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Abstract

We study graphs with spectral radius at most $\frac{3}{2}\sqrt{2}$ and refine results by Woo and Neumaier [On graphs whose spectral radius is bounded by $\frac{3}{2}\sqrt{2}$, *Graphs Combinatorics* **23** (2007), 713-726]. We study the limit points of the spectral radii of certain families of graphs, and apply the results to the problem of minimizing the spectral radius among the graphs with a given number of vertices and diameter. In particular, we consider the cases when the diameter is about half the number of vertices, and when the diameter is near the number of vertices. We prove certain instances of a conjecture posed by Van Dam and Kooij [The minimal spectral radius of graphs with a given diameter, *Linear Algebra Appl.* **423** (2007), 408-419] and show that the conjecture is false for the other instances.

1 Introduction

In [6], the problem was raised to determine the minimal spectral radius of graphs with a given number of vertices and diameter. While the case of minimizing the spectral radius (given the number of vertices and diameter) seems a hard problem, Van Dam [5] and independently Hansen and Stevanović [7] solved the analogous maximization problem completely. In order to tackle the minimization problem, we study graphs with spectral radius at most $\frac{3}{2}\sqrt{2}$. Properties of such graphs were first studied by Woo and Neumaier [12], and some recent work is done by Wang et al. [11]. In Section 3, we shall refine the results of Woo and Neumaier. In particular, we shall show that the graphs under consideration are subgraphs of so-called m-Laundry graphs and m-Urchin graphs. Related to this we study limit points of the spectral radii of certain graph sequences, using methods developed already in the seminal papers of Hoffman and Smith [8, 9]. Some special attention is given to graph sequences whose spectral radii have limit point $\sqrt{2+\sqrt{5}}$.

In Section 4, we shall apply the obtained refinement to (partly) solve the problem of minimizing the spectral radius of graphs with given number of vertices and diameter in case the diameter is about half the number of vertices. In Section 5 we do the same for the case that the diameter D is near the number of vertices n. We prove a conjecture of Van Dam and Kooij [6] for the cases $e = 4$ and 5, where $e = n - D$, whereas we show that the conjecture is false for larger e. Instead, we pose some new conjectures. We remark that the case $e = 4$ was independently solved by Yuan, Shao, and Liu [13].

2 Preliminaries

All the graphs considered in this paper are undirected and simple. By $V(G)$ and $E(G)$ we denote the vertex set and edge set, respectively, of a graph G. Let $\Phi(G)$ denote the characteristic polynomial of G, where whenever necessary we use an indeterminate x, so that $\Phi(G)(x) = \det(xI - A)$, where A is the adjacency matrix of G. By $\rho(G)$ we denote the spectral radius of G, i.e., the largest root of $\Phi(G)$. By $D(G)$ we denote the diameter of G.

If $e = uv$ is an edge of G, we denote by $G \setminus e$ the graph obtained from G by deleting e and by $G \setminus \{u, v\}$ the graph obtained from G by deleting the vertices u and v and all the edges incident to at least one of u and v. In general for a vertex subset W of $V(G)$, we denote by $G \setminus W$ the graph obtained from G by deleting the vertices in W and all the edges incident to at least one vertex in W. An edge uv is called a *bridge* if the deletion of uv causes an increase of the number of components of G. We say a graph H is a subgraph of G if $V(H) \subset V(G)$ and $E(H) \subset E(G)$; it is a proper subgraph if at least one of these inclusions is proper. The following three lemmas are well-known. The first is a consequence of the theory of Perron-Frobenius, cf. [1, Thm. 3.1.1.v], while the latter two were proven by Schwenk, cf. [3, 2.7.9].

Lemma 2.1. *If H is a proper subgraph of a connected graph G, then $\rho(H) < \rho(G)$.*

Lemma 2.2. *Let u be a vertex of degree 1 in a graph G where the only neighbor of u is v. Then*

$$\Phi(G) = x\Phi(G \setminus \{u\}) - \Phi(G \setminus \{u, v\}).$$

Lemma 2.3. *If uv is a bridge of a graph G, then*

$$\Phi(G) = \Phi(G \setminus uv) - \Phi(G \setminus \{u, v\}).$$

A *path of length* l from a vertex u to a vertex v in G is a sequence of $l + 1$ distinct vertices starting with u and ending at v such that consecutive vertices are adjacent. A path P is called a *pendant path* of G if one of the end vertices of P is connected to a vertex w in $G \setminus P$ and the others are not connected on any vertex in $G \setminus P$.

If uv is an edge of a graph G, denote by $G_{u,v}$ the graph obtained from G by subdividing the edge uv by one vertex. More precisely, the vertex set of $G_{u,v}$ is $V(G) \cup \{w\}$, where $w \notin V(G)$ is a new vertex which will be adjacent to both u and v. Also, all the edges of G will be kept in $G_{u,v}$ with the exception of the edge uv.

An *internal path* of G is a sequence of distinct (except possibly $x_1 = x_k$) vertices $x_1, \dots, x_k$ such that $x_i x_{i+1} \in E(G)$ for each $1 \le i \le k - 1$, and where x_1 and x_k have degrees at least 3, and each of the other vertices has degree 2.

Let $\tilde{D}_n$ be the graph obtained from a path $0 \sim 1 \sim \cdots \sim n-2$ by adding a pendant vertex at vertex 1 and a pendant vertex at vertex $n-3$. Hoffman and Smith [9] proved the following result about subdiving an edge on an internal path.

Lemma 2.4. *Let uv be an edge of a connected graph G. If uv is on an internal path of G, then $\rho(G_{u,v}) < \rho(G)$ unless $G = \tilde{D}_n$.*

We remark that subdividing an edge on an internal path of $\tilde{D}_n$ does not change its spectral radius, which equals 2.

Next, we recall some results on graphs with small spectral radius. The first two are classical results by Smith [10], and the third result is by Brouwer and Neumaier [2]. The results require the following definitions. We denote by $T_{k,l,m}$ the graph with $k+l+m+1$ vertices consisting of three paths with k, l, and m edges, respectively, where these paths have one end vertex in common. These graphs are called T-shape trees. The graph $H_{i,j,k}, i, k \ge 2, j \ge 1$ is the graph on $i + j + k + 1$ vertices, obtained from a path of $i + j + k - 1$ vertices, by adding pendant vertices at the i-th and $i + j$-th vertex. These are examples of H-shape trees.

Theorem 2.5. *The only connected graphs on n vertices with spectral radius smaller than 2 are the path P_n, the graph $D_n = T_{1,1,n-3}$, and the graphs $E_6 = T_{1,2,2}$ ($n = 6$), $E_7 = T_{1,2,3}$ ($n = 7$), and $E_8 = T_{1,2,4}$ ($n = 8$).*

Theorem 2.6. *The only connected graphs on n nodes with spectral radius equal to 2 are the n-gon C_n, the graph $\tilde{D}_{n-1} = H_{2,n-5,2}$, and the graphs $\tilde{E}_6 = T_{2,2,2}$ ($n = 7$), $\tilde{E}_7 = T_{1,3,3}$ ($n = 8$), and $\tilde{E}_8 = T_{1,2,5}$ ($n = 9$).*

Theorem 2.7. *Let G be a connected graph. Then $2 < \rho(G) \le \sqrt{2+\sqrt{5}}$ (≈ 2.0582) if and only if G is one of the graphs $T_{1,2,m}, m \ge 6$; $T_{1,3,m}, m \ge 4$; $T_{1,l,m}, m \ge l \ge 4$; $T_{2,2,m}, m \ge 3$; $T_{2,3,3}$; $H_{i,j,k}$, $j \ge i+k \ge 5$; $H_{3,j,k}$, $j \ge k+2$; $H_{2,j,k}$, $j \ge k-1 \ge 2$; $H_{2,1,3}$; $H_{3,4,3}$; $H_{3,5,4}$; $H_{4,7,4}$; $H_{4,8,5}$.*

After Woo and Neumaier [12], we call a tree with maximum degree 3 such that all vertices of degree 3 lie on a path an *open quipu*; a *closed quipu* is a connected graph with maximum degree 3 such that all vertices of degree 3 lie on a circuit, and no other circuit exists; and a *dagger* $T_0(n)$ is obtained from a path with $n+1$ vertices by adding three pendant vertices at one of its end vertices. Woo and Neumaier [12] introduced this terminology for the following result.

Theorem 2.8. *A graph G whose spectral radius $\rho(G)$ satisfies $2 < \rho(G) \leq \frac{3}{2}\sqrt{2}$ (≈ 2.1213) is either an open quipu, a closed quipu, or a dagger.*

Like in [6], we let $P^{m_1,m_2,\cdots,m_t}_{n_1,n_2,\cdots,n_t,p}$ denote the graph with diameter $p-1$ obtained from a path P : $0 \sim 1 \sim \cdots \sim p-1$ on p vertices with pendant paths of n_i vertices added at vertex m_i of the path P. This implies that $n_1 \leq m_1$ and $n_t \leq p - m_t - 1$. We will call the pendant paths of n_i vertices added at vertex m_i of the path P *inner pendant paths* for $2 \leq i \leq t-1$. The other two pendant paths of n_1 and n_t vertices added at vertex m_1 and m_t, respectively, and another two pendant paths: $0 \sim 1 \sim \cdots \sim m_1$, and $m_t \sim m_t+1 \sim \cdots \sim p-1$ on m_1+1 and $p-m_t$ vertices, respectively will be called *outer pendant paths*. Note that these graphs are open quipus.

