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Research article

The bounds of the energy and Laplacian energy of chain graphs

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Abstract: Let G be a simple connected graph of order n with m edges. The energy $\varepsilon(G)$ of G is the sum of the absolute values of all eigenvalues of the adjacency matrix A. The Laplacian energy is defined as $LE(G) = \sum_{i=1}^{n} |\mu_i - \frac{2m}{n}|$, where $\mu_1, \mu_2, \ldots, \mu_n$ are the Laplacian eigenvalues of a graph G. In this article, we obtain some upper and lower bounds on the energy and Laplacian energy of chain graph. Finally, we attain the maximal Laplacian energy among all connected bicyclic chain graphs by comparing algebraic connectivity.

Keywords: chain graph; energy; Laplacian energy; vertex cover number; algebraic connectivity
Mathematics Subject Classification: 05C50, 05C09, 05C92

1. Introduction

In 2008, Bhattacharya et al. [5] and Bell et al. [4] discovered that bipartite chain graphs whose largest eigenvalues within the connected bipartite graph is maximal, and named therein as double nested graphs. After that, many scholars began to study some mathematical properties of chain graphs. Andelic et al. provide that some upper and lower bounds on index of chain graphs [3]. And Alazemi et al. proved that any chain graph has its least positive eigenvalue greater than $\frac{1}{2}$ [2]. Hence Zhang et al. proposed that upper bounds on Laplacian spectral radius of chain graphs [13]. Das et al. studied the energy and Laplacian energy of chain graphs [8]. In this paper, we further study some bounds of energy and Laplacian energy of chain graphs.

We consider finite undirected connected graphs without loops and multiple edges. Let G be a such graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|E(G)| = m$. Let d_i be the degree of the vertex v_i for $i = 1, 2, \ldots, n$. The minimum vertex degrees of G are denoted by $\delta(G)$. Let $N_G(v_i)$ be the adjacent set of the vertex v_i, then $d_i = |N_G(v_i)|$. If G has distinct vertices v_i and v_j with $N_G(v_i) = N_G(v_j)$, then v_i and v_j are duplicates and (v_i, v_j) is a duplicate pair.

Let $A(G)$ be the adjacency matrix of G, and $rank(G)$ be the rank of the adjacency matrix $A(G)$. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ the eigenvalues of $A(G)$. We denote $S(G) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ as the spectrum of G.

The energy of graph G is defined as [11]

$$\varepsilon(G) = \sum_{i=1}^{n} |\lambda_i|.$$

For its basic properties and application, including various lower and upper bounds, see the [17], the recent paper [1, 7, 8, 11, 12, 20] and the references cited therein.

The Laplacian matrix of graph G is defined as $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees. The matrix $L(G)$ has non-negative eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \mu_n = 0$, and the Laplacian spectrum of graph G be denoted by $LS(G) = \{\mu_1, \mu_2, \ldots, \mu_n\}$. The Laplacian energy of G is defined as [10]

$$LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|.$$

It can also be defined as

$$LE(G) = 2S_{\sigma}(G) - \frac{4m\sigma}{n}, \tag{1.1}$$

where σ $(1 \leqslant \sigma \leqslant n)$ be the largest positive integer such that $\mu_\sigma \geq \frac{2m}{n}$ and $S_k(G) = \sum\limits_{i=1}^{k} \mu_i$.

For its basic properties, including various lower and upper bounds, see [7, 8, 10, 18, 19] and the references cited therein. The Laplacian energy found applications not only in theoretical organic chemistry [12, 21], but also in image processing [22] and information theory [16].

In the class of bipartite graphs of fixed order and size those having maximal spectral radius of adjacency/Laplacian/signless Laplacian matrix are chain graphs. Thus, they can be significant in modeling some bipartite networks with large spectral radius. Their applications involve ecological networks, in which graphs with nested properties are considered [14] and are used in some applications for economic network modeling.

We now introduce the structure of a (connected) chain graph. The vertex set of any chain graph consists of two color classes, which are U and V. Both of them are divided into h non-empty units $U_1, U_2, \ldots, U_h$ and $V_1, V_2, \ldots, V_h$, respectively. All the vertices in U_s are joined by edges to all vertices in $\bigcup_{k=1}^{h+1-s} V_k$, for $s = 1, 2, \ldots, h$. Therefore, if $u_i \in U_{s+1}$ and $u_j \in U_s$, then $N_G(u_i) \subset N_G(u_j)$, or if $v_i \in V_{t+1}$ and $v_j \in v_t$, then $N_G(v_i) \subset N_G(v_j)$.

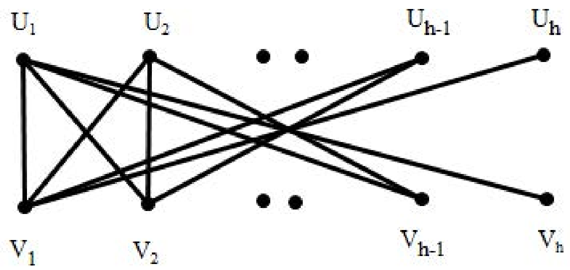

Figure 1. Structure of $G(m_1, \ldots, m_h; n_1, \ldots, n_h)$.

