MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **70** (2013) 205-220

ISSN 0340 - 6253

Diameter of Fullerene Graphs with Full Icosahedral Symmetry

Vesna Andova[a,b1], **Riste Škrekovski**[b2]

[a] *Faculty of Electrical Engineering and Information Technologies, Ss Cyril and Methodius Univ., Ruger Boskovik, P. O. Box 574, 1000 Skopje, Macedonia*
E-mail: vesna.andova@gmail.com

[b] *Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 21, 1111 Ljubljana, Slovenia*
E-mail: skrekovski@gmail.com

(Received September 28, 2012)

Abstract

Fullerene graphs are 3-connected cubic planar graphs with only pentagonal and hexagonal faces. A class of fullerene graphs with icosahedral symmetry is called icosahedral fullerenes, and they are determined by a vector (i, j), $0 \leq i \leq j$ and $j > 0$. For $i = j$ or $i = 0$, the fullerenes are of full icosahedral symmetry. We show that the diameter of an (i, j)-icosahedral fullerene graph of full icosahedral symmetry is $4i + 6j - 1$. We conclude the paper by stating a conjecture on the diameter of any fullerene graph.

1 Introduction

Fullerenes are polyhedral carbon molecules, where atoms are arranged in pentagons and hexagons. The most symmetric is the famous buckminsterfullerene, C_{60}, whose discovery in 1985 marked the birth of fullerene chemistry [15]. The name was a homage to Richard Buckminster Fuller, whose geodetic dome it resembles. From the

[1]Corresponding author. Supported by Ad Futura grant.
[2]Partly supported by ARRS Research Program P1-0297.

very beginning, fullerenes have been attracting attention of diverse research communities.

Fullerenes can also be seen as graphs, vertices represent atoms and edges represent bonds between atoms. A *fullerene graph* is a 3-connected cubic planar graph with only pentagonal and hexagonal faces. By the Euler formula, there are precisely 12 pentagons, but there is no restriction on the number of hexagons. Grünbaum and Motzkin [13] showed that fullerene graphs on n vertices exist for all even $n \geq 24$ and for $n = 20$, i.e., there exists a fullerene graph with α hexagons where α is any integer distinct from 1. Although the number of pentagonal faces is negligible compared to the number of hexagonal faces, their layout is crucial for the shape of a fullerene graph. There is a class of fullerene graphs of tubular shape, called *nanotubes*. The ends of the tube are capped with a subgraph containing six pentagons and possibly some hexagons. There are fullerene graphs where no two pentagons are adjacent, i.e., each pentagon is surrounded by five hexagons. Those fullerene graphs satisfy the *isolated pentagon rule* or shortly IPR, and they are the most stable fullerenes. If the centers of the pentagonal faces form an icosahedra, the fullerene is called *icosahedral fullerene*. The dodecahedron is the only icosahedral fullerene that does not satisfy the IPR.

The *distance* between two vertices $u, v \in V(G)$ in a connected graph G is the length of a shortest path between them, and it is denoted by $d(u, v)$. The *distance between the faces* F_1 and F_2 is the minimal distance between the vertices from F_1 and F_2 or $d(F_1, F_2) = \min\{d(u, v) \,|\, u \in V(F_1),\, v \in V(F_2)\}$. A *diameter* of a connected graph G, $\mathrm{diam}(G)$, is the maximum distance between two vertices of G, i.e., $\mathrm{diam}(G) = \max\{d(u, v) \,|\, u, v \in V(G)\}$. The vertices $u, v \in V(G)$ are *diametral* vertices if $d(u, v) = \mathrm{diam}(G)$, and any shortest path between them is called a *diametral* path. A vertex v that belongs to the border of a pentagonal face is called a *pentagonal* vertex. A vertex that is not pentagonal is called *hexagonal*. A *hexagonal patch* is a simply connected set of hexagons in the (oriented) plane with all interior vertices having valency 3, at most two of the boundary vertices have valency 1 while all the other vertices have valency 2 or 3. A *bisector* of an edge (a segment) in the hexagonal grid is the line orthogonal to the edge passing trough its midpoint.

A number of graph-theoretical invariants were examined as potential stability predictors with various degrees of success [1, 7, 9, 14, 17]. As a result, we have achieved a fairly thorough understanding of fullerene graphs and their properties. For more results and questions on fullerenes see [6, 8, 10, 11, 16].

