Graphs of order $n$ and diameter $2(n - 1)/3$ minimizing the spectral radius

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Abstract

The spectral radius of a graph is the largest eigenvalue of its adjacency matrix. A minimizer graph is such that minimizes the spectral radius among all connected graphs on $n$ vertices with diameter $d$. The minimizer graphs are known for $d \in \{1, 2\} \cup \{n/2, 2n/3 - 1\} \cup \{n - k \mid k = 1, 2, ..., 8\}$. In this paper, we determine all minimizer graphs for $d = 2(n - 1)/3$.

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1 Introduction

All graphs considered in this paper are undirected and simple. Let $G$ be a graph. The greatest distance between any two vertices in $G$ is the diameter of $G$, denoted by $d(G)$, or simply by $d$. An internal path of a graph is a path whose internal vertices have degree 2 and the two end vertices have degree at least 3. An internal path is closed if its two end vertices coincide. The characteristic polynomial of $G$, simply denoted by $\phi_G$, is defined by $\phi_G(\lambda) = \det(\lambda I - A(G))$, where $A(G)$ is the adjacency matrix of $G$ and $I$ is an identity matrix. The largest root of $\phi_G$ is the spectral radius of $G$, denoted by $\rho(G)$.

Hoffman and Smith [6, 7, 12] completely determined all connected graphs $G$ with $\rho(G) \leq 2$. Cvetković et al. [3], Brouwer and Neumaier [11] characterized all connected graphs $G$ with $2 < \rho(G) \leq \sqrt{2 + \sqrt{5}}$.

Figure 1: A dagger

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A **dagger** is obtained by adding a pendent path to the center of a star of order 4, see Figure 1; an **open quipu** is a tree with maximum degree 3 such that all vertices of degree 3 lie on a path; a **closed quipu** is a unicyclic graph with maximum degree 3 such that all vertices of degree 3 lie on the cycle. An open (or closed) quipu can be written in the form of $P^{(m_0,m_1,...,m_r)}_{(k_0,k_1,...,k_r,k_{r+1})}$ (or $C^{(m_1,...,m_r)}_{(k_1,...,k_r)}$) with all $k_i, m_i \geq 0$ and $r \geq 0$ (or $r \geq 1$), where for $r \geq 1$ and $1 \leq i \leq r$, $k_i$ measures the number of internal vertices on the $i$th internal path, while $k_0, k_{r+1}, m_0$ and $m_i$ stand for the lengths of the indicated pendent paths respectively, see Figures 2 and 3. These terminologies were first introduced by Woo and Neumaier [14] for the following result.

![Figure 2: The open quipu $P^{(m_0,m_1,...,m_r)}_{(k_0,k_1,...,k_r,k_{r+1})}$](image)

![Figure 3: The closed quipu $C^{(m_1,...,m_r)}_{(k_1,...,k_r)}$](image)

**Lemma 1.1** [14] A graph $G$ whose spectral radius satisfies $2 < \rho(G) \leq 3/\sqrt{2}$ is either an open quipu, a closed quipu, or a dagger.

A **minimizer** graph of order $n$ with diameter $d$ is such a graph that has the minimal spectral radius among all simple connected graphs on $n$ vertices with diameter $d$. The problem to determine the minimizer graphs was raised by van Dam and Kooij [5] concerning a model of virus propagation in networks. They solved this problem explicitly for $d \in \{1, 2, \lfloor n/2 \rfloor, n-3, n-2, n-1\}$, where the minimizer graph is a complete graph for $d = 1$, a star for $d = 2$ and $n$ large enough, a cycle for $d = \lfloor n/2 \rfloor$ and $n > 6$, a path for $d = n-1$, $P^{(1)}_{(1,n-3)}$ for $d = n-2$, and $P^{(1,1)}_{(1,n-6,1)}$ for $d = n-3$. All the minimizer graphs on $n \leq 20$ vertices were also obtained in [5].
Lemma 2.2 Let \( G \) be a graph. Then the following statements hold.

1. If \( G_2 \) is a proper subgraph of \( G_1 \), then \( \rho(G_1) > \rho(G_2) \).
2. If \( G_1 \) is connected and \( G_2 \) is a proper spanning subgraph of \( G_1 \), then \( \rho(G_1) > \rho(G_2) \) and \( \phi_{G_2}(\lambda) > \phi_{G_1}(\lambda) \) for all \( \lambda \geq \rho(G_1) \).
3. If \( \phi_{G_2}(\lambda) > \phi_{G_1}(\lambda) \) for all \( \lambda \geq \rho(G_1) \), then \( \rho(G_2) < \rho(G_1) \).
4. If $\phi_{G_1}(\rho(G_2)) < 0$, then $\rho(G_1) > \rho(G_2)$.