If $n_s = |U_s|$ and $m_s = |V_s|$ for $s = 1, 2, \ldots, h$, then G is denoted by $G(m_1, \ldots, m_h; n_1, \ldots, n_h)$, as shown in Figure 1. And

$$m = m_1 \sum_{i=1}^{h} n_i + m_2 \sum_{i=1}^{h-1} n_i + \cdots + m_h n_1 = \sum_{i=1}^{h} a_i m_i,$$

$$m = n_1 \sum_{i=1}^{h} m_i + n_2 \sum_{i=1}^{h-1} m_i + \cdots + n_h m_1 = \sum_{i=1}^{h} b_i n_i,$$

where

$$a_i = \sum_{k=1}^{h+1-i} n_k, b_i = \sum_{k=1}^{h+1-i} m_k.$$

Moreover,

$$n = \sum_{k=1}^{h} m_k + \sum_{k=1}^{h} n_k.$$

The second smallest Laplacian eigenvalue of a graph is well known as the algebraic connectivity. It has been proved that the second smallest Laplacian eigenvalue $\mu_{n-1} = 0$ if and only if G is disconnected. The algebraic connectivity is often applied in theoretical chemistry, control theory, combinatorial optimization and other fields [15].

As usual, K_n, $K_{p,q}(p + q = n)$ and $K_{1,n-1}$, denote, respectively, the complete graph, the complete bipartite graph and the star on n vertices. For other undefined notations and terminology from graph theory, the readers are referred to [6].

The paper is organized as follows. In Section 2, we list some previously known results. In Section 3, we get some upper and lower bounds on $\varepsilon(G)$ of a chain graph G. In Section 4, we establish an upper bound on $LE(G)$ of the chain graphs in terms of vertex cover number. In Section 5, we attain the maximal Laplacian energy of the bicyclic chain graph G by comparing the algebraic connectivity.

2. Preliminaries

This section lists some known results to be used in this paper.

Lemma 2.1. *[8] Let B be a $p \times p$ real symmetric matrix and B_k be its leading $k \times k$ submatrix. Then for $i = 1, 2, \ldots, k$,*

$$\lambda_{p-i+1}(B) \leqslant \lambda_{k-i+1}(B_k) \leqslant \lambda_{k-i+1}(B),$$

where $\lambda_i(B)$ is the i-th largest eigenvalue of B.

Lemma 2.2. *[9] Let G be a graph with vertices $\{v_1, v_2, \ldots, v_k\} \subseteq V(G)$ having same set of adjacent vertices, then G has at least $k - 1$ equal eigenvalues 0.*

Lemma 2.3. *[18] Let $G \ncong K_n$. Then $\mu_{n-1} \leqslant \delta(G)$.*

Lemma 2.4. *[10] Let A and B be real symmetric matrices of order n. Then for any $1 \leqslant k \leqslant n$,*

$$\sum_{i=1}^{k} \lambda_i(A + B) \leqslant \sum_{i=1}^{k} \lambda_i(A) + \sum_{i=1}^{k} \lambda_i(B),$$

where $\lambda_i(M)$ denotes the i-th largest eigenvalue of the matrix M.

Lemma 2.5. *[1] If G is a connected bipartite graph of rank r, then*

$$\varepsilon(G) \geq \sqrt{(r+1)^2 - 5}.$$

Lemma 2.6. *[11] If G is a connected bipartite graph of rank r, then*

$$LE(G) \geq 2\left(\varepsilon(G) - r\right).$$

Lemma 2.7. *[8] Let $G \cong G(m_1, \ldots, m_h; n_1, \ldots, n_h)$ be a chain graph of order n. Then*

$$\varepsilon(G) \geq 2\sqrt{n-1},$$

with equation holds if and only if $G \cong K_{1,n-1}$.

Lemma 2.8. *[8] Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. If G has $k-1$ duplicate pairs (v_i, v_{i+1}), where $i = 1, 2, \ldots, k-1$, then G has at least $k-1$ equal Laplacian eigenvalues and they are all equal to the cardinality of the neighbor set.*

3. Bounds on the energy of chain graphs

Theorem 3.1. *Let $G \cong G(m_1, \ldots, m_h; n_1, \ldots, n_h)$ be a chain graph of order n. Then*

$$\varepsilon(G) \leqslant 2\sqrt{hm} \tag{3.1}$$

with equation holds if and only if $G \cong K_{n_1,m_1}$, where $n_1 + m_1 = n$.

