MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **70** (2013) 73-78

ISSN 0340 - 6253

The Smallest Eigenvalue of Fullerene Graphs – Closing the Gap

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(Received October 4, 2012)

Abstract

The icosahedral isomer of C_{60} has the maximum smallest eigenvalue amongst all fullerenes on 60 or more vertices. This settles in affirmative a decade old conjecture.

1 Introduction

A number of spectral invariants of fullerene graphs have been examined recently as possible predictors of fullerene stability. Among the most promising were the separator [1], the smallest eigenvalue [2, 3] and the bipartite edge frustration [4]. The initial approach was mostly computational and empirical. It lead to an accumulation of data that revealed certain patterns that, in turn, prompted several researchers (and at least one computer program) to propose a number of conjectures about various spectral invariants of fullerenes; each of the references cited above contains at least one such conjecture, and the conjecture-making software *Graffiti* formulated many more [5]. Most of the human-made conjectures have been settled in affirmative through an interplay of theoretical and computational methods [1, 6–9]. One of them, however, has been established only for large fullerenes, leaving a gap that this note aims to close.

In order to make the note self-contained, we remind the reader of the basic concepts.

A **fullerene graph** is a planar, 3-regular and 3-connected graph that has only pentagonal and hexagonal faces.

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 $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G)$. The largest eigenvalue of a fullerene graph is not really interesting, since it is always equal to 3. However, the other extremal eigenvalue, the smallest one λ_n, is of significant interest, since it was found to correlate to some extent with fullerene stability.

A **Laplacian eigenvalue** of a graph G is an eigenvalue of its Laplacian matrix $L(G) = D(G) - A(G)$, where $D(G)$ is a diagonal matrix with the degrees of vertices of G on the diagonal. In the fullerene case, $L(G) = 3I - A(G)$. The largest Laplacian eigenvalue of G we denote by $\mu_\infty(G)$.

For other graph-theoretic and graph spectra-related terminology we refer the reader to any of standard monographs, such as, e. g., [10] or [11]. For fullerene graphs the reader might wish to consult the standard reference by Fowler and Manolopoulos [12].

2 Main results

The conjecture we consider here was formulated a decade ago by Fowler, Hansen and Stevanović [2, 3].

Conjecture 1

Amongst all fullerenes with 60 or more vertices, the icosahedral isomer C_{60} (60 : 1812) has the maximum smallest eigenvalue. ■

(The smallest eigenvalue of the icosahedral C_{60}, also known as the buckminsterfullerene, is equal to $-\frac{3+\sqrt{5}}{2} = -\phi^2$, where ϕ is the Golden Ratio.)

The authors checked the validity of their conjecture for small cases by computing and tabulating the smallest eigenvalues of all fullerene graphs on at most 100 vertices. A further verification for all fullerenes on at most 140 vertices followed in a paper concerned with some conjectures about Ramanujan fullerenes [7]. The authors of the conjecture also proved that it is valid for all isolated pentagon (IP) isomers [3], thus establishing the conjecture for an infinite class of graphs.

The next step was made possible by a connection between the quantity called the bipartite edge frustration and the largest Laplacian eigenvalue of a graph. The **bipartite edge frustration** $\varphi(G)$ of a graph G is the smallest number of edges that must be deleted from G in order to make it bipartite. The number of remaining edges, denoted by $\mathrm{bip}(G)$, is related to $\mu_\infty(G)$, the largest Laplacian eigenvalue of G via the following theorem ([11], p. 293).

Theorem A

Let G be a graph on n vertices. Then $\text{bip}(G) \le \frac{n}{4}\mu_\infty(G)$. ■

As fullerene graphs are 3-regular, we have $\mu_\infty(G) = 3 - \lambda_n(G)$, and Theorem A reads as follows.

Theorem A'

Let G be a fullerene graph on n vertices. Then $\lambda_n(G) \le -3 + \frac{4}{n}\varphi(G)$. ■

It was shown in [4] that for each n such that there is a fullerene graph on n vertices, there also is a fullerene graph with $\varphi(G) = 6$. Hence, an infinite class of non-IP fullerenes was found that satisfies Conjecture 1. In the same paper it was shown that for isomers with full icosahedral symmetry group the bipartite edge frustration can be exactly computed; for such a fullerene G_n one has $\varphi(G_n) = \sqrt{\frac{12}{5}n}$. The empirical results suggested that no other fullerene exceeds that limit. So, the authors of [4] advanced the following conjecture.