As we conjecture at the end of the paper that fullerenes with full icosahedral symmetry have the smallest diameter and perhaps these fullerenes are the most stable since they are the most spherical ones [3]. From this point of view, we suspect that the diameter could be used as a measure of stability, in a way that smaller diameter could imply more stable fullerene.

From the results in [2] we derive the upper and lower bound of the diameter of a fullerene graph.

Theorem 1.1. *Let G be a fullerene graph with n vertices. Then,*

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

For more precise results on diameter of fullerene graphs consider [2]. As it was shown in [2], the diameter of the nanotubes is linear in the number of vertices. On the other hand, the diameter of a fullerene graph G on n vertices having icosahedral symmetry is small, i.e., it is of order $\Theta(\sqrt{n})$.

In this paper we determine the diameter of an icosahedral fullerene graph with full icosahedral symmetry, and prove that each pentagonal vertex is diametral. Hexagonal vertices on the other side are not necessarily diametral. Even more, for an arbitrary vertex $x \in V(G)$ there is a pair of diametral pentagonal vertices $u, v \in V(G) \setminus \{x\}$ and a diametral path between them passing through x.

In order to determine the diameter of a fullerene graph with full icosahedral symmetry, we consider the two cases: $(0,i)$- and (i,i)-icosahedral fullerene graphs, where $0 < i$.

2 Construction of icosahedral fullerene graphs

The common feature of all icosahedral fullerenes is their geometrical shape. Icosahedral fullerene graphs are a class of fullerene graphs where the midpoints of all 12 pentagons form a regular icosahedron. The simplest icosahedral fullerene graph is the dodecahedron, C_{20}. Creating bigger icosahedral fullerene graphs means adding hexagons around each pentagon in C_{20} wisely. Caspar and Klug [4] and Coxeter [5] suggested a method that works with the icosahedral fullerene graph dual: *geodesic domes*, i.e., triangulations of the sphere with vertices of degree 5 and 6. Their method is filling the triangular faces of the icosahedron with equilateral triangles from the hexagonal tessellation of the plane.

Goldberg [12] used a hexagonal lattice to determine the vertices of the icosahedron triangular faces. Even more, Goldberg showed that the number of vertices n in a polyhedra of icosahedral symmetry can be related to two integers i and j by the following equation, conveniently called the *Goldberg equation*

$$n = 20(i^2 + ij + j^2). \tag{1}$$

The integers i and j in the Goldberg equation can be considered as components of a two-dimensional *Goldberg vector* $\vec{G} = (i, j)$. To avoid the mirror effect, we always assume that $0 \le i \le j$ and $0 < j$.

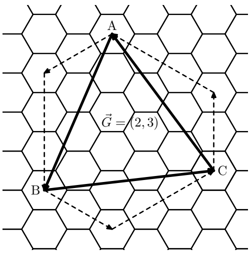

Figure 1. Construction of a $(2, 3)$-triangle, the face of a $(2, 3)$-icosahedral fullerene graph. The vertices of the equilateral triangle ABC are centers of pentagons.

Soon after the discovery of C_{60}, Goldberg vector turned out to be very useful in constructing bigger icosahedral fullerenes. This vector determines the distance and positions of the vertices of the (i, j)-triangle in the hexagonal lattice. See Figure 1 for a construction method of an (i, j)-triangle. Precisely 20 such (i, j)-triangles produce an (i, j)-icosahedral fullerene in a manner shown on Figure **??**. In other words, Goldberg vector defines the way of adding hexagons around each pentagonal face. The vertices of the triangle are centers of the 12 pentagons in the fullerene. The pair of the triangles ABC and $EB'C'$, as shown on Figure **??**, is a pair of opposite triangles. There are exactly 10 such pairs. The pentagons with centers in A and E (Figure **??**) are called *antipodal* pentagons (similarly, the pentagons with centers in B and B', as well as those with centers C and C' are antipodal).

