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Sharp upper bounds on the spectral radius of the signless Laplacian matrix of a graph

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ABSTRACT

Let $G = (V, E)$ be a simple connected graph. Denote by $D(G)$ the diagonal matrix of its vertex degrees and by $A(G)$ its adjacency matrix. Then the signless Laplacian matrix of G is $Q(G) = D(G) + A(G)$. In this paper, we obtain some new and improved sharp upper bounds on the spectral radius $q_1(G)$ of the signless Laplacian matrix of a graph G.

1. Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{1, 2, \ldots, n\}$ and edge set $E(G)$, where $|V(G)| = n$ is the order and $|E(G)| = m$ is the size of G. When i is adjacent to j, we denote this fact by $i \sim j$. For $v_i \in V(G)$, the degree (= number of first neighbors) of the vertex v_i is denoted by d_i. The minimum vertex degree is denoted by δ, the maximum by Δ_1 and the second maximum by Δ_2. Assuming that the degrees are ordered as $d_1 \geqslant d_2 \geqslant \cdots \geqslant d_n$, then $\Delta_1 = d_1,\ \Delta_2 = d_2$ and $\delta = d_n$. The average degree of the neighbors of vertex i is $m_i = \frac{1}{d_i}\sum_{j:j\sim i} d_j$. The eigenvalues of G are the eigenvalues of the adjacency matrix $A(G)$, given as $\lambda_1(G) \geqslant \lambda_2(G) \geqslant \ldots \geqslant \lambda_n(G)$, where, $\lambda_1(G)$ is called the index of G. Consider $D(G)$ as the diagonal matrix of vertex degrees of G. The Laplacian matrix of G is $L(G) = D(G) - A(G)$, its eigenvalues are as displayed as $\mu_1(G) \geqslant \mu_2(G) \geqslant \ldots \geqslant \mu_{n-1}(G) \geqslant \mu_n(G)$ and $\mu_1(G)$ is the spectral radius of Laplacian matrix of graph G. Since $L(G)$ and $A(G)$ are well known, there are many results on their spectra, (see [4,8,10–12,16,20,21,24]).

The matrix $Q(G) = D(G) + A(G)$ was introduced in the classical book of Cvetković, Doob and Sachs on "Spectra of Graphs" [6], but without a name being given to it at that time. Later it was called "quasi-Laplacian matrix" and more recently "signless Laplacian" [3,5,13–15]. Let $q_1(G)$ be the spectral radius of $Q(G)$. Since G is a connected graph then $Q(G)$ is a nonnegative, symmetric and irreducible matrix. Some researchers [25,27] have observed that

$$\mu_1(G) \leqslant q_1(G) \tag{1}$$

and

$$2\lambda_1(G) \leqslant q_1(G). \tag{2}$$

These relations immediately imply that any lower bound on $\mu_1(G)$ is a valid lower bound on $q_1(G)$ and that doubling any lower bound on $\lambda_1(G)$ also yields a valid lower bound on $q_1(G)$. A number of upper bounds on $\mu_1(G)$ given as functions of the

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degree and of the average degree of the neighbors of a vertex have been proposed in the literature. In [2,23], it was gathered some of them and these bounds are

$$\mu_1(G) \leqslant \max_{i \in V}\{2d_i\}, \quad [23] \tag{3}$$

$$\mu_1(G) \leqslant \max_{i \in V}\{d_i + m_i\}, \quad [22], \tag{4}$$

$$\mu_1(G) \leqslant \max_{i \in V}\left\{d_i + \sqrt{d_i m_i}\right\}, \quad [23,29], \tag{5}$$

$$\mu_1(G) \leqslant \max_{i \in V}\left\{\sqrt{2d_i(d_i + m_i)}\right\}, \quad [19], \tag{6}$$

$$\mu_1(G) \leqslant \max_{i \in V}\left\{\frac{d_i + \sqrt{d_i^2 + 8d_i m_i}}{2}\right\}, \quad [17,23], \tag{7}$$

$$\mu_1(G) \leqslant \max_{i \sim j}\{d_i + d_j\}, \quad [1], \tag{8}$$

$$\text{and } \mu_1(G) \leqslant \max_{i \sim j}\left\{\frac{d_i + d_j + \sqrt{(d_i - d_j)^2 + 4m_i m_j}}{2}\right\}, [9,28]. \tag{9}$$

In the above bounds (3),(4),(5) and (7),(8),(9) are valid for $q_1(G)$ (see [2,3,11,23,26]). In this paper, we obtain some new and improved sharp upper bounds on it.

