# The structure of trivalent graphs with minimal eigenvalue gap

Barry Guiduli $^1$ 

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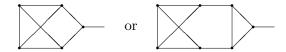
 $<sup>^1\</sup>mathrm{Research}$  partially supported by an IREX fellowship.

#### Abstract

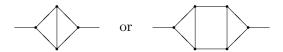
Let G be a connected 3-regular graph on n vertices ( $n \ge 10$ ) such that among all connected 3-regular graphs on n vertices, G has the largest possible second eigenvalue. We show that G must be reduced path-like, i.e. G must be of the form:



where the ends are one of the following:



(the right-hand end block is the mirror image of one of the blocks shown) and the middle blocks are one of the following:



This partially solves a conjecture implicit in a paper of Bussemaker et al. [3].

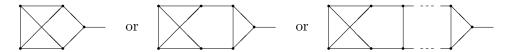
#### 1 Introduction

We let G be a connected trivalent graph on n vertices, and A its adjacency matrix. Let  $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ , be the eigenvalues of A, also called the eigenvalues of G. They are real,  $\lambda_1 = 3$  and  $\lambda_2 < 3$ . The difference between  $\lambda_1$  and  $\lambda_2$  is called the eigenvalue gap. The eigenvalue gap was first investigated by Fiedler in 1973, who called it the algebraic connectivity (see [4]). The intuition is that the gap is large if and only if the graph has large "connectivity". This was formalized by Alon and Milman [2] and Alon [1] who bounded the isoperimetric ratio (a measure of connectivity) above and below, respectively, by functions of the eigenvalue gap (see their respective papers). We show that the trivalent graph on n vertices with maximal second eigenvalue must look like a path. We formalize this with the following definitions.

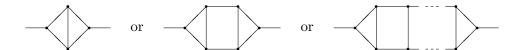
**Definition:** A 3-regular graph is said to be *path-like* if it has the form:



where each end block is one of the following:



(the right-hand end block is the mirror image of one of the blocks shown) and each middle block is one of the following:



**Definition:** We define a three regular graph to be *reduced path-like* if it is path-like, the end blocks are of the first two types, and the middle blocks are of the first two types.

Let  $H_n$  be the reduced path-like graph on n vertices with middle blocks of the first type and one end block of the first type. The other end block is then forced by the value of n. (Notice that  $H_n$  only makes sense for  $n \ge 10$  and even.)

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Conjecture 1 (Bussemaker et al. [3]) For  $n \ge 10$ , the graph  $H_n$  is the unique connected 3-regular graph with maximum second eigenvalue.

We do not prove the conjecture, instead we prove the following result which supports the conjecture.

**Theorem 1** Let G be a connected 3-regular graph on n vertices ( $n \geq 10$ , even), such that among all connected 3-regular graphs on n vertices, G has maximal possible second eigenvalue. Then G is reduced path-like.

(Note: for n < 10, reduced path-like form does not make sense. For the exact graphs achieving the maximum second eigenvalue, see the paper of Bussemaker et al. [3])

We make one more elementary definition and then outline the proof of the theorem.

**Definition:** An elementary move in a graph is a switching of parallel edges: let  $a \sim b$  and  $c \sim d$  in G,  $a \not\sim c$ ,  $b \not\sim d$  (here  $\sim$  and  $\not\sim$  denote adjacency and non-adjacency in G), then the elementary move SWITCH(a, b, c, d) removes the edges  $\{a, b\}$  and  $\{c, d\}$  and replaces them with the edges  $\{a, c\}$  and  $\{b, d\}$ .

We prove the theorem in two parts. First we show that if G is not already minimal path-like, we may transform it into such a graph by elementary moves, never decreasing the second eigenvalue (and assuming it is maximal, never increasing it). Throughout the transformation, we maintain connectivity. We then show that the eigenvector for the second eigenvalue is strictly decreasing from left to right (when the graph is drawn path-like, as above). It then follows that any elementary move will decrease the second eigenvalue, thus showing that G must have been minimal path-like to begin with.

#### 2 General set-up

Let G be a connected 3-regular graph on n vertices. Let A be the adjacency matrix of G. The largest eigenvalue of G is 3 with eigenvector j, the all one's

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vector. The second eigenvalue,  $\lambda_2$ , is given by the maximum of the Rayleigh quotient:

$$\lambda_2 = \max_{x \perp \mathbf{j}} \frac{x^t A x}{||x||}.$$

Let  $\mu: V \longrightarrow \mathbf{R}$  be an eigenvector for the second eigenvalue, considered as a weighting on the vertices; for  $v \in V$  we write  $\mu_v = \mu(v)$ . For convenience, we may assume the vertex set is  $[n] = \{1, 2, \dots, n\}$  and that the vertices are numbered so that  $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ . We call this a *proper labeling* of the vertices (with respect to the eigenvector for the second eigenvalue).

