MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **96** (2026) 669–691
ISSN: 0340–6253
doi: 10.46793/match.96-2.32325

Settling the Andova and Škrekovski Conjecture for Spherical Fullerene Graphs $G_{i,ki}$

Thiago M. D. Silva[a], **Diego S. Nicodemos**[b,c], **Vitor S. Ponciano**[c,d,*], **Simone Dantas**[d]

[a] *SLB, Brazil.*
[b] *Colégio Pedro II, Brazil.*
[c] *State University of Rio de Janeiro, Brazil*
[d] *Fluminense Federal University, Brazil.*

thiagoomenez@gmail.com, diegonicorj@gmail.com, vitor_ponciano@id.uff.br, sdantas@id.uff.br

(Received December 5, 2025)

Abstract

Despite being composed exclusively of pentagonal and hexagonal faces, fullerene graphs (planar, cubic, and 3-connected) exhibit surprising properties. One of the most studied characteristics is the graph diameter, which remains difficult to determine in general. In 2012, Andova and Škrekovski formulated a conjecture regarding this parameter. They proposed that for a fullerene graph with n vertices, the diameter satisfies $\mathrm{diam}(G) \geq \lfloor (5n/3)^{1/2} \rfloor - 1$.

This conjecture is inspired by the study of a family of spherical fullerene graphs $G_{i,j}$, with $i, j \in \mathbb{N}^*$ and $i \leq j$, which also possess icosahedral symmetry. However, in 2023, Silva et al. proved the existence of infinite families of fullerene graphs with icosahedral symmetry, say $G_{i,2i}$, that contradict this conjecture. Thus, a natural question that arises is whether every graph $G_{i,j}$, when j is

*Corresponding author.

a multiple of i, satisfies the conjecture. In this paper, we provide a negative answer to this question and develop new techniques for determining the diameter of this family of graphs. These results completely settle this conjecture for this entire family of graphs.

1 Introduction

Fullerene graphs were defined to model a specific allotrope of carbon, called fullerene. In September 1985, Harold Kroto went to Rice University, where he began working with Richard Smalley and Robert Curl on carbon vaporization and the study of long-chain carbon molecules. Within days, on September 12, they discovered the structure of C_{60}, a molecule composed of 60 carbon atoms [5]. This structure consists of 60 vertices and 32 faces (12 pentagons and 20 hexagons) and was named *buckyball* or *fullerene*, in honor of architect Buckminster Fuller, whose geodesic dome has a design similar to that of Figure 1. For this groundbreaking discovery, Kroto, Curl, and Smalley were awarded the Nobel Prize in Chemistry in 1996 [8].

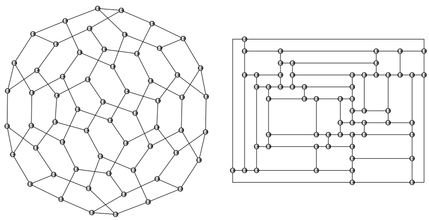
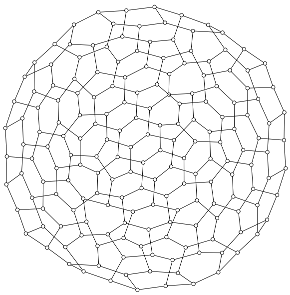


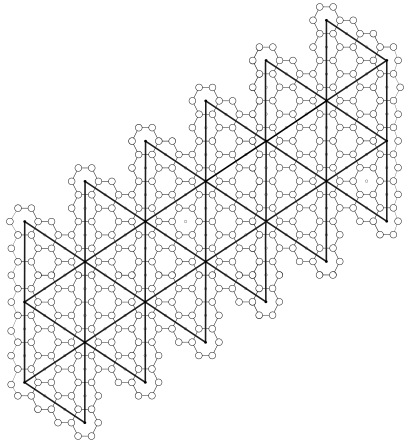
Figure 1. The structure of the C_{60} fullerene graph and its planar representation.

A *fullerene graph* is a planar, cubic, and 3-connected graph with only pentagonal and hexagonal faces. A specific class of fullerene graphs, called *icosahedral fullerene graphs*, was introduced by Andova and Škrekovski [1] in 2013. Each graph $G_{i,j}$ in this class is built from 20 copies of an (i, j)-triangle within a hexagonal tessellation of the plane. The vector $\overrightarrow{G} = (i, j)$, with $0 \leq i \leq j$ and $j > 0$, specifies the relative positions and distances of the vertices in a single triangle, providing a precise construction of the full icosahedral structure.

Fullerene graphs with complete icosahedral symmetry, specifically of



(a) $G_{0,3}$



(b) Planar representation of $G_{0,3}$

Figure 2. Fullerene graph with icosahedral symmetry $G_{0,3}$.

the types $G_{i,i}$ or $G_{0,i}$, $i > 0$, are not only highly symmetric but also perfectly spherical (see an example of $G_{0,3}$ in Figure 2). Based on these properties, Andova and Škrekovski [1] determined their diameters and conjectured that these values provide a lower bound for the diameter of all fullerene graphs.

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

Surprisingly, Nicodemos and Stehlik [7] showed that the conjecture fails for an infinite collection of nanodiscs, providing a clear counterexample. But in the same year, these authors analyzed fullerene graphs with icosahedral symmetry of type $G_{i,j}$, where $j \geq \frac{11i}{2}$, identifying yet another family that conforms to Conjecture 1; and initially suggesting that the conjecture might hold for all icosahedral cases [6].

Silva, Nicodemos, and Dantas [3] refuted this idea and established that spherical graphs of $G_{i,2i}$ do not satisfy Andova and Škrekovski's conjecture. They discussed properties of spherical fullerene graphs and of the hexagonal lattice itself, which simplified the proofs of results first introduced in [6]. Their key property showed that all graphs $G_{i,j}$ admit a reduction of the form $G_{i-\phi,j-\phi}$, where $\phi \leq i$, such that their triangular faces are entirely contained within those of $G_{i,j}$. Moreover, by setting $\phi = i$, this property establishes a specific relation among $G_{i,j}$, $G_{i-1,j-1}$, and $G_{0,j-i}$, forming a chain of reductions of $G_{i,j}$. This, in turn, implies that $\text{diam}(G_{i,j}) \geq \text{diam}(G_{0,j-i})$.

The results presented so far are summarized in Table 1 and represent the state of the art for this problem.

Condition	Formula	Ref.
$i = 0$	$\text{diam}(0, j) = 6j - 1$	[1]
$i = 1$	$\text{diam}(1, j) = 6j + 1$	[6]
$i = j$	$\text{diam}(j, j) = 10j - 1$	[1]
$j = 2i$	$\text{diam}(i, 2i) = 7j = 14i$	[3]
$j \geq \frac{11i}{2}$	$diam(G_{i,j}) \geq \left\lfloor \sqrt{\frac{5n}{3}} \right\rfloor - 1$	[3,6]

Table 1. Diameter $\text{diam}(i, j)$ of fullerene graphs with icosahedral symmetry $G_{i,j}$, $0 \leq i \leq j$.

From the results for $G_{i,2i}$, a natural question that arises is whether every graph $G_{i,j}$ with j being a multiple of i indeed satisfies the conjecture.