2. Sharp upper bounds for the spectral radius of the signless Laplacian matrix of a graph

We first list some known results which will be used in this paper.

Lemma 1 [18]. *Let M be irreducible non-negative matrix. Then $\rho(M)$ is an eigenvalue of M and there is a positive vector X such that $MX = \rho(M)X$.*

Lemma 2 [5]. *Let $M = (m_{ij})$ be an $n \times n$ non-negative matrix and let $R_i(M)$ be the ith row sum of M, i.e., $R_i(M) = \sum_{j=1}^{n} m_{ij} (1 \leqslant i \leqslant n)$. Then*

$$\min\{R_i(M) : 1 \leqslant i \leqslant n\} \leqslant \rho(M) \leqslant \max\{R_i(M) : 1 \leqslant i \leqslant n\}. \tag{10}$$

If M is irreducible, then each equality holds if and only if $R_1 = R_2 = \cdots = R_n$.

Theorem 3 [30]. *Let $A = (a_{ij})$ be an $n \times n$ irreducible non-negative matrix. Then*

$$\min\left\{\sqrt{\frac{\sum_{j=1}^{n} a_{ij} M_j}{R_i}},\ 1 \leqslant i \leqslant n\right\} \leqslant \rho(A) \leqslant \max\left\{\sqrt{\frac{\sum_{j=1}^{n} a_{ij} M_j}{R_i}},\ 1 \leqslant i \leqslant n\right\}, \tag{11}$$

where $R_i = \sum_{j=1}^{n} a_{ij},\ M_i = \sum_{j=1}^{n} a_{ij} R_j,\ M_i' = \frac{M_i}{R_i}$ and $\rho(A)$ denotes the spectral radius of A. Moreover, if A^2 is irreducible, then any equality holds in (11) if and only if $M_1' = M_2' = \cdots = M_n'$; and if A^2 is reducible, then any equality holds in (11) if and only if there exist the permutation matrix P such that

$$PAP^T = \begin{pmatrix} 0_r & A_1 \\ A_2 & 0_{n-r} \end{pmatrix},$$

and $M'_{\sigma(1)} = \cdots = M'_{\sigma(r)},\ M'_{\sigma(r+1)} = \cdots = M'_{\sigma(n)}$, where σ is a permutation on the set $\{1, 2, \ldots, n\}$ which corresponds to the permutation matrix P.

Corollary 4 [30]. *Let $A = (a_{ij})$ be an $n \times n$ irreducible non-negative matrix. Then*

$$\min\{M_i' : 1 \leqslant i \leqslant n\} \leqslant \rho(A) \leqslant \max\{M_i' : 1 \leqslant i \leqslant n\}, \tag{12}$$

where M_i' be as in Theorem 3. Then equality holds in (12) if and only if $M_1' = M_2' = \cdots = M_n'$.

Corollary 5 [30]. *Let $A = (a_{ij})$ be an $n \times n$ irreducible non-negative matrix. Then*

$$\min\left\{\sqrt{M_i} : 1 \leqslant i \leqslant n\right\} \leqslant \rho(A) \leqslant \max\left\{\sqrt{M_i} : 1 \leqslant i \leqslant n\right\}, \tag{13}$$

where M_i be as in Theorem 3. Moreover, if A^2 is irreducible, then any equality holds in (13) if and only if $R_1 = R_2 = \cdots = R_n$; and if A^2 is reducible, then any equality holds in (13) if and only if there exist the permutation matrix P such that

$$PAP^T = \begin{pmatrix} 0_r & A_1 \\ A_2 & 0_{n-r} \end{pmatrix},$$

and $R_{\sigma(1)} = \cdots = R_{\sigma(r)},\ R_{\sigma(r+1)} = \cdots = R_{\sigma(n)}$, where σ is a permutation on the set $\{1, 2, \ldots, n\}$ which corresponds to the permutation matrix P.

