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A sharp lower bound for the least eigenvalue of the signless Laplacian of a non-bipartite graph

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Dedicated to the memory of Francis K. Bell (1944–2006).

Abstract

We prove that the minimum value of the least eigenvalue of the signless Laplacian of a connected non-bipartite graph with a prescribed number of vertices is attained solely in the unicyclic graph obtained from a triangle by attaching a path at one of its endvertices.

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1. Introduction

Let G be a simple graph with vertices $1, \ldots, n$, of degrees $d_1, \ldots, d_n$, respectively. Let A be the (0, 1)-adjacency matrix of G, and let D be the diagonal matrix $\mathrm{diag}(d_1, \ldots, d_n)$. The matrix $D - A$ is the Laplacian of G, while $D + A$ is called the *signless Laplacian* of G. The least eigenvalue of $D - A$ is zero, and the second least is known as the algebraic connectivity of G.

Computer investigations of graphs with up to 11 vertices [5] suggest that the spectrum of $D + A$ performs better than the spectrum of A or $D - A$ in distinguishing non-isomorphic graphs, but relatively few articles on $D + A$ have appeared in the literature. Several references may be found in the papers [3,4]. The latter lists 30 computer-generated conjectures concerning the eigenvalues of $D + A$, and establishes various inequalities such as bounds on the largest eigenvalue of $D + A$. Here we are concerned with the least eigenvalue of $D + A$, denoted by $\kappa(G)$.

If R is the vertex-edge incidence matrix of G then

$$RR^{\mathrm{T}} = D + A, \quad R^{\mathrm{T}}R = A(L(G)) + 2I, \tag{1}$$

where $A(L(G))$ is the adjacency matrix of the line graph $L(G)$. In particular, $D + A$ is positive semi-definite, and so always $\kappa(G) \geqslant 0$. From [3, Theorem 2.2.4] we know that, for a connected graph G, we have $\kappa(G) = 0$ if and only if G is bipartite, and that in this case $\kappa(G)$ is a simple eigenvalue. In [6], $\kappa(G)$ was studied as a measure of non-bipartiteness of a graph.

Conjecture 24 of [4] asserts the following:

If G is a connected non-bipartite graph of order $n(n \geqslant 4)$, then $\kappa(G) \geqslant \kappa(E_{3,n-3})$, where $E_{e,f}$ is the unicyclic graph on $e + f$ vertices obtained by coalescing a vertex in the cycle C_e with an endvertex of the path P_{f+1}.

Here we confirm this conjecture, which remained unproved in [4] notwithstanding the theoretical arguments presented there as further supporting evidence. Preliminary requirements are given in Section 2. In Section 3, we establish several useful properties of an eigenvector corresponding to $\kappa(G)$ in the case that $\kappa(G)$ is minimal among the graphs in question. These properties are used in Section 4 to show that $G = E_{3,n-3}$.

We note in passing that for $n \geqslant 3e - 1$, the graph $E_{e,n-e}$ is the unique graph with least algebraic connectivity among the connected graphs with n vertices and girth e [7].

2. Preliminaries

We extend the notation of Section 1 by writing $\phi(x, G) = \det(xI - A)$ and $\xi(x, G) = \det(xI - D - A)$. From the relations (1) we obtain the following, since the non-zero eigenvalues of RR^{T} and $R^{\mathrm{T}}R$ coincide.

Theorem 2.1. *Let G be a graph with n vertices and m edges. Then*

$$\phi(x, L(G)) = (x + 2)^{m-n}\xi(x + 2, G). \tag{2}$$

The following theorem can be found, for example, in [1, p. 159].

Theorem 2.2. *Let $G \cdot H$ be the graph obtained from disjoint graphs G and H by coalescing the vertex u of G with the vertex v of H. Then*

$$\phi(x, G \cdot H) = \phi(x, G)\phi(x, H - v) + \phi(x, G - u)\phi(x, H) - x\phi(x, G - u)\phi(x, H - v).$$

We write $GuvH$ for the graph obtained from disjoint graphs G and H by adding an edge joining the vertex u of G to the vertex v of H. We write G_u for the graph obtained from G by adding a pendant edge at u. Now the line graph $L(GuvH)$ is the coalescence (at uv) of $L(G_u)$ and $L(H_v)$, and so two applications of Theorem 2.2 yield:

Corollary 2.3. *With the notation above,*

$$\phi(x, L(GuvH)) - \phi(x, L(Guv'H)) = \phi(x, L(G))(\phi(x, L(H_v)) - \phi(x, L(H_{v'}))).$$

We write $Q = D + A$, with eigenvalues $q_1, q_2, \ldots, q_n$, where $q_1 \geqslant q_2 \geqslant \cdots \geqslant q_n$. We refer to the q_i as the Q-eigenvalues of G, and to corresponding eigenvectors as Q-eigenvectors of G. We write $q_i = q_i(G)$, so that $q_n(G) = \kappa(G)$. The Q-eigenvalues of an edge-deleted subgraph of G interlace those of G, as can be seen from (2) by applying the (standard) Interlacing Theorem to $L(G)$:

Theorem 2.4. *Let e be an edge of the graph G. Let $q_1, q_2, \ldots, q_n$ $(q_1 \geqslant q_2 \geqslant \cdots \geqslant q_n)$ and $s_1, s_2, \ldots, s_n (s_1 \geqslant s_2 \geqslant \cdots \geqslant s_n)$ be the Q-eigenvalues of G and $G - e$, respectively. Then*

$$0 \leqslant s_n \leqslant q_n \leqslant \cdots \leqslant s_2 \leqslant q_2 \leqslant s_1 \leqslant q_1.$$

Given a connected non-bipartite graph G, we may delete edges from G to obtain an odd-unicyclic graph, that is, a unicyclic graph G' whose cycle has odd length. By interlacing, $\kappa(G') \leqslant \kappa(G)$, and so among the connected non-bipartite graphs on n vertices, the minimal value of $\kappa(G)$ is attained in an odd-unicyclic graph; moreover, if $\kappa(G)$ is minimal then $\kappa(G) = \kappa(G')$ for some odd-unicyclic graph G', and G can be obtained from G' by adding edges. Accordingly we shall focus our attention first on odd-unicyclic graphs with n vertices ($n \geqslant 4$). For such a graph G, we have $0 < \kappa(G) < 1$ from Theorem 2.1, because $-2 < \lambda(L(G)) < -1$, where $\lambda(L(G))$ is the least eigenvalue of $A(L(G))$ (see [2, Theorem 5.2.2]). It was noted in [4] that

$$\frac{1}{12n^2} \leqslant q_n(E_{e,n-e}) \leqslant q_{n-1}(P_n) = 2\left(1 - \cos\frac{\pi}{n}\right) = 4\sin^2\left(\frac{\pi}{2n}\right)$$

and so

$$\frac{1}{12n^2} \leqslant \kappa(E_{e,n-e}) < \frac{\pi^2}{n^2}.$$

3. The form of a particular eigenvector

For a non-zero vector $\mathbf{x} = (x_1, \ldots, x_n)^\top \in \mathbb{R}^n$, let $R(\mathbf{x})$ be the Rayleigh quotient $\mathbf{x}^\top Q\mathbf{x}/\mathbf{x}^\top\mathbf{x}$. Recall that $\kappa(G) \leqslant R(\mathbf{x})$, with equality if and only if $\mathbf{x}$ is a Q-eigenvector of G corresponding to $\kappa(G)$. We use this observation to prove the following lemma, where we write $r \sim s$ to indicate that vertices r and s are adjacent.

Lemma 3.1. *Let r, s, t be vertices of the graph G such that $r \sim s, r \nsim t$. Let G' be the graph obtained from G by replacing the edge rs with rt, and let $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\top$ be a Q-eigenvector of G corresponding to $\kappa(G)$. If $(x_t - x_s)(2x_r + x_s + x_t) \leqslant 0$ then $\kappa(G') \leqslant \kappa(G)$, with equality if and only if $x_r = -x_s = -x_t$.*

Proof. We may take $\mathbf{x}$ to be a unit vector. Then we have

$$\kappa(G') - \kappa(G) \leqslant \mathbf{x}^{\mathrm{T}}(Q' - Q)\mathbf{x} = (x_t - x_s)(2x_r + x_s + x_t) \leqslant 0,$$

where Q' is the signless Laplacian of G'. If $\kappa(G') = \kappa(G) = \kappa$ then $(x_t - x_s)(2x_r + x_s + x_t) = 0$ and $\mathbf{x}$ is a Q-eigenvector of G' corresponding to κ. In this situation, the eigenvalue equations

$$\kappa x_u = d_u x_u + \sum_{v \sim u} x_v (u = r, s, t)$$

for both G and G' yield $x_s = x_t$, $x_r + x_s = 0$ and $x_r + x_t = 0$, respectively. □

We refer to the modification in Lemma 3.1 as the rotation $rs \mapsto rt$.

Now let $\widehat{G}$ be an odd-unicyclic graph on n vertices for which the least Q-eigenvalue κ is minimal, and let C denote the cycle in $\widehat{G}$. The length of C is the girth of $\widehat{G}$, denoted by g.

Lemma 3.2. *The graph $\widehat{G}$ has a Q-eigenvector $\mathbf{x} = (x_1, \ldots, x_n)^\top$ corresponding to κ with the following properties*:

(i) $x_p \geqslant 0$ *and* $x_q \geqslant 0$ *for some edge* pq *of* C;
(ii) $x_u x_v \leqslant 0$ *for any other edge* uv *of* $\widehat{G}$;
(iii) *if* $x_p x_q = 0$ *then either* x_p *or* x_q *is non-zero.*

Proof. To start with, let $\mathbf{x}$ be any Q-eigenvector corresponding to κ. Since C is an odd cycle, we cannot have $x_u x_v < 0$ for every edge uv of C, and so $x_p x_q \geqslant 0$ for some edge pq of C. Replacing $\mathbf{x}$ with $-\mathbf{x}$ if necessary, we deduce statement (i).