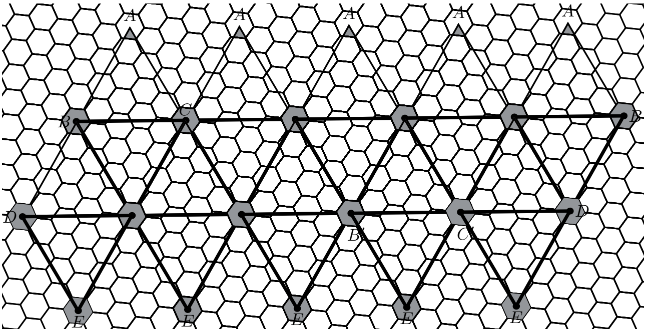

Figure 2. A $(2,3)$-icosahedral fullerene. Its triangular faces are constructed as on Figure 1. The vertices with a same name coincide. The vertices of each triangular are centers of the pentagons. The pentagons with center A and center E are antipodal pentagons, and the triangles ABC and $EB'C'$ form a pair of opposite triangles.

The *(full) icosahedral group* $\mathbf{I}_h$, is the point group of symmetries of the icosahedron and dodecahedron. This group is equivalent to the group direct product $\mathbf{A}_5 \times \mathbb{Z}_2$ of the alternating group $\mathbf{A}_5$, and cyclic group $\mathbb{Z}_2$. The (i,i)- and $(0,i)$-icosahedral fullerene graphs, $i > 0$, have full icosahedral symmetry group, i.e., every element of this class of graphs has a symmetry group $\mathbf{I}_h$.

3 Some properties of a hexagonal lattice

As we already saw in the previous section, icosahedral fullerenes can be represented in a hexagonal lattice. Due to this fact, we present some properties of a hexagonal lattice needed in the next sections.

Tilling a plane with hexagons, means adding hexagons in three different directions, denoted by $\vec{i}$, $\vec{j}$ and $\vec{k}$ on Figure 3. Without loss of generality we can assume that one of the directions is horizontal, say $\vec{k}$. Now, every vertex a is incident to precisely one edge normal to $\vec{k}$, i.e., is incident to a vertical edge e_a. Also, a is incident to a hexagonal face h_a, not containing e_a. We say that a is a *top vertex* if the vertical edge e_a is above the hexagon h_a. If the vertical edge e_a is below the hexagon h_a, then we say that a is a *bottom vertex*. For example in Figure 3 (a), the vertex a is a top vertex, and the vertex b is a bottom vertex.

Let a and b be two different vertices in a hexagonal lattice. We can assume that a is up and right from b, or they are in a same line of hexagons (in some of the directions $\vec{i}$, $\vec{j}$ or $\vec{k}$). Let h_a and h_b be the hexagons defined above for a and b respectively. The lines parallel to $\vec{i}$, $\vec{j}$ and $\vec{k}$ passing trough the centers of h_a and h_b form three different parallelograms, the smallest one is the *parallelogram determined by the vertices a and b*. In the case when a and b belong to the same line of hexagons, this parallelogram is a segment.

The parallelogram determined by the vertices a and b defines a unique (hexagonal) parallelogram patch. Depending on the type of the vertices a and b, there are three types of (hexagonal) parallelogram patches, as shown on Figure 3.

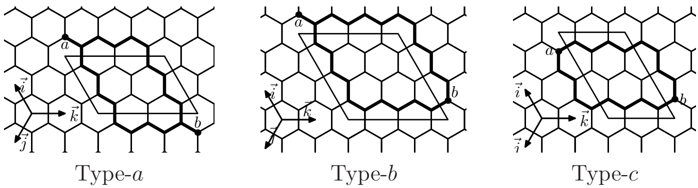

Figure 3. All three types of parallelogram patches defined by the vertices a and b in a hexagonal lattice. *Type-a*: the vertex a is top vertex and b is bottom vertex. *Type-b*: both of the vertices are of the same type. *Type-c*: The vertex a is bottom vertex and the vertex b is top vertex.

The first property determines the distance, i.e., one of the shortest paths between any two vertices in a hexagonal lattice.

Property 3.1. *Let a and b be two vertices in a hexagonal lattice, defining a (hexagonal) parallelogram patch $\mathcal{P}$. One of the shortest paths between the vertices a and b*

consists of consecutive bordering edges of $\mathcal{P}$*.*

Moreover, every vertex from the (hexagonal) parallelogram patch belongs to a shortest path between the vertices determining the patch.

