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Research Article

Spectral determination of trees with large diameter and small spectral radius

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Abstract: Yuan, Shao and Liu proved that the H-shape tree $H'_n = P^{1,n-6}_{1,2;n-3}$ minimizes the spectral radius among all graphs with order $n \geqslant 9$ and diameter $n-4$. In this paper, we achieve the spectral characterization of all graphs in the set $\mathscr{H}' = \{H'_n\}_{n\geqslant 8}$. More precisely we show that H'_n is determined by its spectrum if and only if $n \neq 8, 9, 12$, and detect all cospectral mates of H'_8, H'_9 and H'_{12}. Divisibility between characteristic polynomials of graphs turns out to be an important tool to reach our goals.

Keywords: adjacency spectrum, spectral characterization, DS-graph, matchings, spectral radius

AMS Subject classification: 05C50

1. Introduction

All graphs in this paper are intended to be simple: no loops, multiple or half edges are allowed. We respectively denote by ν_G, ε_G and $A(G)$, the order, the size and the adjacency matrix of a graph $G = (V_G, E_G)$. The *spectrum* $\mathrm{sp}(G)$ of G is the multiset of eigenvalues of $A(G)$, i.e. the roots of the characteristic polynomial of G $\phi(G) = \phi(G, \lambda) := \det(\lambda I - A(G))$. Since $A(G)$ is symmetric, its eigenvalues

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are real and we denote them by $\rho(G) = \lambda_1(G) \geqslant \lambda_2(G) \geqslant \cdots \geqslant \lambda_{\nu_G}(G)$. The maximum eigenvalue $\rho(G)$ of G is called the *index* of G. The Perron-Froebenius theorem ensures that $\rho(G)$ is also equal to the spectral radius of G, i.e. the number $\max\{|\lambda_i(G)| \mid 1 \leqslant i \leqslant \nu_G\}$.

Two graphs G and H are said to be cospectral if $\phi(G) = \phi(H)$ (or, equivalently, $\mathrm{sp}(G) = \mathrm{sp}(H)$). If this is the case we write $G \sim H$. By $[G]$ we denote the *cospectral class* determined by G under the equivalence relation $\sim$. A *cospectral mate* of G is a graph $H \in [G]$ nonisomorphic to G. A graph G is said to be *determined by its spectrum* (or DS for short) when G has no cospectral mates or, equivalently, when $\mathrm{sp}(G) = \mathrm{sp}(H)$ only if G and H are isomorphic. *Spectrally characterizing* a graph G tantamounts to detect all graphs in $[G]$.

Understanding the 'distinguishing power' of the spectrum is a well-established topic in spectral graph theory [17, 22]: in fact, taking up the challenge launched by Haemers and van Dam in [21], many scholars tried to study $[G]$, for G belonging to specific families of graphs. For instance, the spectral characterization has been performed for the T-shaped trees [24], the starlike trees [8, 14], the daggers [16] and the trees with spectral radius at most $\mathfrak{h} := \sqrt{2+\sqrt{5}}$ [7, 19]. Few partial results have been obtained for the H-shape graphs [10, 15] (see the next paragraph for the definitions).

We now fix some notation. $G \cup H$ denotes the disjoint union of the graphs G and H, and kG stands for the disjoint union of k copies of G. For any vertex $u \in G$, $G - u$ is the graph obtained from G by deleting v and its incident edges.

Let P_n and C_n respectively denote the path and the cycle with n vertices. We label their vertices by $0, 1, \ldots, n-1$ assuming that consecutive integers correspond to adjacent vertices. For $0 < m_1 < \cdots < m_t < r-1$, we denote by $P^{m_1,m_2,\ldots,m_t}_{n_1,n_2,\ldots,n_t;r}$ the graph obtained from P_r by attaching at its vertex m_i a pendant path of n_i edges for each $i = 1, 2, \ldots, t$. Similarly, for $0 \leqslant m_1 < \cdots < m_t \leqslant r-1$, we denote by $C^{m_1,m_2,\ldots,m_t}_{n_1,n_2,\ldots,n_t;r}$ the graph obtained from C_r by attaching at its vertex m_i a pendant path of n_i edges for each $i = 1, 2, \ldots, t$ (see Fig. 1). After [25], the graphs of type $P^{m_1,m_2,\ldots,m_t}_{n_1,n_2,\ldots,n_t;r}$ and $C^{m_1,m_2,\ldots,m_t}_{n_1,n_2,\ldots,n_t;r}$ are respectively known as *open* and *closed quipus*, and they can be structurally characterized as the trees (resp., unicyclic graphs) with maximum vertex degree 3 such that the vertices of degree 3 all lie on a path (resp., a cycle). Open quipus with $t = 1$ are also known as T-shape graphs; whereas open quipus with $t = 2$ are sometimes called H-shape or Π-shape trees (see Fig. 2). Closed quipus with just one pendant path are called lollipops or tadpole graphs.

In this paper we carry out the spectral determination of the graphs in the family

$$\mathscr{H}' := \{H'_n\}_{n\geqslant 8}, \qquad \text{where } H'_n = P^{1,n-6}_{1,2;n-3} \text{ (see Fig. 2).}$$

Our works is part of a larger project concerning the spectral determinations of the graphs $G_{n,D}$'s minimizing the spectral radius in the set of graphs with n vertices and diameter D. Van Dam and Kooij [23] conjectured that the open quipu

$$OQ_{n,e} = P^{\lfloor \frac{e-1}{2} \rfloor, n-e-\lceil \frac{e-1}{2} \rceil}_{\lfloor \frac{e-1}{2} \rfloor, \lceil \frac{e-1}{2} \rceil; n-e+1}$$

is one of those minimizer for $D = n - e$ and n large enough, identifying $G_{n,D}$ when $D \in \{1, 2, \lfloor \frac{n}{2} \rfloor, n-3, n-2, n-1\}$.
After [3, 23, 26], we know that the van Dam-Kooji conjecture holds for $1 \leq e \leq 5$, whereas it fails for $e \geqslant 6$ (see [3, 11–13]).
The spectral determination of $G_{n,D}$ with $D \in \{n-1, n-2, n-3\}$ has been performed in [7]: the path $G_{n,n-1} = P_n$, and the *snake* $G_{n,n-2} = P^{1}_{1;n-1}$ ($n \geqslant 4$) are DS, whereas the *double snake* $G_{n,n-3} = P^{1,n-4}_{1,1,n-2}$ is not (see [7, Theorem 3]). Cioaba et al. [3] proved that for n sufficiently large, the graph $G_{n,n-5}$ belongs to the family

$$\mathscr{H} = \left\{ H_n := P^{2,n-7}_{2,2;n-4} \mid n \geqslant 10 \right\}.$$

