On the Diameter and Some Related Invariants of Fullerene Graphs[*]

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Abstract

Fullerene graphs are 3-connected 3-regular planar graphs with only pentagonal and hexagonal faces. We show that the diameter of a fullerene graph G of order n is at least $\frac{\sqrt{24n-15}-3}{6}$ and at most $n/5 + 1$. Moreover, if G is not a $(5,0)$-nanotube its diameter is at most $n/6+5/2$. As a consequence, we improve the upper bound on the saturation number of fullerene graphs. We also report an improved lower bound on the independence number and an upper bound on the smallest eigenvalue of fullerene graphs, confirming some conjectures for large fullerene graphs.

1   Introduction

Fullerenes are polyhedral molecules made entirely of carbon atoms. They come in wide variety of sizes and shapes. The most symmetric is the famous buckminsterfullerene, C_{60}, whose discovery in 1985 marked the birth of fullerene chemistry [24]. The name was a

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homage to Richard Buckminster Fuller, whose geodetic dome it resembles. In 1991, the buckminsterfullerene was pronounced the "Molecule of the year" by the Science magazine. From the very beginning, fullerenes have been attracting attention of diverse research communities. The experimental work was paralleled by theoretical investigations, applying the methods of graph theory to the mathematical models of fullerene molecules called fullerene graphs. One of the main driving forces behind that work has been a desire to identify structural properties characteristic for stable fullerenes, i.e., for fullerene isomers verified in macroscopic quantities. A number of graph-theoretical invariants were examined as potential stability predictors with various degrees of success [1, 11, 6]. As a result, we have achieved a fairly thorough understanding of fullerene graphs and their properties. However, some problems and questions still remain open [3, 25, 14]. Special place among them have several interesting conjectures made by *Graffiti*, a conjecture making software [10]. The main goal of this paper is to consider several of those open questions starting from our results on the fullerene diameters and a recent result on the bipartite edge frustration [9].

2   Definitions and preliminaries

A *fullerene graph* is a 3-connected 3-regular planar graph with only pentagonal and hexagonal faces. By Euler's formula, it follows that the number of pentagonal faces is always twelve. Grünbaum and Motzkin [19] showed that fullerene graphs with n vertices exist for all even $n \geq 24$ and for $n = 20$. 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. If all pentagonal faces are equally distributed, we obtain fullerene graphs of icosahedral symmetry, whose smallest representative is the dodecahedron. On the other hand, there is a class of fullerene graphs of tubular shapes, called nanotubes.

Nanotubical graphs or simply *nanotubes* are fullerene graphs with additional structural properties. They are cylindrical in shape, with the two ends capped with a subgraph containing six pentagons and possibly some hexagons. The cylindrical part of the nanotube can be obtained from a planar hexagonal grid by identifying objects lying on two parallel lines. The way the grid is wrapped is represented by a pair of integers (p_1, p_2). The numbers

p_1 and p_2 denote the coefficients of the linear combination of the unit vectors a_1 and a_2 such that the vector $p_1 a_1 + p_2 a_2$ joins pairs of identified points, i.e., the integers p_1 and p_2 denote the number of unit vectors along two directions in the honeycomb crystal lattice of the nanotube. Nanotubes with $p_2 = 0$ are called *zig-zag* nanotubes, and the ones with $p_1 = p_2$ are called *armchair* nanotubes.
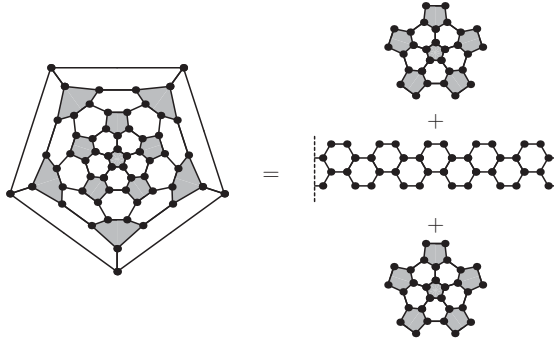

Figure 1: Buckminsterfullerene is the smallest nanotube of type $(5,5)$.

The *distance* between two vertices $u, v \in V(G)$ in a connected graph G is the length of any shortest path between these vertices, and it is denoted by $d(u,v)$. A *diameter* of connected graph G, $\mathrm{diam}(G)$, is the maximum distance between two vertices of G, i.e., $\mathrm{diam}(G) = \max\{d(u,v) \,|\, u,v \in V(G)\}$. While the diameter of fullerene graphs having icosahedral symmetry is small, the diameter of nanotubes is linear in the number of vertices. In this paper we establish lower and upper bounds for the diameter of fullerene graphs and use the results to improve the upper bound on their saturation number and settling the relationship between the independence number and the diameter.

The important definitions for dealing with lower and upper bounds are the O, Ω and Θ notations.

O-notation: For non-negative functions, $f(n)$ and $g(n)$, if there exists an integer n_0 and a constant $c > 0$ such that for all integers $n > n_0$, $f(n) \leq c \cdot g(n)$, then $f(n) = O(g(n))$.

Ω-notation: For non-negative functions, $f(n)$ and $g(n)$, if there exists an integer n_0 and a constant $c > 0$ such that for all integers $n > n_0$, $f(n) \geq c \cdot g(n)$, then $f(n) = \Omega(g(n))$.

Θ-notation: For non-negative functions, $f(n)$ and $g(n)$, $f(n)$ is theta of $g(n)$ if and only if $f(n) = O(g(n))$ and $f(n) = \Omega(g(n))$. This is denoted as $f(n) = \Theta(g(n))$.

We have mentioned that the study of fullerene graphs has been motivated by a search for invariants that will correlate with their stability. Among the more promising candidates were the three that we introduce next.