Similarly, let $C^{m_1,m_2,\cdots,m_t}_{n_1,n_2,\cdots,n_t,p}$ denote the graph obtained from a cycle C : $0 \sim 1 \sim \cdots \sim p-1 \sim 0$ on p vertices with pendant paths of n_i vertices added at vertex m_i of the cycle C. These graphs are closed quipus. In particular, we let $\widehat{C}_n$ denote the graph $C^0_{1,n}$.

For the purpose of this paper, we are going to call the graph $P^{2,3,4,\cdots,n-4,n-3}_{2,1,1,\cdots,1,2,n}$ the *Laundry graph* on $2n-2$ vertices, denoted by $\mathcal{L}_{2n-2}$ and to call the graph $C^{0,1,2,\cdots,n-1}_{1,1,1,\cdots,1,n}$ the *Urchin graph* on $2n$ vertices, denoted by $\mathcal{U}_{2n}$. More generally, we will define the *m-Laundry graph* and the *m-Urchin graph* for integers $m \geq 1$. The m-Laundry graph is obtained from the Laundry graph by replacing all inner pendant paths (of length one) by pendant paths of length m and the four outer pendant paths (of length two) by pendant paths of length $m+1$. In other words, the m-Laundry graph is $P^{m+1,m+2,\cdots,n-m-3,n-m-2}_{m+1,m,\cdots,m,m+1,n}$. Note that the 1-Laundry graph is the usual Laundry graph. Similarly, the m-Urchin graph is obtained from the Urchin graph by replacing all pendant paths of length one by pendant paths of length m, i.e., it is $C^{0,1,2,\cdots,n-1}_{m,m,m,\cdots,m,n}$.

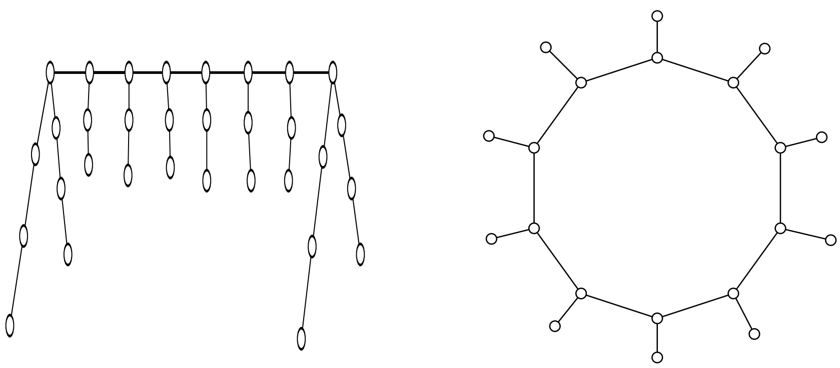

Figure 1: 2-Laundry graph and 1-Urchin graph

3 Refinement of Woo and Neumaier's theorem

In this section we are going to refine Theorem 2.8 using the m-Laundry graphs and the m-Urchin graphs. We define

$$\rho_m := \lim_{n\to\infty} \rho(T_{m,n,n}) \quad \text{and} \quad \theta_{k,m} := \lim_{n\to\infty} \rho(T_{k,m,n}).$$

Note that these limits exist because the sequences are increasing (by Lemma 2.1) and bounded (by the largest degree (3) for example; note however that the next lemma implies that the spectral radius of every T-shape tree is at most $\frac{3}{2}\sqrt{2}$). For notational purpose we define $\lambda := \lambda(x) = \frac{x+\sqrt{x^2-4}}{2}$. The following lemma will be used to show our main results. Recall that $T_0(n)$ is a dagger graph, and $\widehat{C}_n$ denotes the graph $C^0_{1,n}$.

Lemma 3.1. *The following statements hold:*

(a) $\lim_{n\to\infty} \rho(T_0(n)) = \frac{3}{2}\sqrt{2}$,

(b) $\rho_1 = \sqrt{2+\sqrt{5}}$,

(c) $\rho(T_{m,n+1,n+1}) = \rho(T_{m+1,m+1,n})$ *for all positive integers m and n,*

(d) $\rho_m = \theta_{m+1,m+1}$,

(e) $\lim_{m\to\infty} \rho(T_{m,m,m}) = \frac{3}{2}\sqrt{2}$,

(f) $\lim_{m\to\infty} \rho(C^{0,2m+1}_{m,m,4m+2}) = \frac{3}{2}\sqrt{2}$,

(g) $\lim_{n\to\infty} \rho(\widehat{C}_n) = \sqrt{2+\sqrt{5}}$.

(h) $\lim_{n\to\infty} \rho(P^{n,n+2}_{1,1,2n+3}) = \frac{3}{2}\sqrt{2}$.

Proof. (a): By [8, Lemma 3.4], $\lim_{n\to\infty} \rho(T_0(n))$ is the largest root of the polynomial $\lambda(x^2-3)-x$, and this is $\frac{3}{2}\sqrt{2}$. Alternatively, see [12, Lemma 3].
(b): See [8, Proposition 3.6].
(c): From Lemma 2.3, we obtain that

$$\begin{aligned}\Phi(T_{m,n+1,n+1}) &= \Phi(P_{m+n+2})\Phi(P_{n+1}) - \Phi(P_m)\Phi(P_{n+1})\Phi(P_n), \text{ and}\\ \Phi(T_{m+1,m+1,n}) &= \Phi(P_{m+n+2})\Phi(P_{m+1}) - \Phi(P_m)\Phi(P_{m+1})\Phi(P_n)\end{aligned}$$

by taking u to be the vertex of degree three and v a neighbor of u on a path of length $n+1$ (for the first equation) or $m+1$ (for the second equation). It follows that the spectral radius of both graphs is the largest root of $\Phi(P_{m+n+2}) - \Phi(P_m)\Phi(P_n)$.
(d): Immediate from (c).
(e): See [12, Lemma 3].
(f): The graph $C^{0,2m+1}_{m,m,4m+2}$ has two internal paths. We obtain as a subgraph $T_{m,m,m} \cup T_{m,m,m}$,

by removing the edges joining the middle vertices on these internal paths. Similar as in the proof of [9, Lemma 3.3], we have

$$\rho(T_{m,m,m}) = \rho(2T_{m,m,m}) \leq \rho(C^{0,2m+1}_{m,m,4m+2}) \leq \rho(2T_{m,m,m}) + \frac{2}{m} = \rho(T_{m,m,m}) + \frac{2}{m}.$$

Now it follows immediately from (e).
(g): Similar as (f), using (b).
(h): Similar as [12, Lemma 3]. □

Proposition 3.2. *For positive integers $k \leq m$,*

$$\theta_{k,m} < \theta_{k,m+1} < \theta_{k+1,k+1} < \frac{3}{2}\sqrt{2}.$$

Proof. Because $T_{k,m,n}$ is a subgraph of $T_{k,m+1,n}$, it follows that $\theta_{k,m} \leq \theta_{k,m+1}$. Moreover, $\theta_{k,m}$ is the largest root of the polynomial $\lambda\Phi(P_{k+m+1}) - \Phi(P_k)\Phi(P_m)$ by [8, Lemma 3.4]. Similarly, $\theta_{k,m+1}$ is the largest root of the polynomial $\lambda\Phi(P_{k+m+2}) - \Phi(P_k)\Phi(P_{m+1})$. Now we claim that the two polynomials have no common root, which implies $\theta_{k,m} < \theta_{k,m+1}$ (which is to be proven). To prove the claim, assume that there exists a common root x, so that

$$0 =_x \lambda\Phi(P_{k+m+1}) - \Phi(P_k)\Phi(P_m) \text{ and} \quad (1)$$
$$0 =_x \lambda\Phi(P_{k+m+2}) - \Phi(P_k)\Phi(P_{m+1}), \quad (2)$$

where $=_x$ indicates that the polynomials are the same when evaluated at x. By combining these two equations we obtain that

$$\Phi(P_{k+m+2})\Phi(P_m) =_x \Phi(P_{k+m+1})\Phi(P_{m+1}).$$

Since $\Phi(P_{m+1}) = x\Phi(P_m) - \Phi(P_{m-1})$ and $\Phi(P_{k+m+2}) = x\Phi(P_{k+m+1}) - \Phi(P_{k+m})$, it follows that

$$\Phi(P_{k+m+1})\Phi(P_{m-1}) =_x \Phi(P_{k+m})\Phi(P_m).$$

Repeating this procedure, we obtain

$$\Phi(P_{k+3})\Phi(P_1) =_x \Phi(P_{k+2})\Phi(P_2).$$

This implies $(x\Phi(P_{k+2}) - \Phi(P_{k+1}))x =_x \Phi(P_{k+2})(x^2 - 1)$ which means that $\Phi(P_{k+2}) =_x x\Phi(P_{k+1})$. Because $\Phi(P_{k+2}) = x\Phi(P_{k+1}) - \Phi(P_k)$, it follows that x is a root of $\Phi(P_k)$. But then it follows from Equations 1 and 2 that x is a root of both $\Phi(P_{k+m+1})$ and $\Phi(P_{k+m+2})$, which is impossible (because it follows easily by induction and the equation $\Phi(P_{l+2}) = x\Phi(P_{l+1}) - \Phi(P_l)$ that paths of consecutive lengths have no common eigenvalue). Thus the claim, and the inequality $\theta_{k,m} < \theta_{k,m+1}$ is proven.