We can now clarify the reconnecting. With respect to a proper labeling, we show that we can reconnect to get vertex 1 adjacent to vertices 2, 3, and 4. We can then reconnect to get 2 adjacent to 3 and 4. This now looks like:



We show that we can continue in this way, getting a path-like graph, with the labels increasing from left to right. The trick is not to disconnect the graph while we are reconnecting, and not to lower the second eigenvalue. We ensure that the eigenvalue does not decrease by choosing our switch carefully.

**Lemma 1** Let G be a connected trivalent graph with maximal  $\lambda_2$ . Let  $\mu: V \longrightarrow \mathbf{R}$  be an eigenvector for  $\lambda_2$ . If there are vertices a, b, c, d in G such that  $a \sim b, c \sim d, a \not\sim c, b \not\sim d, \mu_a \geq \mu_d$ , and  $\mu_c \geq \mu_b$ , then SWITCH(a, b, c, d) does not decrease the second eigenvalue.

**Proof:** We may assume that  $\|\mu\| = 1$ , then  $\lambda_2 = \mu^t A \mu$ , where A is the adjacency matrix of G. Let A' be the adjacency matrix of the graph after the reconnection. In light of the Rayleigh quotient, it suffices to show that

$$\mu^t A' \mu \ge \mu^t A \mu$$
.

This follows immediately from

$$\mu^t A' \mu - \mu^t A \mu = \mu^t (A' - A) \mu = 2\mu_a \mu_c + 2\mu_b \mu_d - 2\mu_a \mu_b - 2\mu_c \mu_d =$$

$$= 2(\mu_a - \mu_d)(\mu_c - \mu_d) \ge 0.$$

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We have the following lemma to help with keeping the graph connected during reconnecting:

**Lemma 2** Let G be a connected 3-regular graph on [n] with maximal  $\lambda_2$ , properly labeled with respect to an eigenvector  $\mu$ . Assume that  $G \setminus [r]$  is disconnected and that each of its components has and edge which is not a cut edge. Then we may reconnect the graph using elementary moves to connect  $G \setminus [r]$ , not changing  $\lambda_2$ .

**Proof:** It suffices to prove the lemma when  $G\setminus [r]$  has two connected components H and K. We will prove the lemma by contradiction. Assume that we cannot reconnect the graph to accomplish our goal. Let  $\{u_1, u_2\}$  be a non-cut edge in H and  $\{v_1, v_2\}$  a non-cut edge in a cycle in K. Because these edges are not cut edges, both SWITCH $(u_1, u_2, v_1, v_2)$  and SWITCH $(u_1, u_2, v_2, v_1)$  would leave G and  $G\setminus [r]$  connected, so it must be the case that these switches decrease  $\lambda_2$ . Based on the previous lemma, this only happens if the weights of one pair are strictly greater than those of the other pair. We may assume that  $\mu_{u_1}, \mu_{u_2} > \mu_{v_1}, \mu_{v_2}$ . Let x be an element in [r] adjacent to K and let  $(v_1, v_2, v_3, \ldots, v_t)$  be a shortest path in G,  $v_t = x$  (we may possibly need to switch the roles of  $v_1$  and  $v_2$ ). For  $1 \leq i < t$ , SWITCH $(u_1, u_2, v_i, v_{i+1})$  and SWITCH $(u_1, u_2, v_{i+1}, v_i)$  would connect H and K, leaving the graph conected, so by induction,  $\mu_{u_1}, \mu_{u_2} > \mu_{v_1}, \mu_{v_2}, \ldots, \mu_{v_t}$ , but this is a contradiction, as  $\mu_x \geq \mu_v$  for all  $v \in H$ .

#### 3 Reconnecting to get minimal path-like

Assume that G is a connected trivalent graph on n vertices,  $n \geq 10$ . We further assume that among all connected trivalent graphs on n vertices, G has maximal second eigenvalue, and that G is properly labeled. During the reconnecting, we will denote G by  $G_k$  to indicate that the first k vertices are in path-like form.

#### 3.1 Getting $G_4$

#### 3.1.1 Connecting 1 to 2.

If  $1 \not\sim 2$  then there is a shortest path  $(1, i_1, \ldots, i_r, 2)$  from 1 to 2, and a neighbor of 1,  $x, x \neq i_1$  and  $x \not\sim i_r$ , so that we may apply SWITCH $(1, x, 2, i_r)$ , not decreasing the second eigenvalue and leaving 1 adjacent to 2 and G connected.

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#### 3.1.2 Connecting 1 to 3.

If  $1 \not\sim 3$  then let  $x \neq 2$  be a neighbor of 1. We may assume (by Lemma 2), that  $G \setminus \{1\}$  is connected. Let  $(x, i_1, \ldots, i_r, 3)$  be a shortest path from x to 3 not passing through 1. Let y be a neighbor of 3 so that  $y \not\sim i_r$ , then SWITCH(1, x, 3, y).