Let $\widehat{T}$ be the tree $\widehat{G} - pq$. The vertices of $\widehat{T}$ may be coloured so that each edge of $\widehat{T}$ joins a black vertex to a white vertex; without loss of generality, p and q are black. If uv is an edge of $\widehat{T}$ such that $x_u x_v > 0$ then we can reduce $R(\mathbf{x})$ by replacing x_w with $-x_w$ for each vertex w in one component of $\widehat{T} - uv$. This contradicts the minimality of $R(\mathbf{x})$, and so we have statement (ii).

To prove (iii), we first claim that $\mathbf{x}$ can be chosen so that x_i is non-negative for all black vertices i and non-positive for all white vertices i. To see this, suppose that, in $\widehat{T}$, k is a vertex closest to p which violates this property, and let j be the predecessor of k in the $p{-}k$ path in $\widehat{T}$. If k is black then $x_k < 0$, $x_j \leqslant 0$ and $x_j x_k \leqslant 0$, whence $x_j = 0$. Similarly, if k is white then $x_j = 0$. Now replace x_w with $-x_w$ for each vertex w in the component of $\widehat{T} - jk$ containing k. Repetition of this process results in a vector $\mathbf{x}' = (x_1', \ldots, x_n')$ whose entries not only have the required signs but also satisfy the eigenvalue equations

$$\kappa x_u' = d_u x_u' + \sum_{v \sim u} x_v' \quad (u = 1, \ldots, n).$$

Therefore, we may assume that $\mathbf{x} = \mathbf{x}'$.

Now suppose by way of contradiction that $x_p = x_q = 0$. Since $x_p = 0$ the eigenvalue equation for $u = p$ shows that $\sum_{i \sim p} x_i = 0$. Now the neighbours of p are q (for which $x_q = 0$) together with white vertices i (for which $x_i \leqslant 0$). Hence $x_i = 0$ for every neighbour of p. Now $\widehat{G}$ is connected, and so if we repeat this argument with eigenvalue equations for successive neighbours, we obtain the contradiction $\mathbf{x} = \mathbf{0}$. This completes the proof. □

In what follows, we take $\mathbf{x}$ to be a unit Q-eigenvector with the properties specified in Lemma 3.2, and we call x_i the weight of vertex i. As above, we assume that black vertices have non-negative weight, and white vertices have non-positive weight. Without loss of generality, we assume that $x_p \leqslant x_q$, so that $x_q > 0$.

Lemma 3.3. *If u is a vertex of $\widehat{G}$ other than p or q, then*

$$|x_u| > x_q \ (\geqslant x_p).$$

Proof. First, let u be a black vertex other than p or q. Suppose, by way of contradiction, that $x_u \leqslant x_q$. Then $x_u - x_q \leqslant 0$, $2x_p + x_q + x_u > 0$ and $x_p + x_q > 0$. By Lemma 3.1 the rotation $pq \mapsto pu$ results in a graph G' such that $\kappa(G') < \kappa(\widehat{G})$, and this contradicts the minimality of $\kappa(\widehat{G})$.

Secondly, let u be any white vertex. From the eigenvalue equation

$$\kappa x_u = d_u x_u + \sum_{v \sim u} x_v$$

we deduce that

$$(d_u - \kappa)|x_u| \geqslant d_u x_q,$$

because the neighbours of u are black. Since $0 < \kappa < 1$ we have $|x_u| > |x_q|$, as required. □

In what follows, we regard $\widehat{G}$ as constructed from the cycle C by attaching a (possibly trivial) rooted tree to each vertex. Let T_i be the rooted tree attached by its root r_i to the ith vertex of C $(i = 1, \ldots, g)$. We now examine how the weights of vertices in the trees T_i are distributed.

Lemma 3.4. *Let $v_0 v_1 \cdots v_k$ be a path in T_i with $v_0 = r_i$. Then*

$$|x_{v_0}| < |x_{v_1}| < \cdots < |x_{v_k}|.$$

Proof. It suffices to show:
$(*)$ $|x_u| > |x_v|$ for all vertices $u (\neq v)$ reachable from r_i via v.