Now we give our main results. Throughout this paper, G will denote a simple connected graph on n vertices unless stated otherwise.

Theorem 6. *Let $b_i \in \mathbb{R}^+,\ 1 \leqslant i \leqslant n$. Also let $b'_i = \frac{1}{b_i}\sum_{j:j\sim i} b_j,\ c_i = b_i(d_i + b'_i),\ c'_i = \frac{\sum_{j:j\sim i} c_j}{c_i}$ and $k_i = d_i + c'_i$. Then*

(a)

$$q_1(G) \leqslant \max_{1\leqslant i\leqslant n}\left\{ \sqrt{d_i k_i + \frac{\sum_{j:j\sim i}\left(d_j c_j + \sum_{k:k\sim j} c_k\right)}{c_i}} \right\}. \tag{14}$$

If Q^2 is irreducible, then equality holds in (14) if and only if $k_1 = k_2 = \cdots = k_n$ and if Q^2 is reducible, then equality holds in (14) if and only if there exists the permutation matrix P such that

$$PQ(G)P^T = \begin{pmatrix} 0_r & Q_1 \\ Q_2 & 0_{n-r} \end{pmatrix},$$

with $k_{\sigma(1)} = k_{\sigma(2)} = \cdots = k_{\sigma(r)}$ and $k_{\sigma(r+1)} = k_{\sigma(r+2)} = \cdots = k_{\sigma(n)}$, where σ is a permutation on the set $\{1, 2, \ldots, n\}$ which corresponds to the permutation matrix P.

(b)

$$q_1(G) \leqslant \max_{i\sim j}\left\{ \frac{d_i + d_j + \sqrt{(d_i - d_j)^2 + 4 b'_i b'_j}}{2} \right\}, \tag{15}$$

with equality holds in (15) if and only if G is either a regular graph or a bipartite semi-regular graph.

(c)

$$q_1(G) \leqslant \max_{1\leqslant i\leqslant n}\{k_i\}, \tag{16}$$

with equality holds in (16) if and only if $k_1 = k_2 = \cdots = k_n$.

(d)

$$q_1(G) \leqslant \max_{1\leqslant i\leqslant n}\left\{ \sqrt{\frac{c_i(d_i + c'_i)}{b_i}} \right\}. \tag{17}$$

If Q^2 is irreducible, then the equality holds in (17) if and only if $d_1 + b'_1 = d_2 + b'_2 = \cdots = d_n + b'_n$; and if Q^2 is reducible, then the equality holds in (17) if and only if there exists the permutation matrix P such that

$$PQ(G)P^T = \begin{pmatrix} 0_r & Q_1 \\ Q_2 & 0_{n-r} \end{pmatrix},$$

with $d_{\sigma(1)} + b'_{\sigma(1)} = d_{\sigma(2)} + b'_{\sigma(2)} = \cdots = d_{\sigma(r)} + b'_{\sigma(r)}$ and $d_{\sigma(r+1)} + b'_{\sigma(r+1)} = d_{\sigma(r+2)} + b'_{\sigma(r+2)} = \cdots = d_{\sigma(n)} + b'_{\sigma(n)}$, where σ is a permutation on the set $\{1, 2, \ldots, n\}$ which corresponds to the permutation matrix P.

Proof. Let $B = diag(b_1, b_2, \ldots, b_n)$ be an $n \times n$ diagonal matrix. Consider the matrix $B^{-1}Q(G)B$. Now the (i,j)th element of $B^{-1}Q(G)B$ is

$$\begin{cases} d_i & \text{if } i = j, \\ \frac{b_j}{b_i} & \text{if } i \sim j, \\ 0 & \text{otherwise}. \end{cases}$$

