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ON THE MAIN SIGNLESS LAPLACIAN EIGENVALUES OF A GRAPH*

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Abstract. A signless Laplacian eigenvalue of a graph G is called a main signless Laplacian eigenvalue if it has an eigenvector the sum of whose entries is not equal to zero. In this paper, some necessary and sufficient conditions for a graph with one main signless Laplacian eigenvalue or two main signless Laplacian eigenvalues are given. And the trees and unicyclic graphs with exactly two main signless Laplacian eigenvalues are characterized, respectively.

Key words. Signless Laplacian eigenvalue, Main eigenvalue, Tree, Unicyclic graph.

AMS subject classifications. 05C50.

1. Introduction. Let M be a square matrix of order n. An eigenvalue λ of M is said to be a main eigenvalue if the eigenspace $\varepsilon(\lambda)$ of λ is not orthogonal to the all-1 vector $\mathbf{j}$, i.e., if it has an eigenvector the sum of whose entries is not equal to zero. An eigenvector $\mathbf{x}$ is a main eigenvector if $\mathbf{x}^{\mathbf{T}}\mathbf{j} \neq 0$. Specially, if $M = A$ is the $(0,1)$-adjacency matrix of a graph G, then the main eigenvalues of A are said to be main eigenvalues of G. A graph with exactly one main eigenvalue is regular. Cvetković [5] proposed the problem of characterizing graphs with exactly k main eigenvalues, $k > 1$. Hagos [9] gave a characterization of graphs with exactly two main eigenvalues. Recently, Hou and Zhou [11] characterized the tree with exactly two main eigenvalues. Hou and Tian [10] determined all connected unicyclic graphs with exactly two main eigenvalues. Zhu and Hu [12] characterized all connected bicyclic graphs with exactly two main eigenvalues. Rowlinson [13] surveyed results relating main eigenvalues and main angles to the structure of a graph, and discussed graphs with just two main eigenvalues in the context of measures of irregularity and in the context of harmonic graphs.

In this paper, we assume that G is a simple connected graph, and consider the main eigenvalues of the signless Laplacian matrix Q of G, where $Q = D + A$ and D is the diagonal matrix of vertex degrees. The main eigenvalues of Q are said to be

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the main signless Laplacian eigenvalues of G. The signless Laplacian appears very rarely in published papers before 2003. Recently, the signless Laplacian has attracted the attention of researchers, see, e.g. [1, 2, 3, 6, 7]. Here, we obtain necessary and sufficient conditions for a graph with one main signless Laplacian eigenvalue or two main signless Laplacian eigenvalues, and then characterize the trees and unicyclic graphs with exactly two main signless Laplacian eigenvalues, respectively.

2. The graphs with one or two main signless Laplacian eigenvalues. In this section, we show that a graph with exactly one main signless Laplacian eigenvalue is regular, and give a characterization of graphs with exactly two main signless Laplacian eigenvalues.

Note that if G is a simple connected graph with signless Laplacian matrix Q, then there is an eigenvector $\mathbf{x} > 0$ of the largest eigenvalue μ_1 of Q such that $Q\mathbf{x} = \mu_1\mathbf{x}$, and $x^T\mathbf{j} \neq 0$ by the Perron-Frobenius theorem. This shows that the largest eigenvalue μ_1 of Q is a main signless Laplacian eigenvalue. So, G has at least one main signless Laplacian eigenvalue.

The following result gives a characterization of graphs with exactly one main signless Laplacian eigenvalue.

Theorem 2.1. *A graph G with exactly one main signless Laplacian eigenvalue if and only if G is regular.*

Proof. If G is k-regular, then $Q\mathbf{j} = 2k\mathbf{j}$. This shows that $\mu_1 = 2k$ is an eigenvalue of Q with an eigenvector $\mathbf{j}$. Since Q is a non-negative irreducible symmetric matrix, $\mu_1 = 2k$ is the largest eigenvalue of Q with the multiplicity 1 by the Perron-Frobenius theorem. And the eigenvectors of other eigenvalues of Q are orthogonal with $\mathbf{j}$. So, Q has exactly one main eigenvalue.