The *bipartite edge frustration* of a graph G, denoted by $\varphi(G)$, is the smallest cardinality of a set of edges of G that need to be removed from G in order to obtain a bipartite spanning subgraph. It was shown [7] that the bipartite edge frustration of a fullerene graph G can be efficiently computed by finding a minimum-weight perfect matching in the pentagon-distance graph of G. In the same reference it was shown that $\varphi(G) \geq 6$ for any fullerene graph G and that this bound is sharp. Furthermore, it was shown that the bipartite edge frustration of fullerene graphs with icosahedral symmetry is proportional to the square root of the number of vertices ([7], Proposition 11 and Corollary 12). The numerical computations reported there suggested that it cannot behave worse than that, and prompted the authors to state the following conjecture.

Conjecture 1. *Let G be a fullerene graph with n vertices. Then $\varphi(G) \leq \sqrt{\frac{12}{5}n}$.*

Recently, Dvořák, Lidický, and Škrekovski [9] proved a theorem with a weaker multiplicative constant.

Theorem 1. *Let G be a fullerene graph with n vertices. Then $\varphi(G) \leq 39.29\sqrt{n}$.*

Another invariant investigated for its stability-predicting potential is the smallest eigenvalue of a fullerene graph. Recall that a real number λ is an *eigenvalue of a graph G* if λ is an eigenvalue of its adjacency matrix $A(G)$. In [13] it was proven that the dodecahedron has maximum smallest eigenvalue among all fullerene graphs and it is equal to $-\sqrt{5}$. It was also shown that the buckminsterfullerene C_{60} has the maximum smallest eigenvalue among all IP fullerene graphs. This observation lead the authors to state the following conjecture on the smallest eigenvalue of fullerene graphs with at least 60 vertices.

Conjecture 2. *Among all fullerene graphs with at least 60 vertices, the buckminsterfullerene has the maximum smallest eigenvalue.*

The Conjectures 1 and 2 are connected *via* a result on Laplacian eigenvalues from the monograph by Godsil and Royle ([16, p. 293]).

Theorem 2. *Let G be a graph with n vertices. Then* $\operatorname{bip}(G) \leq \frac{n}{4}\mu_\infty(G)$.

Here $\operatorname{bip}(G)$ denotes the maximum number of edges in a bipartite spanning subgraph of G (hence the number of edges in G minus the bipartite edge frustration), and $\mu_\infty(G)$ is the largest Laplacian eigenvalue of G. We refer the reader to Chapter 13 of the above monograph for more on Laplacian eigenvalues; it suffices for our purposes to note that for 3-regular graphs $\mu_\infty(G) = 3 - \lambda_n(G)$, where $\lambda_n(G)$ is the smallest eigenvalue of G.

Another invariant tested as a possible stability predictor is the independence number [11]. A set $I \subseteq V(G)$ is *independent* if no two vertices from I are adjacent in G. The cardinality of any largest independent set in G is called the *independence number* of G and denoted by $\alpha(G)$. A sharp upper bound on the independence number of fullerene graphs was established in [5] as $\alpha(G) \leq \frac{n}{2} - 2$. It was obtained using the fact that all fullerene graphs are 2-extendable. No sharp lower bound on the independence numbers has been reported so far – the best known result $\alpha(G) \geq \frac{3}{8}n$ [20] is no better than the lower bound for triangle-free planar cubic graphs, and numerical evidence suggests that it is far from being sharp. In fact, numerical results suggest a bound of the type $\alpha(G) \geq \frac{n}{2} - C\sqrt{n}$. Those observations were formalized in a pair of conjectures in a recent Ph.D. thesis by S. Daugherty ([3, p. 96]). The first one states that the minimum possible independence number is achieved on the icosahedral fullerenes that also figure prominently in Conjecture 1. The second one [3, Conjecture 5.5.2] states the precise form of the conjectured lower bound. Notice that the constant $3/\sqrt{15}$ is exactly one half of the constant $\sqrt{12/5}$ of Conjecture 1.

Conjecture 3. *Let G be a fullerene graph with n vertices. Then* $\alpha(G) \geq \frac{n}{2} - 3\sqrt{n/15}$.

The relations between diameter and the independence number of fullerenes appear in Conjecture 912 of Graffiti [14]:

Conjecture 4. *For every fullerene graph G, it holds that* $\alpha(G) \geq 2(\operatorname{diam}(G) - 1)$.

For more on independence in fullerenes and in particular in icosahedral fullerenes we refer the reader to [17, 18].

The last invariant considered here, the saturation number, is related to matchings. Recall that a *matching* in G is a collection M of edges of G such that no two edges from M have a vertex in common. If a matching M covers all vertices of G we say that M is a *perfect matching*. Every perfect matching is also a *maximum matching*, i.e., a matching of maximum cardinality. The existence of perfect (and hence maximum) matchings in fullerene graphs has been established long time ago, and there are many papers concerned with their structural and enumerative properties [5, 21, 23]. Another class of matchings, the maximal matchings, have received much less attention so far, in spite of being potentially useful as mathematical models of dimer absorption. A matching M is *maximal* if it cannot be extended to a larger matching of G. The *saturation number* of G is the cardinality of any smallest maximal matching of G. We denote it by $s(G)$. The saturation number of fullerene graph was studied in [5, 8], where the following bounds were established.

Theorem 3. *There exists an absolute constant C such that*

$$\frac{3n}{10} \leq s(G) \leq \frac{n}{2} - C \log_2 n \,,$$

for any fullerene graph G with n vertices.

The upper bound of the above theorem will be improved using the results of Section 3.

3 Lower bound on the diameter

A well known result on the degree-diameter problem states that the number of vertices in a planar graph with maximum degree 3 grows at most exponentially with diameter [15].

Proposition 4. *Let G be a planar graph with maximum degree 3 and a given diameter $\operatorname{diam}(G)$. Then, G has at most $2^{\operatorname{diam}(G)+1} - 1$ vertices.*

This results in a logarithmic lower bound on the diameter in terms of the number of vertices.