We prove this by induction on r $(0 \leqslant r \leqslant d)$, where d is the maximum distance from r_i of a vertex in T_i, and $d(r_i, v) = d - r$. Note first that $(*)$ is satisfied vacuously when v is an endvertex, in particular when $r = 0$. Now suppose that $(*)$ holds when $d(r_i, v) = d - r$ $(0 \leqslant r \leqslant d - 1)$, and let w be the penultimate vertex of the r_i-v path in T_i. From the eigenvalue equation

$$\kappa x_v = d_v x_v + \sum_{j \sim v} x_j,$$

we deduce that $(d_v - \kappa)|x_v| = \sum_{j \sim v} |x_j|$, whence

$$\frac{1}{d_v} \sum_{j \sim v} |x_j| < |x_v|.$$

By our induction hypothesis, $|x_j| > |x_v|$ for all neighbours j of v other than w. Hence $|x_w| < |x_v|$ and $(*)$ holds also when $d(r_i, v) = d - r - 1$. The result follows. □

One of our techniques will be to prune some trees T_i while extending others, and to this end we prove:

Lemma 3.5. *If ab and cd are two non-adjacent edges in T_i $(i \in \{1, \ldots, g\})$, say with $d(r_i, a) < d(r_i, b)$ and $d(r_i, c) < d(r_i, d)$, then the intervals $[|x_a|, |x_b|]$ and $[|x_c|, |x_d|]$ are disjoint.*

Proof. If ab and cd lie in the same path between a root r_i and an endvertex then the result follows from Lemma 3.4. If not, we distinguish two cases:

Case (i): b and d belong to different colour classes. Then

$$(x_d - x_a)(2x_b + x_a + x_d) > 0 \quad \text{and} \quad (x_b - x_c)(2x_d + x_b + x_c) > 0,$$

for otherwise Lemma 3.1 shows that we can reduce κ by rotating ba to bd or dc to db. (Note that both inequalities are strict because $x_a + x_b \neq 0$ and $x_c + x_d \neq 0$ by Lemma 3.4.) But then, in view of the colouring, we have

$$(|x_d| - |x_a|)(|x_a| + |x_d| - 2|x_b|) > 0 \quad \text{and} \quad (|x_c| - |x_b|)(2|x_d| - |x_b| - |x_c|) > 0.$$

Without loss of generality, we may assume that $|x_a| \leqslant |x_c|$. But then $|x_d| > |x_a|$, and the first of the above inequalities yields $|x_b| < \frac{1}{2}(|x_a| + |x_d|)$. Hence $|x_b| < |x_d|$, and also $2|x_d| - |x_b| - |x_c| > 0$. Now the second inequality yields $|x_c| > |x_b|$, and we have $|x_a| < |x_b| < |x_c| < |x_d|$.

Case (ii): b and d are in the same colour class. As in case (i) we have

$$(x_c - x_a)(2x_b + x_a + x_c) > 0 \quad \text{and} \quad (x_a - x_c)(2x_d + x_a + x_c) > 0$$

for otherwise κ can be reduced by rotating ba to bc or dc to da. But then $(2x_b + x_a + x_c)(2x_d + x_a + x_c) < 0$. In view of the colouring we deduce that

$$(2|x_b| - |x_a| - |x_c|)(2|x_d| - |x_a| - |x_c|) < 0.$$

Without loss of generality, we may assume that $|x_b| \leqslant |x_d|$. Then we have $2|x_b| - |x_a| - |x_c| < 0$, and $2|x_d| - |x_a| - |x_c| > 0$. Hence $|x_b| < \frac{1}{2}(|x_a| + |x_c|)$. Next, $|x_a| < |x_c|$ (for otherwise, $|x_b| < |x_a|$, a contradiction), and consequently, $|x_b| < |x_c|$. Thus again we have $|x_a| < |x_b| < |x_c| < |x_d|$. This completes the proof. □

4. The structure of the extremal unicyclic graph

We retain the notation of the previous section, and we first prove the following crucial restriction on the girth of $\widehat{G}$:

Lemma 4.1. *The girth of* $\widehat{G}$ *is* 3.

Proof. By way of contradiction, suppose that $g \geqslant 5$. Let u and v be the vertices of C adjacent to p and q, respectively. Then

$$(x_v - x_u)(2x_p + x_u + x_v) > 0$$

for otherwise, by Lemma 3.1, we can reduce κ by rotating pu to pv. Similarly

$$(x_u - x_v)(2x_q + x_u + x_v) > 0$$

for otherwise we can reduce κ by rotating qv to qu. (Note that by Lemma 3.3, $|x_p| \neq |x_u|$ and $|x_q| \neq |x_v|$.) Hence $2x_p + x_u + x_v$ and $2x_q + x_u + x_v$ are of opposite sign. Since $x_p \leqslant x_q$, it follows that $2x_q + x_u + x_v > 0$, or equivalently (since u and v are white vertices) that $x_q > \frac{1}{2}(|x_u| + |x_v|) \geqslant \min\{|x_u|, |x_v|\}$, a contradiction to Lemma 3.3. This completes the proof. □

By Lemma 4.1, C is a triangle, and in what follows, r denotes its third vertex. We show next that no (non-trivial) tree is attached to C at p.

Lemma 4.2. *The vertex p has degree* 2.