If G has exactly one main signless Laplacian eigenvalue, then the largest eigenvalue μ_1 is the unique main eigenvalue of Q. Let ξ be a eigenvector of μ_1, $\mathbf{V_1} = \varepsilon(\mu_1)$ the eigenspace of μ_1. Then $\mathbf{V_1}$ is the space spanning by ξ. If $\mathbf{V_2}$ is the space spanning by eigenvectors of all eigenvalues of Q different from μ_1, and $\mathbf{V_3}$ is the space spanning by $\mathbf{j}$, then $dim(\mathbf{V_2}) = n-1$ and $dim(\mathbf{V_3}) = 1$. Since Q is a real symmetric matrix, $\mathbf{V_1}$ is the orthogonal complement of $\mathbf{V_2}$. And $\mathbf{V_3}$ is also the orthogonal complement of $\mathbf{V_2}$ since μ_1 is the unique main eigenvalue of Q. So, $\mathbf{V_1} = \mathbf{V_3}$, and $\xi = a\mathbf{j}$ for some real $a \neq 0$. From $Q\xi = \mu_1\xi$, the row sums of Q are equal, and G is regular. ☐

Now, we discuss the characterization of graphs with exactly two main signless Laplacian eigenvalues.

For any positive semi-definite matrix M of order n, all its eigenvalues are non-negative. Let $\mu_1 > \mu_2 > \cdots > \mu_r$ be the eigenvalues of M with multiplicities

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$n_1, n_2, \ldots, n_r$, respectively, where $n_1 + n_2 + \cdots + n_r = n$. $\{\xi_{i1}, \xi_{i2}, \ldots, \xi_{in_i}\}$ is a standard and orthogonal basis of the eigenspace $\varepsilon(\mu_i)$, $i = 1, 2, \ldots, r$. If $P = [\xi_{11}, \ldots, \xi_{1n_1}, \xi_{21}, \ldots, \xi_{2n_2}, \ldots, \xi_{r1}, \ldots, \xi_{rn_r}]$, $P_i = [0, \ldots, \xi_{i1}, \ldots, \xi_{in_i}, 0, \ldots, 0]$ and $\mathbf{j} = [1, 1, \ldots, 1]^T$, then

$$P^T M P = \begin{pmatrix} \mu_1 I_{n_1\times n_1} & 0 & \cdots & 0 \\ 0 & \mu_2 I_{n_2\times n_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mu_r I_{n_r\times n_r} \end{pmatrix}.$$

Let

$$E_i = \begin{pmatrix} 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ \vdots & \vdots & I_{n_i\times n_i} & \vdots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 \end{pmatrix}$$

and $Q_i = PE_iP^T$. Then

$$Q_i\mathbf{j} = PE_iP^T\mathbf{j} = P_iP_i^T\mathbf{j}, \tag{2.1}$$

and M has the spectral decomposition

$$M = \mu_1 Q_1 + \mu_2 Q_2 + \cdots + \mu_r Q_r,$$

where

$$Q_iQ_j = \begin{cases} \mathbf{0} & i \neq j; \\ Q_i & i = j. \end{cases}$$

And, for any polynomial $f(x) = a_0x^n + a_1x^{n-1} + \cdots + a_{n-1}x + a_n$,

$$\begin{aligned} f(M) = \;& a_0(M)^n + a_1(M)^{n-1} + \cdots + a_{n-1}M + a_nI \\ = \;& a_0 \textstyle\sum_{i=1}^r \mu_i^n Q_i + a_1 \sum_{i=1}^r \mu_i^{n-1} Q_i + \cdots \\ & + a_{n-1} \textstyle\sum_{i=1}^r \mu_i Q_i + a_n \sum_{i=1}^r Q_i \\ = \;& \textstyle\sum_{i=1}^r f(\mu_i) Q_i. \end{aligned} \tag{2.2}$$

Lemma 2.2. *Let μ_1, μ_2, …, μ_t $(1 \le t \le r)$ be the main eigenvalues of a positive semi-definite matrix M of order n, and $m(x) = (x-\mu_1)(x-\mu_2)\cdots(x-\mu_t)$. Then*

(i) $m(M)\mathbf{j} = 0$;

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(ii) If $f(x)$ is a polynomial with real coefficients and $f(M)\mathbf{j} = 0$, then $m(x)|f(x)$.

Proof. (i) From (2.2), we know that $m(M) = \sum_{i=1}^{r} m(\mu_i)Q_i = \sum_{i=t+1}^{r} m(\mu_i)Q_i$. And

$$m(M)\mathbf{j} = \sum_{i=t+1}^{r} m(\mu_i)Q_i\mathbf{j}.$$

Since $\mu_{t+1}, \ldots, \mu_r$ are not the main eigenvalues of M, and from (2.1), $Q_i\mathbf{j} = 0$ for $i = t+1, \ldots, r$. So, $m(M)\mathbf{j} = \sum_{i=t+1}^{r} m(\mu_i)Q_i\mathbf{j} = 0$.