In [2], it has been proved that all graphs in $\mathscr{H}$ are DS apart from H_{10}, H_{13} and H_{15}. The search for $G_{n,n-4}$ was carried out by Yuan, Shao and Liu [26]: for $n \geqslant 9$, the only graph attaining the minimimal spectral radius among the graphs with n vertices and diameter $n-4$ is the H-shape tree H'_n (note that $2 = \rho(C_8) < \rho(H'_8)$). In the statement of Theorem 1, which is our main result, and throughout the paper, $\mathbb{N}_{\geqslant a}$ denotes the set $\{n \in \mathbb{N} \mid n \geqslant a\}$.

Theorem 1. *For $n \geqslant 8$, let H'_n be the graph $P^{1,n-6}_{1,2;n-3}$. Then, up to isomorphism,*

$$[H'_8] = \left\{H'_8,\ P_1 \cup C^{0}_{1;6}\right\}, \quad [H'_9] = \left\{H'_9, P^{1,2}_{1,1;7}\right\}, \quad [H'_{12}] = \left\{H'_{12}, P^{2,6}_{1,1;10}\right\},$$

and $[H'_n] = \{H'_n\}$ *for* $n \in \mathbb{N}_{\geqslant 8} \setminus \{8, 9, 12\}$.

From Theorem 1, we realize that all graphs in $\mathscr{H}'$ are DS apart from three exceptions, exactly as it happens for the family $\mathscr{H}$ (see [2]).
As in [2], a graph G is said to be *divisible* by a graph H if $\phi(H)$ divides $\phi(G)$. The proof of Theorem 1, performed in Section 4, allows to appreciate how useful divisibility between graphs can be in order to establish whether a graph is DS or not. In fact, Theorem 2 turns out to be one of the key-tools for carrying out the required case analysis.

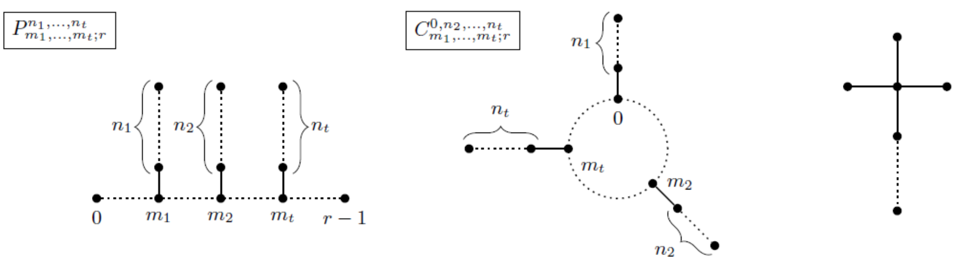

Figure 1. **Open quipus, closed quipus and daggers**

2. Preliminaries and basic tools

We start by recalling a result from [21], the seminal paper for all subsequent works on spectral characterizations.

Proposition 1. [21, Proposition 1] *The path P_n is DS for every positive integer n.*

In order to prove that a graph is DS, it is useful to have at hand as many as possible algebraic invariants shared by cospectral graphs. We summarize few of them in the following proposition.

Proposition 2. [21, Lemma 4] *Let G and H be two cospectral graphs. Then,*
(i) $\nu_G = \nu_H$ *and* $\varepsilon_G = \varepsilon_H$.
(ii) *G is bipartite if and only if H is bipartite.*
(iii) *G is k-regular if and only if H is k-regular.*
(iv) *G is k-regular with girth g if and only if H is k-regular with girth g.*
(v) *G and H have the same number of closed walks of any fixed length.*

Proposition 3. [5, 20] *Let $\mathscr{G}_{<2}$ be the set of connected graphs whose index is less than 2. Then,*

$$\mathscr{G}_{<2} = \left\{P_n(n \geq 1),\ P^1_{1;n-1}(n \geq 4)\right\} \cup \left\{P^1_{2;k-1} \mid k = 5, 6, 7\right\}.$$

Proposition 4. [5, 20] *Let $\mathscr{G}_2$ be the set of connected graphs whose index is 2. Then,*

$$\mathscr{G}_2 = \left\{C_n\ (n \geq 3),\ P^{1,n-4}_{1,1;n-2}\ (n \geq 6),\ K_{1,4},\ P^2_{2;5},\ P^2_{1;8},\ P^3_{1;7}\right\},$$

where $K_{1,4}$ is the star graph with 4 pendant vertices.

Throughout the paper we denote by $\mathfrak{h}$ the number $\sqrt{2+\sqrt{5}}$, known in literature as the (adjacency)-Hoffman limit value.

Proposition 5. [1, 4] *The set $\mathscr{G}_{(2,\mathfrak{h})}$ of connected graphs whose index is in the interval $(2, \mathfrak{h})$ only contains T-shape and H-shape graphs. More precisely, $\mathscr{G}_{(2,\mathfrak{h})} = \mathcal{T} \cup \mathcal{H}$, where*

$$\mathcal{T} = \left\{P^1_{c;4} \;\middle|\; c > 5\right\} \cup \left\{P^1_{c;b+2} \;\middle|\; b > 2,\ c > 3\right\} \cup \left\{P^2_{c;5} \;\middle|\; c > 2\right\} \cup \left\{P^2_{3;6}\right\}$$

and

$$\mathcal{H} = \left\{P^{1,2}_{1,1;5},\ P^{2,6}_{1,1;9},\ P^{2,7}_{1,1;11},\ P^{3,10}_{1,1;14},\ P^{3,11}_{1,1;16}\right\} \cup \left\{P^{a,a+b}_{1,1;a+b+c+1} \;\middle|\; a > 0, c > 0, b \geq b^*(a,c)\right\},$$

$$\textit{with } b^*(a,c) = \begin{cases} c & \text{for } a = 1, \\ c+3 & \text{for } a = 2, \\ a+c+2 & \text{for } a > 2. \end{cases}$$

Proposition 6. [25, Theorem 1] *The connected graphs with spectral radii in the interval* $(\mathfrak{h}, 3\sqrt{2}/2]$ *are either open quipus or closed quipus or daggers (see Fig. 1).*

We write $H \subseteq G$ (resp., $H \subset G$) if H is a subgraph (resp., proper subgraph) of the graph G.