**Lemma 2.3** [7] Let $uv$ be an edge of a connected graph $G$ of order $n$, and denote by $G_{u,v}$ the graph of order $n+1$ obtained from $G$ by subdividing the edge $uv$ once, i.e., replacing the edge $uv$ by a new vertex $w$ and two new edges $uw,vw$. Then the following two properties hold.

(i) If $uv$ does not belong to an internal path of $G$ and $G \neq C_n$, then $\rho(G_{u,v}) > \rho(G)$.

(ii) If $uv$ belongs to an internal path of $G$ and $G \neq P_{(1,1)}^{(1,n-6,1)}$, then $\rho(G_{u,v}) < \rho(G)$.

The following lemma indicates the effect of edge transfers on the spectral radii of graphs. The result for $k-l \geq j$ were stated in [10] without a proof. For completeness, we include a proof here.

**Lemma 2.4** [10] Let $j,k \geq 0$ and $l > 0$ be integers. Let $u$ and $v$ be two vertices (possibly $u = v$ for $j = 0$) of degree at least 2 and connected by an induced path of length $j$ in a graph $G$. Denote by $G^{(j)}_{k,l}$ the graph obtained from $G$ by adding two pendant paths of lengths $k$ and $l$ to vertices $u$ and $v$ respectively, see Figure 4. If $k-l \geq j-1$, then

$$
\phi_{G^{(j)}_{k,l}}(\lambda) \leq \phi_{G^{(j)}_{k+1,l-1}}(\lambda) \text{ for } \lambda \geq \rho(G^{(j)}_{k+1,l-1}), \tag{1}
$$

$$
\rho(G^{(j)}_{k,l}) \geq \rho(G^{(j)}_{k+1,l-1}), \tag{2}
$$

with each equality if and only if $j = 0$ and $k = l - 1$.

![Figure 4: The graph $G^{(j)}_{k,l}$](image)

**Proof.** The strict inequalities in Eqs. (1) and (2) for $j = 0$ and $k-l \geq 0$ were proven in [10, Theorem 5]. It is easy to see that the equalities hold if $j = 0$ and $k = l - 1$ since the two graphs $G^{(0)}_{l-1,l}$ and $G^{(0)}_{l,l-1}$ are isomorphic. Now we assume $j > 0$ and then $u \neq v$. Applying Lemma 2.1, we have

$$
\phi_{G^{(j)}_{k,l}} - \phi_{G^{(j)}_{k+1,l-1}} = \lambda \phi_{G^{(j)}_{k+1,l-1}} - \phi_{G^{(j)}_{k+1,l-2}} - \left(\lambda \phi_{G^{(j)}_{k+1,l-2}} - \phi_{G^{(j)}_{k+1,l-1}}\right).
$$

$$
= \phi_{G^{(j)}_{k-1,l-1}} - \phi_{G^{(j)}_{k-1,l-2}} = \ldots
$$

$$
= \phi_{G^{(j)}_{k-l+1,1}} - \phi_{G^{(j)}_{k-l+2,0}} = \phi_{G^{(j)}_{k-l,0}} - \phi_{G^{(j)}_{k-l+1,0} - v}.
$$

The graph $G^{(j)}_{k-l+1,0} - v$ has two pendant paths of lengths $k-l+1$ and $j-1$ at the vertex $u$. Deleting these two pendant paths results in a subgraph $H$ and $G^{(j)}_{k-l+1,0} - v = H^{(0)}_{k-l+1,j-1}$.
Suppose that $k - l \geq j - 1$. Applying this lemma to $H_{k-l,j}^{(0)}$, we have

$$
\phi_{H_{k-l,j}^{(0)}}(\lambda) \leq \phi_{H_{k-l+1,j-1}^{(0)}}(\lambda) = \phi_{G_{k-l+1,0}^{(j)}}(\lambda) \text{ for } \lambda \geq \rho(G_{k-l+1,0}^{(j)} - v),
$$

$$
\rho(H_{k-l,j}^{(0)}) \geq \rho(G_{k-l+1,0}^{(j)} - v).
$$

Note that the graph $H_{k-l,j}^{(0)}$ is isomorphic to a proper spanning subgraph of $G_{k-l,0}^{(j)}$. By Lemma 2.5 we get

$$
\phi_{G_{k,l}^{(j)}}(\lambda) - \phi_{G_{k+1,l-1}^{(j)}}(\lambda) \leq \phi_{G_{k-l,0}^{(j)}}(\lambda) - \phi_{H_{k-l,j}^{(0)}}(\lambda) < 0,
$$

for $\lambda \geq \rho(G_{k-l,0}^{(j)})$, which implies that $\rho(G_{k+1,l-1}^{(j)}) > \rho(G_{k-l,0}^{(j)})$. □

Woo and Neumaier [14] noted that no (finite) graph has spectral radius exactly $3/\sqrt{2}$ since this is not an algebraic integer. A dagger on vertices with diameter $n-3$ and its spectral radius approaches increasingly to $3/\sqrt{2}$ as $n$ goes to infinity. However, some quipus have spectral radii greater than $3/\sqrt{2}$. Lemma 2.1 was refined in [8] as follows.