(ii) From (2.2) and $Q_i\mathbf{j} = 0$, for $i = t+1, \ldots, r$,

$$f(M)\mathbf{j} = \sum_{i=1}^{r} f(\mu_i)Q_i\mathbf{j} = \sum_{i=1}^{t} f(\mu_i)Q_i\mathbf{j}.$$

Since $f(M)\mathbf{j} = 0$, $\sum_{i=1}^{t} f(\mu_i)Q_i\mathbf{j} = 0$. For $k = 1, 2, \ldots, t$, we have

$$Q_k(\sum_{i=1}^{t} f(\mu_i)Q_i\mathbf{j}) = f(\mu_k)Q_k\mathbf{j} = 0.$$

So, $f(\mu_k) = 0$ for $k = 1, 2, \ldots, t$ and $m(x)|f(x)$. $\square$

A number α is an algebraic integer if there is a monic polynomial $f(x)$ with integral coefficients such that $f(\alpha) = 0$.

LEMMA 2.3. [8] *An $\alpha \in \mathbb{Q}$ is an algebraic integer if and only if α is an integer.*

LEMMA 2.4. [8] *If α and β are algebraic integers, then $\alpha \pm \beta$ and $\alpha\beta$ are also algebraic integers.*

THEOREM 2.5. *Let G be non-regular. Then G has exactly two main signless Laplacian eigenvalues μ_1 and μ_2 if and only if $(Q - \mu_1 I)(Q - \mu_2 I)\mathbf{j} = 0$.*

Proof. Let $\mu_1, \ldots, \mu_t$ be the main eigenvalues of Q, and $m(x) = (x - \mu_1) \cdots (x - \mu_t)$.

If $(Q - \mu_1 I)(Q - \mu_2 I)\mathbf{j} = 0$, then $f(Q)\mathbf{j} = 0$ for $f(x) = (x - \mu_1)(x - \mu_2)$, and $m(x)|f(x)$ by Lemma 2.2. So, $m(x) = (x - \mu_1)(x - \mu_2)$ or $(x - \mu_1)$ or $(x - \mu_2)$, and $t \leq 2$. But G is non-regular, $t = 2$ from Theorem 2.1.

If G has exactly two main signless Laplacian eigenvalues μ_1 and μ_2, then $(Q - \mu_1 I)(Q - \mu_2 I)\mathbf{j} = 0$ from Lemma 2.2. $\square$

In the following, we give an alternative characterization of graphs with exactly two main signless Laplacian eigenvalues.

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In order to find all graphs with exactly two main eigenvalues, Hou and Tian [10] introduced a 2-walk (a,b)-linear graph. For a graph G, the degree of vertex v is denoted by $d(v)$, the number of walks of length 2 of G starting at v is $s(v) = \sum_{u \in N_G(v)} d(u)$, i.e., the sum of the degrees of the vertices adjacent to v, where $N_G(v)$ is the set of all neighbors of v in G. A graph G is called 2-walk (a,b)-linear if there exist unique integer numbers a, b with $a^2 - 4b > 0$ such that $s(v) = ad(v) + b$ holds for every vertex $v \in V(G)$. Hagos [9] showed that a graph G has exactly two main eigenvalues if and only if G is 2-walk linear.

Like a 2-walk (a,b)-linear graph, we definite a 2-walk (a,b)-parabolic graph. A graph G is called 2-walk (a,b)-parabolic if there are uniquely a positive integer a and a non-negative integer b with $a^2 - 8b > 0$ such that $s(v) = -d^2(v) + ad(v) - b$ holds for every vertex $v \in V(G)$.

Theorem 2.6. *A graph G has exactly two main signless Laplacian eigenvalues if and only if G is a 2-walk (a,b)-parabolic graph.*

Proof. If G is a 2-walk (a,b)-parabolic graph, then there are uniquely a positive integer a and a non-negative integer b such that $a^2 - 8b > 0$ and $s(v) = -d^2(v) + ad(v) - b$ for any $v \in V(G) = \{v_1, v_2, \ldots, v_n\}$. So, $s(v_i) + d^2(v_i) - ad(v_i) + b = 0$, and

$$\begin{aligned} \tfrac{1}{2}(A+D)^2\mathbf{j} - aA\mathbf{j} + b\mathbf{j} &= \mathbf{0} \\ \tfrac{1}{2}Q^2\mathbf{j} - \tfrac{1}{2}aL^+\mathbf{j} + b\mathbf{j} &= \mathbf{0} \\ Q^2\mathbf{j} - aQ\mathbf{j} + 2b\mathbf{j} &= \mathbf{0}. \end{aligned}$$

