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Spectral Properties of Fullerene Graphs

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Abstract

We use a result from the theory of geometric representation of graphs to show that the separator of a fullerene graph on n vertices cannot exceed $24/n$, thus improving the best currently known upper bound of $1 - 3/n$. The result is then combined with a recently established upper bound on the smallest eigenvalue of fullerene graphs to show that there are only finitely many Ramanujan fullerenes. That settles down a conjecture on fullerenes made by the *Graffiti* software.

1 Introduction

Fullerene graphs are mathematical models of fullerenes, polyhedral molecules made of carbon atoms with only pentagonal and hexagonal faces. The study of fullerene graphs goes back all the way to the very beginnings of the fullerene chemistry. It has been mainly driven by a need to find structural invariant(s) that could explain why only a tiny fraction of possible fullerene structures have been actually observed. A number of spectral invariants such as, e.g., the separator [16], the smallest eigenvalue [9], and the bipartivity [5] have been examined as possible stability predictors. In the course of that research it was discovered that fullerene graphs also posses some properties that make them interesting outside of the context of fullerene chemistry. As a result, a number of conjectures were proposed about their various properties. Some of those conjectures were made by *Graffiti*, an automated conjecture generating software developed by S. Fajtlowicz since 1986 [7]. Several of those conjectures turned out to be correct, among them two concerned with the separator of fullerenes that were proved in a paper by Stevanović and Caporossi [16]. Some of the conjectures were disproved by various authors, and several of them are still open. The aim of this paper is to further integrate the above lines of research. We first use a result from the theory of geometric representation of graphs to prove a better upper bound on the fullerene separator, and then combine it with a recently improved upper bound on the smallest eigenvalue of fullerenes in order to answer in affirmative a question about the number of Ramanujan fullerenes implicit in *Graffiti* conjectures.

2 Definitions, conjectures, and preliminary results

We start by defining the basic terms. For the general graph-theoretic terminology we refer the reader to any of standard monographs, such as, e. g., [4] or [14]. For fullerene graphs the reader might wish to consult the standard reference by Fowler and Manolopoulos [10]

A **fullerene graph** is a planar, 3-regular and 3-connected graph that has only pentagonal and hexagonal faces. Such graphs on p vertices exist for all even $p \geq 24$ and for $p = 20$ [13].

An **eigenvalue** of a graph G is an eigenvalue of its adjacency matrix $A(G)$. The set of all eigenvalues of a graph is called its **spectrum**. We denote the eigenvalues of G by $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. The largest eigenvalue of a fullerene graph is not really interesting, since it is always equal to 3. However, the other two extremal eigenvalues, the second largest λ_2 and the smallest one λ_n are both of significant interest. Instead of λ_2 one usually considers the quantity called the **separator** of G and defined as $s(G) = 3 - \lambda_2$. The separator of G is also called the **spectral gap** of G. Both the separator [5] and the smallest eigenvalue [9] were found to correlate to some extent with fullerene stability.

The *Graffiti* software stated several conjectures about fullerene graphs. Two of them were concerned with the separator.

Conjecture 895 The separator of a fullerene is at most 1.

Conjecture 896 The separator of a fullerene with n vertices is at most $1 - \frac{3}{n}$.

Both conjectures were proved in a paper by Stevanović and Caporossi [16] using the interlacing theorem. They were also able to prove that the dodecahedron has the largest separator among all fullerenes. In the next section we will prove a stronger upper bound without resorting to the interlacing theorem.

The separator and other spectral invariants figure in several other *Graffiti* conjectures about fullerenes. Some of them are concerned with the so called Ramanujan fullerenes or ramafullerenes.

A **Ramanujan graph** is a finite regular graph of degree k whose all eigenvalues (except k and possibly $-k$) have modulus at most $2\sqrt{k-1}$. Ramanujan fullerenes or **ramafullerenes** are then those with $\lambda_1 = 3$ and $|\lambda_i| \leq 2\sqrt{2}$ for all other values of i. The fullerenes that fail to satisfy the Ramanujan criterion only at the lower end of the spectrum are called positive ramafullerenes; those that violate the criterion only at the upper end are analogously called negative ramafullerenes. Several *Graffiti* conjectures about fullerenes were considered in a paper by Fowler *et al.* [12], where the authors conjectured that the number of ramafullerenes is finite and that none of them has more than 84 vertices.

Conjecture 3 [12] All ramafullerenes have 84 or fewer vertices.