Proof. We note first that we cannot have both $d_p > 2$ and $d_q > 2$. For otherwise there exists a vertex u outside C adjacent to p, and a vertex v outside C adjacent to q. Then we obtain a contradiction exactly as in the proof of Lemma 4.1.

To prove that $d_p = 2$, assume to the contrary that $d_p > 2$. Then $d_q = 2$ and the eigenvalue equations applied at vertices p and q read:

$$\kappa x_p = d_p x_p + x_q + x_r + \sum\nolimits' x_w \quad \text{and} \quad \kappa x_q = 2x_q + x_p + x_r,$$

where $\sum'$ denotes the sum over all neighbours w of p other than q and r. Thus $\kappa(x_p - x_q) = (x_p - x_q) + (d_p - 2)x_p + \sum' x_w$. Since $x_w \leqslant 0$ and $|x_w| > x_p$ for all $w \neq q, r$, we find that $(d_p - 2)x_p + \sum' x_w = (d_p - 2)|x_p| - \sum' |x_w| < 0$. But then $(1 - \kappa)(x_q - x_p) < 0$, and we have $x_p > x_q$, a contradiction. This completes the proof. □

We shall see later that also $d_q = 2$. First we show how Lemma 3.5 helps us to prune the trees T_i.

Lemma 4.3. *For each i, T_i consists of a path, with r_i as an endvertex, and possibly some pendant edges attached at vertices of this path.*

Proof. Let w be a vertex of T_i at maximal distance m from the root r_i, and let v be the unique neighbour of w. We may assume that $m \geqslant 2$. Let $P_1 = u_0u_1 \cdots u_{m-1}u_m$ be the path between $r_i(= u_0)$ and $w(= u_m)$. Note that all neighbours of $v(= u_{m-1})$ other than u_{m-2} are pendant vertices. Consider now a vertex u_k with $k \leqslant m - 2$. Suppose that $P_2 = v_0v_1v_2$ is a path in T_i starting at $v_0 = u_k$, with v_1 and v_2 not belonging to P_1. To apply Lemma 3.5, consider the edges u_ku_{k+1}, $u_{k+1}u_{k+2}$ in P_1, and v_0v_1, v_1v_2 in P_2, together with the corresponding intervals $I_i = [|x_{u_{k+i}}|, |x_{u_{k+i+1}}|]$ $(i = 0, 1)$, and $J_j = [|x_{v_j}|, |x_{v_{j+1}}|]$ $(j = 0, 1)$. By Lemma 3.5, we have $I_0 \cap J_1 = \emptyset$, whence $u_{k+1} < v_1$; and $I_1 \cap J_0 = \emptyset$, whence $v_1 < u_{k+1}$, a contradiction. We conclude that no path of length greater than one is attached at u_k. It follows that T_i has the form described. □

We now focus our attention on the vertex q.

Lemma 4.4. *In the tree attached at q any vertex other than q is adjacent to q.*

Proof. We note first that $d_r > 2$. Otherwise, the eigenvalue equations at p and r yield

$$\kappa x_p = 2x_p + x_q + x_r \quad \text{and} \quad \kappa x_r = 2x_r + x_p + x_q,$$

whence $\kappa = 1$, a contradiction. Hence r has a neighbour r' not on C. Now suppose by way of contradiction that q' and q'' are two vertices not on C with q' and q'' at distance one and two from q, respectively. Consider the paths qrr' and $qq'q''$. With these paths in the role of P_1 and P_2 from the proof of Lemma 4.3, we obtain the same contradiction as there. This completes the proof. □

We are now ready to prove that $d_q = 2$, thereby proving that only the tree attached at r is non-trivial.

Lemma 4.5. *The vertex q has degree* 2.

Proof. Suppose by way of contradiction that q has a neighbour u not on C, and let v be a neighbour of r not on C. (Recall that $d_r > 2$, as we saw in the previous proof.) By Lemma 4.4, u is an endvertex and so the eigenvalue equations at u and v yield:

$$\kappa x_u = x_u + x_q \quad \text{and} \quad \kappa x_v = d_v x_v + \sum_{w \sim v} x_w.$$

In view of the colouring, we deduce that

$$x_q = (1-\kappa)|x_u| \quad \text{and} \quad (d_v - \kappa)|x_v| = \sum_{w \sim v} |x_w|.$$

From the latter equation we find that $(1-\kappa)|x_v| > |x_r|$, since $|x_w| > |x_v|$ for all $w \neq r$ (by Lemma 3.4). Hence $(1-\kappa)|x_v| > |x_r| > x_q = (1-\kappa)|x_u|$, which in turn yields $|x_v| > |x_u|$.