Let $f(x) = x^2 - ax + 2b$. Then $f(Q)\mathbf{j} = \mathbf{0}$, and $f(x) = 0$ has two real roots since $a^2 - 8b > 0$. Moreover, G is non-regular since one has $s(v) = -d^2(v) + 2kd(v) - 0$ and $s(v) = -d^2(v) + (2k+1)d(v) - k$ for a k-regular graph, i.e., $(a,b) = (2k,0)$ or $(2k+1,k)$ is not unique. From Theorem 2.5, G has exactly two main signless Laplacian eigenvalues.

On the other hand, if G has exactly two main signless Laplacian eigenvalues μ_1 and μ_2, then by Theorem 2.5,

$$(Q^2 - (\mu_1 + \mu_2)Q + \mu_1\mu_2 I)\mathbf{j} = \mathbf{0},$$

i.e.,

$$(D+A)^2\mathbf{j} - (\mu_1 + \mu_2)(D+A)\mathbf{j} + \mu_1\mu_2\mathbf{j} = \mathbf{0}.$$

So, $d^2(v) + s(v) - (\mu_1 + \mu_2)d(v) + \frac{\mu_1\mu_2}{2} = 0$ for all $v \in V(G)$. Let $\mu_1 + \mu_2 = a$ and $\mu_1\mu_2 = 2b$, then $s(v) = -d^2(v) + ad(v) - b$, and $a > 0$, $b \geq 0$ and $a^2 - 8b > 0$ since $\mu_1 \neq \mu_2$ are the eigenvalues of the positive semi-definite matrix Q. Note that G is

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non-regular by Theorem 2.1, there are $u, v \in V(G)$ such that $d(u) \neq d(v)$. From $s(u) = -d^2(u) + ad(u) - b$ and $s(v) = -d^2(v) + ad(v) - b$, we have

$$a = \frac{s(u) - s(v)}{d(u) - d(v)} + d(u) + d(v),$$

$$b = \frac{s(u) - s(v)}{d(u) - d(v)} d(v) + d(u)d(v) - s(v), \tag{2.3}$$

and a, b are rational numbers and unique. Because μ_1, μ_2 are the roots of monic polynomial $det(\lambda I - Q) = 0$ with integral coefficients, μ_1, μ_2 are algebraic integers. By Lemmas 2.3 and 2.4, a, b are integers. □

3. Trees with exactly two main signless Laplacian eigenvalues. In this section, we determine all trees with exactly two main signless Laplacian eigenvalues.

Let $G = (V, E)$ be a tree with $n \geq 3$ vertices and the maximum degree Δ. If G has exactly two main signless Laplacian eigenvalues, then from Theorem 2.6, there exist uniquely a positive integer a and a non-negative integer b such that such that $a^2 - 8b > 0$ and

$$s(v) = -d^2(v) + ad(v) - b \tag{3.1}$$

for any $v \in V(G)$.

Case 1. $b = 0$.

Let $v_1 \in V$ with degree $d(v_1) = 1$, and v_2 is its unique adjacent vertex. Then $d(v_2) = s(v_1) = -1 + a$ by (3.1), and

$$a = d(v_2) + 1 \leq \Delta + 1. \tag{3.2}$$

Let $v_0 \in V$ with degree $d(v_0) = \Delta$, then $\Delta = d(v_0) \leq s(v_0) = -d^2(v_0) + ad(v_0) = -\Delta^2 + a\Delta$, and $\Delta \leq a - 1$, i.e.,

$$a \geq \Delta + 1 \tag{3.3}$$

with equality if and only if G is a star with the center v_0. From (3.2) and (3.3), we have $a = \Delta + 1$. So, $G = S_n$ is a star.

Case 2. $b = 1$.