In this paper, we fully resolve this problem by showing that the only graphs $G_{i,ki}$ that do not satisfy Conjecture 1 are those with $k \in \{2, 3, 4, 5\}$, which completely settles Conjecture 1 for this infinite family of graphs.

2 Preliminaries

Let $G = (V(G), E(G))$ be an undirected, finite and simple graph where $V = V(G)$ is the set of vertices of G, and $E = E(G)$ is the set of edges of G. A *path* P between two vertices v_0, $v_{n-1} \in V(G)$ is a finite sequence of distinct vertices of $V(G)$ that can be arranged in a linear order $P = (v_0, v_1, \ldots, v_{n-1})$ in such a way that two vertices are adjacent if and only if they are consecutive in the linear sequence. The length of a path P

is the number of edges in P. The *distance* $d(u,v)$ between two vertices $u,v \in V(G)$ is the number of edges in a shortest path connecting u and v in G (if this path does not exist, $d(u,v)=\infty$). The diameter of a graph G is the length $max_{u,v}d(u,v)$ of the longest shortest path between two vertices $u,v \in V(G)$. Thus, we define *antipodal vertices* as the pairs of vertices that are the furthest apart in a graph, with their distance being equal to the graph's diameter.

Let $i,j \in \mathbb{N}^*$ with $i \leq j$. We define the *fullerene graph* $G_{i,j}$ *as a spherical fullerene with icosahedral symmetry.* The construction of $G_{i,j}$ is based on the *hexagonal lattice.* Consider the infinite hexagonal lattice in the plane and the centers of its hexagons. We define a *unit* as the line segment that joins the centers of two consecutive hexagons in a given direction. Now, choose a reference center. From this center, the main operation consists of moving i units in one direction, passing through the centers of the hexagons, and then j units in a second direction, with the angle between these directions being 120°.

Corollary 1. (Goldberg [4]) *Let $G_{i,j}$, with $0 \leq i \leq j$, be a fullerene graph with icosahedral symmetry. The numbers of vertices and edges are given by $n(G_{i,j}) = 20(i^2+ij+j^2)$ and $m(G_{i,j}) = 30(i^2+ij+j^2)$, respectively.* ∎

A direct consequence of the *Euler relation*, $|V|+|F|=|E|+2$, where $|V|$ is the number of vertices, $|F|$ is the number of faces and $|E|$ is the number of edges of G, ensures that every fullerene graph has exactly 12 pentagonal faces. From now on, to avoid ambiguity, with the vertices of the fullerene graph, we refer to the centers of the hexagons (or pentagons) as *nodes* and the line segments between nodes as *links.*

The boundary of the planar unfolding generated by i and j reconstructs the surface of a regular icosahedron. The labeled vertices serve as a guide for assembling the regular icosahedron, since identical labels indicate the same vertex in the reconstructed solid. A local view of the surface of this regular icosahedron, in the hexagonal lattice, reveals a solid whose surface is composed of hexagons (arising from the hexagonal lattice) and twelve pentagons determined by the vertices $a,b,c,d,e,f,a',b',c',d',e',f'$.

We refer to Figure 3 for an example of the construction of graph $G_{i,j}$ with $i = 3$ and $j = 6$, where pentagonal faces are filled in gray, and solid lines correspond to links between nodes. The dashed lines show the following construction process. We note that the triangular face abc is obtained from an arbitrary node a.

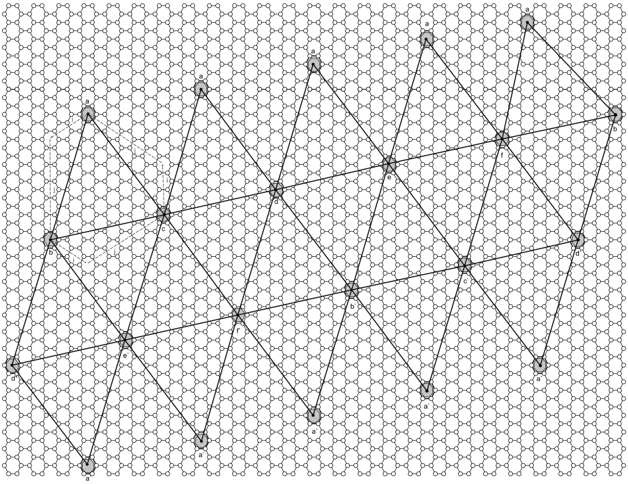


Figure 3. Vector $\overrightarrow{G} = (3, 6)$ generates fullerene graphs with icosahedral symmetry $G_{3,6}$. Pentagonal faces are filled in gray, and solid lines are links between nodes. Dashed lines show the construction process. Hexagons filled in gray with the same label appear distinct in the planar representation but correspond to a single pentagonal face in the reconstructed three-dimensional graph.

Starting at node a, move $i = 3$ units in one direction and then $j = 6$ units in a second direction, with the angle between the two directions equal to 120°; this reaches node b. We repeat this process starting at b (counterclockwise) until we reach node c, and, from c, we return to node a. Thus, we obtain one of the 20 triangular faces (whose vertices are the nodes of 12 pentagons), which generate the fullerene graphs with icosahedral symmetry. We observe that the nodes labeled a (resp. a') correspond to the same node in the three-dimensional fullerene structure. In the planar representation, these nodes appear as distinct, but in the three-dimensional realization of the graph, they correspond to a single node because their corresponding pentagonal faces (filled in gray) on the boundary are identified. This identification closes the surface and enables the computation of the graph's diameter, defined as the mininum (geodesic) distance between such antipodal vertices in the three-dimensional structure.

See an example in Figure 4 of part of the planar representation of the fullerene graph with icosahedral symmetry generated by the vector $\overrightarrow{G} = (3, 6)$, denoted by $G_{3,6}$. The edges of the fullerene graph highlighted in thick lines represent the shortest path between the antipodal nodes a and a' in the three-dimensional structure.

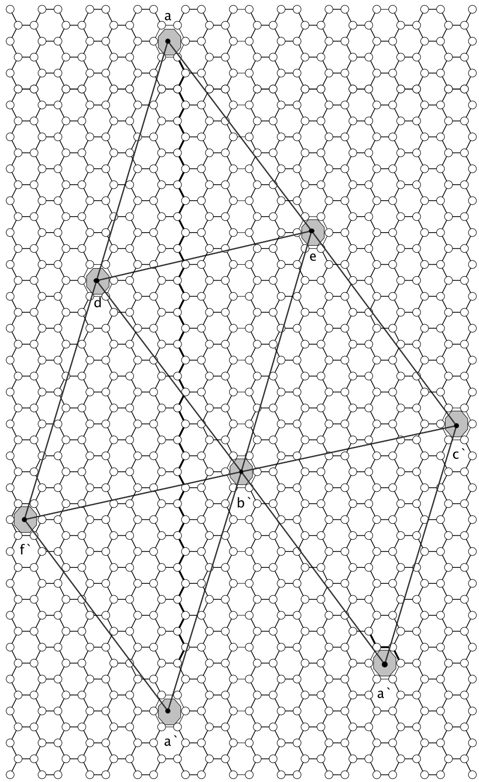


Figure 4. Part of the planar representation of graph $G_{3,6}$. The diameter of the fullerene graph with icosahedral symmetry $G_{3,6}$ is 42. Pentagonal faces are filled in gray, and those with the same label a' correspond to the same face in the reconstructed three-dimensional graph. The edges of $G_{3,6}$ within the shortest path between the antipodal vertices a and a' are highlighted in thick lines.