**Lemma 2.5** [8] Let $G$ be a graph on $n$ vertices ($n \geq 13$) with spectral radius less than $3/\sqrt{2}$. If $G$ is an open quipu then its diameter $d$ satisfies $d \geq (2n - 4)/3$, where the bound is tight. If $G$ is a closed quipu then its diameter $d$ satisfies $n/3 < d \leq 2(n - 1)/3$, where the lower bound is asymptotically tight and only the closed quipu $C_{(k)}^{(0)}$ with $d = 2k + 2$ and $n = 3k + 4$ takes the upper bound.

Let $\delta_1(x)$ be the indicator function of being 1, i.e., $\delta_1(x) = 1$ if $x = 1$ and 0 otherwise. The following lemmas from [8] give necessary conditions for open quipus with spectral radius at most $3/\sqrt{2}$.

**Lemma 2.6** Suppose an open quipu $P_{(m_0, m_1, \ldots, m_r)}^{(m_0, m_1, \ldots, m_r)}$ (with $r \geq 2$) has spectral radius less than $3/\sqrt{2}$. Then the following statements hold.

1. For $2 \leq i \leq r - 1$, we have $k_i \geq m_{i-1} + m_i + 1 - \left[ \frac{\delta_1(m_{i-1}) + \delta_1(m_i)}{2} \right]$.

2. We have $k_1 \geq m_0 + m_1 - \left[ \frac{3\delta_1(m_0) + \delta_1(m_1)}{2} \right] - \left[ \frac{\delta_1(m_0-1) + \delta_1(m_1-1)}{2} \right]$.

3. We have $k_r \geq m_r + m_{r-1} - \left[ \frac{3\delta_1(m_r) + \delta_1(m_{r-1})}{2} \right] - \left[ \frac{\delta_1(m_r-1) + \delta_1(m_{r-1}-1)}{2} \right]$.

**Lemma 2.7** Suppose that an open quipu $P_{(m_0, m_1, \ldots, m_r)}^{(m_0, m_1, \ldots, m_r)}$ (with $r \geq 2$) satisfies

1. $k_i \leq m_{i-1} + m_i + 2 - \left[ \frac{\delta_1(m_{i-1}) + \delta_1(m_i)}{2} \right]$ for $2 \leq i \leq r - 1$;

2. $k_1 \leq m_0 + m_1 - \left[ \frac{3\delta_1(m_0) + \delta_1(m_1) + \delta_1(m_0-1)}{2} \right]$.

3. $k_r \leq m_r + m_{r-1} - \left[ \frac{3\delta_1(m_r) + \delta_1(m_{r-1}) + \delta_1(m_r-1)}{2} \right]$.

Then we have $\rho(P_{(m_0, m_1, \ldots, m_r)}^{(m_0, m_1, \ldots, m_r)}) > 3/\sqrt{2}$. 

5
Denote by $\rho_k$ the spectral radius of $P_{(k,k)}^{(k)}$. Then $\rho_1 = \sqrt{3}$ and $\rho_2 = 2$. Note that $P_{(k,k)}^{(k+1)}$ is a proper subgraph of $P_{(k+1,k+1)}^{(k+1)}$. By Lemma 2.2 and [14, Lemma 3], we have

$$\rho_k < \rho_{k+1} < 3/\sqrt{2}.$$  \hspace{1cm} (3)

Moreover, the following lemma from [8] shows that the graphs we desire in Theorem 1.1 share the same spectral radius.

**Lemma 2.8** [8] For any non-negative integers $i, j$ satisfying $i + j \geq 2$, all open quipus $P_{(i,j)}^{(i-1,j-1)}$ and all closed quipus $C_{(i+j+1,i+j+1)}^{(i+j+1,i+j+1)}$ have the same spectral radius $\rho_{i+j}$.