It is easy to see that the inequality (14) holds from Theorem 3 as

$$R_i = \sum_{j=1}^{n} a_{ij} = d_i + \frac{1}{b_i}\sum_{j:j\sim i} b_j = \frac{c_i}{b_i},$$

$$M_i = d_i R_i + \sum_{j:j\sim i} \frac{b_j}{b_i} R_j = \frac{1}{b_i}\left(d_i c_i + \sum_{j:j\sim i} c_j\right) = \frac{k_i c_i}{b_i}$$

and

$$\sum_{j=1}^{n} a_{ij} M_j = d_i M_i + \sum_{j:j\sim i} a_{ij} M_j = \frac{d_i k_i c_i}{b_i} + \sum_{j:j\sim i} \frac{k_j c_j}{b_i}.$$

Moreover, the proof of the second part of (a) is directly follows from Theorem 3.

Next, we prove that (15) holds. From Lemma 1, there exists a positive eigenvector $\mathbf{X} = (x_1, x_2, \ldots, x_n)^T$ of $B^{-1}Q(G)B$ corresponding to $q_1\left(B^{-1}Q(G)B\right)$. We can assume that one of the eigencomponents, say x_i, is equal to 1 and the other eigencomponents are less than or equal to 1, i.e., $x_i = 1$ and $x_k \leqslant 1, 1 \leqslant k \leqslant n$. Also, let $x_j = \max_k\{x_k : k \sim i\}$. From

$$\left(B^{-1}Q(G)B\right)X = q_1(G)X, \tag{18}$$

we have

$$q_1(G) = d_i + \frac{1}{b_i}\sum_{k:k\sim i} b_k x_k \leqslant d_i + \frac{1}{b_i}\sum_{k:k\sim i} b_k x_j \tag{19}$$

and

$$q_1(G)x_j = d_j x_j + \frac{1}{b_j}\sum_{k:k\sim j} b_k x_k \leqslant d_j x_j + \frac{1}{b_j}\sum_{k:k\sim j} b_k. \tag{20}$$

From (19) and (20), we have

$$q_1(G)^2 - (d_i + d_j)q_1(G) + d_i d_j - \left(\frac{1}{b_i}\sum_{k:k\sim i} b_k\right)\left(\frac{1}{b_j}\sum_{k:k\sim j} b_k\right) \leqslant 0.$$

Thus we have

$$q_1(G) \leqslant \frac{d_i + d_j + \sqrt{(d_i - d_j)^2 + 4b'_i b'_j}}{2}.$$

Hence (15) holds.

Moreover, one can see easily that the equality holds in (15) for regular graph or for bipartite semiregular graph. (16) and (17) with equality follow from Corollaries 4 and 5, respectively. The proof is complete. □

Remark 7. From Theorem 6, we have the following known results.

1. Taking $b_i = 1$ in (15), we have upper bound (8).
2. Taking $b_i = d_i$ in (15), we have upper bound (9).
3. Taking $b_i = 1$ in (16), we have upper bound (4).
4. Taking $b_i = 1$ in (17), we have upper bound (6).

In particular, from Theorem 6, we have the following results.

Corollary 8. *For a graph G, as depicted previously, the following inequalities hold:*

$$q_1(G) \leqslant \max_i\left\{\sqrt{d_i(d_i + m_i) + s_i}\right\}, \tag{21}$$

$$q_1(G) \leqslant \max_i\left\{\sqrt{d_i\left(d_i + \frac{s_i}{d_i + m_i}\right) + \frac{\sum_{j:j\sim i} d_j[d_j(d_j + m_j) + s_j]}{d_i(d_i + m_i)}}\right\} \tag{22}$$

and

$$q_1(G) \leqslant \max_i\left\{d_i + \frac{s_i}{d_i + m_i}\right\}, \tag{23}$$

where $s_i = \sum_{j:j\sim i} \frac{d_j(d_j+m_j)}{d_i}$.

Proof. Taking $b_i = 1$ and $b_i = d_i$ in (14) and $b_i = d_i$ in (16), respectively, we have the required results. □

Remark 9. Since Corollary 8 is a consequence of Theorem 6, it is easy to conclude that the equality conditions in (14) and (16) are also hold.