Property 3.2. *Let* a *and* b *be two vertices in a hexagonal lattice. Let* x *be a vertex from the (hexagonal) parallelogram patch determined by* a *and* b*. Then, there is a shortest path between* a *and* b *that contains* x*.*

Notice that, if a vertex x does not belong to a (hexagonal) parallelogram patch determined by the vertices a and b, then there is no shortest path between a and b containing x.

The final property of a hexagonal lattice needed is obvious.

Property 3.3. *Let* a *and* b *be adjacent vertices in a hexagonal lattice. Let* p *be the bisector of the edge* ab *dividing the lattice into two sections. The section containing the vertex* a *also contains all the vertices closer to* a *than to* b *(and vice versa).*

4 Diameter of full icosahedral-symmetry fullerene graphs

From the structure of the icosahedral fullerene graphs it is clear that the most distant vertices are vertices in opposite triangles. Even more the maximal distance between two pentagonal vertices will be achieved for antipodal pentagon vertices. Combining these observations lead to the main result.

In order to determine the diameter of full icosahedral-symmetry fullerene graphs, we apply Property 3.3 and find vertices from the fullerene graph closer to a specific pentagonal vertex than to any other vertex from the same pentagon. There are also vertices equally distanced from two adjacent pentagonal vertices, a and b, but closer to a and b than to any other vertex from the same pentagon. We show that every pentagonal vertex is diametral, but that does not hold for all hexagonal vertices.

4.1 Diameter of $(0,i)$-icosahedral fullerene graphs

First we calculate the diameter of a $(0,i)$-icosahedral fullerene graph, $i>0$. In this case, unlike the others, every hexagonal vertex belongs to a diametral path between any pair of diametral pentagon vertices.

Theorem 4.1. *The diameter of a* $(0,i)$*-icosahedral fullerene graph* G*, with* $i>0$ *is* $\mathrm{diam}(G)=6i-1$.

Proof. Let v be a pentagonal vertex. Due to the symmetry, we can assume that $v=a$ as shown on Figure 4. We want to determine the closest vertex (vertices) to the vertex a from the antipodal pentagon. In order to do that, we apply Property 3.3 twice, once on each edge incident to a.

From the structure of a $(0,i)$-icosahedral fullerene graphs, it is obvious that the bisector of the bordering edge of a pentagon overlaps with an edge of a $(0,i)$-triangle. Therefore, we find two different bisectors of a pentagonal edge. As a result of this "phenomenon", there are vertices that are equally distanced from the vertices a and b, since they are at the same time on the "left" and on the "right" side from the bisector of the edge ab.

Consider that the vertices of the fullerene are grouped in ten sections A, B, $\ldots$, CD and DE as depicted in Figure 4. All the vertices left from the bisector of the edge ab, i.e., the sections A, AE, AB are closer to the vertex a than to b. At the same time the vertices on the right side of the bisector (the sections B, AB, BC) are closer to b. This implies that the vertices from the section AB are equally distant from the vertices a and b.

The same analysis can be done for all five pentagonal vertices. Combining all of these analysis, we conclude that the vertices from the section A are closer to the vertex a than to any other pentagonal vertex from the same pentagon. The vertices in the section AB (resp. AE) are at same distance from the vertex a and from the vertex b (resp. from the vertex a and the vertex e), but closer to a and b (resp. a and e) than to any other vertex from the same pentagon (Figure 4).

Now, it is clear that the closest antipodal pentagon vertices to the vertex a are c' and d'. The union of the sections A and AB is the parallelogram defined by the vertices a and d', respectively the union of the sections A and AE is the parallelogram defined by the vertices a and c'. Observe that the parallelogram patch defined by these vertices (a and d' or a and c') is of type-a. Due to the symmetry of the graph, the same holds for the vertices a and c'.

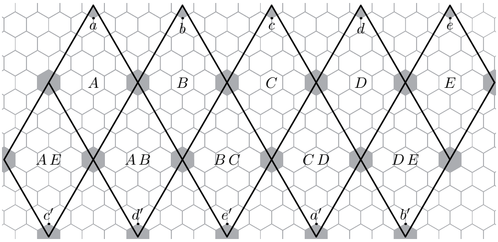

Figure 4. A $(0,4)$-icosahedral fullerene graph, and the sections of vertices closer to a specific pentagonal vertex. The vertices in the section A are closer to the vertex a, those vertices in the sections AB and AE are equally distanced to a and b, respectively to a and e. The diametral vertex of the vertex a is the vertex a'.