The finiteness of the numbers of ramafullerenes follows from a result by Alon and Milman [1]; we will prove later that indeed all of them have at most 84 vertices. For some additional results on Ramanujan graphs we refer the reader to [2].

3 Main results

Crucial for our goal will be an observation on the eigenvalue gap of the Laplacian of planar graphs.

For a given graph G its **Laplacian matrix** $L(G)$ is defined as $L(G) = D(G) - A(G)$, where $D(G) = diag[\delta_1, \ldots, \delta_n]$. (Here δ_i denotes the degree of vertex i.) A real number μ is a **Laplacian eigenvalue** of G if μ is an eigenvalue of $L(G)$. The set of all Laplacian eigenvalues of G is the Laplacian spectrum of G; we denote its elements by $\mu_1 \leq \mu_2 \leq \ldots \leq \mu_n$. We refer the reader to Chapter 13 of [11] for more on Laplacian eigenvalues; it suffices for our purposes to note that for 3-regular graphs $\mu_i(G) = 3 - \lambda_i(G)$. Again, the smallest Laplacian eigenvalue is not interesting since it is always equal to zero, but the second smallest is exactly equal to the separator of G.

Fullerene graphs are planar and 3-connected. It is well known that each such graph can be represented by touching circles. The result is known as Koebe's theorem or a coin representation:

Koebe's theorem: Let G be a 3-connected planar graph. Then one can assign to each vertex i a circle C_i in the plane so that their interiors are disjoint and two vertices are adjacent if and only if the corresponding circles are tangent.

The above result is taken from a recent monograph on the geometric representations of graphs [15]; we refer the reader to Chapter 6 of that book for a proof. Among several applications and consequences of Koebe's theorem there is one concerned with the spectral gap of Laplacians of planar graphs.

Theorem ([15], p. 88)
Let G be a connected planar graph on n vertices with maximum degree Δ. Then the second smallest Laplacian eigenvalue of G is at most $\frac{8\Delta}{n}$.

The proof is simple and follows directly from Koebe representation of G on the unit sphere. By reformulating the above theorem in terms of fullerene graphs we obtain one of our main results.

Corollary 1
Let G be a fullerene graph on n vertices. Then the separator of G is at most $\frac{24}{n}$. ∎

Hence the second largest eigenvalue of a fullerene graph is greater than $3 - \frac{24}{n}$. It is clear that it will exceed $2\sqrt{2}$ for n large enough, and a simple calculation yields that no ramafullerene can exist on 140 or more vertices. The maximum separators of fullerene graphs on at most 100 vertices were computed and reported in [12]; a decreasing trend reported there is also followed by the maximum separators of fullerenes on $102 \leq n \leq 138$ vertices, as can be seen from Fig. 1. The fullerene graphs were generated by using the *fullgen* program of the *CaGe* package [3] and their spectra were computed by using standard EISPACK routines in double precision. Hence we have confirmed the claim of Conjecture 3.

Corollary 2
All ramafullerenes have 84 or fewer vertices. ∎

The same argument gives us also the finiteness of the set of positive ramafullerenes. Our calculations confirm that there are altogether 161 positive ramafullerenes and

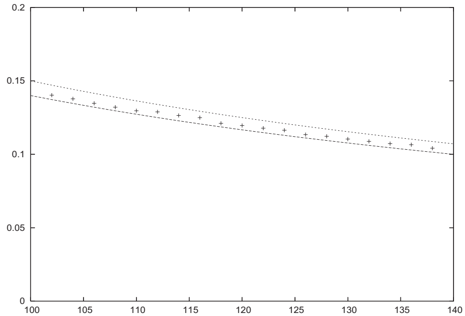

Figure 1: Maximum separators of fullerene graphs on $102 \leq n \leq 138$ vertices.

that none of them has isolated pentagons. Hence all of them were reported in [12]. Figure 1 also gives us some idea on the quality of our upper bound on the separator. One can see from it that all computed values of maximum separators remain between two curves; one of them represents the function $14/n$, the other one is $15/n$. It seems that the upper bound $s(G) \leq \frac{24}{n}$ correctly estimates the asymptotic behavior of the largest separator.

The case of negative ramafullerenes is a bit more complicated. It was shown recently [6] that the smallest eigenvalue of a fullerene graph on n vertices satisfies the inequality $\lambda_n \leq -3 + \frac{C}{\sqrt{n}}$. Hence for large enough values of n it will fall below $-2\sqrt{2}$. However, the exact value of C is still unknown; it is conjectured to be equal to $8\sqrt{3/5}$ [6]. The upper bound on λ_n is poorer than the lower bound for λ_2; this fact is reflected in much larger number of negative ramafullerenes reported in [12]. However, their number must be finite.