Lemma 10 [7]. *Let G be a connected graph. Then* $d_1 + m_1 = d_2 + m_2 = \cdots = d_n + m_n$ *if and only if G is a regular graph or G is a regular bipartite graph.*

Theorem 11. *Let G be a connected graph. Then*

$$q_1(G) \leqslant \max_{1\leqslant i\leqslant n}\{d_i + b_i'\} \tag{24}$$

and

$$q_1(G) \leqslant \max_i \left\{ \frac{d_i + \sqrt{d_i^2 + \frac{4c_ic_i'}{b_i}}}{2} \right\}, \tag{25}$$

where $b_i \in \mathbb{R}^+$, $b_i' = \frac{1}{b_i}\sum_{j:j\sim i} b_j$, $c_i = b_i(d_i + b_i')$, $c_i' = \frac{\sum_{j:j\sim i} c_j}{c_i}$. *Moreover, both the equality hold if and only if* $d_1 + b_1' = d_2 + b_2' = \cdots = d_n + b_n'$.

Proof. Let $X = (x_1, x_2, \ldots, x_n)^T$ be an eigenvector corresponding to the eigenvalue $q_1(G)$ of $B^{-1}Q(G)B$. We assume that one eigencomponent x_i is equal to 1 and the other eigencomponents are less than or equal to 1, that is, $x_i = 1$ and $0 < x_k \leqslant 1$, for all k.

From the ith equation of (18), we have

$$q_1(G)x_i = d_ix_i + \sum_{j:j\sim i} \frac{b_jx_j}{b_i},$$

$$\text{i.e.,}\ \ q_1(G) = d_i + \sum_{j:j\sim i} \frac{b_jx_j}{b_i}. \tag{26}$$

From above the first bound follows. Moreover, the equality holds in (24) if and only if $d_i + b_i'$ $(1 \leqslant i \leqslant n)$ is a constant. Again from the jth equation of (18),

$$q_1(G)x_j = d_jx_j + \sum_{k:k\sim j} \frac{b_kx_k}{b_j}.$$

Multiplying both sides of (26) by $q_1(G)$ and substituting this value $q_1(G)x_j$, we get

$$\begin{aligned} q_1^2(G) &= d_iq_1(G) + \sum_{j:j\sim i}\left\{\frac{b_j}{b_i}\left[d_jx_j + \sum_{k:k\sim j}\frac{b_kx_k}{b_j}\right]\right\} \\ &= d_iq_1(G) + \sum_{j:j\sim i}\frac{b_jd_j}{b_i}x_j + \frac{1}{b_i}\sum_{j:j\sim i}\sum_{k:k\sim j} b_kx_k \leqslant d_iq_1(G) + \sum_{j:j\sim i}\frac{b_jd_j}{b_i} + \sum_{j:j\sim i}\frac{b_jb_j'}{b_i}\ \text{as}\ x_j, x_k \leqslant 1 \\ &= d_iq_1(G) + \sum_{j:j\sim i}\frac{b_j\left(d_j + b_j'\right)}{b_i} = d_iq_1(G) + \frac{c_ic_i'}{b_i} \end{aligned} \tag{27}$$

from above the second bound follows.

Now suppose that the equality holds in (25). Then all inequalities in the above argument must be equalities. From equality in (27), we get $x_j = 1$ for all j such that $j \sim i$ and $x_k = 1$ for all k such that $k \sim j$ and $j \sim i$. From this one can easily show that $x_i = 1$ for all $i \in V$. Thus we have $d_1 + b_1' = d_2 + b_2' = \cdots = d_n + b_n'$.

Conversely, one can easily see that the equality holds in (25) for $d_1 + b_1' = d_2 + b_2' = \cdots = d_n + b_n'$. □

Corollary 12. *Let G be a connected graph. Then*

$$q_1(G) \leqslant \max_{1\leqslant i\leqslant n}\left\{ \frac{d_i + \sqrt{d_i^2 + \frac{8d_im_ib_\ell}{b_i}}}{2} \right\}, \tag{28}$$

where $b_i' = \frac{1}{b_i}\sum_{j:j\sim i} b_j,\; b_\ell = \max_{1\leqslant i\leqslant n} b_i$ *and* $m_i = \frac{1}{d_i}\sum_{j:j\sim i} d_j$.

