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On Two *Graffiti* Conjectures about Fullerene Graphs

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Abstract

We use recently obtained lower bounds on the independence number of fullerene graphs to settle in affirmative a conjecture of the *Graffiti* software about the relationship between the independence number and the face independence number of a fullerene graph. We also consider another *Graffiti* conjecture, concerned with the relationship of the independence number and the radius of a fullerene graph, and show that it is not valid.

1 Introduction

The main goal of this note is to settle two conjectures of the *Graffiti* software about fullerene graphs. One of them, concerned with the independence numbers of fullerenes and their duals, was already attacked and partially solved by Fajtlowicz some twelve years ago. We are not aware of any partial results about the other one, relating the independence number of a fullerene to its radius. In both cases, the progress was made possible by some recently established lower bounds on the independence number of fullerene graphs [11] that follow from a result about their odd cycle transversals.

We start by providing some context on the considered conjectures. They were made by *Graffiti*, a conjecture-making software designed some thirty years ago by S. Fajtlowicz [8] and subsequently developed by him and some of his former collaborators. It evolved through several versions, most of them with colorful names such as *Minuteman* [9], *Dalmatian* and *Pony Express* [10]; together they produced over a thousand of non-trivial conjectures and inspired tens, by now maybe even hundreds, of research papers. Some of the conjectures are still unsolved. We encourage the reader to consult a survey paper by E. DeLaVina [4] and references therein for more on the history of *Graffiti* project and for pointers to various lists of conjectures. For our purpose, the most interesting are the ones concerned with fullerene graphs generated by the *Minuteman* version. Several of them have been proved or disproved by various authors [5, 7, 15, 20], and in this paper we settle two more.

2 Definitions, conjectures, and preliminary results

In this section we define the basic terms and state relevant conjectures. For any general graph-theoretic terms not defined here we refer the reader to any of standard textbooks or monographs, such as, e. g., [17] or [19]. For more context and background on fullerene graphs the reader might wish to consult the standard reference by Fowler and Manolopoulos [14]

A **fullerene graph** is a planar, 3-regular and 3-connected graph that has only pentagonal and hexagonal faces. Such graphs on n vertices exist for all even $n \geq 24$ and for $n = 20$ [16].

An **independent set** in a graph G is a set I of vertices of G such that no two vertices from I are adjacent. The cardinality of any largest independent set of G is called the **independence number** of G and denoted by $\alpha(G)$.

For a planar graph G we denote its dual by G^*. If two faces of a fullerene graph G intersect, they intersect in a whole edge. Hence an independent set in G^* corresponds to a set of disjoint faces in G. The independence number of G^* is then called the **face independence number** of G and denoted by $\alpha^*(G)$.

The first conjecture we consider in this paper is concerned with the relationship between the independence number and the face independent number of a fullerene graph. In the Fajtlowicz's original formulation it reads as follows.

Conjecture 1005

Let F be a fullerene with independence a and maximum number of disjoint faces b. Then $2b \leq a$. ■

It appeared at the end of a list of conjectures produced by the *Pony Express* version [10], almost exclusively concerned with benzenoid graphs. An alternative formulation is more compact.

Conjecture 1005

Let G be a fullerene graph. Then $\alpha(G) \geq 2\alpha^*(G)$. ■

The other conjecture relates the independence number of a fullerene to one of its distance-based invariants, namely to its radius. For vertices u, v of a graph G, their **distance** $d(u, v)$ is defined as the number of edges in any shortest path in G connecting u and v. For a fixed u, the maximum value of $d(u, v)$ over all vertices v is called the **eccentricity** of u. The maximum eccentricity over all vertices in G is the **diameter** of G, denoted by $\mathrm{diam}(G)$. The **radius** of G, denoted by $\mathrm{rad}(G)$, is the minimum value of the eccentricity over all vertices of G. Obviously, $\mathrm{rad}(G) \leq \mathrm{diam}(G) \leq 2\,\mathrm{rad}(G)$.

For some recent results on distance-related properties of fullerene graphs we refer the reader to the series of papers by Andova *et al.* [1–3] and by one of the present authors [6].