Corollary 5. *Let G be a planar cubic graph with n vertices. Then,*

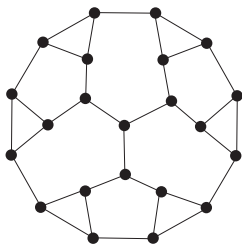$$\operatorname{diam}(G) \geq \lceil \log_2(n+1) \rceil - 1 \,.$$

Figure 2: An example of Ψ_3.

To illustrate corollary 5, we will now show an example of family of graphs Ψ with logarithmic diameter. A full balanced binary tree T_n on n layers is defined as $V(T_n) = \{t_1, t_2, ..., t_{2^n-1}\}$, $E(T_n) = \{(t_i, t_{\lfloor i/2 \rfloor}); 1 < i < 2^n\}$. Now take three full balanced binary trees A_n, B_n, C_n with vertices $a_i, b_i, c_i; 0 < i < 2^n$, respectively and edges as defined above.

For any $n \in \mathbb{N}$, the graph Ψ_n is defined on vertices $V(\Psi_n) = V(A_n) \cup V(B_n) \cup V(C_n) \cup \{\psi\}$ and on edges

$$
\begin{aligned}
E(\Psi_n) = {} & E(A_n) \cup E(B_n) \cup E(C_n) \\
& \cup \quad \{(\psi, a_1), (\psi, b_1), (\psi, c_1)\} \\
& \cup \quad \{(a_{i-1}, a_i); 2^{n-1} < i < 2^n\} \\
& \cup \quad \{(b_{i-1}, b_i); 2^{n-1} < i < 2^n\} \\
& \cup \quad \{(c_{i-1}, c_i); 2^{n-1} < i < 2^n\} \\
& \cup \quad \{(a_{2^n-1}, b_{2^n-1}), (b_{2^n-1}, c_{2^n-1}), (c_{2^n-1}, a_{2^n-1})\}.
\end{aligned}
$$

It is easy to see, that when n is big enough, the diameter of Ψ_n is $2n$, which is logarithmic in terms of $|V(\Psi_n)|$. Figure 2 shows an example of Ψ_3. Note that for $n > 3$, the distance between a_{2^n-1}, b_{2^n-1} is logarithmic.

The logarithmic character of the bound can be attributed to the presence of faces of large size. It would be reasonable to expect that better lower bounds exist for polyhedral graphs with bounded face size. Surprisingly, no such bounds seem to be available in the literature.

However, as mentioned above, fullerene graphs only have pentagonal and hexagonal faces, and we use this fact to show that the diameter is at least of order $\Omega(\sqrt{n})$. Crucial

for our result is a simple observation that in an infinite hexagonal grid, the number of vertices at equal distance from a selected vertex grows linearly with the distance. In what follows we investigate how that behavior is affected by the presence of pentagonal defects. The basic idea is intuitively clear, but in order to formalize it we first introduce some terminology.

Let G be a fullerene graph and let $N_k(x) = \{v \in V(G) \mid d(v,x) = k\}$ be a set of vertices at distance k from a vertex x. We call $N_k(x)$ a k-ring and a vertex in a k-ring is a k-ring vertex. It is easy to see that for $k \geq 1$ it holds

$$v \in N_k(x) \Rightarrow N(v) \subset N_{k-1}(x) \cup N_k(x) \cup N_{k+1}(x),$$

where $N(x)$ is the set of all neighbors of x and $N_0(x) = x$. For a chosen x and an arbitrary k-ring vertex $v \neq x$, we define the value of v as

$$\mu(v) = \sum_{u \in N(v) \cap N_{k+1}(x)} \frac{1}{|N(u) \cap N_k(x)|},$$

where $k = d(v,x)$. Observe that the value $\mu(v)$ represents a measure of the number of vertices that v contributes to the $(k+1)$-ring. Hence, the number of vertices at distance k from x is

$$|N_k(x)| = \sum_{v \in N_{k-1}(x)} \mu(v). \tag{1}$$

Notice that a $(k+1)$-ring vertex u adjacent to two k-ring vertices contributes $\frac{1}{2}$ to the value of each neighbor in the k-ring.

Lemma 6. *Let G be a fullerene graph and let $x \in V(G)$. Then,*

$$|N_k(x)| \leq |N_{k-1}(x)| + 3,$$

for $k \geq 1$.

Proof. The lemma obviously holds for $k = 1$, so we assume that $k > 2$ in the sequel. Let G be a fullerene graph embedded in the plane and x an arbitrary vertex of G. By (1), the statement of the lemma is equivalent to

$$|N_k(x)| = \sum_{u \in N_{k-1}(x)} \mu(u) \leq |N_{k-1}(x)| + 3.$$

In the proof we will make use of the following observation. Let $P = uvwz$ be an induced path in G such that u is an $(i+3)$-ring vertex, v an $(i+2)$-, w an $(i+1)$-, and z an i-ring vertex, respectively. Moreover, let P be incident with a face f. Then, the vertex z has another $(i+1)$-ring neighbor w', and the vertex u has another $(i+2)$-ring neighbor v' such that v' is adjacent to w', for otherwise the length of f would be at least 7 (see Fig. 3). We say that u and z are *extreme for* f.
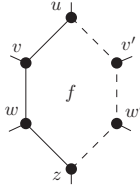

Figure 3: A face incident with the vertices from four distinct rings.

Since every k-ring vertex has at least one neighbor in the $(k-1)$-ring, its value is at most 2. We show that only the neighbors of x may have value 2.

Claim 1. *Let v be a vertex such that $\mu(v) = 2$. Then $d(v,x) = 1$.*

Suppose, to the contrary, that v is a k-ring vertex, for $k > 1$, with $\mu(v) = 2$. Then, v has precisely two neighbors u_1, u_2 in the $(k+1)$-ring, and v is the only k-ring neighbor of u_1 and u_2. Let w be the $(k-1)$-ring neighbor of v. Consider the other two neighbors of w, z_1 and z_2. At least one of them, say z_1, is in the $(k-2)$-ring. Now, consider the face f incident to the vertices v, w, and z_1. Notice that either u_1 or u_2, say u_1, is also incident with f. Hence, u_1 and z_1 are extreme for f, thus u_1 has another k-ring neighbor incident with f, a contradiction. This establishes Claim 1.