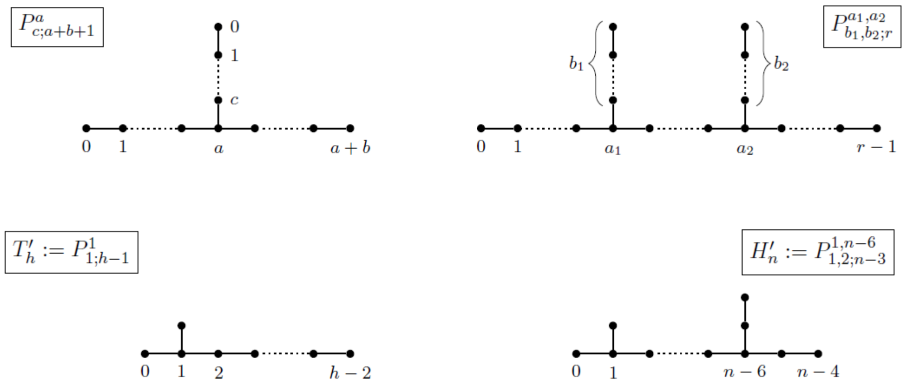

Figure 2. **T-shape and H-shape graphs**

Proposition 7. [5, Theorems 0.6 and 0.7] *Let G be a connected graph and $H \subset G$. Then, $\rho(H) < \rho(G)$.*

For $v \in V_G$, let $G - v$ be the graph obtained from G by deleting v and its incident edges. The following proposition describes the phenomenon known as 'interlacing'.

Proposition 8. [5, Theorem 0.10] *Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ and $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_{n-1}$ be the eigenvalues of the graphs G and $G - v$ respectively. Then, $\lambda_1 \geqslant \mu_1 \geqslant \lambda_2 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_{n-1} \geqslant \lambda_n$.*

Denoted by $d(v)$ the vertex degree of $v \in V_G$ in G, an *internal path* of G is a (possibly closed) walk $v_1 \ldots v_k$ such the $\min\{d(v_1), d(v_k)\} \geqslant 3$ and $d(v_i) = 2$ for $2 \leqslant i \leqslant k-1$. We also recall that *subdividing an edge* $uv \in E_G$ means inserting a new vertex z in V_G and replacing uv with uz and zw. The two parts of the following proposition come from Proposition 7 and [9] respectively.

Proposition 9. *Let uv be an edge of a connected graph G and let G_{uv} be the graph obtained from G by subdividing the edge $uv \in E_G$. Then,*

(i) *if uv is not in an internal path of G and G is not a cycle, then $\rho(G_{uv}) > \rho(G)$;*

(ii) *if uv belongs to an internal path of G and $G \notin \{P^{1,n-4}_{1,1;n-2} \mid n \geqslant 6\}$, then $\rho(G_{uv}) < \rho(G)$.*

For $h > k \geqslant 8$ the graph H'_h is obtained from H'_k by subdividing $h-k$ times an edge in an internal path. Thus, the following corollary immediately comes from Proposition 9

Corollary 1. *$\rho(H_h) > \rho(H_k)$ for all $h > k \geqslant 8$.*

Let v be a vertex of a graph G. As it is usual, we denote by $N_G(v)$ the *neighborhood* of v, i.e. the set $\{w \in V_G \mid vw \in E_G\}$.

Proposition 10. [18, Theorems 2 and 3] *Let $\mathscr{C}(v)$ (resp., $\mathscr{C}(e)$) be the set of all cycles of a graph G containing the vertex $v \in V_G$ (resp., the edge $e = uw \in E_G$). The following identities of polynomials*

$$\phi(G) = \lambda\phi(G-v) - \sum_{v' \in N_G(v)} \phi(G-v-v') - 2\sum_{C \in \mathscr{C}(v)} \phi(G - V(C)) \tag{1}$$

and

$$\phi(G) = \phi(G-e) - \phi(G-u-w) - 2\sum_{C \in \mathscr{C}(e)} \phi(G - V(C)) \tag{2}$$

hold for every $v \in V_G$ and for every $e = uw \in E_G$ (note that $\phi(H) = 1$ if H is the null graph P_0).

Equations (1) and (2) are usually called *Schwenk formulæ*.
Let k be a positive integer. We recall that a k-matching in a graph G is a set of k independent edges. We denote by $M_k(G)$ the number of k-matchings in a graph G, and by Δ_G its maximum vertex degree. The following result follows from the Sachs's Coefficient Theorem for characteristic polynomials of graphs (see [5, Theorem 1.3]).

Proposition 11. *Let G and H be two cospectral graphs.*

(i) *If neither G nor H contains quadrangles as subgraphs, then $M_2(G) = M_2(H)$.*

(ii) *If neither G nor H contains quadrangles or hexagons as subgraphs, then $M_3(G) = M_3(H)$.*

In the following statement, k_G denotes the number of vertices with degree 3 in a fixed graph G.

Proposition 12. *Let G be a graph with N triangles and degree sequence $(d_1, d_2, \ldots, d_{\nu_G})$.*

(i) *The number of 2-matchings in G is $M_2(G) = \binom{\varepsilon_G}{2} - \sum_{i=1}^{\nu_G} \binom{d_i}{2}$.*

(ii) *If T is a tree with maximal degree $\Delta_T = 3$, then $M_2(T) = \dfrac{\nu_T^2 - 5\nu_T}{2} + 3 - k_T$.*

If, instead, G is a closed quipu, then $M_2(G) = \dfrac{\nu_G^2 - 3\nu_G}{2} - k_G$.