Corollary 13. *Let G be a connected graph. Then*

$$q_1(G) \leqslant \max_{1\leqslant i\leqslant n}\left\{\frac{d_i + \sqrt{d_i^2 + \frac{4}{d_i}\sum_{j:j\sim i} d_j(d_j + m_j)}}{2}\right\}.$$

The equality holds if and only if G is a regular graph or G is a regular bipartite graph.

Proof. Taking $b_i = d_i$ in (25), the above bound follows. By Lemma 10 and Theorem 11, the above equality holds if and only if G is a regular graph or G is a regular bipartite graph. □

Corollary 14. *Let G be a connected graph. Then*

$$q_1(G) \leqslant \max_{1\leqslant i\leqslant n}\left\{d_i + \frac{1}{\sqrt{d_i}}\sum_{j:j\sim i}\sqrt{d_j}\right\}, \tag{29}$$

with equality if and only if $d_i + \frac{1}{\sqrt{d_i}}\sum_{j:j\sim i}\sqrt{d_j}$ $(1 \leqslant i \leqslant n)$ *is a constant.*

Proof. Taking $b_i = \sqrt{d_i}$ in (24), the result follows. □

Remark 15. From the Cauchy–Schwarz inequality, it is easy to see that bound (29) is always better than bound (5).

Remark 16. From Theorem 11 and Corollary 12, respectively, we have the following known results:

1. Taking $b_i = 1$ and $b_i = d_i$ in (24), we have upper bounds (3) and (4).
2. Taking $b_i = 1$ in (25) and (28), we have upper bound (7).

Let Γ be the class of graphs $H = (V, E)$ such that H is connected graph with $V(H) = \{1\} \cup V_1 \cup V_2$,

$$d_1 = \Delta_1, \quad V_1 = \{k \in N_1 : d_k = \delta\}, \quad V_2 = \{k \notin N_1 : d_k = \Delta_2\}$$

and

$$(\Delta_2 - \delta)(2\Delta_2 - \Delta_1) = \Delta_1 - \Delta_2.$$

The spectral radius of the signless Laplacian matrix of $H \in \Gamma$ is given by:

$$q_1(H) = 2\Delta_2 = \frac{\Delta_1 + 2\delta - 1 + \sqrt{(\Delta_1 - 2\delta + 1)^2 + 4\Delta_1}}{2}.$$

Denote by H_{n-1,Δ_2}, a connected graph with maximum degree $n-1$ and the second maximum degree Δ_2 such that $\Delta_2 = \delta < n-1$ (δ is minimum vertex degree). Thus H_{n-1,Δ_2} is a $(n-1, \Delta_2)$-semiregular graph with $\Delta_2 < n-1$. One can see easily that the spectral radius of the signless Laplacian matrix of H_{n-1,Δ_2} is given by the following equation

$$q_1^2 - (n + 2\Delta_2 - 2)q_1 + 2(n-1)(\Delta_2 - 1) = 0.$$

Thus the spectral radius of the signless Laplacian matrix of H_{n-1,Δ_2} is given by

$$q_1 = \frac{n + 2\Delta_2 - 2 + \sqrt{(n - 2\Delta_2)^2 + 4(n-1)}}{2}.$$

We now give another upper bound on the spectral radius of the signless Laplacian matrix of a graph.

Theorem 17. *Let G be a connected graph with maximum degree* Δ_1 *and second maximum degree* Δ_2*. Then*

$$q_1 \leqslant \max_{i\sim j}\left\{\frac{d_i + 2d_j - 1 + \sqrt{(d_i - 2d_j + 1)^2 + 4d_i}}{2}\right\}, \tag{30}$$

with equality holds in (30) if and only if G is isomorphic to a regular graph or $G \cong H_{n-1,\Delta_2}$ *or* $G \in \Gamma$.