Proof. By Lemma 2.2, the eigenvalue 0 with multiplicity $\sum_{i=1}^{h}(n_i + m_i - 2)$ of $A(G)$, and the remaining eigenvalues are the eigenvalues of the following matrix,

$$C = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 & m_1 & m_2 & \cdots & m_{h-1} & m_h \\ 0 & 0 & \cdots & 0 & 0 & m_1 & m_2 & \cdots & m_{h-1} & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & m_1 & m_2 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & m_1 & 0 & \cdots & 0 & 0 \\ n_1 & n_2 & \cdots & n_{h-1} & n_h & 0 & 0 & \cdots & 0 & 0 \\ n_1 & n_2 & \cdots & n_{h-1} & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ n_1 & n_2 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ n_1 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{2h}$ be the eigenvalues of C. Then

$$\varepsilon(G) = \sum_{i=1}^{2h} |\lambda_i|.$$

Since G be a bipartite graph, we have λ_i and $-\lambda_i$ are eigenvalues of G. Thus we have

$$\varepsilon(G) = 2\sum_{i=1}^{h}\lambda_i.$$

Obviously,

$$\sum_{i=1}^{2h}\lambda_i^2 = Tr(C^2) = 2\sum_{i=1}^{h}\sum_{j=1}^{h-i+1} m_j n_i = 2m,$$

that is,

$$\sum_{i=1}^{h}\lambda_i^2 = \sum_{i=1}^{h}\sum_{j=1}^{h-i+1} m_j n_i = m.$$

So

$$\begin{aligned}\varepsilon(G) &= 2\sqrt{\sum_{i=1}^{h}\lambda_i^2 + 2\sum_{1\leqslant i<j\leqslant h}\lambda_i\lambda_j}\\ &\leq 2\sqrt{\sum_{i=1}^{h}\lambda_i^2 + \sum_{i=1}^{h}(h-1)\lambda_i^2}\\ &= 2\sqrt{h\sum_{i=1}^{h}\lambda_i^2}\\ &= 2\sqrt{hm}.\end{aligned}$$

First we assume that $h = 1$. Then $G \cong K_{n_1,m_1}$, where $n_1 + m_1 = n$. So $S(G) = \{\pm\sqrt{m_1 n_1}, 0, \cdots, 0\}$ and $\varepsilon(G) = 2\sqrt{m_1 n_1} = 2\sqrt{m}$. Hence the equation holds in (3.1).

Next we assume that $h \geq 2$. By the definition of chain graph, $G(1, 1; 1, 1)$, that is, P_4 is an induced subgraph of G. By Lemma 2.1, we get $\lambda_2(G) \geq \lambda_2(P_4) > 0$. Since G is connected, by Perron-Frobenius theorem we have $\lambda_1(G) > \lambda_2(G)$. Hence the inequality $2\sum_{1\leqslant i<j\leqslant h}\lambda_i\lambda_j \leq \sum_{i=1}^{h}(h-1)\lambda_i^2$ is strict. This completes the proof. □

Theorem 3.2. *Let $G \cong G(m_1, \ldots, m_h; n_1, \ldots, n_h)$ be a chain graph of order n. Then*

$$\varepsilon(G) \geq \sqrt{(2h+1)^2 - 5}. \tag{3.2}$$

Proof. By calculating the matrix C in the proof of Theorem 3.1, we get

$$\det(C) = (-1)^h \prod_{i=1}^{h} m_i n_i \neq 0.$$

Therefore, all the eigenvalues of matrix C are non-zero. Hence $r(G) = 2h$. Using Lemma 2.5, we can get result in (3.2). □

4. Bounds on the Laplacian energy of chain graphs

In this section, we give an upper bound on $LE(G)$ of chain graphs in terms of vertex cover number. Also, the lower bound follows from a known lower bound for Laplacian energy of any graph in terms of rank and energy.

Theorem 4.1. *Let $G \cong G(m_1, \ldots, m_h; n_1, \ldots, n_h)$ be a chain graph of order n, and $a_1 \geq b_1$. Then*

$$LE(G) \leq \begin{cases} 2(m + b_1) - \frac{4m}{n}, & \text{if } \frac{2m}{n} \geq b_1, \\ 2b_1(n-2) - 2m + \frac{8m}{n}, & \text{if } \frac{2m}{n} < b_1, \end{cases} \tag{4.1}$$

with equation holds if and only if $G \cong K_{1,n-1}$.

Proof. Let $\Gamma = \{v_{11}, v_{12}, \ldots, v_{1m_1}, v_{21}, v_{22}, \ldots, v_{2m_2}, \ldots, v_{h1}, v_{h2}, \ldots, v_{hm_h}\}$ be a vertex cover set of the graph G, where v_{ij} is the j-th vertex in V_i. Hence $\{v_{i1}, v_{i2}, \ldots, v_{im_i}\} \in V_i$. We can assume that G_{ij} are spanning subgraphs of G such that $V(G) = V(G_{i1}) = V(G_{i2}) = \cdots = V(G_{im_i})$, and the edge set of G_{ij} is defined as

$$E(G_{ij}) = \left\{ v_{ij}U_k : U_k \subseteq N_G(v_{ij}) \right\}.$$

Since $|N_G(v_{i1})| = |N_G(v_{i2})| = \cdots = |N_G(v_{im_i})| = a_i$,

$$G_{ij} = K_{1,a_i} \cup (n - a_i - 1)K_1,$$

we have

$$E(K_{m_i,a_i}) = E(G_{i1}) \cup E(G_{i2}) \cup \cdots \cup E(G_{im_1}),$$

so

$$L(K_{m_i,a_i}) = L(G_{i1}) + L(G_{i2}) + \cdots + L(G_{im_1}), \quad i = 1, 2, \ldots, h.$$

