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On the separator of fullerenes[1]

by

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ABSTRACT

The separator of a graph is the difference between the two largest eigenvalues of its adjacency matrix. The program *Graffiti*, developed by S. Fajtlowicz, posed the conjecture that the separator of fullerenes is at most 1. Here we prove this conjecture by using the *interlacing theorem* in an interesting manner and then extend this method to show that the dodecahedron has the largest separator amongst all fullerenes.

1 Introduction

The program *Graffiti*, developed by Siemion Fajtlowicz, was introduced in 1986. Early descriptions of *Graffiti* can be found in a series of papers [2, 3, 4, 5, 6]. For a given set of invariants, it automatically generates conjectures and test them on a database of examples. The most interesting conjectures are collected in the file *Written on the Wall* [7] and proposed to mathematical community. More than 70 graph theorists have been working on those conjectures, among which are some of the most widely known mathematicians of the field.

There are now over 900 conjectures developed through *Graffiti*, many in graph theory and related areas of chemistry, but others in geometry, number theory, and other fields. Also, some of the world's most distinguished graph theorists have worked on the conjectures generated by *Graffiti*,

Among the most exciting products of *Graffiti* are conjectures in chemistry on the structure of fullerenes, which when viewed as graphs are planar cubic graphs having only faces of size 5 or 6. In this paper, we focus on Conjectures 895 and 896 from [7].

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

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

We will first prove Conjecture 895 by using the *interlacing theorem* and then extend the same method to prove that the dodecahedron has the largest separator ($3 - \sqrt{5} \approx 0.7639$) amongst all fullerenes. Conjecture 896 is then an easy consequence of this result.

2 Proof of Conjecture 895

To prove this conjecture, we will use famous Cauchy's *interlacing theorem*. For further references to this theorem see [1, p.19].

Theorem 1 (The interlacing theorem) *Let H be an induced subgraph of graph G. If the eigenvalues of G are $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$, and the eigenvalues of H are $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_m$, then $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$ for $i = 1, 2, \ldots, m$.*

In particular, we will only use the inequality $\lambda_2 \geq \mu_2$ in our proofs.

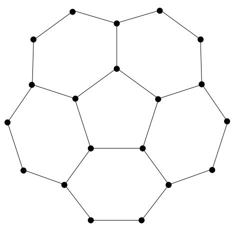
Theorem 2 (Conjecture 895) *The separator of a fullerene is at most* 1.

Proof Let F be an arbitrary fullerene, and let λ_2 denotes the second largest eigenvalue of F. Since a fullerene is a 3-regular graph, its largest eigenvalue equals 3. Thus, in order to prove that the separator of F is less than or equal to 1, we show that λ_2 is greater than or equal to 2.

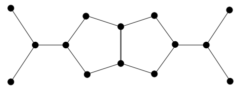
For this purpose we find a set S_1 of graphs with second largest eigenvalue greater than or equal to 2 and such that any fullerene must have at least one induced subgraph in S_1. From the *interlacing theorem*, λ_2 is then also greater than or equal to 2.

To complete the proof, we have depicted one possible set S_1 of graphs in Table 1. If a fullerene F has a pentagon surrounded by hexagons, then it contains the graph I_1 as an induced subgraph. Otherwise, F contains at least two pentagons sharing an edge and must then contain the graph I_2 as an induced subgraph. ■

In Table 1, we have denoted by μ_2 the second largest eigenvalue of the corresponding graph.



I_1, $\mu_2 = 2.0953$



I_2, $\mu_2 = 2$

Table 1: The set S_1.

3 The dodecahedron has the largest separator

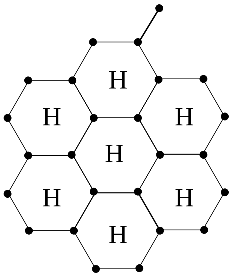
Theorem 3 *The dodecahedron has the largest separator amongst all fullerenes.*

Proof The second largest eigenvalue of the dodecahedron is $\sqrt{5}$, hence the separator equals $3 - \sqrt{5} \approx 0.7639$. Notice further that the dodecahedron is the unique fullerene having only pentagons and no hexagons as its faces.

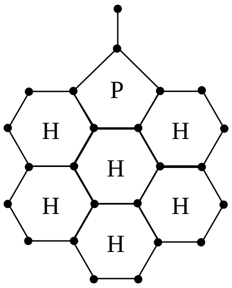
In order to show that the dodecahedron has the smallest second largest eigenvalue (i.e. the largest separator) amongst all fullerenes, we will slightly modify the idea used in proof of Conjecture 895. Namely, this time we will find a set S_2 of graphs such that each fullerene which contains a hexagon (and that means all fullerenes except dodecahedron) has at least one induced subgraph in S_2 and such that each graph from S_2 has the second largest eigenvalue greater than $\sqrt{5}$. Then from the *interlacing theorem* every fullerene but the dodecahedron, has the second largest eigenvalue greater than $\sqrt{5}$.