The inequality $\theta_{k,m+1} < \theta_{k+1,k+1}$ easily follows from the inequalities $\theta_{k,m} < \theta_{k,m+1}$ and the fact that $\theta_{k+1,k+1} = \rho_k = \lim_{n\to\infty} \rho(T_{k,n,n})$.

From Lemma 3.1(e) it follows that ρ_k is at most $\frac{3}{2}\sqrt{2}$. The above inequalities imply that ρ_k is strictly increasing, so that $\theta_{k+1,k+1} < \frac{3}{2}\sqrt{2}$. □

Lemma 3.3. *For $m \geq 1$, we have $\rho_m = \lambda + \lambda^{-1}$, where λ is the largest root of the equation $\lambda^{2m+4} - 2\lambda^{2m+2} + 1 = 0$.*

Proof. As before, $\rho_m = \theta_{m+1,m+1}$, which is the largest root of the polynomial $\lambda\Phi(P_{2m+3}) - \Phi(P_{m+1})\Phi(P_{m+1})$ by [8, Lemma 3.4]. From the characteristic polynomial of the path in [3, p. 73], we deduce that $\Phi(P_m) = \frac{\lambda^{m+1}-\lambda^{-m-1}}{\lambda-\lambda^{-1}}$. From this, and the fact that $x = \lambda + \lambda^{-1}$, the required result can be obtained. □

For $m = 1$, the equation $\lambda^{2m+4} - 2\lambda^{2m+2} + 1 = 0$ has largest root $\sqrt{\frac{1+\sqrt{5}}{2}}$, giving $\rho_1 = \theta_{2,2} = \sqrt{2+\sqrt{5}} \approx 2.0582$. We further remark that $\theta_{2,3} \approx 2.0763, \rho_2 = \theta_{3,3} \approx 2.0936, \theta_{3,4} \approx 2.1013$, and $\frac{3}{2}\sqrt{2} \approx 2.1213$.

Theorem 3.4. *For a positive integer m, let μ be a real number such that $\mu < \theta_{m+1,m+2}$. Then any graph G on n vertices with spectral radius at most μ is a subgraph of an m-Laundry graph or a subgraph of an m-Urchin graph, for n large enough.*

Proof. By Theorems 2.5 and 2.6, any graph with spectral radius at most 2 is a subgraph of C_n or a subgraph of $\tilde{D}_n$ if $n \geq 9$. So we may assume that the spectral radius of G is greater than 2. Since $\mu < \theta_{m+1,m+2}$, there exists a positive integer N_1 such that $\mu < \rho(T_{m+1,m+2,n})$ for all $n \geq N_1$. And by Lemma 3.1(a), there exists a positive integer N_2 such that the spectral radius of a dagger graph with n vertices is strictly greater than μ for all $n \geq N_2$. Let $N := \max\{N_1, N_2\}$. Since $\rho(G) < \frac{3}{2}\sqrt{2}$, the graph G is either an open quipu or a closed quipu, or a dagger, by Theorem 2.8. However, if we take $n \geq N$, then G cannot be a dagger graph. Hence we have two cases, namely either G is an open quipu or a closed quipu.

Case 1. *The graph G is an open quipu.*
Let $p - 1$ denote the diameter of G. If $n \geq (2N + m + 2)^2$, then G can be expressed as $G = P^{m_1,m_2,\cdots,m_t}_{n_1,n_2,\cdots,n_t,p}$ with $p \geq 2N + m + 2$. We have that $n_1 \leq m_1$ and $n_1 \leq m+1$; if $n_1 > m+1$ then $T_{m+1,m+2,N}$ is a subgraph of G, and this means $\rho(G) \geq \rho(T_{m+1,m+2,N})$, a contradiction. If $n_1 = m + 1$, then $m_1 = m + 1$; otherwise G contains $T_{m+1,m+2,N}$ as a subgraph. By the same argument, it holds $n_t \leq p - m_t - 1$ and $n_t \leq m + 1$. If $n_t = m + 1$, then $m_t = p - m - 2$.

Now we are going to consider inner pendant paths of G. Suppose that the inner pendant path at vertex m_i has length at least $m + 1$ for some $2 \leq i \leq t - 1$. Since $p \geq 2N + m + 2$, and G cannot have $T_{m+1,m+2,N}$ as a subgraph, without loss of generality it satisfies $i = 2$, $m_1 = n_1 = m$, $m_2 = m + 1$ and $n_2 \geq m + 1$. However, subdividing the edge m_1m_2 gives a graph with smaller spectral radius containing as a subgraph $T_{m+1,m+2,N}$ which gives a contradiction. Therefore it follows that the graph G is a subgraph of an m-Laundry graph.

Case 2. *The graph G is a closed quipu.*
Since G is a closed quipu, it can be written as $C^{m_1,m_2,\cdots,m_t}_{n_1,n_2,\cdots,n_t,p}$. If necessary we subdivide edges on internal paths of G to get a similar graph $G' = C^{m'_1,m'_2,\cdots,m'_t}_{n_1,n_2,\cdots,n_t,p'}$ with $p' \geq N + m + 3$. Then the length of any pendant path should have length at most m, i.e. $n_i \leq m$ for all $1 \leq i \leq t$, since, if there exists a pendant path with length at least $m + 1$, then G' contains $T_{m+1,m+2,N}$ as a subgraph, so that $\rho(G) \geq \rho(G') \geq \rho(T_{m+1,m+2,N})$, a contradiction. Therefore the graph G is a subgraph of an m-Urchin graph. □

Let $\{G_i\}_{i\geq 1}$ be a sequence of quipus. Let $t_i := t_i(G_i)$ be the number of vertices of degree three in G_i and $\ell_i := \ell_i(G_i)$ be the minimal length of all maximal internal paths in G_i.

Proposition 3.5. *Let $\{G_i\}_{i\geq 1}$ be a sequence of graphs such that G_i is a subgraph of a Laundry graph and $t_i \geq 2$, or G_i is a subgraph of an Urchin graph and $t_i \geq 1$. Then $\lim_{i\to\infty} \rho(G_i) = \sqrt{2+\sqrt{5}}$ implies that $\ell_i \to \infty$ $(i \to \infty)$.*

Proof. First observe that $\sqrt{2+\sqrt{5}}$ cannot be an eigenvalue of a graph, so the number of vertices of G_i must tend to infinity. Suppose that there is a constant h such that $\ell_i \leq h$ for all i. The idea of the proof is to show that there is a graph H that is a subgraph of G_i whenever i is large enough, and that has spectral radius larger than $\sqrt{2+\sqrt{5}}$. This would settle the proof. In fact, we will not exactly show the above, as we may assume without loss of generality that $\ell_i = h$ for all i, because we can always subdivide edges on internal paths. The graph H will also depend on whether G_i is open or closed, as follows. If G_i is a subgraph of a Laundry graph, then there is a k such that G_i contains $P^{1,h+1}_{1,1,2+h+k}$ as a subgraph for large enough i, where k is much larger than h. If G_i is a subgraph of an Urchin graph, then it contains $\widehat{C}_h$ as a subgraph. The spectral radii $\rho(P^{1,h+1}_{1,1,2+h+k})$ and $\rho(\widehat{C}_h)$ are indeed strictly larger than $\sqrt{2+\sqrt{5}}$ by Theorem 2.7. □

We think that in general the converse of Proposition 3.5 does not hold. It is also not so easy to extend Proposition 3.5 to m-Laundry graphs and m-Urchin graphs. However, we get the following results by adding a stronger condition.

Lemma 3.6. *Let $Q_m(t,l)$ be the open quipu with t vertices of degree three, for which its four outer pendant paths have length $m+1$, all of its inner pendant paths have length m, and all of its internal paths have length $2l+1$. Let $\{t_i\}_{i\geq 1}$ and $\{l_i\}_{i\geq 1}$ be integer sequences such that $t_i \geq 2$ for all i. Then $\lim_{i\to\infty} \frac{t_i}{l_i} = 0$ implies that $\lim_{i\to\infty} Q_m(t_i,l_i) = \rho_m$.*

Proof. Let $\widetilde{Q}_m(t_i,l_i)$ be the graph obtained from $Q_m(t_i,l_i)$ by deleting the edges joining the middle vertices of each internal path. Then it is obvious that $\rho(\widetilde{Q}_m(t_i,l_i)) \leq \rho(Q_m(t_i,l_i))$. Moreover, each component of $\widetilde{Q}_m(t_i,l_i)$ is of the form T_{m,l_i,l_i} or $T_{m+1,m+1,l_i}$. Because $\lim_{i\to\infty} \frac{t_i}{l_i} = 0$ implies that $l_i \to \infty$ $(i\to\infty)$, it therefore follows by Lemma 3.1(d) that $\lim_{i\to\infty} \rho(\widetilde{Q}_m(t_i,l_i)) = \rho_m$. By the method of the proof of [9, Lemma 3.3] (notice a small typo therein), we have

$$\rho(Q_m(t_i,l_i)) \leq \rho(\widetilde{Q}_m(t_i,l_i)) + \frac{2(t_i-1)}{l_i}.$$

Since $t_i/l_i \to 0$ $(i\to\infty)$, we obtain that

$$\lim_{i\to\infty} \rho(Q_m(t_i,l_i)) = \lim_{i\to\infty} \rho(\widetilde{Q}_m(t_i,l_i)) = \rho_m.$$

□

Lemma 3.7. *Let $C_m(t,l)$ be the closed quipu with t vertices of degree three, for which all of its pendant paths have length m, and all of its internal paths have length $2l+1$. Let $\{t_i\}_{i\geq 1}$ and $\{l_i\}_{i\geq 1}$ be integer sequences such that $t_i \geq 1$ for all i. Then $\lim_{i\to\infty} \frac{t_i}{l_i} = 0$ implies that $\lim_{i\to\infty} C_m(t_i,l_i) = \rho_m$.*

Proof. Similar as that of Lemma 3.6. □

For a closed quipu G with at least one vertex of degree 3, we define the *depth*, denoted by $r(G)$, as the minimal value r such that it is a subgraph of an r-Urchin graph. For open quipus, the definition of depth is more complicated because of the special role of the outer pendant paths.