By Figure 1,

$$E(G) = E(K_{m_1,a_1}) \cup E(K_{m_2,a_2}) \cup \cdots \cup E(K_{m_i,a_i}),$$

then we can see easily that

$$L(G) = L(K_{m_1,a_1}) + L(K_{m_2,a_2}) + \cdots + L(K_{m_i,a_i}).$$

Note that

$$S_k(G_{i1}) = S_k(G_{i2}) = \cdots = S_k(G_{im_i}) \leq a_i + k,$$

where $S_k(G)$ is the sum of the k largest Laplacian eigenvalues of graph G.

By Lemma 2.4, we get

$$\begin{aligned} S_k(G) &\leq m_1 S_k(G_{11}) + m_2 S_k(G_{21}) + \cdots + m_h S_k(G_{h1}) \\ &\leq m_1(a_1 + k) + m_2(a_2 + k) + \cdots + m_h(a_h + k) \\ &= \sum_{i=1}^{h} m_i a_i + k \sum_{i=1}^{h} m_i \\ &= m + kb_1. \end{aligned}$$

So from (1.1), we get

$$LE(G) = 2S_{\sigma}(G) - \frac{4m\sigma}{n} \leq 2(m + \sigma b_1) - \frac{4m\sigma}{n} = 2m + 2\sigma\left(b_1 - \frac{2m}{n}\right).$$

Since G is connected, $1 \leq \sigma \leq n-1$. So it suffices to consider the following two cases.

Case1. $\frac{2m}{n} \geq b_1$.

Then we have

$$LE(G) \leq 2m + 2b_1 - \frac{4m}{n} = 2(m + b_1) - \frac{4m}{n}.$$

Case2. $\frac{2m}{n} < b_1$.

By Lemma 2.3, we get $\mu_{n-1} \leq \delta(G) \leq \frac{2m}{n}$. Thus it must be $1 \leq \sigma \leq n-2$. Hence

$$LE(G) \leq 2m + 2(n-2)\left(b_1 - \frac{2m}{n}\right) = 2b_1(n-2) - 2m + \frac{8m}{n}.$$

Next we prove that the equality holds.

If $G \cong K_{1,n-1}$, we get $b_1 = m_1 = 1, n_1 = n-1$, and $S(G) = \{0, 1^{n-2}, n\}$. Then

$$LE(K_{1,n-1}) = \sum_{i=1}^{n}\left|\mu_i - \frac{2m}{n}\right| = 2n - \frac{4(n-1)}{n} = 2(m + b_1) - \frac{4m}{n}. \qquad \square$$

Theorem 4.2. *Let $G \cong G(m_1, \ldots, m_h; n_1, \ldots, n_h)$ be a chain graph of order n. Then*

$$LE(G) \geq 4(\sqrt{n-1} - h). \tag{4.2}$$

Proof. By Theorem 3.2, we get $r(G) = 2h$. Using Lemmas 2.6 and 2.7, we get result in (4.2). $\square$

5. Laplacian energy of bicyclic chain graphs

Let G be a connected bicyclic chain graph. We have $m = n + 1$, and $h = 2$ or $h = 3$. If $h = 2$, then $G \cong G(1, 1; 3, n-5)$ or $G \cong G(1, 2; 2, n-5)$. If $h = 3$, then $G \cong G(1, 2, k-3; 1, 1, n-k-2)$, where $4 \leq k \leq n-3$ (Figure 2). In this section, we will attain the maximal Laplacian energy of all connected bicyclic chain graphs.

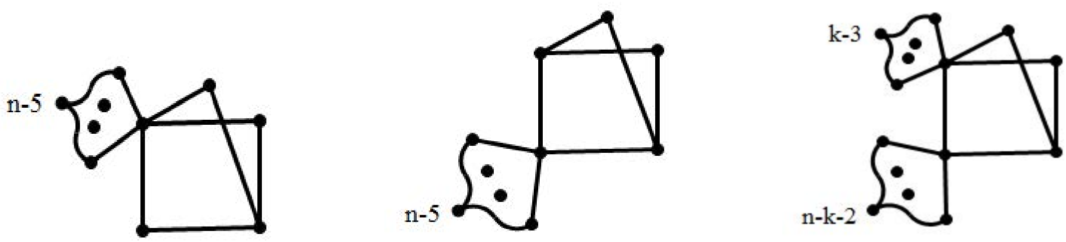

Figure 2. Graphs $G(1, 1; 3, n-5)$, $G(1, 2; 2, n-5)$ and $G(1, 2, k-3; 1, 1, n-k-2)$.

Lemma 5.1. *Let G be a connected bicyclic chain graph* ($n \geq 8$).

