move from a hexagonal face to another, one needs a path with length

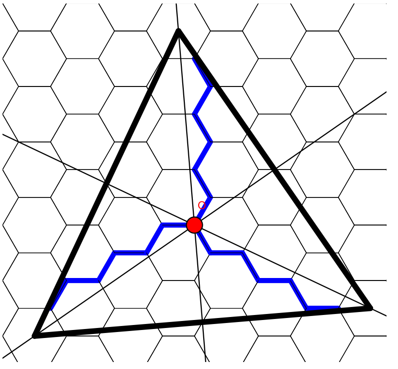


Figure 4: Triangle of $G_{3,4}$. Since $4-3 \equiv 1(\mod 3)$, the center O is a vertex. The shortest paths between O and the pentagonal vertices are depicted in blue.

2. Thus, a path between O and p has length $2i$. Finally, Theorem 11 establishes a lower bound for the diameter of all fullerene graphs $G_{i,i+1}$.

Theorem 11. *Let $G = G_{i,j}$ be a fullerene graph with icosahedral symmetry. If $j = i+1$, then $diam(G_{i,i+1}) = 10i + 4$.*

By Corollary 2, $n = 60i^2 + 60i + 20 > 60i^2$, $i > 0$. Using induction on $i > 0$, we can show that $diam(G_{i,i+1}) = 10i + 4 \geq \left\lfloor \sqrt{\frac{5\times(60i^2+60i+20)}{3}} \right\rfloor - 1$. Thus, Theorem 11 assures that Conjecture 1 is valid for $G_{i,i+1}$.

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Simone Dantas
Instituto de Matemática e Estatística
Universidade Federal Fluminense
Niterói, Brazil
sdantas@id.uff.br

Vinícius Linder
Instituto de Matemática e Estatística
Universidade Federal Fluminense
Niterói, Brazil
vlinder@id.uff.br

Diego Nicodemos
Colégio Pedro II
Rio de Janeiro, Brazil.
nicodemos@cos.ufrj.br

Thiago M. D. Silva
Departamento de Matemática
Pontifícia Universidade Católica do Rio de Janeiro
Rio de Janeiro, Brazil
thiagoomenez@mat.puc-rio.br