(iii) *The number of 3-matchings in G is*

$$M_3(G) = \binom{\varepsilon_G}{3} - (\varepsilon_G - 2)\sum_{i=1}^{\nu_G}\binom{d_i}{2} + 2\sum_i \binom{d_i}{3} + \sum_{ij\in E(G)} (d_i-1)(d_j-1) - N.$$

Proof. Part (i) is elementary: the number $M_2(G)$ is obtained by subtracting the number of pairs of dependent edges from the total number of pairs of edges. Part (ii) is essentially Lemma 2.10 in [24]. For Part (iii), see [6, Theorem 1]. □

The several types of H-shape trees are depicted in Fig. 3, where dotted lines correspond to paths with at least two edges. In other words, the set of the H-shape trees is the disjoint union $\bigsqcup_{i=1}^{12} \mathcal{T}_i$ where, for instance,

$$\mathcal{T}_4 = \left\{ P^{1,c}_{1,a;a+b} \mid a > 2,\ b > 2,\ c \geqslant 2 \right\} \quad \text{and} \quad \mathcal{T}_9 = \left\{ P^{1,c}_{1,2;b+2} \mid b > 2,\ c \geqslant 2 \right\}.$$

Proposition 12 and some calculations allow to classify the H-shape trees by means of the number of their 3-matchings.

Corollary 2. *Let T be an H-shape tree with n vertices, and let $f(n) = (n^3 - 12n^2 + 35n)/6$. Then,*

$$M_3(T) = \begin{cases} f(n), & \text{for} \quad T \in \mathcal{T}_1; \\ f(n)+1, & \text{for} \quad T \in \mathcal{T}_2 \cup \mathcal{T}_3; \\ f(n)+2, & \text{for} \quad T \in \mathcal{T}_4 \cup \mathcal{T}_5 \cup \mathcal{T}_6; \\ f(n)+3, & \text{for} \quad T \in \mathcal{T}_7 \cup \mathcal{T}_8 \cup \mathcal{T}_9; \\ f(n)+4, & \text{for} \quad T \in \mathcal{T}_{10} \cup \mathcal{T}_{11}; \\ f(n)+5, & \text{for} \quad T \in \mathcal{T}_{12}. \end{cases}$$

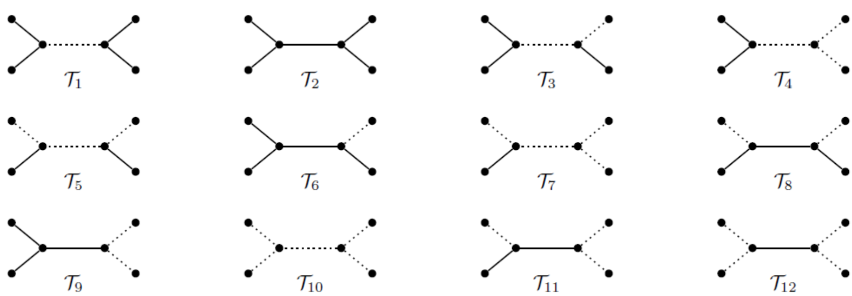

Figure 3. **The several types of H-shape trees**

In [2] the authors called a graph G *recursive* if G belongs to a sequence of graphs $\{G_n\}_{n\geqslant h}$ such that $\nu_{G_n} = n$ and

$$\phi(G_{n+2}) = \lambda\phi(G_{n+1}) - \phi(G_n).$$

The following proposition provides the algebraic machinery to understand which items, in a sequence of recursive graphs, is divided by a path of fixed length. In fact, Proposition 13 is one of the main tools to prove our Theorem 2.

Proposition 13. [2, Lemma 3.3] *Let $\{g_n(\lambda)\}_{n\geqslant 0}$ be a sequence of polynomials, whose elements satisfy*

$$g_{n+2}(\lambda) = \lambda g_{n+1}(\lambda) - g_n(\lambda) \qquad \text{for all } n \geqslant 0.$$

Then,

(i) $g_n(\lambda) = \phi(P_k)\, g_{n-k}(\lambda) - \phi(P_{k-1})\, g_{n-k-1}(\lambda)$ *for* $1 \leqslant k \leqslant n-1$;

(ii) *for each positive* i, $\phi(P_n) \mid g_{n+1+i}(\lambda)$ *if and only if* $\phi(P_n) \mid g_i(\lambda)$.

3. Spectral properties of the H-shape tree H'_n

Let $n \geqslant 8$. For sake of conciseness, we set $\rho'_n := \rho(H'_n)$ and $\mathcal{G}_{<\mathfrak{h}} = \mathcal{G}_{<2} \cup \mathcal{G}_2 \cup \mathcal{G}_{(2,\mathfrak{h})}$. The elements of the three sets $\mathcal{G}_{<2}$, $\mathcal{G}_2$ and $\mathcal{G}_{(2,\mathfrak{h})}$ are listed in Propositions 3, 4 and 5.