Now $(x_u - x_r)(2x_v + x_u + x_r) > 0$ by Lemma 3.1, for otherwise we can reduce κ by rotating vr to vu. In view of the colouring, we have $(x_u - x_r)(2|x_v| - |x_r| - |x_u|) > 0$. Since the second factor is positive, we have $x_u > x_r$. Again, $(x_u - x_r)(2x_p + x_u + x_r) > 0$, for otherwise we can reduce κ by rotating pr to pu. We conclude that $2x_p + x_u + x_r > 0$, equivalently $2x_p > |x_r| + |x_u|$, a contradiction to Lemma 3.3. This completes the proof. □

We shall prove several results based on the comparison of characteristic polynomials, which will enable us to complete the proof of our main result. Recall that, by Eq. (2), for any unicyclic graph G we have $\phi(x, L(G)) = \xi(x+2, G)$, and so $\lambda(L(G)) = \kappa(G) - 2$, a fact used implicitly below. We shall also need the following observation.

Lemma 4.6. *Let G be a connected graph with an odd-unicyclic subgraph H. If $\lambda(L(G)) = \lambda(L(H))$ then G has a Q-eigenvector $(z_1, \ldots, z_n)^\top$ corresponding to $\kappa(G)$ such that $z_u + z_v = 0$ for all edges uv of G not in H.*

Proof. Let $\mathbf{y}$ be a unit eigenvector of $L(H)$ corresponding to $\lambda(L(H))$. Then

$$\lambda(L(H)) = \mathbf{y}^\top A(L(H))\mathbf{y} = \begin{pmatrix} \mathbf{y} \\ \mathbf{0} \end{pmatrix}^\top A(L(G)) \begin{pmatrix} \mathbf{y} \\ \mathbf{0} \end{pmatrix} \geqslant \lambda(L(G)).$$

Since $\lambda(L(G)) = \lambda(L(H))$, $\binom{\mathbf{y}}{\mathbf{0}}$ is an eigenvector of $L(G)$ corresponding to $\lambda(L(G))$. Now G is odd-unicyclic [2, Theorem 5.2.2(i)] and so the map $\mathbf{v} \mapsto R^\top \mathbf{v}$ is an isomorphism from the eigenspace $\mathscr{E}_Q(\kappa(G))$ to the eigenspace $\mathscr{E}_{A(L(G))}(\lambda(L(G)))$ (cf. [2, Lemma 2.2.3]). Let $\binom{\mathbf{y}}{\mathbf{0}} = R^\top \mathbf{z}$. Then $\mathbf{z}$ is a Q-eigenvector $(z_1, \ldots, z_n)^\top$ of G corresponding to $\kappa(G)$ such that $z_u + z_v = 0$ for all edges uv of G not in H. □

We introduce some further notation concerning $\widehat{G}$. Let $T \sim (= T_r)$ be the tree attached to C at r, let u be a vertex of T other than r, and let w be the penultimate vertex of the r-u path in T. We write $T(u)$ for the component of $T - wu$ containing u.

Lemma 4.7. *The tree T has no vertex $u(\neq r)$ such that $d_u > 2$ and $T(u) = K_{1,h}$ $(h \geqslant 2)$.*

Proof. Suppose by way of contradiction that $\widehat{G} = HwuS$, where H is odd-unicyclic and S is a star $K_{1,h}$ $(h \geqslant 2)$ with central vertex u. Let v be an endvertex of S, and let G^* be the graph obtained from $\widehat{G}$ by rotating wu to wv. Let

$$\Delta(x) = \phi(x, L(\widehat{G})) - \phi(x, L(G^*)).$$

By Corollary 2.3 we have

$$\Delta(x) = \phi(x, L(H))(\phi(x, K_{h+1}) - \phi(x, K_h \cdot K_2)).$$

Using Theorem 2.2 to calculate $\phi(x, K_s \cdot K_2)$, we find that

$$\Delta(x) = -(h-1)(x+1)^{h-2}(x+2)\phi(x, L(H)).$$

It follows that $(-1)^n\Delta(x) > 0$ for $x \in (-2, \lambda(L(H))$. By the Interlacing Theorem, we have $\lambda(L(\widehat{G}) \leqslant \lambda(L(H))$ and $\lambda(L(G^*)) \leqslant \lambda(L(H))$. It follows that $\lambda(L(G^*)) \leqslant \lambda(L(\widehat{G}))$, and so $\kappa(G^*) \leqslant \kappa(\widehat{G})$. By the minimality of $\kappa(\widehat{G})$, we have $\kappa(G^*) = \kappa(\widehat{G}) = \kappa$, and then $\kappa = \kappa(L(H))$. Hence $\lambda(L(\widehat{G})) = \lambda(L(H))$. By Lemma 4.6, $\widehat{G}$ has a Q-eigenvector $\mathbf{z} = (z_1, \ldots, z_n)^\top$ corresponding to κ such that $z_u + z_v = 0$. Hence $|z_u| = |z_v|$. Now we may take $\mathbf{x}$ to be constructed from $\mathbf{z}$ as in Lemma 3.2, and then $|x_u| = |x_v|$, contradicting Lemma 3.4. This completes the proof. $\square$