The problem of verifying Conjecture 1 has been studied for more than ten years, and a closely related line of research aims to precisely determine the diameter of the icosahedral fullerene graphs $G_{i,j}$.

Andova and Škrekovski [1] determined bounds for this parameter when G is a fullerene graph with n vertices, and established that:

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

Later, Nicodemos [6] proved that $diam(G_{1,j}) = 6j+1$. Furthermore, $diam(G_{i,j}) \geq \lfloor\sqrt{5n/3}\rfloor - 1$ for $j \geq 11i/2$ was shown, thereby establishing the validity of the conjecture for both families of graphs.

However, in 2023, Silva, Nicodemos, and Dantas [3] proved the existence of infinite families of fullerene graphs with icosahedral symmetry that do not satisfy the conjecture, establishing that $diam(G_{i,2i}) = 14i$. This result was obtained through a key property that every graph $G_{i,j}$ admits a reduction of the form $G_{i-\phi,\, j-\phi}$, with $\phi \leq i$, such that its triangular faces are entirely contained within the triangular faces of $G_{i,j}$. This generates a chain of reductions that leads to the following result.

Lemma 1 (Silva, Nicodemos and Dantas [3]). *For every fullerene graph with icosahedral symmetry $G_{i,j}$, with $0 < i < j$:*

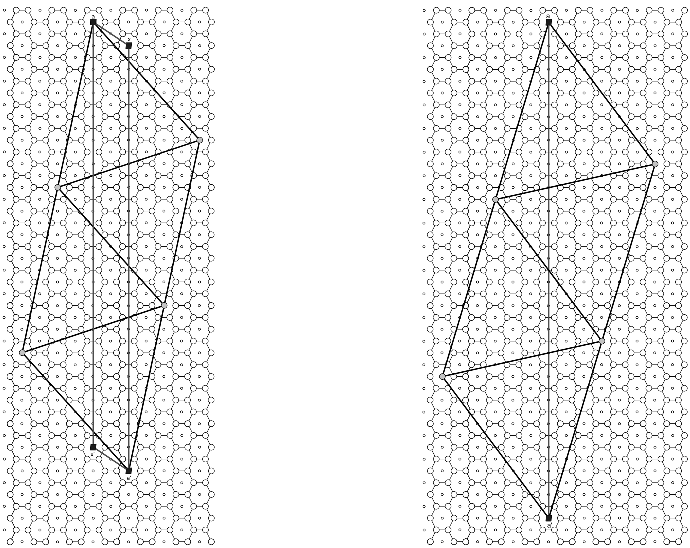
$$diam(G_{i,j}) \geq diam(G_{0,j-i}) = 6j-6i-1. \qquad \blacksquare$$

Another property of spherical graphs $G_{i,j}$ constructed using the hexagonal lattice is the existence of a *parallelogram patch* between the antipodal pentagonal vertices.

We refer to Figure 5 to explain the construction of this parallelogram patch. Let a and a' be antipodal pentagonal nodes. If $j > 2i$, then there is a parallelogram patch connecting the nodes of the pentagonal antipodal faces a and a', whose side length is $j-2i$. Starting at node a, we rotate the vector $\overrightarrow{i}$ counterclockwise by 120°, obtaining the vector $\overrightarrow{p}$. Following direction $\overrightarrow{p}$, we construct the *side length* of the parallelogram patch by moving $j-2i$ units to reach node x.

When $j = 2i$, the hexagons between a and a' form a linear stack, which we regard as a *degenerate parallelogram patch* ($a = x$ and $a' = x'$). According to [1], the minimum path between the pentagonal antipodal nodes must lie within this parallelogram patch. Figure 5 depicts the parallelogram patch of $G_{2,6}$ and the degenerated one of $G_{3,6}$.

Property 1 (Silva, Nicodemos and Dantas [3])**.** *For every fullerene graph with icosahedral symmetry $G_{i,j}$ such that $j \geq 2i$, there exists a parallelogram patch whose side length equals $j - 2i$.*



(a) $G_{2,6}$ (b) $G_{3,6}$

Figure 5. Part of the planar representation of graphs: (a) the parallelogram patch of $G_{2,6}$; and (b) the degenerated parallelogram patch of $G_{3,6}$. The square nodes are the vertices of the respective parallelograms, say a, x, a', and x'.

Property 1 indicates that the diameters of graphs $G_{i,j}$ such that $j \geq 2i$ might be computed using a similar method, as the constructed parallelogram patch contains the minimum path between the antipodal pentagonal vertices [1]. Therefore, it is natural to study the diameter of graphs such that $j \geq 2i$.

3 Parametric construction of the lattice

In this section, we analyze the problem from a different perspective by establishing the geometric and vector framework needed for the metric analysis of fullerene graphs. Since the surface of a fullerene is locally isomorphic to a planar hexagonal lattice, we simplify the complex task of computing geodesics in 3D by mapping it to a 2D real vector-coordinate system. Our goal is to formalize the construction of $G_{i,j}$ using this new methodology.

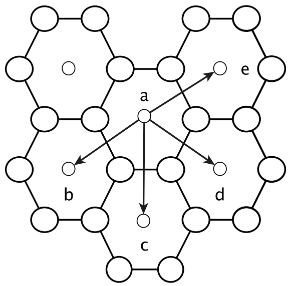


Figure 6. Basic direction vectors: $\overrightarrow{ab} = \overrightarrow{d_1}$, $\overrightarrow{ac} = \overrightarrow{v}$, $\overrightarrow{ad} = \overrightarrow{d_3}$, $\overrightarrow{ae} = \overrightarrow{d_2}$.

First, we define an origin node and a set of direction vectors that represent the possible moves between adjacent carbon atoms (see Figure 6).

This vector framework describes the path between any two nodes as a linear combination of basic moves, thereby facilitating the derivation of closed-form expressions for the diameter and other structural properties of Goldberg polyhedra.

Let $a \in \mathbb{R}^2$ be an origin node, and let $i, j \in \mathbb{R}$ be step scalars. We consider four basic direction vectors in $\mathbb{R}^2$: the upper-left diagonal vector $\overrightarrow{ab} = \overrightarrow{d_1}$; the vertical vector $\overrightarrow{ac} = \overrightarrow{v}$; the lower-right diagonal vector $\overrightarrow{ae} = \overrightarrow{d_2}$; and the upper-right diagonal vector $\overrightarrow{ad} = \overrightarrow{d_3}$.