Let $P_k = v_1 v_2 \cdots v_k$ is a longest path of G. Then $d(v_2) = s(v_1) = -1 + a - 1 = a - 2$ by (3.1), and

$$\begin{aligned} s(v_2) &= -d^2(v_2) + ad(v_2) - 1 \\ &= -(a-2)^2 + a(a-2) - 1 \\ &= 2a - 5. \end{aligned}$$

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Since $P_k = v_1v_2 \cdots v_k$ is a longest path of G, the adjacent vertices of v_2 are pendant vertices except v_3. So, $s(v_2) = \sum\limits_{v \in N_G(v_2)} d(v) = d(v_3) + d(v_2) - 1$ and

$$\begin{aligned} d(v_3) &= s(v_2) - d(v_2) + 1 \\ &= (2a-5) - (a-2) + 1 \\ &= a - 2 = d(v_2). \end{aligned}$$

By (3.1), we have $s(v_3) = s(v_2) = 2a - 5 = d(v_2) + d(v_3) - 1$. This shows that the adjacent vertices of v_3 are pendant vertices except v_2. So, $G = S_{\frac{n}{2},\frac{n}{2}}$ is a double star.

Case 3. $b \geq 2$.

Let $P_k = v_1v_2 \cdots v_k$ is a longest path of G, then $d(v_2) \geq 2$. By (3.1), $d(v_2) = s(v_1) = -1 + a - b$, and $a - b \geq 3$.

Since $P_k = v_1v_2 \cdots v_k$ is a longest path of G, the adjacent vertices of v_2 are pendant vertices except v_3.

$$\begin{aligned} d(v_3) &= s(v_2) - (d(v_2) - 1) \\ &= (-(a-b-1)^2 + a(a-b-1) - b) - (d(v_2) - 1) \\ &= (-(a-b-1)^2 + a(a-b-1) - b) - (a-b-2) \\ &= ab - b^2 - 2b + 1 \end{aligned}$$

and

$$\begin{aligned} d(v_3) - d(v_2) &= (ab - b^2 - 2b + 1) - (a - b - 1) \\ &= ab - b^2 - b - a + 2 \\ &= (b-1)(a-b-2) > 0. \end{aligned}$$

So, $d(v_3) > d(v_2) = a - b - 1 \geq 2$. And no pendant vertex is adjacent to v_3; Otherwise, let u be a pendant vertex adjacent to v_3. Then $d(v_3) = s(u) = -1 + a - b$ by (3.1), contradicting with $d(v_3) > a - b - 1$.

For any $x \in N_G(v_3) \backslash \{v_2, v_4\}$, since x is not a pendant vertex, there is $y \in V(G) \backslash \{v_3\}$ such that $xy \in E(G)$, and y is a pendant vertex by the longest path $P_k = v_1v_2 \cdots v_k$. Then

$$d(x) = s(y) = -1 + a - b = d(v_2), \quad \forall x \in N_G(v_3) \backslash \{v_2, v_4\}.$$

So,

$$\begin{aligned} s(v_3) = \textstyle\sum_{z \in N_G(v_3)} d(z) &= \textstyle\sum_{x \in N_G(v_3) \backslash \{v_2, v_4\}} d(x) + d(v_2) + d(v_4) \\ &= (d(v_3) - 2)d(v_2) + d(v_2) + d(v_4) \end{aligned}$$

and

$$d(v_4) = s(v_3) - (d(v_3) - 1)d(v_2).$$

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By (3.1), $s(v_3) = -d^2(v_3) + ad(v_3) - b$. Note that $d(v_2) = a - b - 1$ and $d(v_3) = ab - b^2 - 2b + 1$,

$$\begin{aligned} d(v_4) &= -d^2(v_3) + ad(v_3) - b - (d(v_3) - 1)d(v_2) \\ &= d(v_3)(-d(v_3) + a - d(v_2)) - b + d(v_2) \\ &= d(v_3)(-ab + b^2 + 3b) + a - 2b - 1 \\ &= d(v_3)b(b - a + 3) + (a - 2b - 1). \end{aligned}$$

If $a-b = 3$, then $d(v_4) = a-2b-1 = 2-b \leq 0$; If $a-b \geq 4$, then $d(v_4) = d(v_3)b(b-a+4)-bd(v_3)+(a-2b-1) \leq -bd(v_3)+(a-2b-1) = -b(ab-b^2-2b+1)+(a-2b-1) = -a(b^2-1)+b^3+2b^2-3b-1 \leq -(b+4)(b^2-1)+b^3+2b^2-3b-1 = -2b^2-2b+3 < 0$. This is impossible.

On the other hand, it is easy to check that $G = S_n$ and $G = S_{\frac{n}{2},\frac{n}{2}}$ are 2-walk $(n, 0)$-parabolic graph and $(\frac{n}{2} + 2, 1)$-parabolic graph, respectively.