By Property 3.2, for every vertex x from the sections A and AB there is a shortest path between a and d' that contains x. From the above, Property 3.1 and the construction of $(0,i)$-triangle (Figure 1), we conclude that the distance between two antipodal pentagons is $6i-3$. Moreover the following holds:

Claim 1. *The distance between a pentagonal vertex $v \in V(G)$ and its closest vertices from the antipodal pentagon is $6i-3$. Moreover, there are precisely two such vertices.*

Notice that a path between the vertices a and e' that goes trough b is comprised by the shortest path between b and e' and the edge ab. This path is of length $6i-2$, and there is no shorter path since the vertex e' is closer to b than to a. Clearly there are paths of length $6i-1$ between the vertices a and a', and these paths are the shortest. If there is shorter path between a and a', then the distance between b and a', or between e and a' is $6i-3$ what contradicts with Claim 1. So, we have that the following claim holds.

Claim 2. *The maximum distance between two pentagonal vertices is $6i-1$.*

Observe that, for every pentagonal vertex v, there is a unique pentagonal vertex

u such that $d(u, v) = 6i - 1$. Next claim determines the upper bound of the distances between pentagonal and hexagonal vertex.

Claim 3. *Let u and v be pentagonal vertices at distance $6i-1$. Let w be an arbitrary vertex. There is a shortest path between u and v that goes trough w.*

In order to prove this claim, let $v = a$ and $u = a'$. If w is in the sections A or AB, by Property 3.2, there is a path P_1 between a and d' of length $6i-3$ that contains the vertex w, so the desired path is $P = P_1 d'e'a'$. If w is in the sections B or BC, there is a path P_2 from b to e' trough w of length $6i - 3$, i.e., $P = abP_2e'a'$ is a path of length $6i - 1$ between a and a' that contains w. If w is in one of the sections C or CD, then the required path comprised of the 2-path abc and a path P_3 from c to a' containing w. By the symmetry of the graph, all the cases are covered, and that proves this claim.

Directly from Claim 3 follows that the distance between any pentagonal and hexagonal vertices is less then $6i - 1$.

Let w_1 and w_2 are two hexagonal vertices. By Claim 3, there are paths between u and v of length $6i - 1$ going trough w_1 and w_2. The union of those two paths gives a closed walk of length at most $2(6i - 1)$. Therefore we have that the distance between any two hexagonal vertices is at most $6i - 1$. So, now we have:

Claim 4. *The distance between any two hexagonal vertices is at most $6i - 1$.*

Finally, this claim completes the proof of the theorem. □

By the icosahedral symmetry of the fullerene graph and the previous theorem follows:

Corollary 4.1. *Let G be a $(0, i)$-icosahedral fullerene graph, $i > 0$. Then, every pentagon vertex in G is diametral. Even more for every pentagonal vertex, there is a unique (pentagonal) vertex at distance* $\operatorname{diam}(G)$.

On the other side, there are hexagonal vertices that are not diametral. Notice that the number of vertices at maximum distance from a hexagonal vertex is not necessarily one as shown in Example 4.1.

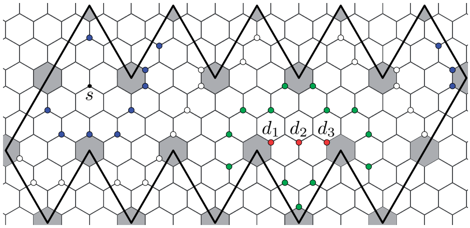

Figure 5. A $(0,3)$-icosahedral fullerene graph. The vertex s is not diametral. Blue vertices are at distance 4 from s, white at distance 8, and green vertices are at distance 12. The most distanced vertices from s are the vertices d_1, d_2, and d_3, which are on distance 15.