Let $v$ be a vertex of graph $G$. In [9], a rooted graph $(G, v)$ was defined as the graph $G$ together with the designated vertex $v$ as a root, and we introduced two parameters $p_{(G,v)}$ and $q_{(G,v)}$ satisfying

$$\phi_G = p_{(G,v)} + q_{(G,v)},$$

$$\phi_{G-v} = x_2 p_{(G,v)} + x_1 q_{(G,v)}.$$  \hspace{1cm} (4)

Here $x_1$ and $x_2$ are the two roots of the equation $x^2 - \lambda x + 1 = 0$, namely

$$x_1 = \frac{\lambda - \sqrt{\lambda^2 - 4}}{2} \quad \text{and} \quad x_2 = \frac{\lambda + \sqrt{\lambda^2 - 4}}{2}.$$  \hspace{1cm} (5)

The fact $x_1 + x_2 = \lambda$, $x_1 x_2 = 1$ will be used deliberately. In this paper, we always assume $\lambda > 2$, then $x_1 < 1 < x_2$. Thus $p_{(G,v)}$ and $q_{(G,v)}$ are well defined, and

$$\left(\begin{array}{c} p_{(G,v)} \\ q_{(G,v)} \end{array}\right) = \frac{1}{x_2 - x_1} \left(\begin{array}{cc} -x_1 & 1 \\ x_2 & -1 \end{array}\right) \left(\begin{array}{c} \phi_G \\ \phi_{G-v} \end{array}\right).$$

Let $P_n$ denote a path of order $n$. As an example in [8, Section 2.2], we have

$$\left(\begin{array}{c} p_{(P_{2k+1},v)} \\ q_{(P_{2k+1},v)} \end{array}\right) = \frac{x_2^{k+1} - x_1^{k+1}}{(x_2 - x_1)^3} \left(\begin{array}{cc} x_2^{k-1} - 2x_1^{k+1} + x_1^{k+3} \\ x_1^{k-1} - 2x_2^{k+1} + x_2^{k+3} \end{array}\right).$$  \hspace{1cm} (6)

where $*$ stands for the center of the odd path $P_{2k+1}$ for $k \geq 0$.

Let $t_{(G,v)} := q_{(G,v)}/p_{(G,v)}$. It was shown in [9] that $t_{(G,v)}$ plays an important role on the spectral radii of open quipus.

**Lemma 2.9** Let $u$ and $v$ be the roots of $P_{(1,3)}^{(1)}$ and $P_{(2,1)}^{(2)}$ respectively as shown in Figure 5. Then we have

$$t\left(\frac{P_{(1,3),u}^{(1)}}{P_{(2,1),v}^{(2)}}\right)(\lambda) < t\left(\frac{P_{(2,1),v}^{(2)}}{P_{(1,3),u}^{(1)}}\right)(\lambda) \text{ for } \lambda > 2.$$  \hspace{1cm} (7)

Figure 5: Two rooted graphs $(P_{(1,3),u}^{(1)})$ and $(P_{(2,1),v}^{(2)})$
Proof. By \(9\) Lemma 2.6] and Eq. (4), we have

\[
\frac{P_{(1,3)}(u)}{Q_{(1,3)}(u)} = \frac{1}{x_2 - x_1} \left( \frac{\lambda - x_1^3}{-x_2} + \frac{x_1^2 - \lambda}{x_2} \right) \left( x_1 \ 0 \right) \left( x_2 \ 0 \right) \left( \frac{P_{(3,i)}}{Q_{(3,i)}} \right)
\]

\[
= \frac{\lambda}{x_2 - x_1} \left( \frac{\lambda - x_1^3}{x_2} + \frac{x_2^3}{x_2} \right),
\]

and

\[
\left( \begin{array}{c}
\frac{P_{(2,1)}(u)}{Q_{(2,1)}(u)}
\end{array} \right) = \left( \begin{array}{cc}
x_1 & 0 \\
0 & x_2
\end{array} \right) \left( \frac{P_{(3,i)}}}{Q_{(3,i)}} \right) = \frac{\lambda^2 - 1}{x_2 - x_1} \left( \frac{\lambda - x_1^3}{x_2} + \frac{x_2^3}{x_2} \right).
\]

Thus we obtain

\[
t_{(1,3)}(\lambda) = \frac{(x_2^3 - \lambda)x_2^3 - x_1^2}{(\lambda - x_1^3)x_2^3 + x_2^3}
\]

\[
t_{(2,1)}(\lambda) = \frac{(x_2^3 - \lambda)x_2^3}{(\lambda - x_1^3)x_2^3}
\]