For an open quipu G with at least two vertices of degree 3, we define the *inner depth* of G, denoted by $\mathrm{ir}(G)$, as the maximal length of its inner pendant paths; if there are no inner pendant paths, we define it as $-\infty$. To define the *outer depth*, we notice that the four outer pendant paths come in two pairs (each pair consists of two paths attached to the same vertex of degree three). If (k_1,m_1) and (k_2,m_2) denote the lengths of the paths in the two pairs, with $k_1 \leq m_1$ and $k_2 \leq m_2$, then the lexicographically largest of these pairs is called the outer depth $\mathrm{or}(G)$. We say G has *depth* r, denoted by $r(G)$, if its outer depth is $(r+1,r+1)$ and its inner depth is at most r, or its inner depth equals r and its outer depth is (k,m) with $k \leq r$.

Theorem 3.8. *Let $\{G_i\}_{i\geq 1}$ be a sequence of quipus of depth $r(G_i) = m$, such that $t_i \geq 2$ if G_i is open and $t_i \geq 1$ if G_i is closed. Then $\lim_{i\to\infty} \frac{t_i}{\ell_i} = 0$ implies that $\lim_{i\to\infty} \rho(G_i) = \rho_m$.*

Proof. First, let us consider the case that all the graphs G_i are open. Consider the graph H_i obtained from G_i by replacing all internal paths of G_i by paths of length ℓ_i (so G_i can be obtained by subdividing edges on internal paths of H_i). Then $\rho(G_i) \leq \rho(H_i)$. Without loss of generality we may assume that ℓ_i is odd. Then H_i is a subgraph of $Q_m(t_i, \frac{\ell_i - 1}{2})$. Hence by Lemma 3.6 we have $\limsup_{i\to\infty} \rho(G_i) \leq \rho_m$.

Consider the graph $\widetilde{G}_i$ obtained from G_i by deleting, on each internal path, the edge joining the middle vertices. Then $\rho(\widetilde{G}_i) \leq \rho(G_i)$ as $\widetilde{G}_i$ is a subgraph of G_i. By considering the components of $\widetilde{G}_i$, we find that $\lim_{i\to\infty} \rho(\widetilde{G}_i) = \rho_m$ because $r(G_i) = m$. Hence $\lim_{i\to\infty} \rho(G_i) = \rho_m$.

For the case that the graphs G_i are subgraphs of m-Urchin graphs, we similarly obtain the result by deleting the edge connecting the middle vertices on each internal path. □

Theorem 3.9. *Let $\{G_i\}_{i\geq 1}$ be a sequence of open quipus with $t_i \geq 2$, of outer depth $\mathrm{od}(G_i) = (k,m)$, with $k \leq m$, and inner depth $\mathrm{id}(G_i) < k$. Then $\lim_{i\to\infty} \frac{t_i}{\ell_i} = 0$ implies that $\lim_{i\to\infty} \rho(G_i) = \theta_{k,m}$.*

Proof. Similar as that of Theorem 3.8. □

For $m = 1$ we have the following two corollaries:

Corollary 3.10. *Let $\{G_i\}_{i\geq 1}$ be a sequence of graphs such that G_i is a subgraph of a Laundry graph.*

(*a*) *If* $t_i = 1$ *for all* i*, then* $\lim_{i\to\infty} \rho(G_i) = \sqrt{2+\sqrt{5}}$ *if and only if for all* n *there exists an integer* I *such that for all* $i \geq I$*,* G_i *is either* T_{1,n_i,k_i} *or* $T_{2,2,n_i}$ *for some* $n_i \geq n$ *and* $k_i \geq n$*.*

(*b*) *If* $t_i = 2$ *for all* i*, then* $\lim_{i\to\infty} \rho(G_i) = \sqrt{2+\sqrt{5}}$ *if and only if for all* n *there exists an integer* I *such that for all* $i \geq I$*,* G_i *is either* $P^{2,\ell_i+2}_{2,2,\ell_i+5}$*,* $P^{2,\ell_i+2}_{2,1,\ell_i+\beta_i+3}$*, or* $P^{\alpha_i,\alpha_i+\ell_i}_{1,1,\ell_i+\alpha_i+\beta_i+1}$ *for some* $\ell_i \geq n$*,* $\alpha_i \geq n$*, and* $\beta_i \geq 1$*.*

(*c*) *If* $t_i \geq 2$ *for all* i *and* $\lim\limits_{i\to\infty} t_i/\ell_i = 0$*, then* $\lim_{i\to\infty} \rho(G_i) = \sqrt{2+\sqrt{5}}$*.*

Proof. (*a*): A subgraph of a Laundry graph with one vertex of degree three is of the form $T_{2,2,n}$ or $T_{1,k,n}$. The result now follows from the facts that $\lim\limits_{n\to\infty} \rho(T_{2,2,n}) = \lim\limits_{n,k\to\infty} \rho(T_{1,k,n}) = \sqrt{2+\sqrt{5}}$, and $\lim\limits_{n\to\infty} \rho(T_{1,k,n}) < \sqrt{2+\sqrt{5}}$ for fixed k.
(*b*): Since G_i is a subgraph of a Laundry graph and $t_i = 2$, the graph G_i has only one internal path, with length ℓ_i, so that it is $P^{\alpha_i,\ell_i+\alpha_i}_{n_1,n_2,\ell_i+\alpha_i+\beta_i+1}$ for some positive integers α_i, β_i, n_1, and n_2 such that $\alpha_i \geq n_1$, $\beta_i \geq n_2$ and $(n_1, n_2) \in \{(1,1),(2,1),(2,2)\}$. Moreover, if $n_1 = 2$ ($n_2 = 2$) then $\alpha_i = 2$ ($\beta_i = 2$). Therefore G_i is of the form $P^{2,\ell_i+2}_{2,2,\ell_i+5}$, $P^{2,\ell_i+2}_{2,1,\ell_i+\beta_i+3}$, or $P^{\alpha_i,\alpha_i+\ell_i}_{1,1,\ell_i+\alpha_i+\beta_i+1}$, where $\alpha_i \geq 1$ and $\beta_i \geq 1$. Without loss of generality me may also assume that $\alpha_i \geq \beta_i$.

Suppose that $\lim_{i\to\infty} \rho(G_i) = \sqrt{2+\sqrt{5}}$. By Proposition 3.5, $\ell_i \to \infty$ ($i \to \infty$). On the other hand, if $\ell_i \to \infty$, then $\rho(P^{2,\ell_i+2}_{2,2,\ell_i+5}) \to \sqrt{2+\sqrt{5}}$ and $\rho(P^{2,\ell_i+2}_{2,1,\ell_i+\beta_i+3}) \to \sqrt{2+\sqrt{5}}$ by Theorem 3.8, whereas by Theorem 3.9, $\rho(P^{\alpha_i,\alpha_i+\ell_i}_{1,1,\ell_i+\alpha_i+\beta_i+1})$ converges to a value smaller than $\sqrt{2+\sqrt{5}}$ if α_i and β_i are bounded. If also $\alpha_i \to \infty$, then $\rho(P^{\alpha_i,\alpha_i+\ell_i}_{1,1,\ell_i+\alpha_i+\beta_i+1}) \to \sqrt{2+\sqrt{5}}$ because G_i contains a subgraph T_{1,α_i,ℓ_i}.
(*c*): This follows immediately from Theorem 3.8. □

Corollary 3.11. *Let* $\{G_i\}_{i\geq 1}$ *be a sequence of graphs such that* G_i *is a subgraph of an Urchin graph. If* $t_i \geq 1$ *for all* i *and* $\lim\limits_{i\to\infty} t_i/\ell_i = 0$*, then* $\lim\limits_{i\to\infty} \rho(G_i) = \sqrt{2+\sqrt{5}}$*.*

Proof. See Theorem 3.8. □

4 Application to diameter D near $\frac{n}{2}$

From now on we will consider graphs which have minimal spectral radius among the graphs with n vertices and diameter D. Such a graph is called a *minimizer graph.* For $n > D \geq 1$, we define $\rho_D(n) := \min\{\rho(G) |\ G \text{ has } n \text{ vertices and diameter } D\}$.