Let $\{\overrightarrow{d_1}, \overrightarrow{v}\}$ be two linearly independent vectors that form a basis for the plane $\mathbb{R}^2$. Thus, the vectors $\overrightarrow{d_2}$ and $\overrightarrow{d_3}$ can be uniquely expressed as linear combinations of $\overrightarrow{d_1}$ and $\overrightarrow{v}$, as follows: $\overrightarrow{d_2} = c_1\overrightarrow{d_1} + c_2\overrightarrow{v}$ and $\overrightarrow{d_3} = c_3\overrightarrow{d_1} + c_4\overrightarrow{v}$, where c_1, c_2, c_3, and $c_4 \in \mathbb{R}$ are scalars whose values are determined by the specific geometry of the lattice.

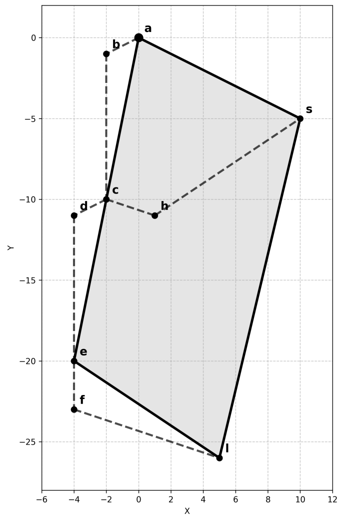


Figure 7. Example of a geometric construction of nodes of graph $G_{i,j}$ from the origin node $a = [0, 0]$.

We refer to Figure 7 for an example, where $i = 1$, $j = 3$, and the linearly independent basis vectors are $\overrightarrow{d_1} = (-2, -1)$ and $\overrightarrow{v} = (0, -3)$. The other vectors are expressed as linear combinations of these two, say $\overrightarrow{d_2} = (3, -1)$ and $\overrightarrow{d_3} = (3, 2)$, such that $\overrightarrow{d_2} = -\frac{3}{2}\overrightarrow{d_1} + \frac{5}{6}\overrightarrow{v}$ and $\overrightarrow{d_3} = -\frac{3}{2}\overrightarrow{d_1} - \frac{1}{6}\overrightarrow{v}$, with $c_1 = -\frac{3}{2}$, $c_2 = \frac{5}{6}$, $c_3 = -\frac{3}{2}$ and $c_4 = -\frac{1}{6}$.

The subsequent nodes of the hexagonal lattice, $\mathcal{L} = \{b, c, d, e, f, h, s, l\}$, are iteratively generated as:

$$\begin{array}{llll} b = a + i\overrightarrow{d_1}, & c = b + j\overrightarrow{v}, & d = c + i\overrightarrow{d_1}, & e = d + j\overrightarrow{v}, \\ f = e + i\overrightarrow{v}, & h = c + i\overrightarrow{d_2}, & l = f + j\overrightarrow{d_2}, & s = h + j\overrightarrow{d_3}. \end{array} \tag{1}$$

This observation leads to the following result.

Lemma 2. *From the previously described vector framework (Equation 1), there exist explicit expressions for each node of the planar representation of $G_{i,j}$ in terms of the origin node a.*

Proof. The formulas for nodes b, c, d, e, and f are obtained by directly substituting the displacement definitions. On the other hand, obtaining nodes h, s, and l requires the explicit substitution of the vectors $\overrightarrow{d_2}$ and $\overrightarrow{d_3}$ by their linear combination in terms of the basis $\{\overrightarrow{d_1}, \overrightarrow{v}\}$, where $\overrightarrow{d_2} = c_1\overrightarrow{d_1} + c_2\overrightarrow{v}$, and $\overrightarrow{d_3} = c_3\overrightarrow{d_1} + c_4\overrightarrow{v}$, where c_1, c_2, c_3, and $c_4 \in \mathbb{R}$ are scalars whose values are determined by the specific geometry of the lattice.

We define vector h iteratively, by setting $h = c + i\overrightarrow{d_2}$. From the calculation of node c, we obtain:

$$\begin{aligned} h &= c + i\overrightarrow{d_2} \\ &= (b + j\overrightarrow{v}) + i\overrightarrow{d_2} \\ &= (a + i\overrightarrow{d_1} + j\overrightarrow{v}) + i(c_1\overrightarrow{d_1} + c_2\overrightarrow{v}) \\ &= a + i\overrightarrow{d_1} + ic_1\overrightarrow{d_1} + j\overrightarrow{v} + ic_2\overrightarrow{v} \\ &= a + i(1 + c_1)\overrightarrow{d_1} + (j + ic_2)\overrightarrow{v} \end{aligned} \tag{2}$$

To compute s from node h, we use $s = h + j\overrightarrow{d_3}$. From Equation 2:

$$\begin{aligned} s &= h + j\overrightarrow{d_3} \\ &= [a + i(1 + c_1)\overrightarrow{d_1} + (j + ic_2)\overrightarrow{v}] + j(c_3\overrightarrow{d_1} + c_4\overrightarrow{v}) \\ &= a + i(1 + c_1)\overrightarrow{d_1} + jc_3\overrightarrow{d_1} + (j + ic_2)\overrightarrow{v} + jc_4\overrightarrow{v} \\ &= a + (i + ic_1 + jc_3)\overrightarrow{d_1} + (j + ic_2 + jc_4)\overrightarrow{v} \end{aligned} \tag{3}$$

By factoring the scalar components, we obtain the final explicit form:

$$s = a + [i(1 + c_1) + jc_3]\overrightarrow{d_1} + [j(1 + c_4) + ic_2]\overrightarrow{v} \tag{4}$$

To express node $l = f + \beta\overrightarrow{d_2}$ in terms of the origin a, we first expand f using the definitions from Equation 1:

$$\begin{aligned} f &= e + i\overrightarrow{v} \\ &= (d + j\overrightarrow{v}) + i\overrightarrow{v} \\ &= (c + i\overrightarrow{d_1} + j\overrightarrow{v}) + i\overrightarrow{v} \\ &= (b + j\overrightarrow{v} + i\overrightarrow{d_1} + j\overrightarrow{v}) + i\overrightarrow{v} \\ &= (a + i\overrightarrow{d_1} + j\overrightarrow{v} + i\overrightarrow{d_1} + j\overrightarrow{v}) + i\overrightarrow{v} \\ &= a + 2i\overrightarrow{d_1} + (2j + i)\overrightarrow{v} \end{aligned}$$

Now, substituting f and $\overrightarrow{d_2} = c_1\overrightarrow{d_1} + c_2\overrightarrow{v}$ into the expression for l:

$$\begin{aligned} l &= f + j\overrightarrow{d_2} \\ &= [a + 2i\overrightarrow{d_1} + (2j+i)\overrightarrow{v}] + j(c_1\overrightarrow{d_1} + c_2\overrightarrow{v}) \\ &= a + (2i + jc_1)\overrightarrow{d_1} + (2j + i + jc_2)\overrightarrow{v} \\ &= a + (2i + jc_1)\overrightarrow{d_1} + [j(2 + c_2) + i]\overrightarrow{v} \end{aligned}$$

■

4 Spherical graphs $G_{i,ki}$

Inspired by the results in the 2D real vector-coordinate system in the previous section, and by the structural properties of the graphs $G_{i,2i}$, it is natural to investigate whether $G_{i,ki}$ satisfies Conjecture 1. To achieve insights into this problem, we study three additional classes of spherical graphs that may cover the problem for all spherical graphs. Before analyzing $G_{i,ki}$ in the hexagonal lattice, we establish a general construction of this family of graphs using the vector framework introduced in Equation 1.