By Claim 1, the maximum value of a k-ring vertex in G, for $k > 1$, is at most $1 + \frac{1}{2} = \frac{3}{2}$. We call a vertex v with $1 < \mu(v) \leq \frac{3}{2}$ *expansive*. Furthermore, Claim 1 also implies that an expansive k-ring vertex, for $k > 1$, has at most one expansive $(k+1)$-ring neighbor. The following claims show that every expansive vertex has a unique expansive predecessor and at most one expansive successor. The only exception are the vertices in the 2-ring, since the vertices of the 1-ring are not expansive.

Claim 2. *An expansive k-ring vertex v has an expansive $(k-1)$-ring neighbor or there is an expansive $(k-2)$-ring vertex z such that $d(v, z) = 2$.*

Suppose that the unique $(k-1)$-ring neighbor w of v is not expansive. Let u_1, u_2 be the $(k+1)$-ring neighbors of v. By Claim 1, we may assume that u_1, say, is adjacent to another k-ring vertex, while u_2 is not. Next, let z_1, z_2 be the other two neighbors of w and, without loss of generality, we assume that z_1 is a $(k-2)$-ring vertex. Since u_2 has only one k-ring neighbor it follows that z_2 is not a $(k-2)$-ring vertex and the vertices u_1, v, w, and z_1 are all incident to some face f. Since z_1 is an extreme vertex for f it has another $(k-1)$-ring neighbor, which means that it is expansive.

Claim 3. *An expansive k-ring vertex v has at most one expansive $(k+2)$-ring vertex at distance 2.*

Suppose, to the contrary, that v has two expansive $(k+2)$-ring vertices at distance 2. Let u_1 and u_2 be the two $(k+1)$-ring neighbors of v. By Claim 1, at least one of u_1 and u_2, say u_2, has another k-ring neighbor v'. Now, we consider the $(k+2)$-ring neighbors of u_1 and u_2. If u_2 has no $(k+2)$-ring neighbor, we are done, since u_1 cannot have two expansive $(k+2)$-ring neighbors by Claim 1. Hence, we may assume that u_2 has an expansive $(k+2)$-ring neighbor t. Then, it has two $(k+3)$-ring neighbors y_1 and y_2. However, they are the extreme vertices of the two faces incident with t, u_2, v, and t, u_2, v', respectively. That means that y_1 and y_2 both have two $(k+2)$-ring neighbors and the value of t is at most 1, hence t is not expansive. Recall that u_1 has at most one expansive $(k+2)$-ring neighbor, so Claim 3 holds.

Observe that all six vertices in the 2-ring may be expansive, therefore, by Claims 2 and 3, it follows that there are at most six expansive vertices in every ring. Hence,

$$|N_k(x)| = \sum_{u \in N_{k-1}(x)} \mu(u) \le 6 \cdot \frac{3}{2} + (|N_{k-1}(x)| - 6) \cdot 1 = |N_{k-1}(x)| + 3,$$

which concludes the proof. ∎

The following theorem gives the lower bound for the diameter of fullerenes.

Theorem 7. *Let G be a fullerene graph. Then,*

$$\text{diam}(G) \ge \frac{\sqrt{24n - 15} - 3}{6}.$$

Proof. Let G be a fullerene graph with n vertices. For every vertex $x \in V(G)$ there exists an integer k such that there is no vertex at distance at least $k+1$ from x, while a vertex at distance k from x exists. By Lemma 6, it is easy to see that the following inequality holds:

$$n = \sum_{i=0}^{k} |N_i(x)| \leq 1 + 3 + \sum_{i=2}^{k} |N_i(x)| = \frac{3}{2}k(k+1) + 1 \,.$$

Since the diameter of G is at least k, we have that

$$\mathrm{diam}(G) \geq k \geq \frac{\sqrt{24n-15}-3}{6} \,.$$

∎

The function of the fullerene diameter is in $\Omega(\sqrt{n})$. However, there are many fullerene graphs with the diameter of order $\Theta(n)$, e.g., nanotubes. We discuss this in the next section.

4 Upper bound on the diameter

In this section we determine the upper bound on the diameter in fullerene graphs. We prove the following theorem.

Theorem 8. *Let F be a fullerene graph with n vertices. Then,*

$$\mathrm{diam}(F) \leq \frac{n}{6} + \frac{5}{2} \,,$$

unless F is a $(5,0)$-nanotube. In that case, we have $n = 10\,k$, $k \in \mathbb{N}$ and

$$\mathrm{diam}(F) = \begin{cases} \frac{n}{5} + 1, & k = 2; \\ \frac{n}{5}, & k \in \{3,4\}\,; \\ \frac{n}{5} - 1, & k \geq 5. \end{cases}$$

Before we continue, we present some additional notation and definitions. Let F be a fullerene graph and let v be an arbitrary vertex in F. We define $L_0^v = \{v\}$ as an initial layer and F_0^v as a set of faces incident with v. Inductively, having defined the sets L_{i-1}^v and F_{i-1}^v, L_i^v is the set of vertices incident with F_{i-1}^v, not contained in L_{i-1}^v. Furthermore, F_i^v is the set of faces incident with L_i^v that are not contained in F_{i-1}^v. For an edge $e = uw$, where $u, w \in V(F)$, we say that it is an *incoming edge* to L_i^v if $u \in L_{i-1}^v$ and $w \in L_i^v$. If e is an incoming edge to L_i^v, then we also say that e is an *outgoing edge* from L_{i-1}^v. The vertex

u is an *outgoing vertex*, and w is an *incoming vertex*, respectively. Notice that a vertex cannot be outgoing and incoming at the same time, and also that the vertices in the last layer are never outgoing (it may also happen that such a vertex is neither incoming).