Example 4.1. *By Theorem 4.1, the diameter of the* $(0,3)$*-icosahedral fullerene is* 17*. Let* s *be a hexagonal vertex from the considered fullerene, as shown on Figure 5. The most distanced vertices from* s *are* d_1*,* d_2*, and* d_3 *and* $d(s,d_i) = 15$*,* $i = 1,2,3$*. The vertex* s *is not diametral, and there are three different vertices at maximal distance from* s*.*

4.2 Diameter of (i,i)-icosahedral fullerene graphs

Another type of fullerene graphs with full icosahedral symmetry are fullerenes with Goldberg vector $\vec{G} = (i,i)$ where $i > 0$. In this section we determine the diameter of such graphs.

Theorem 4.2. *The diameter of an* (i,i)*-icosahedral fullerene graph* G *where* $i > 0$ *is* $\operatorname{diam}(G) = 10i - 1$.

Proof. Similarly as in the proof of Theorem 4.1 we show that every pentagonal vertex is diametral. Due to the symmetry of the graph we can chose any pentagonal vertex, let say vertex a as shown on Figure 6.

First we will determine the vertices closer to a than to any other vertex from the same pentagon. Apply Property 3.3 for the vertices a and b, later apply the same property for the vertices a and e. It is clear that the vertices c' and d' are equally distanced from the vertex a, and at the same time they are the closest vertices to a from the antipodal pentagon (see Figure 6). The parallelogram patch defined by the vertices a and c' (or d') is of type-c.

The bisector of the edge ab passes trough the center of a pentagon, in this case the point x_1, and brakes into two lines. This can easily be seen if we rotate the triangle $x_1x_3x_4$ such that the points x_4 and x_5 are identified. In such way we get the vertices equally distanced form a and b. The vertices right from the line x_2x_4 do not belong in the parallelogram patch defined by a and d', but belong to the parallelogram patch defined by b and e', therefore they are closer to b than to a. In the same manner we find the vertices closer to a than to e, as well as vertices equally distanced from them, but closer to a and e than to any other vertex from the same pentagon. The sections of vertices closer to a different pentagonal vertices of the same pentagon are illustrated on Figure 6. The construction of an (i, j)-icosahedral fullerene graph, Property 3.1 and the previous observation give the following claim.

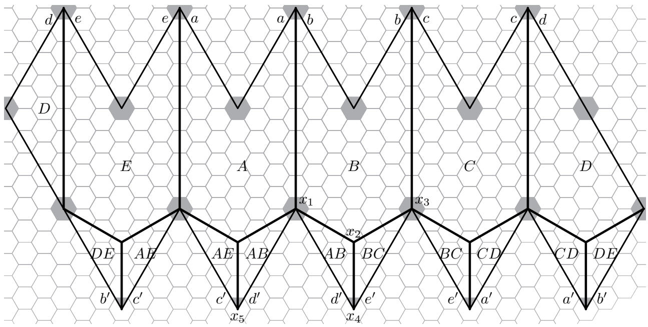

Figure 6. A $(3, 3)$-icosahedral fullerene graph. The vertices in the section A are closer to the vertex a than to any other vertex from the same pentagon. The vertices in the section AB (resp. AE) are equally distanced to a and b (resp. to a and e), but closer to a and b (resp. a and e) than to any other vertex from the same pentagon. The diametral vertex of the vertex a is the vertex a'.

Claim 1. *The distance between two antipodal pentagons is* $10i - 3$.

Notice, that by Property 3.2 all the vertices from the sections A, AB and AE, belong to a shortest path between a and c' or between a and d'. So, there are paths of length $10i - 1$ between a and a' and these paths are the shortest. One such path is comprised by a 2-path abc and one of the shortest paths between the vertices c and a'. By this and Claim 1 we have the following.

Claim 2. *The maximum distance between any two pentagonal vertices is* $10i - 1$.

Notice that the distance between the vertex a and any other hexagonal vertex is less than $10i - 1$. If the hexagonal vertex x belongs in the sections B or BC (resp. E or DE), the distance $d(x, b) < 10i - 3$ (resp. $d(x, e) < 10i - 3$). So the shortest path between a and x is comprised by the edge ab (resp. ae) and the shortest path between b and x (resp. e and x). Similarly if the vertex x belongs to the sections C or CD (resp. D or CD), the shortest path between the vertices a and x is comprised by the 2-path abc (resp. aed) and the shortest path between c and x (resp. d and x). Similarly as the case of $(0, i)$-icosahedral fullerene graphs, $i > 0$, for every pentagonal vertex v there is a unique pentagonal vertex u at maximal distance from v. The distance between these two vertices in (i, i)-icosahedral fullerene graph $i > 0$ is $d(u, v) = 10i - 1$. Next we should determine the distance between any two hexagonal vertices.