Proposition 14. *For each $n \geqslant 8$, the number ρ'_n belongs to the interval $\big(\mathfrak{h}, 3/\sqrt{2}\big)$.*

Proof. By definition, the number ρ'_8 is the largest root of $\phi(H'_8) = x^2(x^2-1)(x^4 - 6x^2 + 7)$. Thus, $\rho'_8 = \sqrt{3+\sqrt{2}} \approx 2.10100$. Applying Corollary 1, we see that $\rho'_n \leqslant \rho'_8 < 3/\sqrt{2} \approx 2.1213$.
In order to see that $\rho'_n > \mathfrak{h}$ for all $n \geqslant 8$ we just note that the intersection $\mathscr{H}' \cap \mathcal{G}_{<\mathfrak{h}}$ is empty; moreover, no simple graph has $\mathfrak{h}$ in its spectrum since the minimal polynomial of $\mathfrak{h}$, i.e. $x^4 - 4x^2 - 1$, has nonreal roots. □

We now list the approximated values of the first few ρ'_n's. As expected from Proposition 14, they all lie in the interval $\big(\mathfrak{h}, 3/\sqrt{2}\big)$.

$$\begin{array}{lll} \rho'_8 \approx 2,10100 & \rho'_{11} \approx 2.06843 & \rho'_{14} \approx 2.06082 \\ \rho'_9 \approx 2.08397 & \rho'_{12} \approx 2.06472 & \rho'_{15} \approx 2.05984 \\ \rho'_{10} \approx 2.07431 & \rho'_{13} \approx 2.06235 & \rho'_{16} \approx 2.05922. \end{array} \tag{3}$$

Curiously enough, all values appearing in (3) are also spectral radii of suitable H-shape trees in $\mathscr{H}$, the family of graphs including the minimizers of the spectral radius for the sets $G_{n,n-5}$ with n sufficiently large (see [2, (16)]). However, despite its intrinsic interest, the apparently large intersection between $\mathrm{sp}(H'_n)$ and $\mathrm{sp}(H_{2n-3})$ is beyond the scope of this article.

Proposition 15. *Among all trees in $\mathcal{T}_4$ with n vertices, only H'_n attains the minimum index.*

Proof. Let G be a graph with n vertices in $\mathcal{T}_4 \setminus \{H'_n\}$. Since G is a tree, then $\varepsilon_G = \varepsilon_{H'_n} = n-1$. Recall that the length of each dotted line in Fig. 3 is at least 2. Let ℓ_1 and ℓ_2 be the lengths of the two longest pendant paths in G. By $G \neq H'_n$ we deduce that at least one of the two inequalities $\ell_1 \geqslant 2$ and $\ell_2 \geqslant 2$ is strict.
Let G' be the graph obtained from G by leaving exactly two edges on the two longest pendant paths, and let G'' be the the graph obtained from G' by inserting the deleted edges (and vertices) in the internal path of G'. Clearly $G'' = H_n$, and $\rho(G) > \rho(G') > \rho_n$. The former inequality comes from Proposition 7, the latter from Proposition 9. □

Proposition 16. *$\lambda_2(H'_n) < 2$ for all $H'_n \in \mathscr{H}'$.*

Proof. By a direct computation, $\lambda_2(H'_8) = 1.52023 < 2$. Let now $n \geqslant 9$, and let u be the vertex of H'_n labelled $n-6$ in Fig. 2. By interlacing and Proposition 3, $\lambda_2(H'_n) \leq \rho(H'_n - u) = \rho(2P_2 \cup P^1_{1;n-6}) < 2$. □

Proposition 17. *For each $n \geqslant 8$, let L_n be the H-shape tree $P^{1,2}_{1,1;n-2}$. Then, $\rho(H'_n) = \rho(L_n)$ if and only if $n = 9$.*

Proof. First of all, note that H'_9 and L_9 are cospectral. In fact,

$$\phi(H'_9) = \phi(L_9) = (x^2-1)(x^6 - 7x^4 + 12x^2 - 2).$$

By a direct computation, $\rho(L_8) = \rho'_{10} > \rho'_8$, and $\rho(L_{10}) \approx 2.08862 > \rho'_{10}$; thus, $\rho(L_n) \neq \rho'_n$ for $n \in \{8, 10\}$.
Now, let $n \geqslant 11$. By Proposition 7 and Corollary 1 it follows that

$$\rho'_n < \rho'_{10} = \rho(L_8) < \rho(L_n).$$ □

Proposition 18. *Let g be the girth of a closed quipu CQ. If $3 \leqslant g \leqslant 5$ then $\rho(CQ) > \rho'_n$ for all $n \geqslant 8$.*

Proof. Since $C^0_{1,g} \subseteq CQ$, we use interlacing, Proposition 9(ii) and Corollary 1, to obtain

$$\rho(CQ) \geqslant \min\{\rho(C^0_{1,3}), \rho(C^0_{1,4}), \rho(C^0_{1,5})\} = \rho(C^0_{1,5}) \approx 2.11491 > \rho'_8 \geqslant \rho'_n$$

for every $n \geqslant 8$. □

We now achieve the recursivity of the graphs in $\mathscr{H}'$ through the same technique used to prove [2, Lemma 4.6].

Proposition 19. *All graphs in the family $\mathscr{H}'$ are recursive. In fact,*

$$\phi(H'_{n+2}) = \lambda\phi(H'_{n+1}) - \phi(H'_n) \quad \text{for all } n \geqslant 8. \tag{4}$$

Proof. We shall make use of the T-shape graph $T'_h := P^1_{1;h-1}$ (see Fig. 2), defined for all $h \geqslant 3$. By plugging in (4) the polynomials

$$\phi(H'_8) = \lambda^8 - 7\lambda^6 + 13\lambda^4 - 7\lambda^2, \quad \phi(H'_9) = \lambda^9 - 8\lambda^7 + 19\lambda^5 - 14\lambda^3 + 2\lambda,$$
$$\text{and} \qquad \phi(H'_{10}) = \lambda^{10} - 9\lambda^8 + 26x^6 - 27\lambda^4 + 9\lambda^2.$$

we see that the claimed equality holds for $n = 8$.