Corollary 2. *[General Vector Form of Lattice Points] Let $\mathcal{P}(a, \alpha, \beta, \mathbb{V})$ be the set of nodes $\{b, c, d, e, f, h, s, l\}$ constructed in Lemma 2, where $\mathbb{V} = \{\overrightarrow{d_1}, \overrightarrow{v}, \overrightarrow{d_2}, \overrightarrow{d_3}\}$ is the set of the four displacement vectors. Any node $x \in \mathcal{P}$ can be expressed in a vector form as $x = a + \overrightarrow{v}_x$, where $\overrightarrow{v}_x$ (the displacement vector from a to x) is a linear combination of vectors in $\mathbb{V}$, computed using scaling factors $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{R}$, as:*

$$\overrightarrow{v}_x = c_1(\alpha, \beta)\overrightarrow{d_1} + c_2(\alpha, \beta)\overrightarrow{v} + c_3(\alpha, \beta)\overrightarrow{d_2} + c_4(\alpha, \beta)\overrightarrow{d_3},$$

with the coefficients c_m are expressed as $c_m(\alpha, \beta) = a_m\alpha + b_m\beta$ such that $a_m \in \mathbb{N}$ and $b_m \in \mathbb{N}$, $m \in \{1, 2, 3, 4\}$. ■

The previous results established the analytic framework for constructing the graph $G_{i,j}$. We now return to the hexagonal lattice to reinterpret these results in their original geometric settings. For each fullerene graph $G_{i,ki}$, there exists a construction $\mathcal{P}(a, i, ki, \mathbb{V})$, where a is the origin node of $G_{i,ki}$. According to Theorem 2, there is an $i-$homothety of $\mathcal{P}(a, i, ki, \mathbb{V})$ of the form $\mathcal{P}(a, 1, k, \mathbb{V})$, which refers to the graph $G_{1,k}$.

Geometrically, this implies that the graph $G_{i,ki}$ can be decomposed into i identical substructures, or blocks, each isomorphic to $G_{1,k}$, arranged consecutively along the hexagonal lattice. From this perspective, Theorem 3 suggests that the diameter of $G_{i,ki}$ should scale linearly with i, since traversing the graph essentially amounts to passing through these blocks one after another. Nevertheless, this intuition must be verified carefully within the geometry of the hexagonal lattice, where boundary identifications may affect distance measurements.

As an example of Theorem 2, graph $G_{2,6}$ is a 2-homothety of graph $G_{1,3}$. Consequently, within $G_{2,6}$, we can stack two blocks of $G_{1,3}$, say $G^z_{1,3}$ with $z \in \{1, 2\}$, as depicted in Figure 9 (center). In this context, the path length $D_{avl}(1, 3)$ (between nodes a and l in block $G_{1,3}$) can be represented as the distance between vertices A_1 and L_1, denoted as $d(A_1, L_1)$, as depicted in Figure 10 in an enlarged view of this block. For each block, the vertices A and L are respectively denoted as the first and last vertices of the block.

The general vector formulation provides the description of all nodes computed in the construction. Using this representation, we can investigate how two constructions are related under specific conditions of the scaling factors α and β.

Theorem 2. *Let $\mathcal{P}_1(a, \alpha_1, \beta_1, \mathbb{V})$ and $\mathcal{P}_2(a, \alpha_2, \beta_2, \mathbb{V})$ be a vector form of lattice nodes, sharing the exact origin a, and the same displacement vectors set $\mathbb{V}$, as presented in 2. If there is $k \in \mathbb{R}$ such that $\alpha_2 = k\alpha_1$ and $\beta_2 = k\beta_1$, then $\mathcal{P}_2$ is a k-homothety (scaling) of $\mathcal{P}_1$, both starting at node a.*

Proof. To demonstrate that $\mathcal{P}_2$ is a homothety of $\mathcal{P}_1$, starting at node a with a factor k, it suffices to show that, for any node $x_1 \in \mathcal{P}_1$ and its corresponding node $x_2 \in \mathcal{P}_2$, $\overrightarrow{ax_2} = k \cdot \overrightarrow{ax_1}$. From Corollary 2, the displacement vector from a to any other node x is a linear combination of $\overrightarrow{d_m} \in \mathbb{V}$, written as:

$$\overrightarrow{ax} = \sum_{m=1}^{4} c_m(\alpha, \beta)\overrightarrow{d_m}, \tag{5}$$

where $c_m(\alpha, \beta) = a_m\alpha + b_m\beta$, $a_m \in \mathbb{N}$ and $b_m \in \mathbb{N}$.

Considering the corresponding node x_2, with parameters $(\alpha_2, \beta_2) = (k\alpha_1, k\beta_1)$, the coefficient c_m of x_2 is:

$$c_m(\alpha_2, \beta_2) = c_m(k\alpha_1, k\beta_1) = a_m(k\alpha_1) + b_m(k\beta_1)$$

Factoring out k, we obtain:

$$c_m(\alpha_2, \beta_2) = k(a_m\alpha_1 + b_m\beta_1) = k \cdot c_m(\alpha_1, \beta_1).$$

Therefore, all coefficients of the vector $\overrightarrow{ax_2}$ scale by k. Substituting this relation into the vector $\overrightarrow{ax_2}$:

$$\begin{aligned}\overrightarrow{ax_2} &= \sum_{m=1}^{4} c_m(\alpha_2, \beta_2)\,\overrightarrow{d}_m \\ &= \sum_{m=1}^{4} (k \cdot c_m(\alpha_1, \beta_1))\,\overrightarrow{d}_m = k \cdot \sum_{m=1}^{4} c_m(\alpha_1, \beta_1)\,\overrightarrow{d}_m = k \cdot \overrightarrow{AX_1}\end{aligned}$$

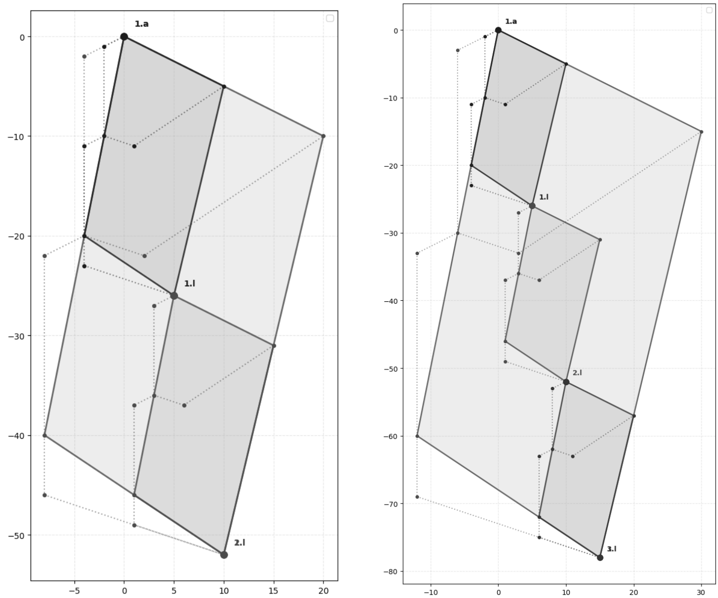
Since the relation $\overrightarrow{ax_2} = k \cdot \overrightarrow{ax_1}$ holds for all corresponding nodes x_1 and x_2 (including a, where $k \cdot \overrightarrow{aa} = \overrightarrow{aa}$), the vector form $\mathcal{P}_2$ is a homothety of $\mathcal{P}_1$ with center at a and scale factor k. ■

Figure 8 illustrates the application of Theorem 2. As shown in the examples, when the parameters α and β are scaled by a factor k, the resulting construction $\mathcal{P}_2$ maintain a k-homothety relationship with $\mathcal{P}_1$, preserving the same origin and displacement vectors.