(1) If $G \cong G(1,1;3,n-5)$*, then* $LE(G) = 6 + \frac{2(n-4)(n+1)}{n} - 2\mu_{n-1}$.

(2) If $G \cong G(1,2;2,n-5)$*, then* $LE(G) = 10 + \frac{2(n-6)(n+1)}{n} - 2\mu_{n-1}$.

(3) If $G \cong G(1,2,k-3;1,1,n-k-2)$*, where* $4 \leq k \leq n-3$*, then* $LE(G) = 10 + \frac{2(n-6)(n+1)}{n} - 2\mu_{n-1}$.

Proof. (1) Let $G \cong G(1,1;3,n-5)$. By Lemma 2.8, we conclude that $2, 2, \underbrace{1, 1, \cdots, 1}_{n-6}$ are the Laplacian eigenvalues of G and the remaining Laplacian eigenvalues of G are satisfying the equation $f_1(x) = 0$, where $f_1(x)$ is the characteristic polynomial of the matrix

$$A_1 = \begin{pmatrix} n-2 & 0 & -3 & 5-n \\ 0 & 3 & -3 & 0 \\ -1 & -1 & 2 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix},$$

that is, $f_1(x) = x\left(x^3 - (4+n)x^2 + (5n-2)x - 3n\right)$.

Let $h_1(x) = x^3 - (4+n)x^2 + (5n-2)x - 3n$. Then we obtain $h_1(0) = -3n < 0$, $h_1(1) = n-5 > 0$, $h_1(2) = 3n-12 > 0$, $h_1(n-1) = -3 < 0$ and $\lim_{x\to\infty} h_1(x) = \infty$. Thus the Laplacian eigenvalues of G are $\mu_1, \mu_2, 2, 2, \underbrace{1, 1, \ldots, 1}_{n-6}, \mu_{n-1}, 0$, where $\mu_1 \geq n-1$, $2 \leq \mu_2 \leq n-1$, $\mu_{n-1} < 1$ and $\mu_1 + \mu_2 + \mu_{n-1} = n+4$.

Therefore

$$LE(G) = \sum_{i=1}^{n} \left|\mu_i - \frac{2(n+1)}{n}\right| = 6 + \frac{2(n-4)(n+1)}{n} - 2\mu_{n-1}. \tag{5.1}$$

(2) Let $G \cong G(1,2;2,n-5)$. By Lemma 2.8, we conclude that $3, 2, \underbrace{1, 1, \cdots, 1}_{n-6}$ are the Laplacian eigenvalues of G and the remaining Laplacian eigenvalues of G are satisfying the equation $f_2(x) = 0$, where $f_2(x)$ is the characteristic polynomial of the matrix

$$A_2 = \begin{pmatrix} n-3 & 0 & -2 & 5-n \\ 0 & 2 & -2 & 0 \\ -1 & -2 & 3 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix},$$

that is, $f_2(x) = x\left(x^3 - (3+n)x^2 + (5n-8)x - 2n\right)$.

Let $h_2(x) = x^3 - (3+n)x^2 + (5n-8)x - 2n$. Then we obtain $h_2(0) = -2n < 0$, $h_2(1) = 2n-10 > 0$, $h_2(3) = 4n-24 > 0$, $h_2(n-2) = -4 < 0$ and $\lim_{x\to\infty} h_2(x) = \infty$. Thus the Laplacian eigenvalues of G are $\mu_1, \mu_2, 3, 2, \underbrace{1, 1, \ldots, 1}_{n-6}, \mu_{n-1}, 0$, where $\mu_1 \geq n-2$, $3 \leq \mu_2 \leq n-2$, $\mu_{n-1} < 1$ and $\mu_1 + \mu_2 + \mu_{n-1} = n+3$.

Therefore

$$LE(G) = \sum_{i=1}^{n} \left|\mu_i - \frac{2(n+1)}{n}\right| = 10 + \frac{2(n-6)(n+1)}{n} - 2\mu_{n-1}. \tag{5.2}$$

(3) Let $G \cong G(1,2,k-3;1,1,n-k-2)$. When $4 \leq k \leq \lceil \frac{n}{2} \rceil$, by Lemma 2.8, we conclude that $2, \underbrace{1, 1, \cdots, 1}_{n-7}$ are the Laplacian eigenvalues of G and the remaining laplacian eigenvalues of G are satisfying equation $f_3(x) = 0$, where $f_3(x)$ is the characteristic polynomial of the matrix

$$A_3 = \begin{pmatrix} n-k & 0 & 0 & -1 & -1 & 2+k-n \\ 0 & 2 & 0 & -1 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ -1 & -2 & 3-k & k & 0 & 0 \\ -1 & -2 & 0 & 0 & 3 & 0 \\ -1 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

that is

$$f_3(x) = x(x-1)\left(x^4 - (n+6)x^3 + (kn+5n-k^2+10)x^2 - (4kn+5n-4k^2+12)x + 6n\right). \tag{5.3}$$