It follows that Eq. (5) is equivalent to

\[
\frac{(x_2^3 - \lambda)x_2^3 - x_1^2}{(\lambda - x_1^3)x_2^3 + x_2^3} < \frac{(x_2^3 - \lambda)x_2^3}{(\lambda - x_1^3)x_2^3},
\]

namely,

\[
(x_2^3 - \lambda)(\lambda - x_1^3) - (x_2 - x_1) < (x_2^3 - \lambda)x_2^3 + (\lambda - x_1^3)x_1^3,
\]

which holds by the following easy calculation,

\[
(x_2^3 - \lambda)(\lambda - x_1^3)(x_2 - x_1) = \left[ \lambda(x_2^3 + x_1^3) - \lambda^2 - 1 \right] (x_2 - x_1)
\]

\[
< \left[ (x_2^3 + x_1^3)^2 - \lambda^2 - 1 \right] (x_2 - x_1)
\]

\[
= (x_2^6 + x_1^6 - x_2^6 - x_2^6 - x_2^6 - 1)(x_2 - x_1)
\]

\[
= x_2^7 - x_2^5 + x_1^3 - x_1^5 - x_1^7
\]

\[
= (x_2^3 - \lambda)x_2^4 + (\lambda - x_1^3)x_1^4,
\]

where the inequality holds by

\[
x_1^3 + x_2^3 = (x_1 + x_2) (x_2^2 - x_1x_2 + x_2^2) = \lambda [(x_1 - x_2)^2 + 1] > \lambda > 2.
\]

The proof is complete. \( \square \)

For a vertex \( v \) of graph \( G \), denote by \( (G, v, i) \) \( (i \geq 0) \) the graph obtained from \( G \) by adding a pendent path of length \( i \) to \( v \). It is clear that \( (G, v) \) can be regarded as \( (G, v, 0) \). Let \( u \) be the other end of the pendent path in \( (G, v, i) \), then by \(9\) Lemma 2.6 (1)],

\[
\phi_{(G, v, i)} = (1, 1) \left( \frac{P_{(G, v, i), u}}{Q_{(G, v, i), u}} \right) = (1, 1) \left( \begin{array}{cc}
x_1 & 0 \\
0 & x_2
\end{array} \right)^i \left( \frac{P_{(G, v)}}{Q_{(G, v)}} \right) = x_1^i P_{(G, v)} + x_2^i Q_{(G, v)}.
\]

Let \( \alpha_{(G, v, i)} := \phi_{(G, v, i+1)} / \phi_{(G, v, i)} \), then the following equality holds accordingly,

\[
\alpha_{(G, v, i)} = \frac{\phi_{(G, v, i+1)}}{\phi_{(G, v, i)}} = \frac{x_1^{i+1} P_{(G, v)} + x_2^{i+1} Q_{(G, v)}}{x_1^i P_{(G, v)} + x_2^i Q_{(G, v)}} = \frac{x_1^{i+1} + x_2^{i+1}}{x_1^i + x_2^i} t_{(G, v)}.
\]
For convenience, we write $\alpha_{(G,v)}$ for $\alpha_{(G,v,0)}$. Let $(G_i, v_i)$ be a (possibly empty) rooted graph for $i = 1, 2, 3$, and let $T_{G_1, G_3}^{G_2}$ be the graph shown in Figure 6. We have the following lemma, which indicates that the spectral radius of $T_{G_1, G_3}^{G_2}$ decreases as $\alpha_{(G_i,v_i)}$ (also $t_{(G_i,v_i)}$) increases for $i = 1, 2, 3$.

**Lemma 2.10** The spectral radius $\rho\left(T_{G_1, G_3}^{G_2}\right)$ is the largest root of the equation

$$\alpha_{(G_2,v_2)} = \frac{1}{\alpha_{(G_1,v_1)}} + \frac{1}{\alpha_{(G_3,v_3)}}. \quad (7)$$

Moreover, let $(G'_i, v'_i)$ be a rooted graph for $i = 1, 2$, then the following holds.

- If $\alpha_{(G_1,v_1)} \left(p\left(T_{G_1, G_3}^{G_2}\right)\right) > \alpha_{(G_i', v'_i)} \left(p\left(T_{G_1, G_3}^{G_2}\right)\right)$, then $p\left(T_{G_1, G_3}^{G_2}\right) < p\left(T_{G_1, G_3}^{G_2}\right)$.
- If $\alpha_{(G_2,v_2)} \left(p\left(T_{G_1, G_3}^{G_2}\right)\right) > \alpha_{(G_2', v'_2)} \left(p\left(T_{G_1, G_3}^{G_2}\right)\right)$, then $p\left(T_{G_1, G_3}^{G_2}\right) < p\left(T_{G_1, G_3}^{G_2}\right)$.

**Lemma 2.10** readily implies the following result.

**Corollary 2.1** For any pair of graphs $G_1$ and $G_2$, $\rho\left(T_{G_1, G_1}^{G_2}\right) = \rho\left(T_{G_2, G_2}^{G_2}\right)$.