Having established how constructions behave under scaling, the following theorem examines a direct consequence of the structural linear scaling of the distance between the antipodal vertices of the pentagon.

Theorem 3. *Let a be the origin of a lattice, let $\mathcal{B} = \{\overrightarrow{d_1}, \overrightarrow{v}\}$ be its vector basis, and let $\alpha, \beta \in \mathbb{R}^+$ be the scaling factors. Let $\overrightarrow{d_2}$ be the displacement vector expressed by the linear combination $\overrightarrow{d_2} = \alpha\overrightarrow{d_1} + \beta\overrightarrow{v}$.*

Let $D_{avl}(\alpha, \beta)$ be the path length (number of links) of the parallelogram patch $a \to v \to l$, where $v = a + (\beta - 2\alpha)\overrightarrow{d_2}$. If the parameters α and β maintain a fixed linear proportion $\beta = k\alpha$ for some constant $k > 0$, then



(a) Construction $\mathcal{P}(1.a, 2, 6, \mathbb{V})$ (b) Construction $\mathcal{P}(1.a, 3, 9, \mathbb{V})$

Figure 8. Examples of k-homothety for constructions $\mathcal{P}(1.a, 2, 6, \mathbb{V})$ and $\mathcal{P}(1.a, 3, 9, \mathbb{V})$. In (a), two *chains* of $\mathcal{P}(a, 1, 3, \mathbb{V})$, $a \in \{1.a, 1.l\}$, fit within $\mathcal{P}(1.a, 2, 6, \mathbb{V})$. In (b), three chains of $\mathcal{P}(a, 1, 3, \mathbb{V})$, $a \in \{1.a, 1.l, 2.l\}$, fit within $\mathcal{P}(1.a, 3, 9, \mathbb{V})$.

the path length D_{avl} scales linearly with α:

$$D_{avl}(\alpha, k\alpha) = \alpha \cdot D_{avl}(1, k)$$

Proof. The total path length D_{avl} is the sum of the norm of the vectors $\overrightarrow{av}$ and $\overrightarrow{vl}$:

$$D_{avl}(\alpha, \beta) = \|\overrightarrow{av}\| + \|\overrightarrow{vl}\|$$

We substitute $\beta = k\alpha$ and express all displacement vectors in terms of the basis $\{\overrightarrow{d_1}, \overrightarrow{v}\}$.

Considering $v = a + (\beta - 2\alpha)\overrightarrow{d_2}$ and the relation $\overrightarrow{d_2} = \alpha\overrightarrow{d_1} + \beta\overrightarrow{v}$:

$$\begin{aligned}\overrightarrow{av} &= (\beta - 2\alpha) \cdot \overrightarrow{d_2} \\ &= (k\alpha - 2\alpha) \cdot (\alpha\overrightarrow{d_1} + \beta\overrightarrow{v}) \\ &= \alpha(k-2) \cdot (\alpha\overrightarrow{d_1} + \beta\overrightarrow{v}) = \alpha \cdot \left[\alpha(k-2)\overrightarrow{d_1} + \beta(k-2)\overrightarrow{v}\right]\end{aligned}$$

Replacing $\overrightarrow{d_2} = \alpha\overrightarrow{d_1} + \beta\overrightarrow{v}$, and $\beta = k\alpha$, in the equation of $\overrightarrow{vl} = (2\alpha \cdot \overrightarrow{d_1}) + ((\alpha + 2\beta) \cdot \overrightarrow{v}) + (2\alpha \cdot \overrightarrow{d_2})$, we have that:

$$\begin{aligned}\overrightarrow{vl} &= 2\alpha\overrightarrow{d_1} + (\alpha + 2k\alpha)\overrightarrow{v} + 2\alpha(\alpha\overrightarrow{d_1} + \beta\overrightarrow{v}) \\ &= 2\alpha\overrightarrow{d_1} + \alpha(1+2k)\overrightarrow{v} + 2\alpha\alpha\overrightarrow{d_1} + 2\alpha\beta\overrightarrow{v} \\ &= \alpha \cdot \left[(2 + 2\alpha)\overrightarrow{d_1} + ((1+2k) + 2\beta)\overrightarrow{v}\right]\end{aligned}$$

Both vectors have the form $\alpha \cdot \overrightarrow{w}(k)$, where $\overrightarrow{w}(k)$ is a constant vector determined only by k, α, β, $\overrightarrow{d_1}$, and $\overrightarrow{v}$. Now, let $\overrightarrow{y}$ be $\overrightarrow{av}$ or $\overrightarrow{vl}$. In $\mathbb{R}^2$, if $\overrightarrow{y} = \alpha \cdot \overrightarrow{w}(k)$, then $\|\overrightarrow{y}\| = \|\alpha \cdot \overrightarrow{w}(k)\| = \alpha \cdot \|\overrightarrow{w}(k)\|$. This follows from the linearity of the norm, $\|c\overrightarrow{u}\| = |c|\|\overrightarrow{u}\|$, and from the fact that $\alpha > 0$.

Again, applying the linearity of the norm, that is $\overrightarrow{av} = \alpha \cdot \overrightarrow{w}_1(k)$ and $\overrightarrow{vl} = \alpha \cdot \overrightarrow{w}_2(k)$, we have:

$$\begin{aligned}D_{avl}(\alpha, k\alpha) &= \|\overrightarrow{av}\| + \|\overrightarrow{vl}\| \\ &= \|\alpha \cdot \overrightarrow{w}_1(k)\| + \|\alpha \cdot \overrightarrow{w}_2(k)\| \\ &= \alpha \cdot \|\overrightarrow{w}_1(k)\| + \alpha \cdot \|\overrightarrow{w}_2(k)\| \\ &= \alpha \cdot (\|\overrightarrow{w}_1(k)\| + \|\overrightarrow{w}_2(k)\|)\end{aligned}$$

The term in parentheses is the path length for $\alpha = 1$, say $D_{avl}(1, k)$. Hence,

$$D_{avl}(\alpha, k\alpha) = \alpha \cdot D_{avl}(1, k)$$

This shows that, by keeping a linear proportion between the scaling factors, the path length $a \to v \to l$ is directly proportional to the factor α. ■

Hence, the path length $D_{avl}(2, 6)$ of graph $G_{2,6}$ includes two times $D_{avl}(1, 3)$. However, we observe that from vertex L_1 in Block 1 to vertex

A_2 in Block 2, we add one edge to connect the paths of these two blocks $G^1_{1,3}$ and $G^2_{1,3}$. Therefore, $D_{avl}(2,6) = D_{avl}(1,3) + 1 + D_{avl}(1,3)$.