Van Dam and Kooij [6] determined $\rho_D(n)$ for $D \in \{1, 2, \lfloor\frac{n}{2}\rfloor, n-3, n-2, n-1\}$. They observed that for $n \geq 7$, the unique minimizer graph with n vertices and diameter $D = \lfloor\frac{n}{2}\rfloor$ is the n-gon C_n.

Now we will apply Theorem 3.8 to determine $\rho_D(n)$ for $D = \frac{n-e}{2}$ with fixed $e \geq 2$ and show that a minimizer graph is a member of one of four families of graphs as described below. Let $\mathcal{C}^{(t)}_s$ be the family of graphs obtained from the cycle C_s by adding pendant vertices at t distinct vertices. Clearly, each member of $\mathcal{C}^{(t)}_s$ has $n = s + t$ vertices, is a subgraph of the Urchin graph $\mathcal{U}_{2s}$, and has diameter between $\lfloor\frac{s}{2}\rfloor + 1$ and $\lfloor\frac{s}{2}\rfloor + 2$ (if $t \geq 1$).

Theorem 4.1. *For given integer $e \geq 2$, $\rho_D(2D+e) \to \sqrt{2+\sqrt{5}}$ as $D \to \infty$. Moreover, a minimizer graph with diameter D and $n = 2D+e$ vertices is in one of the four families $\mathcal{C}^{(t)}_{n-t}, e+1 \leq t \leq e+4$, for n large enough.*

Proof. Let $e \geq 2$ be fixed. For $n \geq 6(e+2)$ such that $n-e$ is even, take the graph $H_n = C^{0,l,2l,\cdots,(e+1)l}_{1,1,\cdots,1,n-(e+2)}$ in $\mathcal{C}^{(e+2)}_{n-e-2}$, where $l = \lfloor \frac{n-e-2}{4(e+2)} \rfloor$. The graph H_n has diameter $\frac{n-e}{2}$. By Corollary 3.11, $\lim_{n\to\infty} \rho(H_n) = \sqrt{2+\sqrt{5}}$ as $t(H_n)/\ell(H_n) = (e+2)/\lfloor \frac{n-e-2}{4(e+2)} \rfloor \to 0$ $(n \to \infty)$. Let G_n be a minimizer graph with n vertices and diameter $D = \frac{n-e}{2}$. Since $\rho(G_n) \leq \rho(H_n)$ we can take $\epsilon > 0$ such that $\rho(G_n) \leq \rho_1 + \epsilon < \theta_{2,3}$ for n large enough. By Theorem 3.4, G_n is a subgraph of a Laundry graph or an Urchin graph, for n large enough. However, G_n cannot be a subgraph of a Laundry graph because $D(G_n) = \frac{n-e}{2}$. Hence for n large enough, G_n is in $\mathcal{C}^{(t)}_{n-t}$, for some t. Therefore, the diameter of G_n is between $\lfloor \frac{n-t}{2} \rfloor + 1$ and $\lfloor \frac{n-t}{2} \rfloor + 2$, hence it follows that $e+1 \leq t \leq e+4$. To finish the proof, we observe that $\rho(G_n) > \sqrt{2+\sqrt{5}}$ by Theorem 2.7. □

Next, we consider the cases where $\frac{n}{2} \leq D \leq \frac{2n}{3}$. In these cases, the graph $C(n,D) := C^{0,n-D}_{D-\lfloor \frac{n}{2} \rfloor, D-\lceil \frac{n}{2} \rceil, 2(n-D)}$ with n vertices and diameter D is a good candidate for a minimizer graph. We observe that for every $\epsilon > 0$ there exists a positive integer N such that for all $n \geq N$ and $\frac{n}{2} \leq D \leq \frac{2n}{3}$, we have $\rho(C(n,D)) < \frac{3}{2}\sqrt{2} + \epsilon$. This observation, which provides a natural upper bound on $\rho_D(n)$, can be shown in a similar way as in the proof of Lemma 3.1 (f).

For fixed $e = 2D-n$ we can get better upper bounds because $\rho(C(2D-e,D)) \to \rho_{\lceil \frac{e}{2} \rceil}$ as $D \to \infty$ by Theorem 3.8. We even conjecture that this is optimal.

Conjecture 4.2. *Let $e \geq 1$. For n large enough and such that $n+e$ is even, the unique minimizer graph G_n with n vertices and diameter $\frac{n+e}{2}$ is $C(n, \frac{n+e}{2}) = C^{0,\frac{n-e}{2}}_{\lfloor \frac{e}{2} \rfloor, \lceil \frac{e}{2} \rceil, n-e}$.*

We shall prove this conjecture for $e \leq 4$. Some more evidence for the conjecture is given by the following lemma.

Lemma 4.3. *Let $e \geq 1$, $n \geq e+4$ and such that $n+e$ is even. If a minimizer graph with n vertices and diameter $\frac{n+e}{2}$ is a subgraph of an $\lceil \frac{e}{2} \rceil$-Urchin graph but not of an $\lceil \frac{e}{2} \rceil$-Laundry graph, then it is $C^{0,\frac{n-e}{2}}_{\lfloor \frac{e}{2} \rfloor, \lceil \frac{e}{2} \rceil, n-e}$.*

Proof. Suppose the minimizer graph G_n is a subgraph of an $\lceil \frac{e}{2} \rceil$-Urchin graph and contains a cycle of length s. Then on one hand $\frac{n+e}{2} = D(G_n) \leq \lfloor \frac{s}{2} \rfloor + n - s$ and on the other hand $\frac{n+e}{2} = D(G_n) \leq \lfloor \frac{s}{2} \rfloor + 2\lceil \frac{e}{2} \rceil$. By combining these inequalities, it follows that $s = n-e$ for e even, and that in this case $C^{0,\frac{n-e}{2}}_{\lfloor \frac{e}{2} \rfloor, \lceil \frac{e}{2} \rceil, n-e}$ is the only graph possible. For odd e, it follows that $n-e-2 \leq s \leq n-e$, and that there are three types of candidate graphs: $C^{0,\frac{n-e}{2}}_{\lfloor \frac{e}{2} \rfloor, \lceil \frac{e}{2} \rceil, n-e}$, $C^{0,\lfloor \frac{n-e-1}{2} \rfloor}_{\lceil \frac{e}{2} \rceil, \lceil \frac{e}{2} \rceil, n-e-1}$, and $C^{0,h,\frac{n-e-2}{2}}_{\lceil \frac{e}{2} \rceil, 1, \lceil \frac{e}{2} \rceil, n-e-2}$ for some h. By applying Lemmas 2.1 and 2.4, it follows that of these candidates, $C^{0,\frac{n-e}{2}}_{\lfloor \frac{e}{2} \rfloor, \lceil \frac{e}{2} \rceil, n-e}$ has the smallest spectral radius. □

To prove the cases $e \leq 4$ we use the following lemma.

Lemma 4.4. *Let $e \geq 1$, $m = \lceil \frac{e}{2} \rceil$, and n be such that $n + e$ is even. Let G be a subgraph of an m-Laundry graph, with n vertices and diameter $D = \frac{n+e}{2}$. Then, possibly after subdividing edges on internal paths, G contains $P^{s,s+m}_{1,1,2s+m+1}$ as a subgraph, for some $s = s(n)$, with $s \to \infty$ as $n \to \infty$.*

Proof. Let t be the number of vertices of degree 3 in G. Then by counting vertices one obtains that $n \leq D+1+tm+2$, from which it follows that $t \geq \frac{n-6}{2m} - 1$. Consider the vertices of degree 3 in their natural order on the path, and let τ be the number of consecutive pairs of such vertices at distance at most m. Then it follows that $\frac{n}{2} + m \geq D \geq 2 + \tau + (t-1-\tau)(m+1)$, from which we derive that $\tau \geq \tau_0(n)$ for some $\tau_0(n)$ for which $\tau_0(n) \to \infty$ as $n \to \infty$. The statement now follows by taking $s(n) = \lfloor \frac{1}{2}\tau_0(n) \rfloor$. □

Theorem 4.5. *For n large enough and odd, the unique minimizer graph G_n with n vertices and diameter $D = \frac{n+1}{2}$ is $\widehat{C}_{n-1} = C(n, \frac{n+1}{2})$. For n large enough and even, the unique minimizer graph G_n with n vertices and diameter $D = \frac{n+2}{2}$ is $C^{0,\frac{n-2}{2}}_{1,1,n-2}$. Moreover, $\rho_D(2D-1) \to \sqrt{2+\sqrt{5}}$ and $\rho_D(2D-2) \to \sqrt{2+\sqrt{5}}$ as $D \to \infty$.*

Proof. We shall only prove the first case ($e = 1$). The other case ($e = 2$) is similar. As mentioned before, $\lim_{n\to\infty} \rho(\widehat{C}_{n-1}) = \sqrt{2+\sqrt{5}}$ according to Theorem 3.8. Since $\rho(G_n) \leq \rho(\widehat{C}_{n-1}) \to \rho_1$ ($n \to \infty$), we have that $\rho(G_n) < \theta_{2,3}$ for n large enough. Then by Theorem 3.4, G_n is a subgraph of a Laundry graph or an Urchin graph, for n large enough. If G_n is a subgraph of a Laundry graph, and has diameter $\frac{n+1}{2}$, then for n large enough, G_n contains $P^{s,s+1}_{1,1,2s+2}$ as a subgraph by Lemma 4.4, where $s = s(n) \to \infty$ as $n \to \infty$. But then $\rho(G_n) \geq \rho(P^{s,s+1}_{1,1,2s+2}) \geq \rho(P^{s,s+2}_{1,1,2s+3}) \to \frac{3}{2}\sqrt{2}$ ($n \to \infty$) according to Lemma 3.1 (h), which gives a contradiction. Thus G_n cannot be a subgraph of a Laundry graph, for n large enough. The result now follows from Lemma 4.3. □

For $n = 11, 13, 15, 17, 19$, it was checked by computer that the unique minimizer graph with n vertices and diameter $\frac{n+1}{2}$ is $\widehat{C}_{n-1}$, see [6, Table 2]. For $n = 9$ and $D = 5$, a minimizer graph is either $\widehat{C}_8$ or $P^{1,3}_{1,2,6}$.