Conjecture 911

Let G be a fullerene graph on n vertices. Then

$$\alpha(G) \geq \mathrm{rad}(G) \log\left(\frac{n}{2} - 1\right).$$

■

We close this section by quoting some results that will enable us to settle the above conjectures. The first one is a lower bound on the independence number of fullerene graphs.

Theorem A ([11])

Let G be a fullerene graph on n vertices. Then $\alpha(G) \geq \frac{n}{2} - \sqrt{\frac{3n}{5}}$. The equality is achieved if and only if G is an icosahedral fullerene. ■

Next result is a general upper bound on the independence number of a planar graph with prescribed minimum degree.

Theorem B ([19], p. 19)

Let G be a connected planar graph on n vertices with minimum degree 5. Then any largest independent set in G has less than $\frac{2n}{5}$ vertices. ■

Finally, we will need an upper bound on the diameter of fullerene graphs.

Theorem C ([1])

Let G be a fullerene graph on n vertices. Then $\mathrm{diam}(G) \leq \frac{n}{6} + \frac{5}{2}$, unless G is a narrow nanotube capped on both ends by hemidodecahedral caps. If G is such nanotube, then G has $10k$ vertices and $\mathrm{diam}(G) \leq \frac{n}{5} - 1$ for $k \geq 5$. ■

(For the remaining cases of short nanotubes, the upper bound is $\frac{n}{5} + 1$ for $k = 2$ (i.e., for the dodecahedron) and $\frac{n}{5}$ for $k = 3, 4$.)

3 Main results

We first treat Conjecture 1005. As mentioned in the introduction, it was partially proved by Fajtlowicz in [10]. He was able to show that it is true for all fullerenes with at least 96 vertices. He relied on the lower bound on the independence number of triangle-free cubic graphs $\alpha(G) \geq \frac{3}{8}n$ that was conjectured by Albertson, Bollobás and Tucker and subsequently proved by Heckman and Thomas [18].

Theorem 1

Let G be a fullerene graph. Then $\alpha(G) \geq 2\alpha^*(G)$.

Proof

We follow the same approach as Fajtlowicz, but use the lower bound of Theorem A instead of the 3/8 bound of Heckman and Thomas. Fajtlowicz observed that the maximum number of disjoint faces D in a fullerene is at most $\frac{n+k}{6}$, where k is the number of pentagons among those faces. Our claim will follow if we prove a stronger inequality, $\frac{n}{2} - \sqrt{\frac{3n}{5}} \geq 2\frac{n+k}{6}$. Since k cannot exceed 12, this inequality reduces to $\frac{n}{6} - \sqrt{\frac{3n}{5}} \geq 4$. This is equivalent to $5n^2 - 348n + 2880 \geq 0$, and this is satisfied for $n \geq 60$. Hence, we have managed to extend the range of validity of Conjecture 1005 down to $n = 60$.

As the next step, we notice that for $n < 60$ a fullerene cannot have 12 disjoint pentagons, since the smallest IPR isomer has 60 vertices. Also, the only fullerene with icosahedral symmetry on less than 60 vertices is the dodecahedron. Hence, we can replace the left hand side by its ceiling and decrease the right hand side to $\frac{11}{3}$. The resulting inequality $\left\lceil \frac{n}{6} - \sqrt{\frac{3n}{5}} \right\rceil \geq \frac{11}{3}$ is valid for all $n > 50$, and this extends the validity of the conjecture down to $n = 52$.

The conjecture is obviously valid for the dodecahedron, i.e., for $n = 20$ case. This leaves us with the range $24 \leq n \leq 50$ in which the validity of Conjecture 1005 is not yet established. In reference [12] one can find several tables containing distributions of independence numbers for all fullerene isomers on at most 120 vertices. We have compared the reported minimum values of independence numbers $\alpha_{min}(G_n)$ with upper bounds b_n

from Theorem B for all fullerene isomers on $24 \leq n \leq 50$ vertices. The results appear in

n	$\alpha_{min}(G_n)$	n^*	b_n	$\alpha^*_{max}(G_n)$
24	9	14	5	4
26	11	15	6	4
28	11	16	**6**	4
30	12	17	6	5
32	13	18	**7**	6
34	14	19	7	6
36	15	20	7	6
38	16	21	8	6
40	16	22	8	7
42	18	23	9	7
44	18	24	9	8
46	19	25	9	8
48	20	26	10	8
50	21	27	10	9