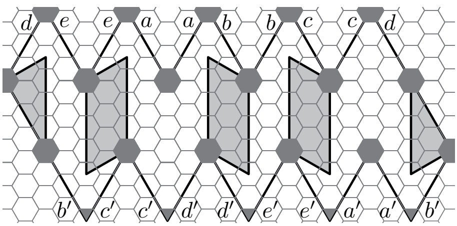

Figure 7. The uncolored part of the fullerene contains the vertices that belong to a shortest path between a and a'. This part is an union of the (hexagonal) parallelogram patches determined by the vertices: a and c', a and d', b and e', c and a', d and a', or the vertices e and b', since every vertex from these parallelograms belongs to a path of length $10i - 1$ between the vertices a and a'. The shaded parallelograms are the sections of vertices that might not belong to a shortest path between the vertices a and a'.

Claim 3. *Let* F_0 *and* F_1 *be antipodal pentagons. Then for any two hexagonal vertices* w_1 *and* w_2*, there is a pair of pentagonal vertices* $v \in V(F_0)$ *and* $u \in V(F_1)$ *at distance* $10i - 1$ *such that there are shortest paths* P_1 *and* P_2 *between* u *and* v *containing* w_1 *and* w_2 *respectively.*

To prove this claim, first let locate the vertices that belong to a shortest path between the vertices a and a'. Clearly all the vertices from the sections A, AB and AE belong to such a path. Further, we have that all the vertices that belong to a shortest path between the vertices b and e' also belong to a path of length $10i - 1$ between a and a'. By Property 3.2, every vertex x from the (hexagonal) parallelogram patch determined by the vertices b and e' belongs to a shortest path P_x between b and e', and the required path is $abP_xe'a'$. Similarly, each vertex from the (hexagonal) parallelogram patch determined by the vertices c and a' belong to a shortest pat between a and a'. This path is comprised by the 2-path abc and the shortest path between c and a' containing the corresponding vertex. Due to the symmetry of the graph we find all the vertices that belong to a shortest path between a and a'. These vertices belong to the uncolored section of the fullerene graph as illustrated on Figure 7. Respectively, the complement of this section contains vertices that might not belong to such a path.

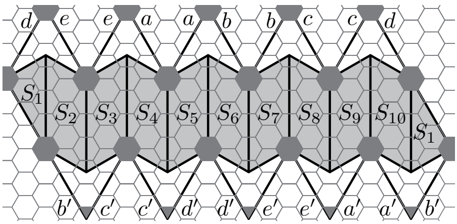

Figure 8. The vertices from the sections sections S_1, S_3, S_6 and S_8 might not belong to a shortest path between a and a', as shown on Figure 7. Using the symmetry of the graph we find that sections of vertices that might not belong to a shortest path between the vertices: b and b' (sections S_3, S_5, S_8 and S_{10}), c and c' (sections S_2, S_5, S_7 and S_{10}), d and d' (sections S_2, S_4, S_7 and S_9), and e and e' (sections S_1, S_4, S_6 and S_9).

By the symmetry of the graph we can find these sections for all five vertices on the border of F_0 as shown on Figure 8. On Figure 7, we can see that if w_1 or w_2 do not belong to none of the shaded sections according to some vertex, let say a, then we can choose $v = a$ and $u = a'$. If only one of the vertices belongs to a shaded section, say section S_1, then v can be one of the vertices $\{b, c, d\}$. Now, let both vertices belong to some of the shaded sections. There are ten such sections (Figure 8). Without loss of generality we can assume that w_1 belongs to the section S_1. We consider two cases:

- If w_2 belongs to some of the sections S_1, S_3, S_5, S_6, S_8 or S_{10}, then we choose $v = d$ and $u = d'$.

- If w_2 belongs to some of the sections S_2, S_4, S_7 or S_9, then $v = b$ and $u = b'$.

This proves the Claim 3. Notice that there are more different possibilities for the choices for u and v.