It was also checked that for $n = 16, 18, 20$, the unique minimizer graph with n vertices and diameter $\frac{n+2}{2}$ is indeed $C^{0,\frac{n-2}{2}}_{1,1,n-2}$, see [6, Table 2]. For $n = 14$ and diameter 8, a minimizer graph is either $C^{0,6}_{1,1,12}$ or $C^{0}_{2,12}$.

We finish this section with the cases $e = 3$ and 4 of Conjecture 4.2.

Theorem 4.6. *For n large enough and odd, a minimizer graph G_n with n vertices and diameter $\frac{n+3}{2}$ is $C^{0,\frac{n-3}{2}}_{1,2,n-3}$, while for n large enough and even, a minimizer graph G_n with n vertices and diameter $\frac{n+4}{2}$ is $C^{0,\frac{n-4}{2}}_{2,2,n-4}$. Moreover, $\rho_D(2D-3) \to \rho_2$ and $\rho_D(2D-4) \to \rho_2$ as $D \to \infty$.*

Proof. Similar as that of Theorem 4.5. □

5 Application to diameter D near n

For $\frac{2n}{3} \leq D \leq n-1$, the graph $T(n, D) := T_{\lfloor \frac{D}{2} \rfloor, \lceil \frac{D}{2} \rceil, n-D-1}$ has n vertices, diameter D and spectral radius $\rho(T(n, D)) < \frac{3}{2}\sqrt{2}$ (because any T-shape tree has spectral radius smaller than

$\frac{3}{2}\sqrt{2})$, which gives a natural upper bound on $\rho_D(n)$ for these cases. Like in the previous section, we will be able to improve on this under certain assumptions.

In [6], the following conjecture was made regarding the graphs of diameter D minimizing the spectral radius for $D = n - e$, where e is fixed and n is large enough.

Conjecture 5.1. *For fixed e, the graph $P^{\lfloor \frac{e-1}{2} \rfloor, n-e-\lceil \frac{e-1}{2} \rceil}_{\lfloor \frac{e-1}{2} \rfloor, \lceil \frac{e-1}{2} \rceil, n-e+1}$ is a minimizer graph with n vertices and diameter $D = n - e$, for n large enough.*

As mentioned earlier, the cases $e = 1, 2, 3$ were settled in [6]. After making some observations for general e, we shall give a short proof of the case $e = 4$, which was solved independently by Yuan, Shao and Liu [13]. More precisely, we will prove that for $n \geq 11$, the unique minimizer graph with n vertices and diameter $n - 4$ is $P^{1,n-6}_{1,2,n-3}$. Finally, we prove the case $e = 5$.

It follows from Theorem 3.8 that for the conjectured minimizer graphs we have that $\lim_{n\to\infty} \rho(P^{\lfloor \frac{e-1}{2} \rfloor, n-e-\lceil \frac{e-1}{2} \rceil}_{\lfloor \frac{e-1}{2} \rfloor, \lceil \frac{e-1}{2} \rceil, n-e+1}) = \rho_{\lceil \frac{e-1}{2} \rceil}$. Here we shall show that Conjecture 5.1 is false for $e \geq 6$, by showing that $\rho_D(D + e) \to \sqrt{2 + \sqrt{5}}$ as $D \to \infty$, and that a minimizer graph must be in one of the families we will describe now.

For $e \geq 5$, let $\mathcal{P}_{n,e}$ be the family of graphs of the form $P^{m_1,\ldots,m_{e-3}}_{n_1,\ldots,n_{e-3},n-e+1}$, with $n_1 = n_{e-3} = 2$, $n_i = 1$ for $1 < i < e - 3$, $m_1 = 2$, $m_{e-3} = n - e - 2$. Also, for $e \geq 4$, $\mathcal{P}'_{n,e}$ consists of graphs of the form $P^{m_1,\ldots,m_{e-2}}_{n_1,\ldots,n_{e-2},n-e+1}$, with $n_1 = 2$, $n_i = 1$ for $1 < i$, $m_1 = 2$, $m_{e-2} = n - e - 1$, and $\mathcal{P}''_{n,e}$ of graphs of the form $P^{m_1,\ldots,m_{e-1}}_{n_1,\ldots,n_{e-1},n-e+1}$, with $n_i = 1$ for all i, $m_1 = 1$, $m_{e-1} = n - e - 1$. All graphs in these three families have n vertices and diameter $D = n - e$.

Theorem 5.2. *For given integer $e \geq 4$, $\rho_D(D + e) \to \sqrt{2 + \sqrt{5}}$ as $D \to \infty$. Moreover, a minimizer graph with diameter D and $n = D + e$ vertices is in one of the three families $\mathcal{P}_{n,e}$, $\mathcal{P}'_{n,e}$, and $\mathcal{P}''_{n,e}$, for n large enough.*

Proof. Let $e \geq 4$ be fixed. For $n \geq 2e$, take the graph $H_n = P^{m_1,\ldots,m_{e-1}}_{n_1,\ldots,n_{e-1},n-e+1}$, with $n_i = 1$ for all i, $m_i = 1 + (i-1)l$ for $i < e - 1$, $m_{e-1} = n - e - 1$ in $\mathcal{P}''_{n,e}$, where $l = \lfloor \frac{n-e-2}{e-2} \rfloor$. By Corollary 3.10(c), $\lim_{n\to\infty} \rho(H_n) = \sqrt{2 + \sqrt{5}}$ as $\ell(H_n) = \lfloor \frac{n-e-2}{e-2} \rfloor \to \infty$ $(n \to \infty)$ and $t(H_n) = e - 1$. Let G_n be a minimizer graph with n vertices and diameter $D = n - e$. Since $\rho(G_n) \leq \rho(H_n)$ we can take $\epsilon > 0$ such that $\rho(G_n) \leq \rho_1 + \epsilon < \theta_{2,3}$ for n large enough. By Theorem 3.4, G_n is a subgraph of a Laundry graph or an Urchin graph, for n large enough. It then follows that G_n must be a subgraph of a Laundry graph because $D(G_n) = n - e$. Hence G_n is of the form $P^{m_1,\ldots,m_{e-3}}_{n_1,\ldots,n_{e-3},n-e+1}$, with $n_1 = n_{e-3} = 2$, $n_i = 1$ for $1 < i < e - 3$, $m_1 \geq 2$, $m_{e-3} \leq n - e - 2$, or of the form $P^{m_1,\ldots,m_{e-2}}_{n_1,\ldots,n_{e-2},n-e+1}$, with $n_1 = 2$, $n_i = 1$ for $1 < i$, $m_1 \geq 2$, $m_{e-2} \leq n - e - 1$, or of the form $P^{m_1,\ldots,m_{e-1}}_{n_1,\ldots,n_{e-1},n-e+1}$, with $n_i = 1$ for all i, $m_1 \geq 1$, $m_{e-1} \leq n - e - 1$. It then follows from Lemmas 2.1 and 2.4 that the inequalities for the m_i should be equalities, i.e., G_n is in one of the families $\mathcal{P}_{n,e}$, $\mathcal{P}'_{n,e}$, and $\mathcal{P}''_{n,e}$, for n large enough. To finish the proof, we observe that $\rho(G_n) > \sqrt{2 + \sqrt{5}}$ by Theorem 2.7. □

Instead of Conjecture 5.1 we pose the following.

Conjecture 5.3. *For fixed $e \geq 5$, a minimizer graph with n vertices and diameter $D = n - e$ is in the family $\mathcal{P}_{n,e}$, for n large enough.*

Computational results comparing the three families of graphs $\mathcal{P}_{n,e}$, $\mathcal{P}'_{n,e}$, and $\mathcal{P}''_{n,e}$ for $e = 5, ..., 9$ support Conjecture 5.3. For $e = 6$ and $e = 7$ we can be more specific as follows.

Conjecture 5.4. *The graph $P_{2,1,2,n-5}^{2,\lceil (D-1)/2\rceil,D-2}$ is the unique minimizer graph with n vertices and diameter $D = n - 6$, for n large enough.*

Conjecture 5.5. *The graph $P_{2,1,1,2,n-6}^{2,\lfloor (D-2)/3\rfloor,D-\lfloor (D-2)/3\rfloor,D-2}$ is the unique minimizer graph with n vertices and diameter $D = n - 7$, for n large enough.*

Next, we shall prove Conjecture 5.1 for the case $e = 4$. For this, we use the following lemma.