From above, we have

Theorem 3.1. *A tree with $n \geq 3$ vertices has exactly two main signless Laplacian eigenvalues if and only if G is the star S_n or the double star $S_{\frac{n}{2},\frac{n}{2}}$.*

It was showed in [11] that the trees with $n \geq 3$ vertices has exactly two main eigenvalues (of adjacent matrix) are S_n, $S_{\frac{n}{2},\frac{n}{2}}$ and T_a. But from Theorem 3.1, we know that T_a is not a tree with exactly two main signless Laplacian eigenvalues, where T_a $(a \geq 2)$ is defined in [11] to be the tree with one vertex v of degree $a^2 - a + 1$ while every neighbor of v has degree a and all remaining vertices are pendant.

4. Unicyclic graphs with exactly two main signless Laplacian eigenvalues. In this section, we determine all unicyclic graphs with exactly two main signless Laplacian eigenvalues.

The unique unicyclic graph with n vertices and the minimum degree $\delta \geq 2$ is the cycle C_n, and it is regular. By Theorem 2.1, it has exactly one main signless Laplacian eigenvalues. So, we only need to consider the unicyclic graphs with the minimum degree $\delta = 1$.

Remark 4.1. If G is a 2-walk (a, b)-parabolic graph with $\delta(G) = 1$, then $a-b \geq 3$ since there is a pendent vertex x with the only incident edge xy in G and $d(y) = s(x) = -1 + a - b \geq 2$.

Let $\mathcal{G}_{a,b} = \{G : G \text{ is a 2-walk } (a, b) - \text{parabolic unicyclic graph with } \delta(G) = 1\}$, and for each $G \in \mathcal{G}_{a,b}$, let G_0 be the graph obtained from G by deleting all pendant vertices. If $v \in V(G_0)$, we use $d_{G_0}(v)$ to denote the degree of the vertex v in G_0.

Lemma 4.2. *If $G \in \mathcal{G}_{a,b}$ and $v \in V(G_0)$, then $d(v) = d_{G_0}(v)$ or $d(v) = a-b-1$.*

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Proof. If there is a pendant x adjacent to v in G, then $d(v) = s(x) = a - b - 1$ by (3.1). Otherwise, $d(v) = d_{G_0}(v)$. $\square$

LEMMA 4.3. *If $G \in \mathcal{G}_{a,b}$, then (i) $\delta(G_0) \geq 2$; (ii) $a - b \geq 4$ and $a \geq 5$.*

Proof. (i) If $\delta(G_0) = 1$, then there is $y \in V(G_0)$ such that $d_{G_0}(y) = 1$, and there must exist a pendant vertex x adjacent to y in G. By (3.1), $d(y) = s(x) = -1 + a - b$, this shows that there are $a - b - 2$ pendant vertices adjacent to y in G. Let z be the unique non-pendant vertex adjacent to y in G, then $s(y) = \sum\limits_{w \in N_G(y)} d(w) = d(z) + (a - b - 2)$. By (3.1), we know

$$\begin{aligned} s(y) &= -d^2(y) + ad(y) - b \\ &= -(a-b-1)^2 + a(a-b-1) - b \end{aligned}$$

and $d(z) = s(y) - (a - b - 2) = -(a - b - 1)^2 + a(a - b - 1) - b - (a - b - 2)$, i.e.,

$$d(z) = ab - b^2 - 2b + 1. \tag{4.1}$$

So,

$$d(z) - d(y) = (ab - b^2 - 2b + 1) - (a - b - 1) = (b - 1)(a - b - 2). \tag{4.2}$$

(I) If $b = 0$, then (4.1) yields $d(z) = 1$. This is impossible since z is a non-pendant vertex adjacent to y in G.

(II) If $b = 1$, then by (4.1) and (4.2), $d(z) = a - 2$ and $d(y) = d(z) = a - 2$.

From (3.1), $s(z) = -(a - 2)^2 + a(a - 2) - 1 = 2a - 5 = d(y) + d(z) - 1$. This shows that all the vertices adjacent to z, except y, are pendant vertices. So, G is a double star with the centers z and y. This is impossible since $G \in \mathcal{G}_{a,b}$.

(III) If $b \geq 2$, then no pendant vertex is adjacent to z in G; Otherwise, $d(z) = s(u) = -1 + a - b \geq 2$, where u is a pendant vertex is adjacent to z. This implies that $d(z) = d(y)$ and $a - b \geq 3$, contradicting with (4.2).