Now, by Claim 3, we have that for every pair of hexagonal vertices, there is a closed walk of length at most $2(10i-1)$ going trough both of the vertices. That gives the following claim.

Claim 4. *The distance between any two hexagonal vertices is not greater than* $10i-1$.

This claim establishes the theorem. □

Theorem 4.1 and Theorem 4.2 can be combined together. Then we obtain the theorem for a diameter of fullerene graphs with full icosahedral symmetry.

Theorem 4.3. *Let G be an (i, j)-icosahedral fullerene graph, such that $0 = i < j$ or $0 < i = j$. Then, the diameter of G is given by* $\mathrm{diam}(G) = 4i + 6j - 1$.

Applying Goldberg equation (1) and Theorem 4.3 we conclude that the diameter of a fullerene graph with full icosahedral symmetry is of order $\Theta(\sqrt{n})$. If we consider an (i, i)-icosahedral fullerene F ($i > 0$) then by (1), $n = 60i^2$. By Theorem 4.3, $\mathrm{diam}(F) = 10i - 1$, i.e., $\mathrm{diam}(F) = 10\sqrt{\frac{n}{60}} - 1 = \sqrt{\frac{5n}{3}} - 1$. As we believe that the icosahedral fullerenes have the smallest diameter, it leads us to conjecture the following:

Conjecture 4.1. *For every fullerene graph F on n vertices holds* $\mathrm{diam}(F) \geq \left\lfloor \sqrt{\frac{5}{3}n} \right\rfloor - 1$.

References

[1] E. Albertazzi, C. Domene, P. W. Fowler, T. Heine, C. Van Alsenoy, F. Zerbetto, Pentagon adjacency as a determinant of fullerene stability, *Phys. Chem. Chem. Phys.* **1** (1999) 2913–2918.

[2] V. Andova, T. Došlić, M. Krnc, B. Lužar, R. Škrekovski, On the diameter and some related invariants of fullerene graphs, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 109–130.

[3] F. Banhart, T. Füller, P. Redlich, P. M. Ajayan, The formation, annealing and self–comression of carbon onions under electron irradiation, *Chem. Phys. Lett.* **269** (1997) 349–355.

[4] D. L. D. Caspar, A. Klug, *Viruses, Nucleic Acids and Cancer*, Williams & Wilkins, Baltimore, 1963.

[5] H. S. M. Coxeter, Virus macromolecules and geodesic domes, in: J. C. Butcher (Ed.), *A Spectrum of Mathematics*, Oxford Univ. Press, Oxford, 1971, pp. 98–107.

[6] S. M. Daugherty, *Independent Sets and Closed-Shell Independent Sets of Fullerenes*, Ph.D. thesis, Univ. Victoria, 2009.

[7] T. Došlić, Bipartivity of fullerene graphs and fullerene stability, *Chem. Phys. Lett.* **412** (2005) 336–340.

[8] T. Došlić, On some structural properties of fullerene graphs, *J. Math. Chem.* **31** (2002) 187–195.

[9] S. Fajtlowicz, C. E. Larson, Graph–theoretic independence as a predictor of fullerene stability, *Chem. Phys. Lett.* **377** (2003) 485–490.

[10] P. W. Fowler, D. E. Manolopoulos, *An Atlas of Fullerenes*, Oxford Univ. Press, Oxford, 1995.

[11] P. W. Fowler, K. M. Rogers, S. Fajtlowicz, P. Hansen, G. Caporossi, Facts and conjectures about fullerene graphs: leapfrog, cylindrical and Ramanujan fullerenes, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer, Berlin, 2000, pp. 134–146.

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

[13] B. Grünbaum, T. S. Motzkin, The number of hexagons and the simplicity of geodesicson certain polyhedra, *Canad. J. Math.* **15** (1963) 744–751.

[14] Y. Ju, H. Liang, J. Zhang, F. Bai, A note on Fowler–Manolopoulos predictor of fullerene stability, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 419–424.

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

[16] J. Malkevitch, Geometrical and combinatorial questions about fullerenes, in: P. Hansen, P. Fowler, M. Zheng (Eds.), *Discrete Mathematical Chemistry*, Am. Math. Soc., Providence, 2000, pp. 261–166.

[17] D. Stevanović, Remarks on Fowler–Manolopoulos predictor of fullerene stability, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 285–292.