Corollary 3

There are finitely many negative ramafullerenes. ■

As we have mentioned, the exact value of the constant C in $\lambda_n(G) \leq -3 + \frac{C}{\sqrt{n}}$ is not known. Even if we assume the conjectured value of $8\sqrt{3/5}$, it still leaves a possibility of existence of negative ramafullerenes on n vertices for all $n \leq 1304$.

However, our computations indicate that the upper bound on λ_n is not very tight. In Table 1 we present the number of negative ramafullerenes on $102 \leq n \leq 140$ vertices. Again, the isomers were generated by using *fullgen* and their spectra computed by using double precision EISPACK routines. One can observe that the decreasing trend present in Table 1 of reference [12] is continued in our Table 1 and that the number of negative ramafullerenes reaches zero at $n = 134$ and stays there for $n = 136$ and 138. However, a lonely negative ramafullerene appears again for 140. As expected, it is the only isomer with the I symmetry group. Our computations indicate that no other negative ramafullerenes appear among the IPR isomers of fullerenes with $140 < n \leq 146$. Since it is evident from Table 1 that the largest negative ramafullerenes have isolated pentagons, it is reasonable to conjecture that there are no negative ramafullerenes on more than 140 vertices.

Conjecture

There are altogether 191480 negative ramafullerenes and none of them has more than 140 vertices. There are exactly 6935 negative ramafullerenes with isolated pentagons. All negative ramafullerenes with more than 120 vertices have isolated pentagons. ■

We conclude with an observation on the separator of the buckminsterfullerene. It follows readily from Corollary 1 that its value of 0.2434 [12] cannot be exceeded for fullerenes on more than 100 vertices. By combining that observation with the values reported in Table 1 of reference [12] we obtain the following result.

Corollary 4

The buckminsterfullerene $C_{60} : I_h$ has the largest separator among all fullerenes with isolated pentagons. ■

n	N_{-}	N_{-} (IPR)	$(\lambda_n)_{max}$	s_{max}
102	4197	544	-2.79111	0.14023
104	2969	616	-2.79533	0.13778
106	2150	818	-2.79759	0.13473
108	1737	899	-2.80012	0.13205
110	1301	870	-2.80045	0.12965
112	960	751	-2.80471	0.12886
114	564	474	-2.80648	0.12644
116	330	304	-2.80664	0.12498
118	224	218	-2.81529	0.12110
120	141	136	-2.81372	0.11959
122	51	51	-2.81758	0.11778
124	33	33	-2.82051	0.11636
126	2	2	-2.82278	0.11341
128	5	5	-2.82466	0.11224
130	6	6	-2.82409	0.11036
132	2	2	-2.82495	0.10880
134	0	0	-2.83103	0.10727
136	0	0	-2.83586	0.10655
138	0	0	-2.83082	0.10413
140	1	1	-2.81168	0.10365

Table 1: Number of negative ramafullerenes N_{-}, negative IPR ramafullerenes N_{-} (IPR), maximum smallest eigenvalue $(\lambda_n)_{max}$, and maximum separator s_{max} for fullerenes on n vertices.

4 Conclusion

We have answered in affirmative several open questions and conjectures concerned with spectral properties of fullerene graphs. In particular, we have proved that the separator of a fullerene graph on n vertices is bounded from above by $\frac{24}{n}$. In an earlier paper [6] we have proved that the smallest eigenvalue of a fullerene graph on n vertices cannot exceed $-3 + \frac{C}{\sqrt{n}}$ for some positive constant C. The difference in quality of those bounds is reflected in the fact that there are many more negative than positive ramafullerenes. Further, we have confirmed that the lists of ramafullerenes and positive ramafullerenes reported in [12] are indeed complete and we have proved that there are only finitely many negative ramafullerenes.

The conjectures about ramafullerenes were made by *Graffiti*, an automated conjecture making software. At the time of writing of this paper several other *Graffiti* conjectures about fullerenes are still open. Particularly interesting are those concerned with relationships between the separator and several other invariants, such as, e.g., the diameter, the radius, and the independence number. It is quite possible that the new and improved upper bound on the separator will open new approaches to those conjectures. We refer the reader to [12] for a list of open conjectures.

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