Let $g(x) = x^4 - (n+6)x^3 + (kn+5n-k^2+10)x^2 - (4kn+5n-4k^2+12)x + 6n$. Then we obtain $g(0) = 6n > 0$, $g(1) = 3k^2 - 3kn + 5n - 7 < 0$, $g(2) = 4(k-2)(2+k-n) < 0$, $g(k) = -(k-2)(k-3)(2k-n) \geq 0$. Since when n is odd, $g(x)$ is same for $k = \lceil \frac{n}{2} \rceil$ and $k = \lfloor \frac{n}{2} \rfloor$, we take a smaller value $k = \lfloor \frac{n}{2} \rfloor$. $g(n-k) = (2+k-n)(2k-n)(-n+3+k) \leq 0$ and $\lim\limits_{x\to\infty} g(x) = \infty$. Thus the Laplacian eigenvalues of G are $\mu_1, \mu_2, \mu_3, 2, \underbrace{1, 1, \cdots, 1}_{n-7}, \mu_{n-1}, 0$, where $\mu_1 \geq n-k$, $k \leq \mu_2 \leq n-k$, $2 < \mu_3 < k$, $\mu_{n-1} < 1$.

Since $\sum\limits_{i=1}^{n} \mu_i = 2m = 2(n+1) = 2n+2$, we get $\mu_1+\mu_2+\mu_3+\mu_{n-1} = n+6$, that is, $\mu_1+\mu_2+\mu_3 = n+6-\mu_{n-1}$.

Therefore

$$LE(G) = \sum_{i=1}^{n} \left|\mu_i - \frac{2(n+1)}{n}\right| = 10 + \frac{2(n-6)(n+1)}{n} - 2\mu_{n-1}. \tag{5.4}$$

When $\lceil \frac{n}{2} \rceil < k < n-3$, letting $k = n-k$ in the Eq (5.3) we get the same characteristic polynomial, so it is equal to the Laplacian energy when $4 \leq k \leq \lceil \frac{n}{2} \rceil$.

When $k = n-3$, $f_3(x) = x(x-1)(x-3)\left(x^3 - (3+n)x^2 + (5n-8)x - 2n\right)$, so it is equal to the Laplacian energy of $G(1,2;2,5)$.

This completes the proof. □

Lemma 5.2. *Let $G_{n,k} \cong G(1,2,k-3;1,1,n-k-2)$, where $4 \leq k \leq \lceil \frac{n}{2} \rceil$. Then $\mu_{n-1}(G_{n,k}) \geq \mu_{n-1}\left(G(1,2,\lceil \frac{n}{2} \rceil - 3;1,1,\lfloor \frac{n}{2} \rfloor - 2)\right)$, with equation holds if and only if $k = \lceil \frac{n}{2} \rceil$. In particular, if n is odd, then $\mu_{n-1}\left(G(1,2,\lceil \frac{n}{2} \rceil - 3;1,1,\lfloor \frac{n}{2} \rfloor - 2)\right) = \mu_{n-1}\left(G(1,2,\lceil \frac{n}{2} \rceil - 4;1,1,\lfloor \frac{n}{2} \rfloor - 1)\right)$.*

Proof. If $k = \lceil \frac{n}{2} \rceil$, then $\mu_{n-1}(G_{n,k}) = \mu_{n-1}\left(G(1,2,\lceil \frac{n}{2} \rceil - 3;1,1,\lfloor \frac{n}{2} \rfloor - 2)\right)$. By Lemma 5.1, we obtain that $\mu_1, \mu_2, \mu_3, \mu_{n-1}$ are the roots of the equation $P(G_{n,k}, x) = 0$, where

$$P(G_{n,k}, x) = x^4 - (n+6)x^3 + (kn+5n-k^2+10)x^2 - (4kn+5n-4k^2+12)x + 6n,$$

and $\mu_1 \geq n-k$, $k \leq \mu_2 \leq n-k$, $2 < \mu_3 < k$, $\mu_{n-1} < 1$.

We need to prove that

$$\mu_{n-1}(G_{n,k}) > \mu_{n-1}\left(G(1,2,\lceil\frac{n}{2}\rceil - 3;1,1,\lfloor\frac{n}{2}\rfloor - 2)\right), \; for\ 4 \leq k \leq \lceil\frac{n}{2}\rceil - 1.$$

Since

$$P(G_{n,k+1}, x) - P(G_{n,k}, x) = x(x-4)(n-2k-1),\ \ for\ 0 < x < 1,$$

we get $P(G_{n,k+1}, x) - P(G_{n,k}, x) \leq 0$. Hence $P(G_{n,k+1}, x) \leq P(G_{n,k}, x)$. So when n is odd and $k = \lceil \frac{n}{2} \rceil - 1$, the equation holds.

Thus we have $\mu_{n-1}(G_{n,k}) > \mu_{n-1}(G_{n,k+1})$, that is,

$$\mu_{n-1}(G_{n,4}) > \mu_{n-1}(G_{n,5}) > \cdots > \mu_{n-1}(G_{n,\lceil \frac{n}{2} \rceil - 1}) \geq \mu_{n-1}(G_{n,\lceil \frac{n}{2} \rceil}). \tag{5.5}$$

Hence $\mu_{n-1}(G_{n,k}) > \mu_{n-1}(G_{n,\lceil \frac{n}{2} \rceil}) = \mu_{n-1}\left(G(1, 2, \lceil \frac{n}{2} \rceil - 3; 1, 1, \lfloor \frac{n}{2} \rfloor - 2)\right)$.