#### 3.1.3 Connecting 1 to 4.

(This is identical to the previous reconnection.) If  $1 \not\sim 4$  then let x be the third neighbor of 1. We may assume (by Lemma 2), that  $G \setminus \{1\}$  is connected. Let  $(x, i_1, \ldots, i_r, 4)$  be a shortest path from x to 4 not passing through 1. Let y be a neighbor of 4 so that  $y \not\sim i_r$ , then SWITCH(1, x, 4, y).

#### 3.1.4 Connecting 2 to 3.

We may assume that  $G \setminus \{1\}$  is connected. Let  $(2, i_1, \ldots, i_r, 3)$  be a shortest path in  $G \setminus \{1\}$ . Let x be the third neighbor of 2 and y the third neighbor of 3. Then either  $x \not\sim i_r$  and SWITCH $(2, x, 3, i_r)$ , or  $i_1 \not\sim y$  and SWITCH $(2, i_1, 3, y)$ . One of these is possible because  $G \setminus \{1\}$  is connected.

#### 3.1.5 Connecting 2 to 4.

We may assume that  $G \setminus [4]$  is connected. Let x be the third neighbor of 2, y the third neighbor of 3, and let u and v be the two other neighbors of 4. If  $3 \sim 4$  then SWITCH(2, x, 4, 3). Otherwise, if  $x \neq u$  and  $x \not\sim u$ , then apply SWITCH(2, x, 4, u). If one of these relations does not hold, try the same for v instead of v. If the same relations hold for v, try to get  $3 \sim 4$  by considering 3 instead of 2 and looking at u and v; then SWITCH(2, x, 4, 3) will work. If none of these are allowed, then  $G \setminus [4]$  has a connected component consisting of just  $\{x, y, u, v\}$ , this set having 2 or 4 points depending on the equalities, and being disconnected from the rest of the graph. This contradicts the fact that  $G \setminus [4]$  is connected (in fact, in this case G has a connected component with 6 or 8 vertices, contradicting the fact that G is connected with at least 10 vertices).

#### 3.2 General Steps

We now introduce general steps that deal with the remaining vertices. We assume at this point that the graph G has the desired connections among

the vertices [r], i.e. we have  $G_r$ . The next three sets of general steps show how to reconnect  $G_r$  to get either  $G_{r+1}$  of  $G_{r+2}$ .

#### 3.2.1 r is odd.

Based on our construction, we only arrive at this case when  $r \sim r-2$  and  $r \sim r-1$ , so there is only one edge leaving the first r vertices, and it leaves from r. We need to connect r to r+1. Let x be the third neighbor of r and y be a neighbor of r+1 the furthest possible from r and SWITCH(r, x, r+1, y). This gives us  $G_{r+1}$ 

### 3.2.2 r is even and the two edges leaving the first r vertices both come from r.

**Step 1.** Connect r to r+1. Let x be the neighbor of r closest to r+1 and let y be the neighbor of r+1 furthest from r. SWITCH(r, x, r+1, y).

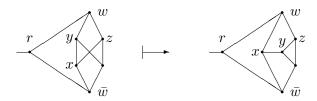
**Step 2.** Connect r to r+2. We may assume that  $G \setminus [r+1]$  is connected. Let x be the third neighbor of r. Let y be the neighbor of r+2 furthest from x in  $G \setminus [r]$ . SWITCH(r, x, r+2, y). This does not disconnect because there is a path from x to one of the other neighbors of r+2 not using the two removed edges.

**Step 3.** Connect r+1 to r+2. We may assume that  $G \setminus [r+2]$  is connected. There are some cases to consider:

CASE I: r+1 and r+2 share two neighbors. Call the neighbors x and y. If  $x \sim y$ , then n=r+4 and we are done as this is  $G_n$ . Otherwise, SWITCH(r+1, x, r+2, y). This leaves  $G_{r+2}$ .



CASE II:  $\operatorname{dist}_{G\setminus[r]}(r+1,r+2)=3$  and both neighbors of r+1 and r+2 are adjacent to each other (then n=r+6). Let x be the smallest among the remaining vertices (i.e. x=r+3), so  $\mu_x$  is largest among the remaining vertices. Let y, z be the two neighbors of x and let w=r+1 or r+2, whichever is adjacent to y and z, and call the other  $\bar{w}$ . Then SWITCH(w,y,x,z) reduces the graph to CASE III.



CASE III:  $\operatorname{dist}_{G\setminus[r]}(r+1,r+2)=2$ . If we arrive at this case then r+1 and r+2 share one neighbor (because of CASE I). Call this neighbor x and let y and z be the other neighbors of r+1 and r+2 respectively. Then either  $x \not\sim y$  and SWITCH(r+1,y,r+2,x), or  $x \not\sim z$  and SWITCH(r+1,x,r+2,z). This leaves  $G_{r+2}$ .