Let now $n \geqslant 9$. Applying (1) with respect to the vertex with label $n-6$ in Fig. 2, we obtain

$$\begin{aligned}
\phi(H'_{n+2}) &= \left(\lambda\phi(P_2)^2 - 2\phi(P_1)\phi(P_2)\right)\phi(T'_{n-3}) - \phi(P_2)^2\phi(T'_{n-4}) \\
&= \left(\lambda\phi(P_2)^2 - 2\phi(P_1)\phi(P_2)\right)\left(\lambda\phi(T'_{n-4}) - \phi(T'_{n-5})\right) \\
&\qquad - \phi(P_2)^2\left(\lambda\phi(T'_{n-5}) - \phi(T'_{n-6})\right) \\
&= \lambda\left((\lambda\phi(P_2)^2 - 2\phi(P_1)\phi(P_2))\phi(T'_{n-4}) - \phi(P_2)^2\phi(T'_{n-5})\right) \\
&\qquad - \left((\lambda\phi(P_2)^2 - 2\phi(P_1)\phi(P_2))\phi(T'_{n-5}) - \phi(P_2)^2\phi(T'_{n-6})\right) \\
&= \lambda\phi(H'_{n+1}) - \phi(H'_n).
\end{aligned}$$

Thus, (4) is proved. □

Theorem 2. *The path P_m $(m \geqslant 1)$ divides H'_n if and only if*

$$(m, n) \in \{(1, h), (2, h) \mid h \in \mathbb{N}_8\} \cup \{(5, 6s + 4) \mid s \in \mathbb{N}\}.$$

Proof. We consider the sequence of polynomials $\{g_i(\lambda)\}_{i\in\mathbb{N}}$, where

$$\begin{aligned}
g_0(\lambda) &= -\lambda^{10} + 7\lambda^8 - 14\lambda^6 + 7\lambda^4 + \lambda^2 &&= -\lambda^2(\lambda^2-1)(\lambda^6 - 6\lambda^4 + 8\lambda^2 + 1), \\
g_1(\lambda) &= -\lambda^9 + 6\lambda^7 - 9\lambda^5 + 2\lambda^3 + 2\lambda &&= -\lambda(\lambda^2-1)(\lambda^6 - 5\lambda^4 + 4\lambda^2 + 2), \\
g_2(\lambda) &= -\lambda^8 + 5\lambda^6 - 5\lambda^4 + \lambda^2 &&= -\lambda^2(\lambda^2-1)(\lambda^4 - 4\lambda^2 + 1), \\
g_3(\lambda) &= -\lambda^7 + 4\lambda^5 - \lambda^3 - 2\lambda &&= -\lambda(\lambda^2-1)(\lambda^4 - 3\lambda^2 - 2), \\
g_4(\lambda) &= -\lambda^6 + 4\lambda^4 - 3\lambda^2 &&= -\lambda^2(\lambda^2-1)(\lambda^2-3), \\
g_5(\lambda) &= -2\lambda^3 + 2\lambda &&= -2\lambda(\lambda^2-1) \\
g_6(\lambda) &= \lambda^6 - 6\lambda^4 + 5\lambda^2 &&= \lambda^2(\lambda^2-1)(\lambda^2-5), \\
g_7(\lambda) &= \lambda^7 - 6\lambda^5 + 7\lambda^3 - 2\lambda &&= \lambda(\lambda^2-1)(\lambda^4 - 5\lambda^2 + 2),
\end{aligned} \tag{5}$$

and

$$g_n(\lambda) = \phi(H'_n) \quad \text{for } n > 7.$$

The equality

$$g_{n+2}(\lambda) = \lambda g_{n+1}(\lambda) - g_n(\lambda) \tag{6}$$

holds for every $n \geqslant 0$. This can be proved by a direct inspection if $0 \leqslant n \leqslant 7$, and by Proposition 19 if $n > 7$.
Since 0 and ± 1 are roots of both $g_0(\lambda)$ and $g_1(\lambda)$, an easy inductive argument using (6) shows that $\phi(P_1) = \lambda$ and $\phi(P_2) = \lambda^2 - 1$ divide $\phi(H'_n)$ for all $n \in \mathbb{N}_{\geqslant 8}$.
Let now $m \geqslant 3$. There exists a unique integral pair (s, i) with $s \geqslant 0$ and $0 \leqslant i \leqslant m$ such that $n = (m+1)s + i$. From Proposition 13 it follows that $\phi(P_m) \mid g_n(\lambda)$ if and only if $\phi(P_m) \mid g_i(\lambda)$, where $0 \leqslant i \leqslant m$. We now distinguish two cases.

Case 1. $3 \leqslant m \leqslant 7$. The polynomials after the second equalities in (5) cannot be further decomposed in the ring $\mathbb{Z}[\lambda]$. Moreover, it is obvious that $\phi(P_m)$ can possibly divide $g_i(\lambda)$ only if $m \leqslant \deg g_i(\lambda)$. Taking into account these two facts, one quickly realizes that, in the considered range, $\phi(P_m) \mid g_i(\lambda)$ if and only if $(m, i) = (5, 4)$. In fact, $g_4(\lambda) = -\lambda\phi(P_5)$.

Case 2. $m \geqslant 8$. For degree reasons, when $0 \leqslant i \leqslant 7$, $\phi(P_m)$ could possibly divide $g_i(\lambda)$ only for $(i, m) \in \{(0, 8), (1, 8), (2, 8), (1, 9), (2, 9), (0, 10)\}$. A direct check shows that no divisibility occurs in any of those six cases. Finally, assume $(m \geqslant) i \geqslant 8$. Since $\deg g_i(\lambda) = |V_{H'_i}| = i$, $\phi(P_m)$ could possibly a factor of $\phi(H'_i)$ only for $m = i$ and, if this were the case, $\phi(P_i) = \phi(H'_i)$. This equality cannot be true since, by Proposition 1, every path is DS. □

We end this section by recalling a proposition by Liu and Huang useful to detect cospectral mates of H-shape trees.

Proposition 20. [15, Equation (2) and Lemma 3.1] *Let $n_4(G)$ be the number of quadrangles in a graph G. If G is cospectral to an H-shape graph with n vertices, then $n_4(G) \leqslant 1$. Moreover, the degree sequence of G is $(1^2, 2^{n-2})$ if $n_4(G) = 1$, whereas it belongs to*

$$\{(0^1, 1^1, 2^{n-3}, 3^1), (1^4, 2^{n-6}, 3^2)\} \qquad \text{if } n_4(G) = 0.$$

4. Proof of Theorem 1

The proof of Theorem 1 still requires three additional lemmas.

Lemma 1. [7, Lemma 4] *For $a, b, c > 1$ the following equalities hold.*

(i) $\phi(P^a_{c,a+b+1}, 2) = a + b + c + 2 - abc$;

(ii) $\phi(P^{a-1,a+b-1}_{1,1,a+b+c-1}, 2) = 4(a + b + c) - 4ac - 2bc - 2ab + abc$.