This completes the proof. □

Lemma 5.3. *Let G be a bicyclic graph of order $n \geq 8$. Then $\mu_{n-1}(G(1, 2; 2, n-5)) > \mu_{n-1}\left(G(1, 2, \lceil \frac{n}{2} \rceil - 3; 1, 1, \lfloor \frac{n}{2} \rfloor - 2)\right)$.*

Proof. When $k = 3$, we get $P(G_{n,k}, x) = f_2(x)$, that is $\mu_{n-1}(G_{n,3}) = \mu_{n-1}(G(1, 2; 2, n-5))$.

By Lemma 5.2, we have $P(G_{n,k+1}, x) \leq P(G_{n,k}, x)$, and $P(G_{n,4}, x) \leq P(G_{n,3}, x)$ still hold.

By inequation (5.5), we obtain

$$\mu_{n-1}(G_{n,3}) > \mu_{n-1}(G_{n,4}) > \cdots > \mu_{n-1}(G_{n,\lceil \frac{n}{2} \rceil - 1}) \geq \mu_{n-1}(G_{n,\lceil \frac{n}{2} \rceil}).$$

Hence $\mu_{n-1}(G(1, 2; 2, n-5)) > \mu_{n-1}(G_{n,\lceil \frac{n}{2} \rceil}) = \mu_{n-1}\left(G(1, 2, \lceil \frac{n}{2} \rceil - 3; 1, 1, \lfloor \frac{n}{2} \rfloor - 2)\right)$ for $n \geq 8$. □

Lemma 5.4. *Let G be a bicyclic graph of order $n \geq 8$. Then $\mu_{n-1}(G(1, 1; 3, n-5)) - \mu_{n-1}\left(G(1, 2, \lceil \frac{n}{2} \rceil - 3; 1, 1, \lfloor \frac{n}{2} \rfloor - 2)\right) > \frac{2}{n}$.*

Proof. For $n = 8$ and $n = 9$, it can be verified by using Maple.

Let $n = 8$, $\mu_{n-1}(G(1, 1; 3, n-5)) = 0.8377$ and $\mu_{n-1}\left(G(1, 2, \lceil \frac{n}{2} \rceil - 3; 1, 1, \lfloor \frac{n}{2} \rfloor - 2)\right) = 0.5858$. Then $\mu_{n-1}(G(1, 1; 3, n-5)) - \mu_{n-1}\left(G(1, 2, \lceil \frac{n}{2} \rceil - 3; 1, 1, \lfloor \frac{n}{2} \rfloor - 2)\right) = 0.2519 > \frac{1}{4}$, so the conclusion is correct.

Let $n = 9$, $\mu_{n-1}(G(1, 1; 3, n-5)) = 0.8169$ and $\mu_{n-1}\left(G(1, 2, \lceil \frac{n}{2} \rceil - 3; 1, 1, \lfloor \frac{n}{2} \rfloor - 2)\right) = 0.5344$. Then $\mu_{n-1}(G(1, 1; 3, n-5)) - \mu_{n-1}\left(G(1, 2, \lceil \frac{n}{2} \rceil - 3; 1, 1, \lfloor \frac{n}{2} \rfloor - 2)\right) = 0.2825 > \frac{2}{9}$, so the conclusion is correct.

Next we prove when $n \geq 10$, the inequality holds.

By Lemma 5.3, we get $\mu_{n-1}(G(1, 2; 2, n-5)) \geq \mu_{n-1}\left(G(1, 2, \lceil \frac{n}{2} \rceil - 3; 1, 1, \lfloor \frac{n}{2} \rfloor - 2)\right)$, so we can prove $\mu_{n-1}(G(1, 1; 3, n-5)) - \mu_{n-1}(G(1, 2; 2, n-5)) > \frac{2}{n}$. Let $\alpha = \mu_{n-1}(G(1, 1; 3, n-5)), \beta = \mu_{n-1}(G(1, 2; 2, n-5))$. Then it is satisfying

$$h_1(x) = x^3 - (4+n)x^2 + (5n-2)x - 3n \ and \ h_1(\alpha) = 0.$$

$$h_2(x) = x^3 - (3+n)x^2 + (5n-8)x - 2n \ and \ h_2(\beta) = 0.$$

By the implicit function existence theorem and Figure 3, when $G \cong G(1, 1; 3, n-5)$, the relation between the decreases of α and the increase of n, and $h_1(x)$ is monotonically increasing on the interval $[0, 1]$. Hence $h_1(0.81) = -3.713 + 0.39n > 0$, $h_1(0.69) = -2.956 - 0.26n < 0$, so $0.69 < \alpha < 0.81$.