An *edge-cut* of graph G is a set of edges $C \subset E(G)$ such that $G - C$ is disconnected. A graph G is *k-edge-connected* if G cannot be separated into two components by removing less than k edges. An edge-cut C of G is *cyclic* if each component of $G - C$ contains a cycle. A graph is *cyclically k-edge-connected* if at least k edges must be removed to disconnect it into two components such that each contains a cycle. For fullerene graphs, Došlić [4] proved the following theorem.

Theorem 9. *Every fullerene graph F is cyclically 5-edge-connected.*

Additionally, Kardoš and Škrekovski [22] proved that the cyclically 5-edge-connected fullerenes are of unique type.

Theorem 10. *If F is a fullerene graph which is not a $(5,0)$-nanotube, it is cyclically 6-edge-connected.*

As every face in F is of length 5 or 6 and every vertex has degree 3, we immediately infer that:

Lemma 11. *For every vertex $x \in L_{i+1}^v$, $i \geq 1$, there exists a vertex $y \in L_i^v$ such that $d(x, y) \leq 2$.*

The inequality in Lemma 11 is tight only when x is an outgoing vertex, otherwise there is a vertex $y \in L_i^v$ adjacent to x. Also, note that if $x \in L_1^v$, then $d(x, v)$ could be 3 (see Figure 4). This together with Lemma 11 gives:

Lemma 12. *Let $x \in L_i^v$. Then $d(v, x) \leq 2i + 1$. Furthermore, if $d(v, x) = 2i + 1$, then v is adjacent with at least one hexagon.*

Now, we show that when L_i^v is small enough, L_{i+2}^v is empty, or in other words we reach the "end" of the fullerene.

Lemma 13. *Let $i \geq 2$ and $|L_i^v| < 12$. Then, $L_{i+2}^v = \emptyset$.*
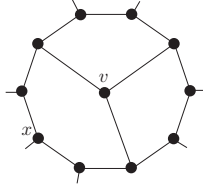
Figure 4: The vertex v is a starting vertex and $L_0^v = \{v\}$. Faces incident to v belong to the set F_0^v. The vertices incident to F_0^v different from v form the fist layer L_1^v. Distance between v and $x \in L_1^v$ is three.

Proof. Suppose first that L_i^v induces an acyclic graph. Then, $F_i^v = \emptyset$ and therefore also $L_{i+1}^v = L_{i+2}^v = \emptyset$. Hence, we may assume that there exists a cycle C in the graph induced by L_i^v. By Theorem 9, there are at least five incoming edges to L_i^v. If the number of incoming edges is precisely five, C is a 5-face, for otherwise F is a $(5,0)$-nanotube. It follows that $L_{i+1}^v = L_{i+2}^v = \emptyset$.

On the other hand, if there are at least six incoming edges to L_i^v and since $|L_i^v| < 12$ we have at most five outgoing edges from L_i^v, witch also means, that there is at most five incoming vertices to L_{i+1}^v. By the same argumentation we infer that the graph induced by L_{i+1}^v is either acyclic or it contains a cycle C' which is a 5-face in F. Either way, L_{i+2}^v is empty. ∎

The following lemma will determine the maximal distance from the last layer with at least 12 vertices L_{k-1}^v to the vertices in the last layer.

Lemma 14. *Let x be a vertex from the last layer in our graph and let k be the smallest number, such that $k \geq 2$ and $|L_k^v| < 12$. Then, there exists a vertex $z \in L_{k-1}^v$ such that $d(z, x) \leq 3$.*

Proof. If L_k^v is the last layer in our graph, we know that by Lemma 11 that $d(z, x) \leq 2$.

Now consider $L_{k+1}^v \neq \emptyset$. By Lemma 13, L_{k+2}^v is an empty set. It follows that there is no outgoing vertices from L_{k+1}^v. Hence, every vertex in L_{k+1}^v is adjacent to some vertex y in L_k^v. Moreover, by Lemma 11 there is a vertex z in L_{k-1}^v such that $d(y, z) \leq 2$, hence $d(x, z) \leq 3$. Note that the vertex y is an outgoing vertex. ∎

Now we are ready to prove Theorem 8.

Proof of Theorem 8. Let F be a fullerene graph. We divide the proof in two parts. In the first, we prove that the diameter of F is at most $\frac{n}{6} + \frac{5}{2}$, if F is not a $(5,0)$-nanotube. In the latter part, we prove the bound for $(5,0)$-nanotubes.

So, assume that F is not a $(5,0)$-nanotube. Let v be an arbitrary vertex of F. We will prove that $d(u, v) \leq \frac{n}{6} + \frac{5}{2}$ for every vertex $u \in V(F)$, which will establish the first part of the theorem.

Let C_m be the number of vertices in $L_k^v \cup L_{k+1}^v$ and let L_k^v be the first layer that contains less then 12 vertices (according to the vertex v), where $k \geq 2$. By Lemma 13, L_k^v or L_{k+1}^v is the last layer of the fullerene. Then, the order n of fullerene F is

$$n = |L_0^v| + |L_1^v| + \sum_{i=2}^{k-1} |L_i^v| + |L_k^v \cup L_{k+1}^v| \geq 1 + |L_1^v| + 12(k-2) + C_m \,,$$

or

$$k \leq \frac{1}{12}(n + 23 - |L_1^v| - C_m)\,. \tag{2}$$

We will now determine the distance from v to an outgoing vertex $x \in L_{k-1}^v$. According to the choice of vertex v, there are two cases:

1. *Let v be adjacent to pentagons only.*

   Obviously, $|L_1^v| = 9$. It also follows from Lemma 12 and from (2), that:

   $$d(v, x) \leq 2k - 2 \leq \frac{1}{6}(n + 2 - C_m) \tag{3}$$

   Later we will see, that this case gives us better bound, but it may happen, that there is no such possible choice of v.

2. *Let v be adjacent to at least one hexagon.*

   Obviously $|L_1^v| \geq 10$. It also follows from Lemma 12 and from (2), that:

   $$d(v, x) \leq 2k - 1 \leq \frac{1}{6}(n + 7 - C_m) \tag{4}$$

So now we have the distance from v to the last layer with at least 12 vertices for both cases above. Determining the distance from an outgoing vertex of this layer to the "end" will establish the proof.

