On the \((1, 2)\)-spectral spread of fullerenes

Dragan Stevanović and Gilles Caporossi

Abstract. Let \(G\) be a simple graph on \(n\) vertices with the eigenvalues (of an adjacency matrix) \(\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n\). For \(1 \leq i < j \leq n\), the \((i, j)\)-spectral spread (or just \((i, j)\)-spread) of \(G\) is defined as the difference \(\lambda_i - \lambda_j\). The program \textit{Graffiti}, developed by S. Fajtlowicz, posed the conjecture that the \((1, 2)\)-spread of fullerenes is at most 1. Here we prove this conjecture by using the \textit{interlacing theorem} in an interesting manner and then extend this method to show that the dodecahedron has the largest \((1, 2)\)-spread amongst all fullerenes.

1. Introduction

The program \textit{Graffiti}, developed by Siemion Fajtlowicz, was introduced in 1986. Early descriptions of \textit{Graffiti} can be found in a series of papers [8, 9, 10, 11, 12]. For a given set of invariants, it automatically generates conjectures and test them on a database of examples. Some such conjectures are collected in the file \textit{Written on the Wall} [13] and proposed to the mathematical community. Many 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 \textit{Graffiti}, many in graph theory and related areas of chemistry, but others in geometry, number theory, and other fields.

Among the most exciting products of \textit{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 [13].

\textbf{Conjecture 895.} The separator of a fullerene is at most 1.

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

\textbf{Remark 1.1.} Note that in these conjectures the term separator is used to denote \((1, 2)\)-spectral spread. We opted for alternative terminology since the term

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separator is already used in a different meaning in the literature. Besides, the difference $\lambda_1 - \lambda_n$ is already named as the spectral spread in the literature, so it was a straightforward generalization to call it a $(1, n)$-spectral spread.

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 $(1, 2)$-spread ($3 - \sqrt{5} \approx 0.7639$) amongst all fullerenes. Conjecture 896 is then an easy consequence of this result.

Conjecture 895 was one among six selected by S. Fajtlowicz for presentation at Graph Theory Day 42. It was proved during the following week at the DIMACS Workshop on Computer-Generated Conjectures from Graph Theoretic and Chemical Databases by the first author, using the interactive component of the system GRAPH [3, 4, 6, 14] for calculations of graph properties; when the result was presented, the second author could simplify the proof on the spot, using the interactive component of AGX [1, 2] for the same purpose. Both authors then collaborated on the present paper.

We note that, unlike Graffiti, system GRAPH is nowadays mostly used as a powerful, yet simple “graph calculator”, enabling users to draw graphs and check their properties. On the other hand, the main purpose of AGX is to find extremal graphs with respect to some optimization function defined on a set of graphs, which can lead to faster discovery of new conjectures either automatically using dedicated routines or interactively. However, for the purpose of this paper, AGX was also used as a “graph calculator”.

2. Proof of conjecture 895

To prove this conjecture, we will use the famous Cauchy’s interlacing theorem. For further references to this theorem see [5, p.19].

**Theorem 2.1** (The interlacing theorem). Let $H$ be an induced subgraph of a graph $G$. If the eigenvalues of $G$ are $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, and the eigenvalues of $H$ are $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_m$, then $\lambda_i \geq \mu_i \geq \lambda_{n-m+i}$ for $i = 1, 2, \ldots, m$.

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

**Theorem 2.2** (Conjecture 895). The $(1, 2)$-spread of a fullerene is at most 1.

<table>
<thead>
<tr>
<th>Table 1. The set $S_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I_1$, $\mu_2 = 2.0953$</td>
</tr>
<tr>
<td>$I_2$, $\mu_2 = 2$</td>
</tr>
</tbody>
</table>
Proof. Let $F$ be an arbitrary fullerene, and let $\lambda_2$ 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 $(1,2)$-spread of $F$ is less than or equal to 1, we show that $\lambda_2$ 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, $\lambda_2$ 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, where we have denoted by $\mu_2$ the second largest eigenvalue of the corresponding graph.