**Proof of Lemma 2.10** By Lemma 2.1, we have

$$\phi_{T_{G_1, G_3}^{G_2}} = \phi_{(G_1,v_1,1)}\phi_{(G_2,v_2,1)}\phi_{(G_3,v_3,1)} - \phi_{(G_1,v_1,1)}\phi_{(G_2,v_2,1)}\phi_{(G_3,v_3,1)} - \phi_{(G_1,v_1,1)}\phi_{(G_2,v_2,1)}\phi_{(G_3,v_3,1)} - \phi_{(G_2,v_2,1)}\phi_{(G_3,v_3,1)}\left(\alpha_{(G_2,v_2)} - \frac{1}{\alpha_{(G_1,v_1)}} - \frac{1}{\alpha_{(G_3,v_3)}}\right).$$

The graphs $G_2$, $(G_1,v_1,1)$, and $(G_3,v_3,1)$ have spectral radius all less than $\rho\left(T_{G_1, G_3}^{G_2}\right)$ since they are proper subgraphs of $T_{G_1, G_3}^{G_2}$. Thus, $\rho\left(T_{G_1, G_3}^{G_2}\right)$ must be the largest root of Eq. (7). The rest of the lemma follows easily from Lemma 2.2.

### 3 Proof of main theorem

**Proof of Theorem 1.1** The theorem holds for $n := 3k + 1 \leq 20$ as checked in [5]. So we can assume that $n > 20$ and $k > 6$. Lemma 2.8 together with Eq. (8) implies that all graphs stated in the theorem have the same spectral radius $\rho_k \in (2, 3/\sqrt{2})$.

By Lemma 2.9, the only closed quipu with diameter $2(n - 1)/3$ and spectral radius less than $3/\sqrt{2}$ is $C_{(2k+1)}^{(k-1)}$. By Lemmas 2.3 and 2.2 and Corollary 2.1, we get

$$\rho\left(C_{(2k+1)}^{(k-1)}\right) > \rho\left(C_{(2k+2)}^{(k-1)}\right) > \rho\left(P_{(k+1,k+1)}^{(k-1)}\right) = \rho\left(P_{(k,k)}^{(k)}\right) = \rho_k.$$
This shows that $C_{(2k+1)}^{(k-1)}$ cannot be a minimizer graph. Note that a dagger of order $n$ has diameter $n - 3 > 2(n - 1)/3$ for $n > 11$. Then by Lemma 1.1 any minimizer graph must be an open quipu with spectral radius less than $3/\sqrt{2}$, which can be written as $P_{(m_0,m_1,\ldots,m_r)}$. Counting the number of vertices and the diameter, we have

$$3k = n - 1 = m_0 + m_r + \sum_{j=0}^{r} m_j + \sum_{i=1}^{r} k_i + r, \quad (8)$$

$$2k = m_0 + m_r + \sum_{i=1}^{r} k_i + r. \quad (9)$$

By Lemma 2.6 we also have

$$l_1 := k_1 + 2 - m_0 - m_1 \geq 0, \quad (10)$$

$$l_r := k_r + 2 - m_{r-1} - m_r \geq 0, \quad \text{and} \quad (11)$$

$$l_i := k_i - m_{i-1} - m_i \geq 0 \text{ for } 2 \leq i \leq r - 1. \quad (12)$$

Summing up these equalities and applying Eqs. (8) and (9), we obtain

$$\sum_{j=1}^{r} l_j = \sum_{i=1}^{r} k_i - m_0 - m_r - 2 \sum_{l=1}^{r-1} m_l + 4$$

$$= 3 \left( m_0 + m_r + \sum_{i=1}^{r} k_i + r \right) - 2 \left( m_0 + m_r + \sum_{j=0}^{r} m_j + \sum_{i=1}^{r} k_i + r \right) + 4 - r$$

$$= 4 - r.$$

This implies that $r \leq 4$. We will show that all open quipus with $r > 1$ internal paths must have spectral radius greater than $\rho_k$, which implies the right minimizer graphs as desired in the theorem. For this purpose, those open quipus with spectral radius at most $3/\sqrt{2}$ need only to be considered. One can check that Lemmas 2.6 and 2.7 exclude most open quipus for minimizer graphs except those shown in Figure 7 whose spectral radii, however, are indeed greater than $\rho_k$, as proven in the following.

**Case 1** $r = 2$. In this case, $l_1 + l_2 = 2$. By symmetry, we have the following two subcases.

**Subcase 1.1** $l_1 = 0$ and $l_2 = 2$.

Eqs. (10) and (11) imply that

$$k_1 = m_0 + m_1 - 2,$$

$$k_2 = m_1 + m_2.$$

Then by Lemma 2.6 (2), we have

$$\left\lceil \frac{3\delta_1(m_0) + \delta_1(m_1)}{2} \right\rceil + \left\lceil \frac{\delta_1(m_0 - 1) + \delta_1(m_1 - 1)}{2} \right\rceil \geq 2.$$