A *single comet* with *head u* and *tail v* consists of a $u - v$ path of length $\geqslant 2$ together with at least one pendant edge at u. Note that the definition embraces paths of length > 2. We refine the argument of Lemma 4.7 to prove:

Lemma 4.8. *The tree T has no vertex u $(\neq r)$ such that $d_u > 2$ and $T(u)$ is a single comet with head u.*

Proof. Suppose by way of contradiction that $\widehat{G} = HwuS$, where H is odd-unicyclic and S is a comet with head u. Let v be the tail of S, and let G^* be the graph obtained from $\widehat{G}$ by rotating wu to wv. Let

$$\Delta(x) = \phi(x, L(\widehat{G})) - \phi(x, L(G^*)).$$

By Corollary 2.3 we have

$$\Delta(x) = \phi(x, L(H))(\phi(x, L(S_u)) - \phi(x, L(S_v))).$$

Let $d_u = h$ and $d(u, v) = m$. Note that S_u (S_v) can be constructed from disjoint graphs P_m and $K_{1,h}$ by adding an edge between an endvertex of P_m and the central vertex (respectively, a pendant vertex) of $K_{1,h}$. Applying Corollary 2.3 again, we have

$$\phi(x, L(S_u)) - \phi(x, L(S_v)) = \phi(x, P_{m-1})(\phi(x, K_{h+1}) - \phi(x, K_h \cdot K_2))$$

and so

$$\Delta(x) = -(h-1)(x+1)^{h-2}(x+2)\phi(x, P_{m-1})\phi(x, L(H)).$$

Hence $(-1)^n\Delta(x) > 0$ when $-2 < x < \lambda'$, where $\lambda' = \min\{\lambda(P_{m-1}), \lambda(L(H))\}$. By the Interlacing Theorem, $\lambda(\widehat{G}) \leqslant \lambda'$ and $\lambda(G^*) \leqslant \lambda'$, and so $\lambda(G^*) \leqslant \lambda(\widehat{G})$. It follows that $\lambda(L(G^*)) \leqslant \lambda(L(\widehat{G}))$, and so $\kappa(G^*) \leqslant \kappa(\widehat{G})$. By the minimality of $\kappa(\widehat{G})$, we have $\kappa(G^*) = \kappa(\widehat{G}) = \kappa$, and we obtain a contradiction as in Lemma 4.7. This completes the proof. $\square$

Using the last two lemmas we now have:

Proposition 4.9. *The tree T consists of a path (with r as an endvertex) and possibly some pendant edges at r.*

Proof. Suppose that T has a vertex $u \neq r$ of degree > 2. Let u be such a vertex for which $d(r, u)$ is maximal, and consider the bridge wu, where w is the penultimate vertex on the path from r to u. Then the graph $T(u)$ is either a star or a comet. These possibilities are excluded by Lemmas 4.7 and 4.8, and so the result follows from Lemma 4.3. □

It follows that if $d_r > 3$ then T is either a star with centre r or a single comet with head r, and it remains to eliminate these possibilities.

Proposition 4.10. *The vertex r has degree* 3.

Proof. For $h \geqslant 0$ and $k \geqslant 1$, let $G_{h,k}$ be the graph obtained from the triangle pqr by adding h pendant edges at r and a pendant path of length k with endvertex r. Let $G(h, k) = L(G_{h,k})$, of order $n = h + k + 3$; and for $h \geqslant 1$ define

$$\Delta(x) = \phi(x, G(h, k)) - \phi(x, G(h - 1, k + 1)).$$

By Corollary 2.3 we have

$$\Delta(x) = \phi(x, P_{k-1})(\phi(x, G(h, 1)) - \phi(x, G(h - 1, 2)),$$

where $\phi(x, P_{k-1})$ is defined as 1 when $k = 1$.

Now $G(h, 1)$, of order $h + 4$, has a clique of order $h + 3$; by the Interlacing Theorem, -1 is an eigenvalue of $G(h, 1)$ of multiplicity $\geqslant h + 1$. But also $G(h, 1)$ has a divisor of order 3 without -1 as an eigenvalue, and we find

$$\phi(x, G(h, 1)) = (x + 1)^{h+1}(x^3 - (h + 1)x^2 - (p + 4)x + 2h).$$

Similarly, considering a divisor of order 5 in $G(h - 1, 2)$, we have (for $h \geqslant 1$):

$$\begin{aligned}\phi(x, G(h - 1, 2)) = (x + 1)^{h-1}(x^5 &- (h - 1)x^4 - 2(h + 2)x^3 \\ &+2(h - 3)x^2 + 3hx - 2(h - 2)).\end{aligned}$$

It follows that (for $h \geqslant 1$):

$$\Delta(x) = (x + 1)^{h-1}\phi(x, P_{k-1})(-(h + 1)x^3 - 3(h + 1)x^2 - 4x + 4(h - 1)).$$

Thus

$$\Delta(x) = -(h + 1)(x + 1)^{h-1}\phi(x, P_{k-1})(x - x_1)(x - x_2)(x + 2),$$

where

$$x_{1,2} = \frac{1}{2}\left(-1 \pm \sqrt{9 - \frac{16}{h + 1}}\right).$$

Hence $(-1)^n\Delta(x) > 0$ when $-2 < x < M$, where $M = \min\{x_2, -2\cos\frac{\pi}{k}\}$.