Similarly, $h_2(0.58) = -5.454 + 0.56n > 0$, $h_2(0.43) = -3.915 - 0.035n < 0$, so $0.43 < \beta < 0.58$. Therefore, $\alpha - \beta > 0.11 > \frac{2}{19}$, that is, when $n \geq 19$, hence the conclusion is correct.

When $10 \leq n \leq 18$, $\alpha - \beta > \frac{2}{n}$ is obvious. The results are shown in Table 1.

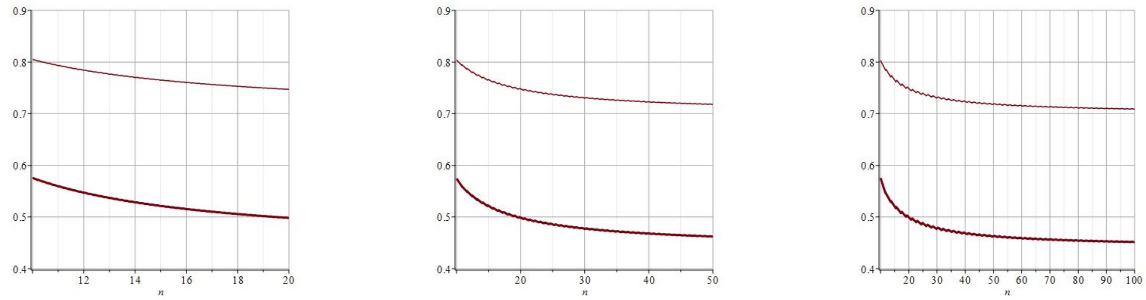

Figure 3. $h_1(x)$ (thin line) and $h_2(x)$ (thick line).

Table 1. The correlation between $\alpha - \beta$ and $\frac{2}{n}$.

n	α	β	$\alpha - \beta$	$\frac{2}{n}$
10	0.8107	0.5735	0.2372	0.200
11	0.7899	0.5566	0.2333	0.182
12	0.7804	0.5438	0.2366	0.167
13	0.7728	0.5332	0.2396	0.154
14	0.7666	0.5248	0.2418	0.143
15	0.7612	0.5176	0.2436	0.133
16	0.7566	0.5116	0.2450	0.125
17	0.7526	0.5064	0.2462	0.118
18	0.7491	0.5020	0.2471	0.111

So we conclude that when $n \geq 8$,

$$\mu_{n-1}(G(1,1;3,n-5)) - \mu_{n-1}\left(G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)\right) > \frac{2}{n}. \qquad \square$$

Theorem 5.1. *Let G be a connected bicyclic chain graph of order $n \geq 8$. Then $G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)$ attains the maximal Laplacian energy. In particular, when n is odd, $LE\left(G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)\right) = LE\left(G(1,2,\lceil \frac{n}{2} \rceil - 4; 1,1,\lfloor \frac{n}{2} \rfloor - 1)\right)$.*

Proof. By Lemma 5.1, we can attain the maximal Laplacian energy by comparing μ_{n-1} in equations (5.1), (5.2) and (5.4). It is obvious that $LE(G(1,2;2,n-5)) < LE\left(G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)\right)$. In particular, when n is odd, $LE\left(G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)\right) = LE\left(G(1,2,\lceil \frac{n}{2} \rceil - 4; 1,1,\lfloor \frac{n}{2} \rfloor - 1)\right)$. So

$$\begin{aligned}
&LE\left(G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)\right) - LE(G(1,1;3,n-5)) \\
=&10 + \frac{2(n-6)(n+1)}{n} - 2\mu_{n-1}\left(G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)\right) \\
&-6 - \frac{2(n-4)(n+1)}{n} + 2\mu_{n-1}(G(1,1;3,n-5)) \\
=&2\left(\mu_{n-1}(G(1,1;3,n-5)) - \mu_{n-1}\left(G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)\right)\right) - \frac{4}{n}.
\end{aligned}$$

Hence by Lemma 5.4, $LE\left(G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)\right) - LE(G(1,1;3,n-5)) > 0$, that is, $LE\left(G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)\right) > LE(G(1,1;3,n-5))$. In conclusion, we get $G(1,2,\lceil \frac{n}{2} \rceil - 3; 1,1,\lfloor \frac{n}{2} \rfloor - 2)$ has the maximal Laplacian energy among all connected bicyclic chain graphs ($n \geq 8$). $\square$

6. Conclusions

In this paper, we introduced the definition of chain graph. We obtain some bounds on $\varepsilon(G)$ of the chain graphs. Since the rank of the chain graphs is $2h$, we can get some bounds on $\varepsilon(G)$ and $LE(G)$ of the chain graphs. We present the upper bound on $LE(G)$ of the chain graphs in terms of vertex cover number. In order to attain the maximal Laplacian energy of bicyclic chain graphs, we compare algebraic connectivity of each kind of bicyclic chain graphs. The problem is still open to discuss what chain graphs give the maximal Laplacian energy for given n and whether it is still related to algebraic connectivity.

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Conflict of interest

The authors declare that they have no conflict of interest in this paper.

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