Lemma 2. *Let $H = P^{a-1,a+b-1}_{1,1,a+b+c-1}$ with $c \geqslant a \geqslant 3$ and $b \geqslant 2$. The equality $\phi(H, 2) = -12$ only holds if (a, b, c) belongs to the set*

$$\mathcal{S} := \{(3, 4, 4), (3, 6, 6), (3, 7, 10), (4, 5, 4), (7, 5, 10), (8, 5, 8)\}. \tag{7}$$

Proof. By Lemma 1, the condition $\phi(H,2)=-12$ is equivalent to $b\,q_1=q_2$, where

$$q_1 := ac-2(a+c)+4 \quad \text{and} \quad q_2 := 4ac-4(a+c)-12.$$

The numbers q_1 and q_2 are both zero or both nonzero. Now, $(q_1,q_2)=(0,0)$ is equivalent to $(ac,a+c)=(10,7)$ which is impossible, since $c\geqslant a\geqslant 3$. Thus, $q_1\neq 0$, and $bq_1=q_2$ is equivalent to

$$b=4+\frac{4(a+c-7)}{q_1}. \tag{8}$$

If $a\geqslant 12$, then $a+c>7$ and $q_1\geqslant 10(c-2)>0$. Therefore, (8) yields

$$0<b-4=\frac{4(a+c-7)}{q_1}\leqslant\frac{4(2c-7)}{10(c-2)}<\frac{4}{5}<1$$

which is false. Therefore, if (8) holds, then $a<12$. The possible cases are listed below. Equation (8) becomes:

(i) $b=8-\dfrac{8}{c-2}$ for $a=3$; thus, $(a,b,c)\in\{(3,4,4),(3,6,6),(3,7,10)\}$;

(ii) $b=6-\dfrac{2}{c-2}$ for $a=4$, leading to $(a,b,c)=(4,5,4)$;

(iii) $b=\dfrac{24}{5}+\dfrac{8}{5(c-2)}$ for $a=7$, having $(a,b,c)=(7,5,10)$ as admissible solution;

(iv) $=\dfrac{14}{3}+\dfrac{2}{(c-2)}$ for $a=8$, resulting in $(a,b,c)=(8,5,8)$.

For a respectively equal to $5,6,9,10$ and 11, Equation 8 becomes

$$b=\frac{16}{3};\quad b=5+\frac{1}{c-2}\quad b=\frac{32}{7}+\frac{16}{7(c-2)};\quad b=\frac{9}{2}+\frac{5}{2(c-2)},\quad b=\frac{40}{9}+\frac{8}{3(c-2)},$$

and none of these five equations have admissible solutions. This ends the proof. □

Lemma 3. *$\phi(H'_n,2)=-12$ for all $n\geqslant 8$.*

Proof. Let $\{g_i(\lambda)\}_{i\geqslant 0}$ be the sequence of polynomials defined along the proof of Theorem 2. The statement is proved through an inductive argument using (10) and the equalities $g_0(2)=g_1(2)=-12$. □

Let G be a graph cospectral to H'_n. Then, $\nu_G = n$ and $\varepsilon_G = n-1$. From Proposition 20, we deduce in particular that $\Delta_G \leqslant 3$.
By Propositions 14 and 16, $\rho(G) \in \big(\mathfrak{h}, 3/\sqrt{2}\big)$ and $\lambda_2(G) < 2$. Since $\mathscr{G}_{<2}$ only contains trees (see Proposition 3), and the component of G having $\rho(G)$ among its eigenvalues is a quipu (by Proposition 6), there are just two possibilities: if G is connected, then G is an open quipu; otherwise $G = CQ \cup T$, where CQ is a closed quipu with $\rho(CQ) = \rho'_n = \rho(G)$ and $T \in \mathscr{G}_{<2}$ (the graph G has at most one acyclic component since, for instance, G has at most 4 pendant vertices by Proposition 20).

Case 1. G is connected. In this case G is an open quipu. By Proposition 20, the degree sequence of G is $(1^4, 2^{n-6}, 3^2)$. This means that G is an H-shape tree. From Proposition 11 and Corollary 2 we deduce that G necessarily belongs to $\mathcal{T}_4 \cup \mathcal{T}_5 \cup \mathcal{T}_6$ (see Fig. 3).

Case 1.1. $G \in \mathcal{T}_4$. By Proposition 15 we know that the only graph with n vertices in $\mathcal{T}_4$ whose spectral radius is $\rho(G) = \rho'_n$ is H_n. Thus, $G = H'_n$.

Case 1.2. $G \in \mathcal{T}_5$. By looking at Fig. 3, we see that there exists a triple of positive integers (a, b, c) with $\min\{a, c\} \geqslant 3$ and $b \geqslant 2$ such that

$$G = P^{a-1,a+b-1}_{1,1;a+b+c-1}.$$

By symmetry, it is not restrictive to assume $a \leqslant c$. Note that $n = \nu_{H'_n} = \nu_G = a+b+c+1$. From Lemmas 2 and 3 we deduce that (a, b, c) belongs to the set $\mathcal{S}$ defined in (7). Now, a direct calculation shows that $\phi(G) = \phi(H'_{a+b+c+1})$ only for $(a, b, c) = (3, 4, 4)$. Thus, $G = P^{2,6}_{1,1;10}$ and $n = 12$.

Case 1.3. $G \in \mathcal{T}_6$. The only graph with n vertices in $\mathcal{T}_6$ is $P^{1,2}_{1,1,n-2}$. By Proposition 17, $\rho(G) = \rho(H'_n)$ occurs only for $n = 9$. The graphs $P^{1,2}_{1,1,n-2}$ and H'_9 are, indeed, cospectral.

Case 2. $G = CQ \cup T$, where CQ is a closed quipu with $\rho(CQ) = \rho'_n = \rho(G)$ and $T \in \mathscr{G}_{<2}$. By Proposition 2(ii) and Proposition 18, the girth g of CQ is even and larger than 5. Thus, the degree sequence of G is either $(0^1, 1^1, 2^{n-3}, 3^1)$ or $(1^4, 2^{n-6}, 3^2)$ by Proposition 20.