It follows that $m_0 = 1$. Also by Lemma 2.7

$$\left\lceil \frac{3\delta_1(m_2) + \delta_1(m_1) + \delta_1(m_2 - 1)}{2} \right\rceil > 0,$$
Then by Lemma 2.6, it follows that all open quipus $P_{(m_0, k_1, k_2, m_2)}^{(m_0, m_1, m_2)}$, except $P_{(1, k-3, k-1, 1)}^{(1, k-2, 1)}$, $P_{(1, k-4, k-1, 2)}^{(1, k-3, 2)}$, and $P_{(1, 1, k-2)}^{(1, 1, k-2)}$ shown in Figure 7(a), have spectral radius greater than $3/\sqrt{2}$. By Lemmas 2.4 and 2.8, however, we have
\[
\rho\left(P_{(1, k-2, 1)}^{(1, k-3, k-1, 1)}\right) > \rho\left(P_{(1, k-1)}^{(1, k-1, k-1)}\right) = \rho_k,
\]
\[
\rho\left(P_{(1, k-3, 2)}^{(1, k-4, k-1, 2)}\right) > \rho\left(P_{(2, k-2)}^{(2, k-1, k-2)}\right) = \rho_k,
\]
\[
\rho\left(P_{(1, 1, k-2)}^{(1, 1, k-2)}\right) > \rho\left(P_{(2, k-2)}^{(2, k-1, k-2)}\right) = \rho_k.
\]

**Subcase 1.2** $l_1 = 1$ and $l_2 = 1$.

Eqs. (10) and (11) imply that
\[
k_1 = m_0 + m_1 - 1,
\]
\[
k_2 = m_1 + m_2 - 1.
\]

Then by Lemma 2.6
\[
\left[\frac{3\delta_1(m_0) + \delta_1(m_1)}{2}\right] + \left[\frac{\delta_1(m_0 - 1) + \delta_1(m_1 - 1)}{2}\right] \geq 1,
\]
\[
\left[\frac{3\delta_1(m_2) + \delta_1(m_1)}{2}\right] + \left[\frac{\delta_1(m_2 - 1) + \delta_1(m_1 - 1)}{2}\right] \geq 1.
\]

It follows that $m_0 = m_2 = 1$ or $m_1 = 1$ since $n > 20$. Also by Lemma 2.7
\[
\left[\left[3\delta_1(m_0) + \delta_1(m_1) + \delta_1(m_0 - 1)\right]/2\right] > 1, \text{ or}
\]
\[
\left[\left[3\delta_1(m_2) + \delta_1(m_1) + \delta_1(m_2 - 1)\right]/2\right] > 1.
\]

It follows that $m_0 = 1$ or $m_2 = 1$. Therefore, combining with Eqs. (8) and (9), we obtain that all open quipus $P_{(m_0, k_1, k_2, m_2)}^{(m_0, m_1, m_2)}$, except $P_{(1, k-2, 1)}^{(1, k-2, k-2, 1)}$ and $P_{(1, 1, k-2)}^{(1, 1, k-2, k-2)}$ shown in Figure 7(a), have spectral radius greater than $3/\sqrt{2}$. 

---

| $k-3$ | $k-2$ | $k-1$ |
|-------|-------|-------|
|       |       |       |

| $k-2$ | $k-1$ | $k-3$ |
|-------|-------|-------|
|       |       |       |

| $k-2$ | $k-1$ | $k-3$ |
|-------|-------|-------|
|       |       |       |

(a)

| $k-3$ | $k-2$ | $k-4$ |
|-------|-------|-------|
|       |       |       |

| $k-2$ | $k-1$ | $k-3$ |
|-------|-------|-------|
|       |       |       |

(b)

Figure 7: Open quipus with diameter $2k$
By Lemmas 2.3 and 2.8 and Corollary 2.1 we get
\[ \rho \left( P(1,k-2,1)_{(1,k-2,2,1)} \right) > \rho \left( P(1,k-2,1)_{(1,k,k,1)} \right) = \rho \left( P(1,k-1)_{(1,k-1,k-1)} \right) = \rho_k. \]

Let \( G := P(1,1)_{(1,1,k-3)} \) and \( H := P(2,2)_{(2,k-2)} \), and let \( x \) and \( y \) be the right most endvertices of \( G \) and \( H \) respectively. Note that
\[ G \cong \left( P(1,3), u, k - 3 \right), \]
\[ H \cong \left( P(2,1), v, k - 3 \right). \]

By Lemma 2.9 and Eq. (6), we have \( \alpha_{(G,x)}(\lambda) < \alpha_{(H,y)}(\lambda) \) for \( \lambda > 2 \). Then by Lemmas 2.10 and 2.8 we have
\[ \rho \left( P(1,1,k-2)_{(1,1,k-2,2,2)} \right) > \rho \left( P(2,k-2)_{(2,k-1,k-2)} \right) = \rho_k, \]
noting that
\[ P(1,1,k-2)_{(1,1,k-2,2,2)} \cong T_{G,P_{k-3}}, \]
\[ P(2,k-2)_{(2,k-1,k-2)} \cong T_{H,P_{k-3}}. \]

**Case 2** \( r = 3 \). We have \( l_1 + l_2 + l_3 = 1 \), which implies that only one of \( l_1 \), \( l_2 \), and \( l_3 \) equals one. By symmetry, we have the following two subcases.