Now suppose by way of contradiction that $d_r > 3$, so that $\widehat{G} = G_{h,k}$ for some $h \geqslant 1$. We have $\lambda(L(\widehat{G})) \leqslant \lambda(L(E_{3,h+k})) \leqslant -2\cos\frac{\pi}{h+k+3}$, and so clearly $\lambda(L(\widehat{G})) < -2\cos\frac{\pi}{k}$. Also

$$-2\cos\frac{\pi}{h + k + 3} \leqslant -2\cos\frac{\pi}{h + 4} < -2\left(1 - \frac{\pi^2}{2(h + 4)^2}\right) < x_2$$

and so $\lambda(L(\widehat{G})) < M$. We conclude that $\lambda(G(h - 1, k + 1) < \lambda(L(\widehat{G}))$, and hence that $\kappa(G_{h-1,k+1}) < \kappa(\widehat{G})$, a contradiction. Thus $d_r = 3$ as required. □

Proposition 4.10 is the final step needed to confirm the original conjecture. Moreover, we can now prove our main result:

Theorem 4.11. *If G is a connected non-bipartite graph on n vertices whose least Q-eigenvalue is minimal*, *then $G = E_{3,n-3}$.*

Proof. It remains to show that $\widehat{G}$ $(= E_{3,n-3})$ is the only connected non-bipartite graph G on n vertices for which $\kappa(G) = \kappa(\widehat{G})$. Otherwise, some such graph G can be obtained from $\widehat{G}$ by adding edges (see Section 2), and by interlacing, $\kappa(\widehat{G} + uv) = \kappa(\widehat{G})$ for any edge uv of G not in $\widehat{G}$. It suffices to derive a contradiction when $G = \widehat{G} + uv$. In this situation, let $\widehat{Q}$, Q be the signless Laplacians of $\widehat{G}$, G respectively, and let $(y_1, \ldots, y_n)^\top$ be a unit Q-eigenvector $\mathbf{y}$ of G corresponding to $\kappa(G)$. Then

$$\kappa(G) = \mathbf{y}^\top Q\mathbf{y} = \mathbf{y}^\top \widehat{Q}\mathbf{y} + y_u^2 + y_v^2 + 2y_u y_v \geqslant \kappa(\widehat{G}) + (y_u + y_v)^2 \geqslant \kappa(\widehat{G}).$$

Since $\kappa(G) = \kappa(\widehat{G})$, we conclude that $y_u + y_v = 0$ and $\mathbf{y}$ is a Q-eigenvector of $\widehat{G}$ corresponding to $\kappa(\widehat{G})$. In particular, $|y_u| = |y_v|$. We may take $\mathbf{x}$ to be constructed from $\mathbf{y}$ as in the proof of Lemma 3.2, so that $|x_u| = |x_v|$. By Lemma 3.4, u and v cannot both lie on the path T, and so without loss of generality we may assume that u is a vertex of T, while $v = q$. Now we have a contradiction to Lemma 3.3, and the proof is complete. □

Finally, we note that our arguments show that, for an odd-unicyclic graph U with n vertices, we have $\lambda(L(U)) \geqslant \lambda(L(E_{3,n-3}))$, with equality if and only if $U = E_{3,n-3}$.

References

[1] D. Cvetković, M. Doob, H. Sachs, Spectra of Graphs, third ed., Johann Ambrosius Barth Verlag, Heidelberg, Leipzig, 1995.

[2] D. Cvetković, P. Rowlinson, S.K. Simić, Spectral Generalizations of Line Graphs, Cambridge University Press, Cambridge, 2004.

[3] D. Cvetković, P. Rowlinson, S.K. Simić, Signless Laplacians of finite graphs, Linear Algebra Appl. 423 (2007) 155–171.

[4] D. Cvetković, P. Rowlinson, S.K. Simić, Eigenvalue bounds for the signless Laplacian, Publ. Inst. Math. (Beograd) 81 (95) (2007) 11–27.

[5] E.R. van Dam, W.H. Haemers, Which graphs are determined by their spectrum, Linear Algebra Appl. 373 (2003) 241–272.

[6] M. Desai, V. Rao, A characterization of the smallest eigenvalue of a graph, J. Graph Theory 18 (1994) 181–194.

[7] S.M. Fallat, S. Kirkland, S. Pati, Minimizing algebraic connectivity over connected graphs with fixed girth, Discrete Math. 254 (2002) 115–142.