CASE IV: Let x and y be neighbors of r+1 and r+2 respectively, such that  $x \not\sim y$  and one is on a path from r+1 to r+2. SWITCH(r+1, x, r+2, y).

## **3.2.3** r is even and the two edges leaving the first r vertices come from r and r-1.

We note that if we arrive at the case, then  $r \sim r-1$ .

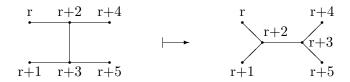
**Step 1.** Connect r-1 to r+1. We may assume that  $G \setminus [r]$  is connected and hence there is a path from r-1 to r+1 in  $G \setminus \{r\}$ . Let x be the third neighbor of r-1 and let y be the neighbor of r+1 furthest from r-1 in  $G_r \setminus \{r\}$ . SWITCH(r-1, x, r+1, y). If  $r \sim r+1$  too, then this is  $G_{r+1}$  and skip the following steps.

**Step 2.** Connect r to r+2. This is the same as step 2 above.

**Step 3.** Connect r+1 to r+2. This is the same as for step 3 above.

#### 3.3 Putting G in minimal path-like form

We may now assume that G is path-like with labels increasing from left to right in a proper labeling (this is what we have acheived in the previous reconnecting). By applying SWITCH(r+1, r+3, r+2, r+4) as often as possible to G, we put G in minimal path-like form without decreasing  $\lambda_2$ .



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## 4 The eigenvector coordinates are strictly decreasing

In the previous section we reconnected the graph to put it in minimal pathlike form with the weights given by  $\mu$  non-increasing from left to right. Assume that the graph is drawn horizontally like the original example in the definition of path-like, with the vertices numbered 1 to n, increasing from left to right. Further, assume that the weights of the vertices given by en eigenvector  $\mu$  of  $\lambda_2$  are non-increasing from left to right. We will show that these weights are in fact strictly decreasing. We may assume that vertices with the same horizontal position have the same weight (we may assume this by noticing that there is a graph automorphism interchanging any two vertices in the same horizontal position, and then averaging the eigenvector). Assume that there are two adjacent vertices in a different horizontal position with the same weight. If this is the case, then we can find two such ones c and d (c to the left of d) so that the left-most neighbor of c, call it a, has greater weight than the right-most neighbor of d, call this f. Let b and e be the other neighbors of c and d, respectively. It is possible that some of these coincide, but here are some important observations: a cannot be to the right or c, f cannot be to the left of d, b cannot be to the right of d, and e cannot be to the left of c. Summarizing what we know about the weights, we have  $\mu_a > \mu_f$  and  $\mu_a \ge \mu_b \ge \mu_c = \mu_d \ge \mu_e \ge \mu_f$ . We show that there exists some  $\epsilon > 0$  such that we may increase  $\mu_c$  by  $\epsilon$  and decrease  $\mu_d$  by  $\epsilon$  (keeping the vector perpendicular to j) to increase the Rayleigh quotient, thus showing that the second eigenvalue was not maximal, and hence arriving at a contradiction. We assume that  $\|\mu\|=1$ , then for the new vector, the Rayleigh quotient is

$$\frac{\lambda_2 + 2\epsilon(\mu_a + \mu_b + \mu_d - \mu_c - \mu_e - \mu_f - \epsilon)}{1 + 2\epsilon(\mu_c - \mu_d + \epsilon)},$$

which is greater than  $\lambda_2$  if

$$\mu_a + \mu_b - \mu_e - \mu_f > \lambda_2 \epsilon$$
.

This is possible, as the left hand side is greater than zero, and taking an appropriate  $\epsilon$ , we arrive at a contradiction.

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#### 5 QED

We need to show that any elementary move will now decrease the Rayleigh quotient, so that G must have been in this shape all along. If we apply SWITCH(a,b,c,d) to rewire without decreasing the Rayleigh quotient, we must find four vertices a,b,c,d such that  $a \sim b$ ,  $c \sim d$ ,  $a \not\sim c$ ,  $b \not\sim d$ , SWITCH(a,b,c,d) does not disconnect G, and  $\mu_a \geq \mu_d$ ,  $\mu_b \geq \mu_c$ . These vertices do not exist in a pathlike graph, with  $\mu$  strictly decreasing from left to right. This completes the proof of Theorem 1.

#### 6 Remarks

I would like to thank my advisor László Babai for bringing this conjecture to my attention and for many useful discussions.

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#### Author's address:

University of Chicago Department of Mathematics 5734 University Ave. Chicago, IL 60637

and

Math. Res. Inst., Hung. Acad. Sci. Reáltanoda utca 13-15.

H-1053 Budapest

E-mail: bdg@cs.elte.hu

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