**Subcase 2.1** \( l_1 = l_3 = 0 \) and \( l_2 = 1 \).

Eqs. (10), (11) and (12) imply that
\[ k_1 = m_0 + m_1 - 2, \]
\[ k_2 = m_1 + m_2 + 1, \]
\[ k_3 = m_2 + m_3 - 2. \]

Then by Lemma 2.6 we have
\[ \left[ \frac{3\delta_1(m_0) + \delta_1(m_1)}{2} \right] + \left[ \frac{\delta_1(m_0 - 1) + \delta_1(m_1 - 1)}{2} \right] \geq 2; \]
\[ \left[ \frac{3\delta_1(m_3) + \delta_1(m_2)}{2} \right] + \left[ \frac{\delta_1(m_3 - 1) + \delta_1(m_2 - 1)}{2} \right] \geq 2. \]

It follows that \( m_0 = m_3 = 1 \). Lemma 2.7 however, implies that all open quipus \( P(1,m_1,m_2,1)_{(1,k_1,k_2,k_3,1)} \) have spectral radius greater than \( 3/\sqrt{2} \).

**Subcase 2.2** \( l_1 = 1 \) and \( l_2 = l_3 = 0 \).

Eqs. (10), (11) and (12) imply that
\[ k_1 = m_0 + m_1 - 1, \]
\[ k_2 = m_1 + m_2, \]
\[ k_3 = m_2 + m_3 - 2. \]

Then by Lemma 2.6 we have
\[ \left[ \frac{3\delta_1(m_3) + \delta_1(m_2)}{2} \right] + \left[ \frac{\delta_1(m_3 - 1) + \delta_1(m_2 - 1)}{2} \right] \geq 2. \]
It follows that \( m_1 = 1 \) or \( m_2 = 1 \), and \( m_3 = 1 \). Also by Lemma 2.7
\[
\left\lceil \left( 3\delta_1(m_0) + \delta_1(m_1) + \delta_1(m_0 - 1) \right)/2 \right\rceil > 1,
\]
which implies that \( m_0 = 1 \). Therefore, combining with Eqs. (8) and (9), we obtain that all open quipus \( P_{(m_0,m_1,m_2,m_3)}^{(m_0,m_1,m_2,m_3)} \), except \( P_{(1,1,k-2,k-4,1)}^{(1,k-3,1,1)} \) and \( P_{(k-3,2,0,1)}^{(1,k-3,1,1)} \) shown in Figure 7 (b), have spectral radius greater than \( 3/\sqrt{2} \).

By Lemma 2.4, however, we get
\[
\rho \left( P_{(1,1,k-2,k-4,1)}^{(1,1,k-3,1,1)} \right) > \rho \left( P_{(1,1,k-2,k-2)}^{(1,1,k-2,k-2)} \right) > \rho_k,
\]
where the last inequality was proved in Subcase 1.2, and
\[
\rho \left( P_{(1,1,k-3,1,1)}^{(1,k-3,2,0,1)} \right) > \rho \left( P_{(1,k-3,2,0,1)}^{(1,k-3,2,2)} \right) > 3/\sqrt{2},
\]
where the last inequality holds since \( k - 2 < k - 3 + 2 \) and \( \delta_1(k - 3) = \delta_1(k - 4) = 0 \) for \( k > 6 \) which fails to satisfy Lemma 2.6 (3).

Case 3 \( r = 4 \). We have \( l_1 + l_2 + l_3 + l_4 = 0 \), which implies that \( l_1 = l_2 = l_3 = l_4 = 0 \). Eqs. (10), (11) and (12) imply that
\[
\begin{align*}
k_1 &= m_0 + m_1 - 2, \\
k_2 &= m_1 + m_2, \\
k_3 &= m_2 + m_3, \\
k_4 &= m_3 + m_4 - 2.
\end{align*}
\]
As above, Lemma 2.6 implies that \( m_0 = m_4 = 1 \). Lemma 2.7 however, implies that all open quipus \( P_{(1,k_1,k_2,k_3,k_4,1)}^{(1,m_1,m_2,m_3)} \) have spectral radius greater than \( 3/\sqrt{2} \). This completes the proof. \( \square \)

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