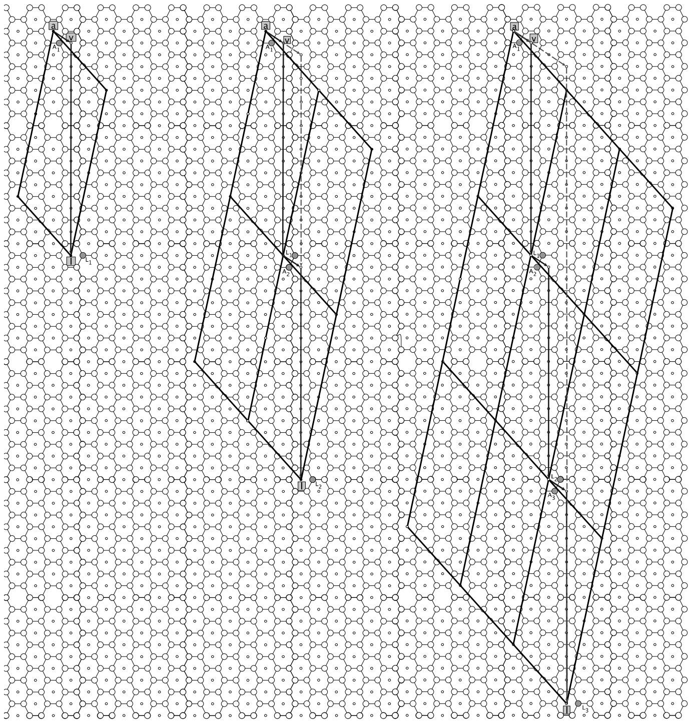


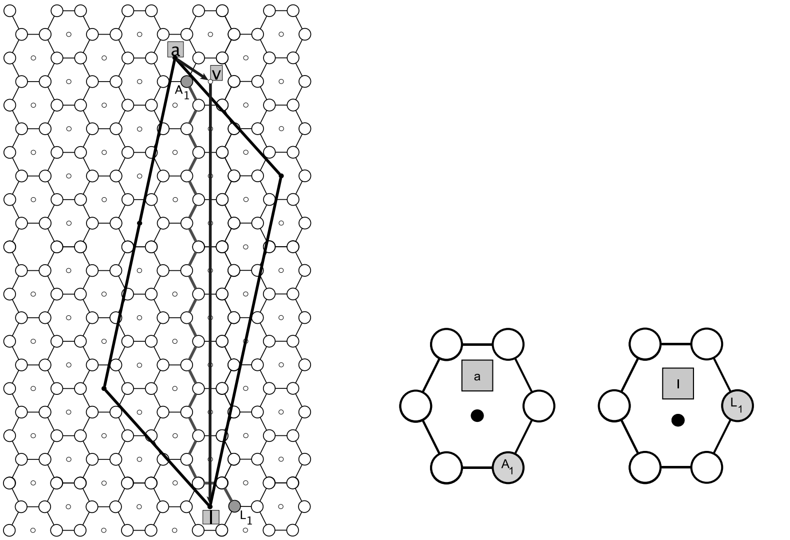
Figure 9. Block of $G_{1,3}$ (left); two blocks $G_{1,3}$ within $G_{2,6}$ (center); and three blocks $G_{1,3}$ within $G_{3,9}$ (right); Arrows in solid lines: corresponding number of links in $D_{avl}(1,3)$ contributing to total path length; Arrows in dashed lines: the respective $D_{avl}(i,j)$. Vertices A_i and L_i, $i \in \{1,2,3\}$ are filled in gray. Note that in the lowest $G_{1,3}$ blocks, the solid lines overlap the dashed lines.

Similarly, Figure 9 (right) shows that $D_{avl}(3,9) = D_{avl}(1,3) + 1 + D_{avl}(1,3) + 1 + D_{avl}(1,3)$, and this leads to the following result:

Theorem 4. *Let $G_{i,j}$ be a fullerene graph with icosahedral symmetry. If $j = ki$ where $k > 2$, then:*

$$diam(G_{i,ik}) = i \cdot diam(G_{1,k}) + (i-1)$$

Proof. The proof proceeds by induction on i, the number of blocks. For



(a) Block 1: The arrows represent the length of the parallelogram patch $a \to v \to l$.

(b) Enlarged view of the hexagons of nodes a and l, containing the first and last vertices, A_1 and L_1 respectively.

Figure 10. Example of the hexagonal lattice with a representation of Block 1, and its respective first and last vertices of $G_{2,6}$

the Base Case ($i = 1$), for a single block, the total distance is, by definition, the internal diameter of the block:

$$\mathrm{diam}(G_{1,k}) = d_G(A_1, L_1) = \alpha$$

Applying the proposed formula for $i = 1$ yields $1 \cdot \alpha + (1 - 1) = \alpha + 0 = \alpha$.

We assume, by the induction hypothesis, that the formula is true for an arbitrary number of blocks $i = t \geq 1$. That is: $\mathrm{diam}(G_{t,tk}) = t \cdot \alpha + (t - 1)$. Now, we prove the property holds for $i = t + 1$.

The total distance up to the end of block $t + 1$ can be decomposed into the distance up to block t, plus the connection and the new block:

$$\mathrm{diam}(G_{t+1,(t+1)k}) = \underbrace{\mathrm{diam}(G_{t,tk})}_{\text{ind. hyp.}} + \underbrace{d_G(L_t, A_{t+1})}_{\text{connection}} + \underbrace{d_G(A_{t+1}, L_{t+1})}_{\text{new block}}$$

Substituting using the Induction Hypothesis, the given definitions, and reorganizing the terms algebraically:

$$\begin{aligned}\operatorname{diam}(G_{t+1,(t+1)k}) &= [t \cdot \alpha + (t-1)] + 1 + \alpha \\ &= t \cdot \alpha + \alpha + t - 1 + 1 \\ &= (t+1)\alpha + ((t+1) - 1)\end{aligned}$$

and this ends the proof. ■

4.1 Verifying the Andova and Škrekovski's conjecture

In this section, we analyze whether the graphs $G_{i,ki}$, for $k \geq 2$, satisfy Andova and Škrekovski's conjecture (Conjecture 1). From Theorem 4 and [6]:

$$diam(G_{i,ki}) = i \cdot diam(G_{1,k}) + i - 1 = 6ki + 2i - 1 \tag{6}$$

To verify the integer values of k such that the graphs $G_{i,ki}$ do not satisfy Andova and Škrekovski's conjecture, it suffices to compute the following:

$$6ki + 2i - 1 < \left\lfloor \sqrt{\frac{5\ n(G_{i,ki})}{3}} \right\rfloor - 1. \tag{7}$$

From Corollary 1, compute $n(G_{i,ki})$ as:

$$n_{G_{i,ki}} = 20\left(i^2 + ki^2 + k^2i^2\right). \tag{8}$$

By substituting Equation (8) in Equation (7), we derive the following:

$$6ki + 2i < \sqrt{\frac{100}{3}\,(i^2 + ki^2 + k^2i^2)}. \tag{9}$$

Noting that Equation 9 is only valid for $i \geq 1$, we obtain:

$$6k + 2 < \sqrt{\frac{100}{3}\,(1 + k + k^2)}. \tag{10}$$

Exploring the values of k that satisfy Equation 10, we find that k falls within the range $[-2, 11/2]$. This result means that for all graphs $G_{i,ki}$ where k equals 2, 3, 4, or 5, Conjecture 1 is false. This finding aligns with the result presented in [6], which asserts that Conjecture 1 holds for all $G_{i,j}$ when $j > 11i/2$. Thus, $G_{i,ki}$, $k \in \{2, 3, 4, 5\}$ are infinite families of spherical fullerene graphs for which Conjecture 1 is not valid.