Lemma 5.6. $\rho(P_{k,1,k+m+2}^{k,k+m}) = \rho(P_{1,k-1,1,2m+5}^{1,m+2,2m+3})$ *for $k \geq 2$ and $m \geq 1$.*

Proof. We rewrite the characteristic polynomials of the two graphs as follows. Using Lemma 2.3 with u being the vertex of degree 3 incident to two paths of length k, we obtain that

$$\Phi(P_{k,1,k+m+2}^{k,k+m}) = \Phi(P_k)\left[\Phi(T_{1,1,m+k}) - \Phi(P_{k-1})\Phi(T_{1,1,m-1})\right].$$

Since P_k is a proper subgraph of $P_{k,1,k+m+2}^{k,k+m}$, it follows that $\rho(P_{k,1,k+m+2}^{k,k+m})$ is the largest root of $\Phi(T_{1,1,m+k}) - \Phi(P_{k-1})\Phi(T_{1,1,m-1})$.

Similarly, using Lemma 2.3 with u being the middle vertex of degree 3, we obtain that

$$\Phi(P_{1,k-1,1,2m+5}^{1,m+2,2m+3}) = \Phi(T_{1,1,m})\left[\Phi(T_{1,1,m+k}) - \Phi(P_{k-1})\Phi(T_{1,1,m-1})\right].$$

Since $T_{1,1,m}$ is a proper subgraph of $P_{1,k-1,1,2m+5}^{1,m+2,2m+3}$, it follows that $\rho(P_{1,k-1,1,2m+5}^{1,m+2,2m+3})$ is also the largest root of $\Phi(T_{1,1,m+k}) - \Phi(P_{k-1})\Phi(T_{1,1,m-1})$. This finishes the proof. □

Theorem 5.7. *For $n \geq 11$, the graph $P_{1,2,n-3}^{1,n-6}$ is the unique minimizer graph with n vertices and diameter $n - 4$.*

Proof. Let G_n denote a minimizer graph with n vertices and diameter $n - 4$, for $n \geq 11$. Lemma 2.4 implies that the spectral radius of $P_{1,2,n-3}^{1,n-6}$ is decreasing with n, so that

$$\rho(G_n) \leq \rho(P_{1,2,n-3}^{1,n-6}) \leq \rho(P_{1,2,8}^{1,5}) \approx 2.0684.$$

Thus, by Theorem 2.8, G_n is a dagger, a closed quipu, or an open quipu. However, if G_n is a dagger, then $\rho(G_n) = \rho(T_0(n-4)) \geq \rho(T_0(7)) \approx 2.1203$, which is a contradiction. Also, if G_n is a closed quipu, then it contains as a subgraph $\widehat{C}_s$, where $s \leq 8$ because the diameter of G_n is $n-4$. Thus, in that case $\rho(G_n) \geq \rho(\widehat{C}_s) \geq \rho(\widehat{C}_8) \approx 2.0840$, which is a contradiction too. So G_n must be an open quipu. If G_n is a T-shape tree, then it contains $T_{3,3,3}$ as a subgraph, hence $\rho(G_n) \geq \rho(T_{3,3,3}) \approx 2.0743$, which is again a contradiction.

Thus, it follows that G_n is either of the form $P_{1,2,n-3}^{m_1,m_2}$, with $m_1 \geq 1$ and $m_2 \leq n-6$, or of the form $P_{1,1,1,n-3}^{m_1,m_2,m_3}$, with $m_1 \geq 1$ and $m_3 \leq n-5$. Lemmas 2.1 and 2.4 then imply that equality should hold in the inequalities for the m_i. Thus, G_n is $P_{1,2,n-3}^{1,n-6}$ or of the form $P_{1,1,1,n-3}^{1,m_2,n-5}$ for some m_2. However, by Lemmas 2.4 and 5.6 (for $k = 2, m = n-7$; note that $P_{1,2,n-3}^{1,n-6} = P_{2,1,n-3}^{2,n-5}$), we have that $\rho(P_{1,1,1,n-3}^{1,m_2,n-5}) > \rho(P_{1,1,1,2n-9}^{1,n-5,2n-11}) = \rho(P_{1,2,n-3}^{1,n-6})$, which finishes the proof. □

For the case $e = 5$, the computations in [6] show that $P^{2,n-7}_{2,2,n-4}$ is the unique minimizer graph with n vertices and diameter $D = n - 5$, for $14 \leq n \leq 20$. For the proof of the conjecture for this case, we use the following lemmas to eliminate two families of candidates.

Lemma 5.8. *Let $k \geq 3$. Then $\rho(P^{2,2k-2,3k-2}_{2,1,1,3k}) = \rho(P^{2,2k-2}_{2,2,2k+1}) = \rho(P^{1,k-1,2k-3}_{1,1,1,2k-1})$.*

Proof. Define $G = P^{2,2k-2,3k-2}_{2,1,1,3k}$ and $H = P^{2,2k-2}_{2,2,2k+1}$. By applying Lemma 2.3 (with bridge $2k - 2 \sim 2k - 1$), we obtain that

$$\begin{aligned}\Phi(H) &= \Phi(P_2)[\Phi(T_{2,2,2k-2}) - x\Phi(T_{2,2,2k-5})]\\ &= \Phi(P_2)[\Phi(P_3)\Phi(T_{2,2,2k-5}) - \Phi(P_2)\Phi(T_{2,2,2k-6}) - x\Phi(T_{2,2,2k-5})]\\ &= \Phi(P_2)[(x^3 - 3x)\Phi(T_{2,2,2k-5}) - (x^2 - 1)\Phi(T_{2,2,2k-6})].\end{aligned}$$

By a different application of Lemma 2.3 (with bridge $k - 1 \sim k$), we derive that

$$\begin{aligned}\Phi(H) &= \Phi(T_{2,2,k-3})[\Phi(T_{2,2,k-2}) - \Phi(T_{2,2,k-4})]\\ &= \Phi(T_{2,2,k-3})\Phi(P_2)[\Phi(P_{k+1}) - x\Phi(P_{k-2}) - \Phi(P_{k-1}) + x\Phi(P_{k-4})]\\ &= \Phi(T_{2,2,k-3})\Phi(P_2)[\frac{1}{x}\Phi(T_{1,1,k-1}) - \Phi(T_{1,1,k-4})].\end{aligned}$$

Now it follows that

$$\begin{aligned}&\Phi(H) \cdot \frac{\Phi(T_{1,1,k+1})\Phi(T_{2,2,k-3}) + x\Phi(T_{2,2,2k-6})}{\Phi(P_2)\Phi(T_{2,2,k-3})}\\ =\ &[(x^3 - 3x)\Phi(T_{2,2,2k-5}) - (x^2 - 1)\Phi(T_{2,2,2k-6})]\Phi(T_{1,1,k+1})\\ &+ [\frac{1}{x}\Phi(T_{1,1,k-1}) - \Phi(T_{1,1,k-4})]x\Phi(T_{2,2,2k-6})\\ =\ &(x^3 - 3x)[\Phi(T_{2,2,2k-5})\Phi(T_{1,1,k+1}) - x\Phi(T_{2,2,2k-6})\Phi(T_{1,1,k-1})]\\ =\ &(x^3 - 3x)\Phi(G).\end{aligned}$$

The last equality follows from applying Lemma 2.3 (with bridge $2k - 3 \sim 2k - 2$), whereas the one-but-last follows from the recursive relations of $\Phi(T_{1,1,i})$ that follow from Lemma 2.2.

Because the largest root of H is larger than the largest root of $\Phi(P_2)(x^3 - 3x)\Phi(T_{2,2,k-3})$, it follows that $\rho(G) = \rho(H)$.

From $\Phi(P^{1,k-1,2k-3}_{1,1,1,2k-1}) = \Phi(T_{1,1,k-3})[\Phi(T_{1,1,k-1}) - x\Phi(T_{1,1,k-4})]$, it finally follows that $\rho(H) = \rho(P^{1,k-1,2k-3}_{1,1,1,2k-1})$. □

Lemma 5.9. *Let $2 \leq m_2 \leq 2k - 4$. Then $\rho(P^{1,m_2,2k-3}_{1,1,1,2k-1}) \geq \rho(P^{1,k-1,2k-3}_{1,1,1,2k-1})$ with equality if and only if $m_2 = k - 1$.*

Proof. Let $r = m_2 - 2$ and $s = 2k - 4 - m_2$. Without loss of generality we may assume that $m_2 \leq k - 1$, so that $r \leq s$. Then

$$\begin{aligned}\Phi(P^{1,m_2,2k-3}_{1,1,1,2k-1}) &= x\Phi(P^{1,2k-3}_{1,1,2k-1}) - \Phi(T_{1,1,r})\Phi(T_{1,1,s})\\ &= x\Phi(P^{1,2k-3}_{1,1,2k-1}) - x^2[\Phi(P_{r+2}) - \Phi(P_r)][\Phi(P_{s+2}) - \Phi(P_s)].\end{aligned}$$

Assume that $m_2 < k-1$, so that $r \le s-2$. It follows that

$$\begin{aligned}\Phi(P^{1,m_2+1,2k-3}_{1,1,1,2k-1}) - \Phi(P^{1,m_2,2k-3}_{1,1,1,2k-1}) &= x[\Phi(P_{r+2}) - \Phi(P_r)][(x^2-2)\Phi(P_{s+1}) - 2\Phi(P_{s-1})] \\ &\quad - x[(x^2-2)\Phi(P_{r+2}) - 2\Phi(P_r)][\Phi(P_{s+1}) - \Phi(P_{s-1})] \\ &= x(x^2-4)[\Phi(P_{r+2})\Phi(P_{s-1}) - \Phi(P_r)\Phi(P_{s+1})].\end{aligned}$$

Because $\Phi(P_m) = \frac{\lambda^{m+1}-\lambda^{-m-1}}{\lambda-\lambda^{-1}}$, one can obtain easily that $\Phi(P_{r+2})\Phi(P_{s-1}) \ge \Phi(P_r)\Phi(P_{s+1})$ for any $x \ge 2$ with equality if and only if $r+1=s$. This implies the desired results. □

Lemma 5.10. *Let $n \ge 15$ and $3 \le m_2 \le n-7$. Then $\rho(P^{2,n-7}_{2,2,n-4}) < \rho(P^{2,m_2,n-6}_{2,1,1,n-4})$.*

Proof. Let $G' = P^{2,m_2,n-6}_{2,1,1,n-4}$ for some $3 \le m_2 \le n-7$.