By (3.1), we have $s(z) = -d^2(z) + ad(z) - b$. And

$$\begin{aligned} s(z) &= \sum_{w \in N_G(z)} d(w) = \textstyle\sum_{w \in N_{G_0}(z)} d(w) \\ &= d(y) + \textstyle\sum_{w \in N_{G_0}(z) \setminus \{y\}} d(w) \\ &\geq d(y) + 2(d(z) - 1) \\ &= a - b - 1 + 2(d(z) - 1). \end{aligned}$$

So,

$$-d^2(z) + ad(z) - b \geq a - b - 1 + 2(d(z) - 1),$$

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$$d^2(z)-(a-2)d(z)+a-3\leq 0,$$

and

$$1\leq d(z)\leq a-3.$$

By (4.1), $ab-b^2-2b+1\leq a-3$, i.e., $b^2+(2-a)b+a-4\geq 0$. Then

$$b\leq\frac{(a-2)-\sqrt{(a-4)^2+4}}{2}\quad\text{or}\quad b\geq\frac{(a-2)+\sqrt{(a-4)^2+4}}{2}$$

From Theorem 2.6, $a^2>8b\geq 16$, i.e., $a>4$, and

$$\frac{(a-2)-\sqrt{(a-4)^2+4}}{2}<\frac{(a-2)-(a-4)}{2}=1.$$

So, $b\geq\frac{(a-2)+\sqrt{(a-4)^2+4}}{2}$. But

$$2\leq d(y)=a-b-1\leq a-\frac{(a-2)+\sqrt{(a-4)^2+4}}{2}-1=\frac{a-\sqrt{(a-4)^2+4}}{2}.$$

We have $a-4\geq\sqrt{(a-4)^2+4}$. This is impossible.

Summarizing (I)-(III) above, we have $\delta(G_0)\geq 2$.

(ii) Because $G\in\mathcal{G}_{a,b}$, $\delta(G)=1$. There is a pendent vertex x and the only edge xy incident with x in G. $d(y)=s(x)=a-b-1$ by (3.1). From (i), $d(y)\geq d_{G_0}(y)+1\geq\delta(G_0)+1\geq 3$. So, $a-b\geq 4$.

Since

$$\begin{aligned}s(y)&=d(y)-d_{G_0}(y)+\textstyle\sum_{w\in N_{G_0}(y)}d(w)\\&\geq d(y)-d_{G_0}(y)+2d_{G_0}(y)\\&\geq a-b-1+2=a-b+1,\end{aligned}$$

by (2.3), we have

$$\begin{aligned}a&=\tfrac{s(y)-s(x)}{d(y)-d(x)}+d(y)+d(x)\\&\geq\tfrac{(a-b+1)-(a-b-1)}{a-b-2}+(a-b-1)+1\\&=\tfrac{2}{a-b-2}+a-b>a-b\geq 4.\end{aligned}$$

So, $a\geq 5$ since a is a integer from Theorem 2.6. $\square$

In the following, we determine all unicyclic graphs with exactly two main signless Laplacian eigenvalues.

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Let G_1 be the unicyclic graph with n vertices obtained by attaching $k \geq 1$ pendant vertices to each vertex of a cycle with length r, where $n = (k+1)r$. It was showed in [10] that G_1 is the only connected graph with exactly two main eigenvalue (of adjacent matrix). G_2 is the unicyclic graph with n vertices obtained from the cycle $u_1u_2 \cdots u_{3t}$ by attaching one pendant vertices to the vertex u_{3s+1} for $s = 0, 1, \ldots, t-1$, where $n = 4t$.

Theorem 4.4. *Let G be a unicyclic graphs with n vertices different from the cycle C_n. G has exactly two main signless Laplacian eigenvalues if and only if G is isomorphic to one of graphs G_1 and G_2.*

Proof. First, it is easy to check that G_1 is a 2-walk $(k+5, 2)$-parabolic graph and G_2 is a 2-walk $(5, 1)$-parabolic graph.

Next, because $G \in \mathcal{G}_{a,b}$ is unicyclic, G_0 is a cycle from Lemma 4.3(i). Let $G_0 = C_r = u_1u_2 \cdots u_ru_1$, then $d(u_i) \in \{d_{G_0}(u_i), a-b-1\} = \{2, a-b-1\}$ from Lemma 4.2, where $1 \leq i \leq r$.