We recall that the first family was introduced by Silva, Nicodemos, and Dantas [3], and considered $k = 2$. They also posed the following conjecture:

Conjecture 2 (Silva, Nicodemos, and Dantas [3])**.** *Let $G_{i,j}$ be a fullerene graph with icosahedral symmetry. If $j = ki$ where $k > 1$, then:*

$$\left| diam(G_{i,ki}) - \left(diam(G_{0,(k-1)i}) + 8i \right) \right| \leq 1. \qquad \blacksquare$$

Our work confirms Conjecture 2, which leads to the following result.

Theorem 5. *If $G_{i,ki}$ is a fullerene graph with icosahedral symmetry, then*

$$diam(G_{i,ki}) = diam(G_{0,(k-1)i}) + 8i.$$

Proof. Recall from Equation (6) that our derived formula for the diameter is:

$$diam(G_{i,ki}) = i \cdot diam(G_{1,k}) + i - 1 = 6ki + 2i - 1. \tag{11}$$

Consider the reference value for the case $i = 0$ given by $diam(G_{0,j}) = 6j - 1$. Substituting $j = (k-1)i$, we obtain:

$$diam(G_{0,(k-1)i}) = 6((k-1)i) - 1 = 6ki - 6i - 1.$$

Now, we evaluate the expression from the conjecture by adding the term $8i$:

$$\begin{aligned} diam(G_{0,(k-1)i}) + 8i &= (6ki - 6i - 1) + 8i \\ &= 6ki + 2i - 1. \end{aligned}$$

Comparing this result with Equation (11), we observe that:

$$diam(G_{i,ki}) - \left(diam(G_{0,(k-1)i}) + 8i \right) = 0,$$

and hence the conjecture is verified. $\blacksquare$

5 Conclusion

In this paper, we settle the Andova and Škrekovski's Conjecture [1] (Conjecture 1), for fullerene graphs with icosahedral symmetry $G_{i,j}$ where j is a multiple of i.

In Table 2, we present the state of the art of the computation of $diam(G_{i,j})$, for $1 \leq i \leq 5$ and $1 \leq j \leq 25$. The notation N/F ("Not Found") indicates that, even for small values of i and j, there is still no study or general formula available.

i \ j	1	2	3	4	5	6	7	8	9	10	11	12	13
0	5	11	17	23	29	35	41	47	53	59	65	71	77
1	9	13	19	25	31	37	43	49	55	61	67	73	79
2	—	19	N/F	28	N/F	39	N/F	51	N/F	63	N/F	75	N/F
3	—	—	29	N/F	N/F	42	N/F	N/F	59	N/F	N/F	77	N/F
4	—	—	—	39	N/F	N/F	N/F	56	N/F	N/F	N/F	79	N/F
5	—	—	—	—	49	N/F	N/F	N/F	N/F	70	N/F	N/F	N/F

i \ j	14	15	16	17	18	19	20	21	22	23	24	25
0	83	89	95	101	107	113	119	125	131	137	143	149
1	85	91	97	103	109	115	121	127	133	139	145	151
2	87	N/F	99	N/F	111	N/F	123	N/F	135	N/F	147	N/F
3	N/F	95	N/F	N/F	113	N/F	N/F	131	N/F	N/F	149	N/F
4	N/F	N/F	103	N/F	N/F	N/F	127	N/F	N/F	N/F	151	N/F
5	N/F	99	N/F	N/F	N/F	N/F	129	N/F	N/F	N/F	N/F	159

Table 2. Diameter diam($G_{i,j}$) of fullerene graphs with icosahedral symmetry $G_{i,j}$, for $1 \leq i \leq 5$ and $1 \leq j \leq 25$, where N/F ("Not Found") indicates that there is no general formula.

Moreover, based on the study of graphs $G_{i,j}$ where j is a multiple of i, we propose a conjecture that the diameter of all graphs $G_{i,j}$ can be computed as the sum of two multiples, $G_{i,ki}$, plus 1. Specifically, since every pair (i, j) can be decomposed into the sum of two pairs $(i_1, k_1 i_1)$ and $(i_2, k_2 i_2)$, we conjecture the following:

Conjecture 3. *If $G_{i,j}$ is a fullerene graph with icosahedral symmetry such that $i = i_1 + i_2$ and $j = k_1 i_1 + k_2 i_2$, with $k_1, k_2 \in \mathbb{N}^*$, then*

$$diam(G_{i,j}) = diam(G_{i_1,k_1 i_1}) + diam(G_{i_2,k_2 i_2}) + 1.$$

***Acknowledgment*:** This work was partially supported by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brasil (CAPES) – Finance Code 001; the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) 311260/2021-7, 422912/2021-2; 409288/2024-1; and the Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro (FAPERJ) Processo SEI-260003/014835/2023, E-26/210.649/ 2023.

References

[1] V. Andova, R. Škrekovski, Diameter of fullerene graphs with full icosahedral symmetry, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 205–220.

[2] S. Dantas, V. Linder, D. Nicodemos, T. M. D. Silva, On the diameter of spherical fullerene graphs, *Mat. Contemp.* **46** (2018) 256–264

[3] T. M. D. Silva, D. S. Nicodemos, S. Dantas, Spherical fullerene graphs that do not satisfy Andova and Škrekovski's conjecture, *Proced. Comput. Sci.* **223** (2023) 316–324.

[4] M. Goldberg, A class of multi-symmetric polyhedra, *Tohoku Math. J.* **43** (1939) 104–108.

[5] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. Smalley, C60: Buckminsterfullerene, *Nature* **318** (1985) 162–163.

[6] D. Nicodemos, *Diameter of Fullerene Graphs and Odd-Cycle Transversals of Fullerene-(3,4,5,6) Graphs*, Ph.D. thesis, COPPE/UFRJ, Rio de Janeiro, 2017.

[7] D. Nicodemos, M. Stehlik, Fullerene graphs of small diameters, *MATCH Commun. Math. Comput. Chem.* **77** (2017) 725–728.

[8] M. A. Shampo, R. A. Kyle, D. P. Steensma, Robert F. Curl Jr–Nobel laureate in chemistry, *Mayo Clinic Proceed.* **85** (2010) 750–751.