The set S_2 is depicted in Table 2. This set consists of all 13 possible combinations of pentagons and hexagons around a central hexagon, together with one pendant vertex attached to one of the faces. Hence, if a fullerene F contains an hexagon, its neighboring faces must form one of the combinations J_1–J_{13} depicted in Table 2. The additional pendant vertex is needed in each of them in order to have the second largest eigenvalue greater than $\sqrt{5}$. This pendant vertex cannot be adjacent to any of other vertices, because in F

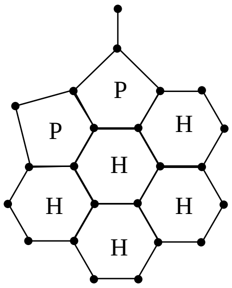
this vertex must lie in two faces together with its neighbor from Table 2, and for these two faces to be formed we will need to use remaining two edges adjacent to the pendant vertex. This shows that the corresponding combination from Table 2 is indeed an induced subgraph of F. ■



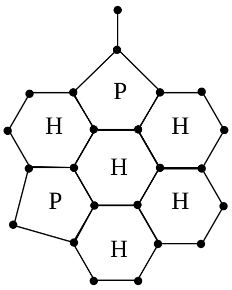
J_1, $\mu_2 = 2.2520$



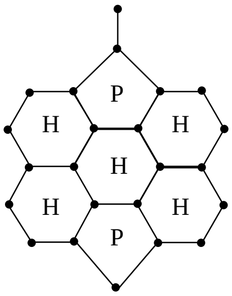
J_2, $\mu_2 = 2.2723$



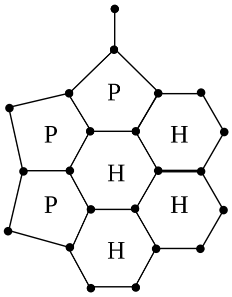
J_3, $\mu_2 = 2.2646$



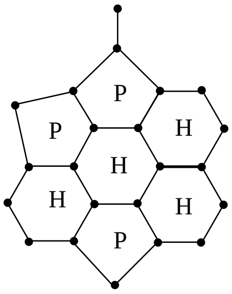
J_4, $\mu_2 = 2.2725$



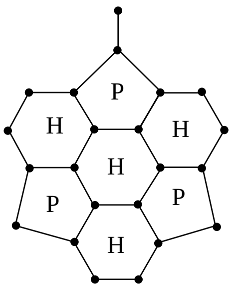
J_5, $\mu_2 = 2.2906$



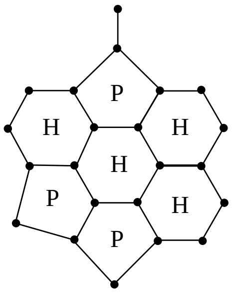
J_6, $\mu_2 = 2.2527$



J_7, $\mu_2 = 2.2828$

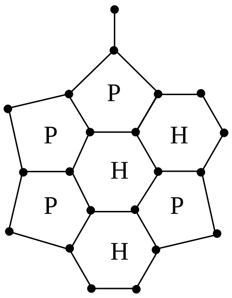


J_8, $\mu_2 = 2.2666$

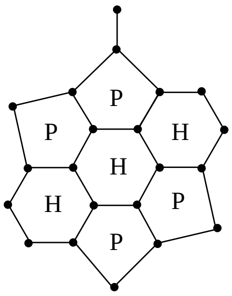


J_9, $\mu_2 = 2.2702$

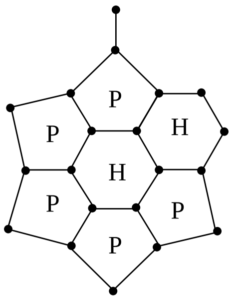
Table 2: The set S_2 (continued on the next page).



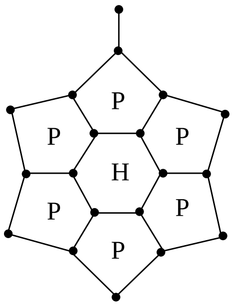
J_{10}, $\mu_2 = 2.2573$



J_{11}, $\mu_2 = 2.2868$



J_{12}, $\mu_2 = 2.2695$



J_{13}, $\mu_2 = 2.2472$

Table 2: The set S_2.

As earlier, in Table 2 we have denoted by μ_2 the second largest eigenvalue of a corresponding graph and for viewing pleasure in each face we have placed a letter "P" or "H" to denote a pentagon or a hexagon, resp.

Conjecture 896 is now easy to prove.

Theorem 4 (Conjecture 896) *The separator of a fullerene with n vertices is at most* $1-\frac{3}{n}$.

Proof From the previous theorem, the separator of any fullerene is at most $3-\sqrt{5} \approx 0.7639$. On the other hand, each fullerene has at least 20 vertices, so $1-\frac{3}{n} \geq 0.85$. Hence the separator of any fullerene is smaller than $1 - \frac{3}{n}$. ∎

References

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[7] Graffiti, *Written on the Wall*, **http://www.math.uh.edu/˜clarson/#fajt**.