Conjecture 2

Let G be a fullerene graph on n vertices. Then $\varphi(G_n) \le \sqrt{\frac{12}{5}n}$. ■

It is clear that Conjecture 2 implies Conjecture 1 *via* Theorem A'. The first step toward turning Conjecture 2 into a theorem was made by Dvořak, Lidický and Škrekovski [13]. They proved a weaker statement.

Theorem B

Let G be a fullerene graph on n vertices. Then $\varphi(G_n) \le 39.29\sqrt{n}$. ■

By applying Theorem B, the validity of Conjecture 1 was established for large enough fullerene graphs. It was done in [8].

Theorem C

Let G be a fullerene graph on n vertices. Then $\lambda_n(G) \le -3 + \frac{157.16}{\sqrt{n}}$. ■

Theorem C implies Conjecture 1 for all fullerene graphs on at least 169292 vertices. Hence, the conjecture was shown to be asymptotically true, but the question still remained about its validity for $142 \le n \le 169290$.

Conjecture 2 was finally proved in a recent paper by Faria, Klein and Stehlík [9].

Theorem D

If G is a fullerene graph on n vertices, then $\varphi(G_n) \leq \sqrt{\frac{12}{5}n}$. Equality holds if and only if $n = 60k^2$ for some $k \in \mathbb{N}$ and $Aut(G) \cong I_h$. ■

The authors of [9] used their result to improve several bounds obtained in [8]. In particular, they obtained a better bound on $\lambda_n(G)$. Their Corollary 7.2 reads as follows.

Theorem E

If G is a fullerene graph on n vertices, then $\lambda_n(G) \leq -3 + 8\sqrt{\frac{3}{5n}}$. ■

Theorem E implies that Conjecture 1 is true for all fullerene graphs on at least $n = 264$ vertices. Thus the gap had been reduced to $142 \leq n \leq 262$. The remaining cases could, in principle, be verified by a direct computation, but the cost and the effort required would still be prohibitively high.

All the progress reported so far had been achieved by gradually improving the upper bound on $\varphi(G)$ and then combining it with Theorem A. However, once Conjecture 2 was proved and became Theorem E, its improving potential was exhausted. Hence, it was time to look at the other side for a result leading to a possible improvement. Fortunately, it turned out that exactly such a result was available in the literature.

Theorem F (Theorem 3.5 of [14])

Let G be a connected cubic graph on n vertices. Then $b(G) \leq \frac{4}{7+\lambda_n(G)}$, where $b(G)$ is the bipartite density of G, $b(G) = \frac{|E(G)|-\varphi(G)}{|E(G)|}$. ■

(In the original formulation Theorem F characterizes also the cases of equality, but none of them matter for fullerene graphs.)

Now, by combining Theorem D with Theorem F, we obtain an improved upper bound on $\lambda_n(G)$. The proof follows by a straightforward computation and we omit the details.

Theorem 1

Let G be a fullerene graph on n vertices. Then $\lambda_n(G) \leq -3 + \frac{16}{\sqrt{15n}-4}$. ■

The right-hand side of the formula from Theorem 1 is a decreasing function of n, and it is easily verified that it falls below the value $-\phi^2$ between $n = 140$ and $n = 141$. Hence no fullerene on more than 140 vertices can have the smallest eigenvalue greater than $-\frac{3+\sqrt{5}}{2}$, the smallest eigenvalue of buckminsterfullerene. By a remarkable coincidence, this exactly fits with the lower end of the gap in Conjecture 1! Hence, we have closed the gap and turned Conjecture 1 into a theorem.

Theorem 2
Amongst all fullerene graphs on 60 or more vertices, the icosahedral isomer of C_{60} (60 : 1812) has the maximum smallest eigenvalue. ■

3 Concluding remark

There is another conjecture in [3], concerned with the minimum smallest eigenvalue of fullerenes, that still remains open. It claims that among all fullerenes on a given number of vertices the one with the minimum smallest eigenvalue has the maximum number of pentagon-pentagon adjacencies. This seems to be consistent with the fact that a large number of pentagon-pentagon adjacencies leads to a low bipartite edge frustration, and hence to large "bipartiteness". It seems natural that the graphs that are in a sense closest to bipartite have the smallest eigenvalue closest to -3.

Acknowledgment: Partial support of the Ministry of Science, Education and Sport of the Republic of Croatia (Grants No. 177-0000000-0884 and 037-0000000-2779) is gratefully acknowledged.

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