Let d_M be the maximal distance between the vertices in the last layer and the outgoing vertices of layer L_{k-1}^v. By Lemmma 14 it follows, that $1 \leq d_M \leq 3$. We will now consider all three cases, to bound the number of vertices in the last layers:

- $d_M = 3$: By Lemma 11, we immediately infer that $L_{k+1}^v \neq \emptyset$, so $|L_{k+1}^v| \geq 1$. Moreover, since $L_{k+1}^v \neq \emptyset$, L_k^v is not acyclic. Now, by Theorem 10 there are at least six incoming vertices in L_k. Since there is at least one vertex in L_{k+1}^v there are also at least three outgoing vertices in L_k. Hence, we have $C_m = |L_k^v \cup L_{k+1}^v| \geq 10$.

- $d_M = 2$: It is obvious that in this case $L_{k+1}^v = \emptyset$. Let $x \in L_k^v$ be such a vertex that the distance to the closest vertex in L_{k-1}^v is two. Since x cannot be outgoing vertex and since $\deg(x) = 3$ it follows that $N(x) \subseteq L_k^v$, so we have $C_m = |L_k^v| \geq 4$.

- $d_M = 1$: In this case it is obvious that in the last layer there is at least one vertex, i.e., $C_m = |L_k^v| \geq 1$.

Finally, we compute the upper bound of the distance between v and a vertex in the last layer and we use that result to compute the bound of the diameter of F.

$$\mathrm{diam}(F) \leq d(v, x) + d_M, \tag{5}$$

where x is an outgoing vertex of L_{k-1}^v. By (3), (4) and (5) we again have two cases, depending on the choice of v.

$$\mathrm{diam}(F) \leq \frac{1}{6}(n + 2 - C_m) + d_M = \frac{n}{6} + C_1 \tag{6}$$
$$\mathrm{diam}(F) \leq \frac{1}{6}(n + 7 - C_m) + d_M = \frac{n}{6} + C_2 \tag{7}$$

Now, we determine the upper bound of the constants C_1, C_2 by plugging the values computed above in (6) and (7), respectively. We infer that $C_1 \leq \frac{5}{3}$ and $C_2 \leq \frac{5}{2}$. This establishes the first part of Theorem 8. Note, that if our fullerene contains diametral vertex, adjacent only to pentagons, then we can use the bound from (6) with constant C_1, which is better than C_2.

Suppose now that F is a $(5,0)$-nanotube with n vertices. Notice that $n \equiv 0 \pmod{10}$ or $n = 10k$, $k \in \mathbb{N}$. The diameter of the graph is determined by the most distanced vertices, and in this case they belong to the different caps and are incident only to 5-faces.

Now, it is easy to compute that the theorem holds for $k \in \{2, 3, 4, 5\}$. For $k > 5$, we prove the theorem by induction on the number of vertices. Let $k \geq 5$ and assume that the theorem holds for $(5, 0)$-nanotubes on $10k$ vertices. A $(5, 0)$-nanotube F' on $10(k + 1)$ vertices can be constructed easily by adding an extra layer of hexagons between already existing hexagonal layers. This construction gives us a $(5, 0)$-nanotube with additional 10 vertices (see Figure 5). By Lemma 11 and the comment after it, we have that the diameter
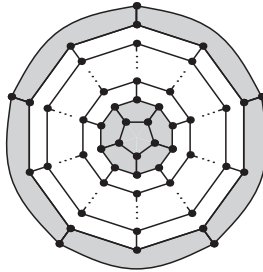

Figure 5: A $(5, 0)$-nanotube.

increases by 2, i.e.,

$$\mathrm{diam}(F') = \mathrm{diam}(F) + 2 = \frac{10k}{5} - 1 + 2 = \frac{10(k + 1)}{5} - 1 \,,$$

and this completes the proof. ∎

5 New bounds on some related invariants

5.1 Improved lower bound on the independence number

Independence number of fullerene graphs attracted a lot of attention not only as a potential stability predictor [11], but also in the context of study of independent sets as possible models for addition of bulky segregated groups such as free radicals or halogen atoms [2]. Sharp upper bounds on the independence number of $n/2 - 2$ for general fullerenes and $n/2 - 4$ for those with isolated pentagons follow by simple counting argument [12]. Lower bounds were gradually improved from (almost) trivial $\alpha(G) \geq n/3$ valid for all 3-chromatic graphs to $\alpha(G) \geq \frac{3}{8}n$ mentioned in section 2 [20]. A better lower bound of type $\alpha(G) \geq$

$\frac{n}{2} - C\sqrt{n}$, for some constant C, was established for icosahedral fullerenes [17]. Using Theorem 1, it can be shown that such bound holds for all fullerene graphs, which goes in favour to Conjecture 3.

Theorem 15. *Let G be a fullerene graph with n vertices. Then,*

$$\alpha(G) \geq \frac{n}{2} - 78.58\sqrt{n}\,.$$

Proof. Let G be a fullerene graph with n vertices. By the upper bound $\varphi(G) \leq 39.29\sqrt{n}$ [9], it follows that the removal of at most $39.29\sqrt{n}$ edges from G results in a bipartite spanning subgraph G'. At least one of the two partition classes of G', call it W', is of size at least $\frac{n}{2}$, and it is an independent set in G'. We know that the set M of removed edges forms a matching [7], and that each edge from M connects two vertices from the same partition class of G'. Even if each edge of M connects two vertices from W' in G, there are at most $39.29\sqrt{n}$ edges in M, and hence the vertices of W' not incident to any edge from M form an independent set in G of cardinality at least $\frac{n}{2} - 2 \cdot 39.29\sqrt{n} = \frac{n}{2} - 78.58\sqrt{n}$. ∎

Theorem 8 and Theorem 15 imply the next corollary.