Proof. Let $\mathbf{X} = (x_1, x_2, \ldots, x_n)^T$ be an eigenvector of $Q(G)$ corresponding to an eigenvalue q_1. We can assume that one eigencomponent x_i is equal to 1 and the other eigencomponents are less than or equal to 1, that is, $x_i = 1$ and $0 < x_k \leqslant 1$, for all k. We have

$$Q(G)\mathbf{X} = q_1\mathbf{X}. \tag{31}$$

Let $x_j = \max_{k:k \neq i} x_k$. From the ith equation of (31),

$$q_1 x_i = d_i x_i + \sum_{k:k\sim i} x_k, \quad \text{i.e., } q_1 \leqslant d_i + d_i x_j. \tag{32}$$

From the jth equation of (31),

$$\begin{aligned} &q_1 x_j = d_j x_j + \sum_{k:k\sim j} x_k,\\ &\text{i.e., } \ q_1 x_j \leqslant d_j x_j + 1 + (d_j - 1)x_j,\\ &\text{i.e., } \ (q_1 - 2d_j + 1)x_j \leqslant 1. \end{aligned} \tag{33}$$

From (32) and (33), we get

$$(q_1 - d_i)(q_1 - 2d_j + 1) \leqslant d_i,$$

i.e.,

$$q_1^2 - (d_i + 2d_j - 1)q_1 + 2d_i(d_j - 1) \leqslant 0,$$

i.e.,

$$q_1 \leqslant \frac{d_i + 2d_j - 1 + \sqrt{(d_i - 2d_j + 1)^2 + 4d_i}}{2}.$$

The first part of the proof is over.

Now suppose that equality holds in (30). Then all inequalities in the above argument must be equalities. In particular, from (32) we get

$$x_k = x_j \text{ for all } k, k \sim i.$$

Also from (33) we get

$$x_k = x_j \text{ for all } k, \quad k \sim j, \ k \neq i \text{ and } i \sim j.$$

Let $V_1 = \{k : x_k = x_j\}$. If $V_1 \neq V(G) \setminus \{i\}$, then there exist vertices $p \in V_1, \ q \notin V_1, \ q \neq i$ such that $p \sim q$ as G is connected. Thus we have $x_q < x_j$ as x_j is the second maximum eigencomponent. For vertex $p \in V(G)$, from above, we must have $x_q = x_j$, a contradiction. Thus $V_1 = V(G) \setminus \{v_i\}$. If $x_j = 1$, then

$$q_1 = 2d_i, \quad i = 1, 2, \ldots, n.$$

Hence G is a regular graph.

Otherwise, $x_j < 1$. Now we consider two cases (i) $d_i = n - 1$, (ii) $d_i < n - 1$.

Case (i) : $d_i = n - 1$. In this case vertex i is adjacent to all the remaining vertices in G. One can see easily that any two vertices j and k in $V(G) \setminus \{i\}, d_j = d_k < n - 1$. Thus we have $\Delta_2 = d_2 = d_3 = \ldots = d_n = \delta$. Hence $G \cong H_{n-1,\Delta_2}$.

Case (ii) : $d_i < n - 1$. In this case $V_1 = \{k \in N_i\}$ and $V_2 = V(G) \setminus (V_1 \cup \{i\})$. One can see easily that any two vertices j and k in $V_1, d_j = d_k$ and also we have $d_r = d_s$, for $r, s \in V_2$. Moreover, we have

$$q_1 = d_1(1 + x_j), \tag{34}$$

$$q_1 = 2d_j - 1 + \frac{1}{x_j} \quad j \in V_1, \tag{35}$$

$$\text{and } q_1 = 2d_k \ k \in V_2. \tag{36}$$

From (34) and (36), we get $d_1 > d_k, \ k \in V_2$. From (35) and (36), we get $d_k > d_j, \ k \in V_2, \ j \in V_1$. Thus we have $d_1 = \Delta_1, \ d_k = \Delta_2$ and $d_j = \delta, k \in V_2$ and $j \in V_1$. Moreover, $(\Delta_2 - \delta)(2\Delta_2 - \Delta_1) = \Delta_1 - \Delta_2$, by (34)–(36).

Hence $G \in \Gamma$.

Conversely, one can see easily that the equality holds in (30) for regular graph or for H_{n-1,Δ_2} or for $G, G \in \Gamma$. □

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