First, let $n = 2k+5$ be odd. In this case, $P^{2,n-7}_{2,2,n-4} = P^{2,2k-2}_{2,2,2k+1} =: H$ and $G' = P^{2,m_2,2k-1}_{2,1,1,2k+1}$. Recall from the previous lemma that $\rho(H)$ is the largest root of $\Phi(T_{2,2,k-2}) - \Phi(T_{2,2,k-4})$.

If $m_2 \le k-1$, then $\rho(G') > \rho(P^{2,m_2}_{2,1,m_2+2}) \ge \rho(P^{2,k-1}_{2,1,k+1}) = \rho(x[\Phi(T_{2,2,k-2}) - \Phi(T_{2,2,k-4})]) = \rho(H)$. If $k \le m_2 \le n-7 = 2k-2$, then subdividing an appropriate number of edges on the internal paths of G' gives the graph $P^{2,2k-2,3k-2}_{2,1,1,3k}$. Thus, $\rho(G') > \rho(P^{2,2k-2,3k-2}_{2,1,1,3k})$. From the previous lemma we have that $\rho(P^{2,2k-2,3k-2}_{2,1,1,3k}) = \rho(H)$ which implies $\rho(G') > \rho(H)$ in this case as well. This proves the assertion for n odd.

Next, let $n = 2k+6$ be even. If $m_2 = n-7$, then G' is obtained from $P^{2,n-7}_{2,2,n-4}$ by replacing one edge and it follows easily (cf. [4, Thm. 6.4.7]) that $\rho(P^{2,n-7}_{2,2,n-4}) < \rho(G')$. Assume finally that $m_2 \le n-8 = 2k-2$, and let $H = P^{2,2k-2}_{2,2,2k+1}$. Because $n > 2k+5$, it follows that $\rho(H) > \rho(P^{2,n-7}_{2,2,n-4})$. Similar as in the case where n is odd, one can now show that $\rho(G') > \rho(H)$, which finishes the proof. □

Lemma 5.11. *Let $n \ge 15$ and $2 \le m_2 < m_3 \le n-7$. Then $\rho(P^{2,n-7}_{2,2,n-4}) < \rho(P^{1,m_2,m_3,n-6}_{1,1,1,1,n-4})$.*

Proof. If $m_2 = 2$, then $P^{1,m_2,m_3,n-6}_{1,1,1,1,n-4}$ is obtained from $P^{2,m_3,n-6}_{2,1,1,n-4}$ by replacing one edge, and as before, it follows that $\rho(P^{1,m_2,m_3,n-6}_{1,1,1,1,n-4}) > \rho(P^{2,m_3,n-6}_{2,1,1,n-4})$. The required result now follows from the previous lemma. Similarly, the result follows if $m_3 = n-7$.

Assume now that $n = 2k+5$ is odd. Since we may assume that $m_3 \le n-8 = 2k-3$, we obtain that

$$\rho(P^{1,m_2,m_3,n-6}_{1,1,1,1,n-4}) > \rho(P^{1,m_2,m_3}_{1,1,1,m_3+2}) \ge \rho(P^{1,m_2,2k-3}_{1,1,1,2k-1}) \ge \rho(P^{1,k-1,2k-3}_{1,1,1,2k-1}) = \rho(P^{2,n-7}_{2,2,n-4}),$$

among others by using Lemmas 5.9 and 5.8.

Assume next that $n = 2k+6$ even. If $m_3 \le n-9$, then similar as above, we obtain that

$$\rho(P^{1,m_2,m_3,n-6}_{1,1,1,1,n-4}) > \rho(P^{1,m_2,m_3}_{1,1,1,m_3+2}) \ge \rho(P^{1,m_2,2k-3}_{1,1,1,2k-1}) \ge \rho(P^{1,k-1,2k-3}_{1,1,1,2k-1}) = \rho(P^{2,n-8}_{2,2,n-5}) > \rho(P^{2,n-7}_{2,2,n-4}).$$

By symmetry, the result follows if $m_2 \ge 4$.

The only case left is when $m_2 = 3$ and $m_3 = n-8$. For this case, we claim that $\rho(P^{1,3,n-8,n-6}_{1,1,1,1,n-4}) > \rho(P^{2,n-8,n-6}_{2,1,1,n-4})$, which together with the previous lemma settles the proof. To prove the claim, we note that by Lemma 2.3, we have that

$$\begin{aligned}\Phi(P^{1,3,n-8,n-6}_{1,1,1,1,n-4}) &= \Phi(T_{1,1,3})\Phi(P^{1,3}_{1,1,n-8}) - x\Phi(T_{1,1,1})\Phi(P^{1,3}_{1,1,n-9}), \\ \Phi(P^{2,n-8,n-6}_{2,1,1,n-4}) &= \Phi(T_{2,2,1})\Phi(P^{1,3}_{1,1,n-8}) - \Phi(P_5)\Phi(P^{1,3}_{1,1,n-9}).\end{aligned}$$

After working out the technical details, we obtain that

$$\Phi(P_{2,1,1,n-4}^{2,n-8,n-6}) - \Phi(P_{1,1,1,1,n-4}^{1,3,n-8,n-6}) = -\Phi(P_{1,1,n-8}^{1,3}) + (x^3 - 3x)\Phi(P_{1,1,n-9}^{1,3}).$$

For $x \geq \rho(P_{2,1,1,n-4}^{2,n-8,n-6}) > 2$, it follows that

$$\Phi(P_{2,1,1,n-4}^{2,n-8,n-6}) - \Phi(P_{1,1,1,1,n-4}^{1,3,n-8,n-6}) > -\Phi(P_{1,1,n-8}^{1,3}) + x\Phi(P_{1,1,n-9}^{1,3}) = \Phi(P_{1,1,n-10}^{1,3}) > 0,$$

and the claim follows. □

Theorem 5.12. *For $n \geq 18$, the graph $P_{2,2,n-4}^{2,n-7}$ is the unique minimizer graph with n vertices and diameter $n-5$.*

Proof. Let G_n denote a minimizer graph with n vertices and diameter $n-5$, for $n \geq 18$. Similar as before, we have that

$$\rho(G_n) \leq \rho(P_{2,2,n-4}^{2,n-7}) \leq \rho(P_{2,2,14}^{2,11}) \approx 2.0710.$$

Thus, by Theorem 2.8, G_n is a dagger, a closed quipu, or an open quipu. By the same arguments as in Theorem 5.7, G_n cannot be a dagger or a T-shape tree. If G_n is a closed quipu, then it contains as a subgraph $\widehat{C}_s$, where $s \leq 10$ because the diameter of G_n is $n-5$. Thus, in that case $\rho(G_n) \geq \rho(\widehat{C}_s) \geq \rho(\widehat{C}_{10}) \approx 2.0743$, which is a contradiction. So G_n must be an open quipu, but not a T-shape tree.

Similar as before, it follows that G_n is $P_{2,2,n-4}^{2,n-7}$ or of the form $P_{1,2,1,n-4}^{1,m_2,n-6}$ for some m_2, or of the form $P_{2,1,1,n-4}^{2,m_2,n-6}$ for some m_2, or of the form $P_{1,1,1,1,n-4}^{1,m_2,m_3,n-6}$ for some m_2 and m_3.

However, by Lemmas 2.4, 5.6 (for $k=3, m=n-8$), and 2.1, we have that $\rho(P_{1,2,1,n-4}^{1,m_2,n-6}) > \rho(P_{1,2,1,2n-11}^{1,n-6,2n-13}) = \rho(P_{3,1,n-3}^{3,n-5}) > \rho(T_{3,3,3}) \approx 2.0743$, so G_n cannot be of the form $P_{1,2,1,n-4}^{1,m_2,n-6}$.

By Lemma 5.10, G_n cannot be of the form $P_{2,1,1,n-4}^{2,m_2,n-6}$, and by Lemma 5.11, it cannot be of the form $P_{1,1,1,1,n-4}^{1,m_2,m_3,n-6}$. Thus, G_n must be $P_{2,2,n-4}^{2,n-7}$. □

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