Corollary 16. *Let G be a fullerene graph with n vertices. If n is sufficiently large, then*

$$\alpha(G) \geq 2(\operatorname{diam}(G) - 1)\,.$$

Proof. Using the bounds in Theorem 8 and Theorem 15 it is not hard to compute that when $n \geq 617\,502$, the following series of inequalities holds:

$$\alpha(G) \geq \frac{n}{2} - 78.58\sqrt{n} \geq 2\left(\frac{n}{5} + 1\right) - 1 \geq 2(\operatorname{diam}(G) - 1)\,.$$

∎

Hence, Corollary 16 settles Conjecture 4, for all fullerenes of sufficiently large order.

5.2 Improved upper bound on the smallest eigenvalue

Recall that the smallest eigenvalue $\lambda_n(G)$ of a 3-regular graph G and the largest Laplacian eigenvalue $\mu_\infty(G)$ of G are related *via* the following relation ([16, p. 280]):

$$\lambda_n(G) = 3 - \mu_\infty(G).$$

By plugging this into Theorem 2 and noting that $\mathrm{bip}(G) = \frac{3}{2}n - \varphi(G)$ we obtain an upper bound on $\lambda_n(G)$ in terms of the bipartite edge frustration of G of the form $\lambda_n(G) \leq -3 + \frac{4}{n}\varphi(G)$. By taking into account an upper bound on $\varphi(G)$ we immediately obtain the following upper bound on the smallest eigenvalue of a fullerene graph with n vertices.

Theorem 17. *Let G be a fullerene graph with n vertices. Then,*

$$\lambda_n(G) \leq -3 + \frac{157.16}{\sqrt{n}}.$$

Since the smallest eigenvalue of C_{60} is $-\phi^2$, where ϕ is the golden ratio $\frac{1+\sqrt{5}}{2}$, an immediate consequence is that Conjecture 2 is true for all fullerene graphs with at least $169\,291$ vertices.

5.3 Improved upper bound on the saturation number

In this subsection we improve the upper bound on the saturation number in fullerene graphs. Using the obtained lower bound on the diameter we are able to improve the logarithmic additive correction of Theorem 3 and to prove the following result.

Theorem 18. *Let G be a fullerene graph with n vertices. Then,*

$$s(G) \leq \frac{n}{2} - \frac{1}{4}(\mathrm{diam}(G) - 2).$$

In particular,

$$s(G) \leq \frac{n}{2} - \frac{\sqrt{24n - 15} - 15}{24}.$$

Proof. Let G be a fullerene graph with n vertices and diameter k. Let x and y be a pair of diametral vertices of G, i.e., $d(x, y) = k$. By Theorem 7, we have that $k \geq \frac{\sqrt{24n-15}-3}{6}$. Let $P = xv_1v_2 \cdots v_{k-1}y$ be a shortest path between x and y. Notice that the vertices v_i, for every even i such that $1 \leq i < k$, form an independent set I. We call a vertex v *even* if $v \in I$, and *odd* if $v \in V(P)\backslash I$. In what follows, we will construct a maximal matching M in $G - I$ such that it will cover all the vertices adjacent to I. The idea is to choose a set of independent edges covering all the neighbors of I with no vertex of I being covered and then extend it to a maximal matching M.

For $i \in \{1, 2, \ldots, k-1\}$, let u_i be the third neighbor of v_i distinct from v_{i-1} and v_{i+1} (for convenience, we define $v_0 = x$ and $v_k = y$), and let w_i^1, w_i^2 be the two neighbors of u_i distinct from v_i.
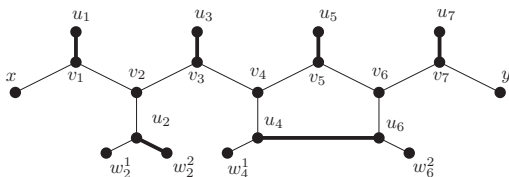
Figure 6: An independent set with three unmatched vertices v_2, v_4, and v_6.

First, we show that all the vertices u_i are distinct. It is easy to see that we obtain a cycle of length less than 5 if u_i is adjacent to v_j, for $j \in \{i-2, i-1, i+1, i+2\}$, which violates the girth condition of fullerene graphs. Moreover, since the vertices v_i are on the shortest path between x and y, we have that $i - 1 \le d(x, u_i) \le i + 1$, and so u_i is not adjacent to v_j, if $|j - i| > 2$. Hence, all u_i are distinct and the edges $u_i v_i$ independent. We add the edges $v_i u_i$, for every odd v_i, to the matching M.

In order to match all the neighbors of the even vertices, it remains to add either the edge $u_i w_i^1$ or the edge $u_i w_i^2$ to M, for all even v_i. First, notice that a vertex u_i may be adjacent to some u_j, for $j \in \{i-3, i+3\}$, that means the edge $u_i u_j$ cannot be in M, since u_j is already covered. Fortunately, since P is a shortest path, both edges $u_i u_{i-3}$ and $u_i u_{i+3}$ cannot appear in G. Therefore, for all such u_i, let $w_i \in \{w_i^1, w_i^2\}$ be distinct from u_j and add the edge $u_i w_i$ to M.

Now, let H be the subgraph of G induced by the edges $u_i w_i^j$, where i is even, $j \in \{1, 2\}$, and $w_i^j \ne u_{i\pm3}$ (observe, that it may happen, that $w_i^j = u_{i\pm2}$, see figure 6). We claim that H has the following properties:

(1) $\Delta(H) \le 2$.

(2) No path component of H starts and ends with u_i's.

We prove each claim separately. Observe that the vertex u_i cannot be of degree 3, since it is adjacent to v_i which is not a vertex of H. So, suppose that some w_i^j is of degree 3 in H. Then, w_i^j must be adjacent to u_{i-2}, u_i, and u_{i+2} as P is a shortest path. But, since no separating cycles of size 5 or 6 exist in fullerene graphs, we infer that w_i^j is of degree at most 2. This proves (1).