Case 2.1. T is a path. By Theorem 2, necessarily $\nu_T \in \{1, 2, 5\}$.

Case 2.1.1. $T = P_1$. In this case the degree sequence of the closed quipu CQ is $(1^1, 2^{n-3}, 3^1)$. In other words, CQ is a lollipop of type $C^0_{t,2s}$ where $t = n-1-2s$ and $2 < s \leqslant (n-2)/2$.
By applying (2) to CQ with respect to an edge incident to the vertex of degree 3, we obtain the identity

$$\phi(C^0_{t,2s}) = \phi(P_{2s+t}) - \phi(P_{2s-2}) - \phi(P_t) - 2\phi(P_t). \tag{9}$$

Since $\phi(P_k, 2) = k+1$, Lemma 3 and (9) yield

$$-12 = \phi(H'_n, 2) = \phi(G, 2) = \phi(P_1, 2)\phi(CQ, 2) = -4st,$$

which holds only for $(s,t) = (3,1)$. In other words, the case $T = P_1$ occurs only if $n = 8$ and $G = P_1 \cup C^0_{1,6}$. A direct computation shows that H'_8 and G are indeed cospectral, their characteristic polynomial being $\lambda^2(\lambda^2-1)(\lambda^4-6\lambda^2+7)$.

Case 2.1.2. $T = P_2$. The degree sequence of CQ is $(1^2, 2^{n-6}, 3^2)$, i.e. CQ is a closed quipu with two pendant paths, and we can write

$$G = P_2 \cup C^{0,m}_{a,b;2s} \qquad \text{with } s > 2 \text{ and } 2(s+1)+a+b = n.$$

We first note that $s \neq 3$, since, by interlacing and Corollary 1,

$$\rho(C^{0,m}_{a,b;6}) \geqslant \rho(C^{0,m}_{1,1;6}) \geqslant \min\left\{\rho(C^{0,1}_{1,1;6}),\ \rho(C^{0,2}_{1,1;6}),\ \rho(C^{0,3}_{1,1;6})\right\} \approx 2.17009 > \rho'_8 \geqslant \rho'_n.$$

Let $e_{i,j}$ denote the number of the edges $e = uv$ with $d(u) = i$ and $d(v) = j$ in the graph CQ. In particular, we set $(x,y) := (e_{3,3}, e_{1,2})$. Obviously, $0 \leqslant x \leqslant 1$ and $0 \leqslant y \leqslant 2$, and it is straightforward to check the equalities

$$e_{1,3} = 2-y, \quad e_{2,3} = 4-2x+y \qquad \text{and} \qquad e_{2,2} = \varepsilon_{CQ}+x-y-6. \tag{10}$$

Recall that $f(n) = (n^3-12n^2+35n)/6$. With the aid of (10) and Proposition 12 we compute

$$M_3(G) = M_3(CQ) + M_2(CQ) = f(n)+x+y+3.$$

This number, by Lemma 2 and Proposition 11, should be equal to $f(n)+2$, implying $x+y=-1$, against the intrinsic nonnegative nature of x and y. Thus, this case does not occur.

Case 2.1.3. $T = P_5$. Since P_5 divides H'_n, the integer n is even. In fact, we have $n = \nu_G \equiv 4 \bmod 6$ by Theorem 2. This time, the degree sequence of CQ is $(1^2, 2^{n-9}, 3^2)$. Thus, we can write

$$G = P_5 \cup C^{0,m}_{a,b;2s} \qquad \text{with } s > 3 \text{ and } 2s+a+b = n-5.$$

For the very same reason explained in Case 2.1.2, the girth of CQ cannot be 6 and, once again, by Proposition 11, $M_3(G) = M_3(H'_n)$. Let $x := e_{3,3}$, $y := e_{1,2}$, $e_{1,3}$, $e_{2,2}$ and $e_{2,3}$ be the numbers defined in Case 2.1.2. Relations (10) hold with $\varepsilon_{CQ} = n-5$. Therefore, by a counting argument and Proposition 12,

$$M_3(G) = M_3(CQ) + 4M_2(CQ) + 3\varepsilon_{CQ} = f(n)+x+y+2.$$

Hence, $M_3(G) = M_3(H'_n)$ if and only if $x + y = 0$, i.e. $CQ = C^{0,k}_{1,1,2s}$ with $2 \leqslant k \leqslant s$. So far, we have proved that ν_{CQ} is even. Consequently $n = \nu_G$ should be odd against Theorem 2. In other words, this case does not occur.

Case 2.2. $T \in \{P^1_{1;h-1}, P^1_{2;k} \mid h \geqslant 4;\ 4 \leqslant k \leqslant 6\}$. In this case, the closed quipu CQ is a (bipartite) lollipop, since it must have exactly one pendant vertex and only one vertex of degree 3. Thus, $CQ = C^0_{t,2s}$. In Case 2.1.1, we already explained why $\phi(CQ, 2) = -2st$. With this information at hand, using Lemma 1(i) we arrive at

$$\phi(G,2) = \begin{cases} -8st & \text{if } T \cong P^1_{1;h-1}; \\ -6st & \text{if } T \cong P^1_{2;4}; \\ -4st & \text{if } T \cong P^1_{2;5}; \\ -2st & \text{if } T \cong P^1_{2;6}. \end{cases} \tag{11}$$

From (11) we see that $\phi(G, 2) = \phi(H'_n, 2) = -12$ only for

$$(G, H'_n) \in \mathcal{U} = \left\{ \left(P^1_{2;5} \cup C^0_{1;6},\ H'_{14}\right),\ \left(P^1_{2;6} \cup C^0_{2;6},\ H'_{16}\right),\ \left(P^1_{2;6} \cup C^0_{1;12},\ H'_{21}\right) \right\}.$$

Yet, each pair in $\mathcal{U}$ contains graphs which are not cospectral, their spectral radius being different. Hence, even this final case does not occur, and the proof of Theorem 1 is over.

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