(i) If $d(u_1) = d(u_2) = \cdots = d(u_r) = a-b-1$, then u_i has $k = a-b-3$ pendant vertices for $1 \leq i \leq r$. So, $G \cong G_1$.

(ii) If there is $u_i \in V(G_0)$ such that $d(u_i) = 2$ for some $i \in \{1, 2, \ldots, r\}$, then by (3.1), we have

$$d(u_{i-1}) + d(u_{i+1}) = s(u_i) = -d^2(u_i) + ad(u_i) - b = -4 + 2a - b. \tag{4.3}$$

Without loss of generality, we assume that $d(u_{i+1}) \geq d(u_{i-1})$. From Lemma 4.3(ii), $d(u_{i-1}) + d(u_{i+1}) = s(u_i) = (a-b-4) + a \geq 5$. Since $d(u_{i-1}), d(u_{i+1}) \in \{d_{G_0}(u_i), a-b-1\} = \{2, a-b-1\}$, we have $d(u_{i+1}) = d(u_{i-1}) = a-b-1$, or $d(u_{i+1}) = a-b-1$ and $d(u_{i-1}) = 2$.

If $d(u_{i+1}) = d(u_{i-1}) = a-b-1$, then $b = 2$ by (4.3). From (3.1), $s(u_{i-1}) = -(a-b-1)^2 + a(a-b-1) - b = 3a - 11$. And

$$s(u_{i-1}) = d(u_{i-2}) + d(u_i) + (d(u_{i-1}) - d_{G_0}(u_{i-1})),$$

i.e., $d(u_{i-2}) = s(u_{i-1}) - d(u_i) - d(u_{i-1}) + d_{G_0}(u_{i-1}) = (3a-11) - 2 - (a-b-1) + 2 = 2a - 8$. From Lemma 4.2, $d(u_{i-2}) = 2a - 8 \in \{a-b-1, d_{G_0}(u_{i-2})\} = \{a-3, 2\}$. We have $a = 5$, and $a - b = 3 < 4$, contradicting with Lemma 4.2(ii).

If $d(u_{i+1}) = a-b-1$ and $d(u_{i-1}) = 2$, then $a = 5$ from (4.3). By (3.1), $s(u_{i+1}) = -(a-b-1)^2 + a(a-b-1) - b = 4 + 2b - b^2$. And

$$s(u_{i+1}) = d(u_{i+2}) + d(u_i) + (d(u_{i+1}) - 2),$$

i.e., $d(u_{i+2}) = s(u_{i+1}) - d(u_i) - d(u_{i+1}) + 2 = (4 + 2b - b^2) - 2 - (a-b-1) + 2 = 3b - b^2$.

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From Lemma 4.2, $d(u_{i+2}) = 3b - b^2 \in \{a - b - 1, d_{G_0}(u_{i-2})\} = \{4 - b, 2\}$. We have $b = 1$ or $b = 2$. And $a - b \geq 4$ from Lemma 4.3. So, $b = 1$ and $d(u_{i+1}) = 3$, $d(u_{i+2}) = 2$.

By (3.1) again,

$d(u_{i+3}) + d(u_{i+1}) = s(u_{i+2}) = -d^2(u_{i+2}) + 5d(u_{i+2}) - 1 = 5$,
and $d(u_{i+3}) = 5 - d(u_{i+1}) = 2$;

$d(u_{i+4}) + d(u_{i+2}) = s(u_{i+3}) = -d^2(u_{i+3}) + 5d(u_{i+3}) - 1 = 5$,
and $d(u_{i+4}) = 5 - d(u_{i+2}) = 3$;

$d(u_{i+5}) + d(u_{i+3}) + 1 = s(u_{i+4}) = -d^2(u_{i+4}) + 5d(u_{i+4}) - 1 = 5$,
and $d(u_{i+5}) = 5 - d(u_{i+3}) - 1 = 2$.

Continuing like this, we have

$$d(u_k) = \begin{cases} 2, & k - i \equiv 0, 2(mod 3); \\ 3, & k - i \equiv 1(mod 3). \end{cases}$$

So, $r \equiv 0(mod 3)$ and $G \cong G_2$. $\square$

The results on main sigenless Laplacian eigenvalues presented in Section 2 are useful to the problem of characterizing graphs with a given number of main sigenless Laplacian eigenvalues. And Theorems 3.1 and 4.4 show that the set of graphs with a given number of main sigenless Laplacian eigenvalues is not identical with the set of graphs a given number of main eigenvalues (of adjacent matrix).

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