Now we show claim (2). Suppose that P' is a path that starts with a vertex u_a and ends with a vertex u_b, for some $a, b \in \{1, 2, \ldots, k-1\}$ and let $a < b$. A vertex u_i has degree 1 in H only if it is adjacent to u_{i-3} or u_{i+3} in G. Thus u_a is adjacent to u_{a-3} or u_{a+3}. Since G has no separating cycles of length at least 6, we conclude that u_a must be adjacent to u_{a-3}. Similarly, u_b must be adjacent to u_{b+3}. So, the path $v_{a-3}u_{a-3}P'u_{b+3}v_{b+3}$ is shorter than the path $v_{a-3}v_{a-2}\ldots v_{b+3}$, contradicting the fact that the path P is a shortest path between x and y.

Finally, we find a matching M' in H that covers all u_i's in H. We consider every component C of H separately. By (1), they are only paths and cycles. If C is a path in H that does not start nor end with u_i, we add every second edge of C to M'. Otherwise, we start with the edge incident to the u_i with which C starts or ends. By (2), it follows that all u_i's of C are covered. If C is an even cycle, we simply add every second edge of C to M'. In case when C is an odd cycle, it contains an edge u_iu_{i+2} for some i. We add u_iu_{i+2} to M' and choose the edges of the path $C - u_iu_{i+2}$ as described above.

In this way, every u_i in H is matched and we add the edges of M' to M. Hence, we have matched all the neighbors of the even vertices. Next, extend M to a maximal matching in G. Since no even vertex is matched by the edges in M, its size is at most

$$|M| \leq \frac{n - |I|}{2} = \frac{n}{2} - \frac{1}{2}\left\lceil \frac{\text{diam}(G) - 2}{2} \right\rceil \leq \frac{n}{2} - \frac{\text{diam}(G) - 2}{4} \leq \frac{n}{2} - \frac{\sqrt{24n - 15} - 15}{24},$$

what establishes the theorem. ∎

6 Concluding remarks

We have established new lower and upper bounds on the diameter of fullerene graphs and combined it with recently established upper bounds on the bipartite edge frustration to derive improved bounds on the independence number, the smallest eigenvalue, and the saturation number of fullerene graphs. It is very likely that the new bounds on the diameter will also be useful in studying other distance-based invariants of fullerene graphs, such as, e.g., the eccentricity and distance sums. The techniques used here can be also applied to other classes of polyhedral graphs, in particular to generalized fullerenes, to their boron-nitrogen analogues, and to other polyhedral graphs with bounded face size.

One of the more immediate goals should be confirming the exact values of constants in Conjectures 1 and 3. An important conjecture on the closed-shell independence number of fullerenes ([3, Conjecture 7.7.1]) will follow immediately from Conjecture 3 if the numerical value of C is confirmed. (The closed-shell independence number $\alpha^-(G)$ is the maximum cardinality of an independent set whose complement has exactly half of its eigenvalues positive. It is conjectured that there are exactly three fullerene graphs whose independence number and closed-shell independence number coincide. At the moment we have a weaker result stating that the number of such fullerenes is finite.) There is some evidence that the closed-shell property is relevant for the stability of fullerenes. A more detailed discussion and a number of open questions can be found in Chapter 7 of [3].

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] O. V. Boltalina, N. A. Galeva, Direct fluorination of fullerenes, *Russ. Chem. Rev.* **69** (2000) 609–621.

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

[4] T. Došlić, Cyclical edge–connectivity of fullerene graphs and $(k, 6)$-cages, *J. Math. Chem.* **33** (2003) 103–112.

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

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

[7] T. Došlić, D. Vukičević, Computing the bipartite edge frustration of fullerene graphs, *Discr. Appl. Math.* **155** (2007) 1294–1301.

[8] T. Došlić, Saturation number of fullerene graphs, *J. Math. Chem.* **43** (2008) 647–657.

[9] Z. Dvořak, B. Lidický, R. Škrekovski, Bipartizing fullerenes, *arXiv:1106.0420v1*, preprint.

[10] S. Fajtlowicz, Written on the Wall (A List of Conjectures of Graffiti), *(available from the author on request)*.

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

[12] P. W. Fowler, S. Daugherty, W. Myrvold, Independence number and fullerene stability, *Chem. Phys. Lett.* **448** (2007) 75–82.

[13] P. W. Fowler, P. Hansen, D. Stevanović, A note on the smallest eigenvalue of fullerenes, *MATCH Commun. Math. Comput. Chem.* **48** (2003) 37–48.

[14] 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.

[15] E. Friedman, R. W. Pratt, New bounds for largest planar graphs with fixed maximum degree and diameter, *preprint*.

[16] C. Godsil, G. Royle, *Algebraic Graph Theory*, Springer, New York, 2001.

[17] J. E. Graver, The independence number of fullerenes and benzenoids, *Eur. J. Combin.* **27** (2006) 850–863.

[18] J. E. Graver, Kekulé structures and the face independence number of a fullerene, *Eur. J. Combin.* **28** (2007) 1115–1130.

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

[20] C. H. Heckman, R. Thomas, Independent sets in triangle-free cubic planar graphs, *J. Combin. Theory B* **96** (2006) 253–275.

[21] F. Kardoš, D. Kral', J. Miškuf, J. S. Sereni, Fullerene graphs have exponentially many perfect matchings, *J. Math. Chem.* **46** (2009) 443–447.

[22] F. Kardoš, R. Škrekovski, Cyclic edge–cuts in fullerene graphs, *J. Math. Chem.* **44** (2007) 121–132.

[23] D. J. Klein, X. Liu, Theorems on carbon cages, *J. Math. Chem.* **11** (1992) 199–205.

[24] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. E. Smalley, C_{60}: Buckminsterfullerene, *Nature* **318** (1985) 162–163.

[25] J. Malkevitch, Geometrical and combinatorial questions about fullerenes, in: P. Hansen, P. Fowler, M. Zheng (Eds.), *Discrete Mathematical Chemistry, DIMACS Series in Discrete Mathematics and Theoretical Computer Science* **51** (2000) 261–166.