Table 1: The smallest value of the independence number of a fullerene on n vertices $\alpha_{min}(G_n)$; the number of vertices in a dual graph n^*; the upper bound from Theorem B b_n; the largest value of the face independence number $\alpha^*_{max}(G_n)$ of a fullerene on n vertices.

columns 2 and 4, respectively, of Table 1. One can see that $\alpha_{min}(G_n) \leq 2b_n$ remains valid throughout the range with only two exceptions: $n = 28$ and $n = 32$. The exceptional cases appear in the table in boldface font. In order to settle those two cases, we have computed the face independence numbers for both isomers on 28 vertices and for all six isomers on 32 vertices. We have found that both isomers on 28 vertices have $\alpha^*(G) = 4$; for C_{32}, we found that five out of six isomers have the face independence number equal to five, while the remaining one has $\alpha^*(G) = 6$. In all cases, the maximum computed face independence number is less than one half of the minimum independence number, and hence Conjecture 1005 is established for all fullerene graphs.

We have also computed face independence numbers for all fullerene graphs on $24 \leq n \leq 50$ isomers. Their maximum values for given n are reported in the fifth column of Table 1. ■

Let us now look at Conjecture 911.

Theorem 2
Conjecture 911 is false for large enough n.

Proof
We look at narrow nanotubes G_n on $n = 10k$ vertices. As mentioned in Theorem C, their diameter is equal to $\frac{n}{5} - 1$. It is clear from their structure that their radius is roughly one-half of the diameter. Hence, $\mathrm{rad}(G_n) \sim \frac{n}{10}$. On the other hand, the independence number of G_n is equal to $\frac{n}{2} - 2$. It is clear now that the right hand side of Conjecture 911 grows superlinearly and that it will exceed the linear growth of the left hand side for large enough n; it suffices to take $n \sim 2 \cdot 10^5$. Hence, the Conjecture is false for very long nanotubes. ■

To be fair to Conjecture 911, one should notice that it remains valid for infinite classes of fullerenes. For example, for icosahedral fullerenes their diameter (and hence also radius) grows as the square root of the number of vertices, while the independence number grows linearly, with a downward correction of the order of $\sqrt{n}$.

4 Conclusion

We have answered some open questions and conjectures concerned with independence properties of fullerene graphs. In particular, we have shown that the independence number of a fullerene graph is at least twice as big as its face independence number. Further, we have found a class of counterexamples to a conjecture relating the independence number of a fullerene and its radius. We have shown that for very long narrow nanotubes, both their radius and their independence number grow linearly with the number of vertices.

At the time of writing of this paper several other *Graffiti* conjectures about independence and distance-related properties of fullerenes are still open. We mention here two that are quite similar to the ones treated here.

Conjecture 908 $\alpha(G) \leq \mathrm{rad}(G)^2$.

Conjecture 909 $\alpha(G) \leq \mathrm{rad}(G)\overline{\ell(G)}$, where $\overline{\ell(G)}$ denotes the average distance in G.

It can be shown that Conjecture 908 is valid for two classes of fullerenes, the narrow nanotubes and the icosahedral isomers. The first class is known to have the largest diameter, while the second one is conjectured [2] to have the smallest diameter among all isomers on the same number of vertices. The same is valid for Conjecture 909. Hence, there are good chances that both are true. The validity of both conjectures can be also shown for nanotubical non-classical fullerenes.

We also mention here Conjecture 843, claiming that the independence number of a fullerene graph on n vertices is greater or equal to $\frac{n}{2} - 8$. At first glance it seems as a very weak conjecture. However, the constant correction of 8 become worse than the square-root correction of Theorem A only for $n \geq 108$.

It would be an interesting thing to see if some of the conjectures could be established also for non-classical fullerenes.

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