If a fullerene $F$ has a pentagon surrounded by hexagons, then it obviously contains the graph $I_1$ as an induced subgraph. Otherwise, $F$ contains at least two pentagons sharing an edge and it must then contain the graph $I_2$ as an induced subgraph. We prove this by supposing that there exists an edge between two of the vertices $L_1, \ldots, L_4, M_1, \ldots, M_4$ of $I_2$ and showing that any choice of the end vertices of this edge leads to a contradiction. The conclusion to which we arrive in each case is that one of the faces, to which the hypothetical edge belongs, either

- has an inappropriate length, i.e. it has either less than 5 or more than 6 edges, or
- it has “double” edges, i.e. there exists an edge such that the same face appears on both of its sides.

Since the number of distinct cases is rather large, we illustrate the proof by considering existence of an edge joining $L_1$ and $L_3$, and of an edge joining $L_1$ and $M_2$. Remaining cases are considered in a similar way.

Suppose first that the vertices $L_1$ and $L_3$ are joined by an edge $e_1$. Let $F_1$ be the face determined by edges $e_1$ and $L_1K_1$. In the face $F_1$, if we go along the edge $e_1$ from $L_1$ to $L_3$, then $F_1$ must also contain edges $L_3K_2, K_2N_2$ and $N_2M_3$. On the other hand, if we go along the edge $e_1$ from $L_3$ to $L_1$, then $F_1$ must also contain edges $L_1K_1, K_1N_1$ and $N_1M_1$. Thus, the face $F_1$ has at least seven edges, which is a contradiction.

Next, suppose that the vertices $L_1$ and $M_2$ are joined by an edge $e_2$. Let $F_2$ be the face determined by edges $e_2$ and $L_1K_1$. In the face $F_2$, if we go along the edge $e_2$ from $L_1$ to $M_2$, then $F_2$ must also contain edges $M_2N_1, N_1K_1$ and $K_1L_2$. On the other hand, if we go along the edge $e_2$ from $M_2$ to $L_1$, then $F_2$ must also contain edges $L_1K_1$ and $K_1L_2$. But then the face $F_2$ appears on both sides of the edge $K_1L_2$, which is a contradiction.  \qed
3. The largest $(1,2)$-spectral spread amongst fullerenes

Theorem 3.1. Amongst all fullerenes, the dodecahedron has the largest $(1,2)$-spectral spread.

Proof. The second largest eigenvalue of the dodecahedron is $\sqrt{5}$, hence the $(1,2)$-spread 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 $(1,2)$-spread) amongst all fullerenes, we will slightly modify the idea used in proof of Conjecture 895. Namely, this time we find a set $S_2$ of graphs such that each fullerene which contains a hexagon (and that means all fullerenes except the 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. It consists of all possible combinations of at least one pentagon and hexagons around a central hexagon, together with one pendant vertex attached to one of the faces. A fullerene $F$ containing a hexagon must contain a hexagon $H$ adjacent to a pentagon, and, hence, neighboring faces of $H$ must form one of the graphs $J_i$, $i = 1, 2, \ldots, 12$, depicted in Table 2. The additional pendant vertex is needed in some of them in order to have the second largest eigenvalue greater than $\sqrt{5}$. Using the technique from the proof of Theorem 2.2, one can prove that $J_i$ is really the induced subgraph of $F$. \qed

As earlier, in Table 2 we have denoted by $\mu_2$ the second largest eigenvalue of a corresponding graph and for viewing pleasure we have placed in each face a letter “P” or “H” to denote a pentagon or a hexagon, resp.

Conjecture 896 is now easy to prove.

Theorem 3.2 (Conjecture 896). The $(1,2)$-spread of a fullerene with $n$ vertices is at most $1 - \frac{3}{n}$.

Proof. From the previous theorem, the $(1,2)$-spread 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 $(1,2)$-spread of any fullerene is smaller than $1 - \frac{3}{n}$. \qed

Acknowledgements

The authors are grateful to an anonymous referee for a valuable suggestion which led to an improvement of terminology used herein.
Table 2. The set $S_2$. 

<table>
<thead>
<tr>
<th>$J_n$</th>
<th>$\mu_2$</th>
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<tr>
<td>$J_{12}$</td>
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References


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