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ON THE SECOND LAPLACIAN SPECTRAL MOMENT OF A GRAPH

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Abstract. Kragujevac (M. L. Kragujevac: On the Laplacian energy of a graph, Czech. Math. J. *56(131)* (2006), 1207–1213) gave the definition of Laplacian energy of a graph G and proved $LE(G) \geqslant 6n-8$; equality holds if and only if $G = P_n$. In this paper we consider the relation between the Laplacian energy and the chromatic number of a graph G and give an upper bound for the Laplacian energy on a connected graph.

Keywords: Laplacian eigenvalues, Laplacian energy, chromatic number, complement

MSC 2010: 05C50

1. Introduction

Let $G = (V,\ E)$ be a simple connected graph with vertex set $V = \{v_1, v_2, \dots, v_n\}$ and edge set E. Denote by d_i the degree of a vertex v_i of the graph G. Without loss of generality, we assume $d_1 \geqslant d_2 \geqslant \dots \geqslant d_n$ and denote by $\pi(G) = (d_1, d_2, \dots, d_n)$ the degree sequence of G. Let $A(G)$ be the adjacency matrix of G and $L(G) = D(G) - A(G)$ the Laplacian matrix of the graph G where $D(G) = \operatorname{diag}(d_1, d_2, \dots, d_n)$ is the diagonal matrix of vertex degrees of G. Denote its Laplacian eigenvalues by $\mu_1(G) \geqslant \mu_2(G) \geqslant \dots \geqslant \mu_n(G) = 0$ (or $\mu_1 \geqslant \mu_2 \geqslant \dots \geqslant \mu_n = 0$).

The energy of a graph G is defined as the sum of the absolute values of all the eigenvalues of $A(G)$. This quantity has a long known chemical application, for details see the surveys ([4]–[6]). Recently, Kragujevac [7] gave the definition of the Laplacian energy of a graph G as

$$LE(G) = \sum_{i=1}^{n} \mu_i^2(G) = \sum_{i=1}^{n-1} \mu_i^2(G). \tag{1}$$

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In fact, the quantity was named "Laplacian energy". However, this quantity is simply the well-known "second spectral moment" (of the Laplacian eigenvalues) or, more colloquially, "second Laplacian spectral moment". Furthermore, Laplacian eigenvalues obey the well-known relations

$$\sum_{i=1}^{n} \mu_i(G) = 2m, \quad \sum_{i=1}^{n} \mu_i^2(G) = 2m + \sum_{i=1}^{n} d_i^2(G) \tag{2}$$

where $m = |E(G)|$. Kragujevac ([7]) proved

$$LE(G) \geqslant 6n - 8,$$

where equality holds if and only if $G = P_n$. In this paper we consider the relation between $LE(G)$ and its chromatic number, and give a strict upper bound of $LE(G)$.

2. The Laplacian energy of G and its chromatic number

In order to obtain our main result in this section, the following notation and lemmas are necessary.

Definition 2.1. For a graph G, the chromatic number of G, denoted by $\chi(G)$, is the minimum number of colors needed to color the vertices of G so that no two adjacent vertices have the same color.

Lemma 2.1 ([1]). *For any graph G with $\chi(G) = k$, G has at least k vertices v_i with $d_i \geqslant k - 1$ $(1 \leqslant i \leqslant k)$.*

Lemma 2.2 ([2]). *For any graph G we have*

$$\chi(G) \leqslant \Delta + 1;$$

the equality holds if and only if $G = C_{2n+1}$ or $G = K_n$.

Lemma 2.3 ([3]). *For any graph G, if G_1 is a subgraph of G,*

$$\mu_i(G_1) \leqslant \mu_i(G).$$

Now, we formulate and prove the result of this section.

Theorem 2.1. *Let G be a connected graph with $\chi(G) = k$. Then*

$$LE(G) \geqslant k^2(k-1),$$

and the equality holds if and only if $G = K_1$, $G = C_3$ or $G = K_n$.

P r o o f. By (1), (2) and Lemma 2.1, we obtain

$$\begin{aligned} LE(G) &= \sum_{i=1}^{n} \mu_i^2(G) = 2m + \sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} d_i + \sum_{i=1}^{n} d_i^2 \\ &\geqslant k(k-1) + k(k-1)^2 = k^2(k-1). \end{aligned}$$

Next, we prove equality. We first prove necessity.

Case 1: $G = K_1$.

$$SP_L(G) = \{0\},\ \chi(G) = k = 1,\ \text{so } LE(G) = 0 = k^2(k-1).$$

Case 2: $G = C_3$.

$$SP_L(G) = \{3,3,0\},\ \chi(G) = k = 3,\ \text{so } LE(G) = 18 = k^2(k-1).$$

Case 3: $G = K_n$.

$$SP_L(G) = \{\underbrace{n,\ldots,n}_{n-1},0\},\ \chi(G) = k = n,\ \text{so } LE(G) = 0 = k^2(k-1).$$

We prove sufficiency.

Case 1: $G = C_{2n+1}$ ($n \geqslant 2$) is an odd cycle; then $\chi(G) = k = 3$. Since P_{2n+1} is a subgraph of G, by Lemma 2.3 we have

$$\begin{aligned} \mu_1(G) &\geqslant \mu_1(P_{2n+1}) \geqslant \mu_1(P_5) = \frac{5+\sqrt{5}}{2}, \\ \mu_2(G) &\geqslant \mu_2(P_{2n+1}) \geqslant \mu_2(P_5) = \frac{3+\sqrt{5}}{2}. \end{aligned}$$

So we obtain

$$\begin{aligned} LE(G) &= \sum_{i=1}^{n} \mu_i^2(G) \geqslant \mu_1^2(G) + \mu_2^2(G) \geqslant \mu_1^2(P_{2n+1}) + \mu_2^2(P_{2n+1}) \\ &\geqslant \mu_1^2(P_5) + \mu_2^2(P_5) = 11 + 4\sqrt{5} > 9. \end{aligned}$$

Case 2: G is neither K_n nor C_{2n+1}.

By Lemma 2.2, we have

$$k < \Delta + 1 < n.$$

Let $\chi(G) = k$, then by Lemma 2.1, G has at least k vertices v_i with $d_i \geqslant k-1$ $(1 \leqslant i \leqslant k)$. So

$$\begin{aligned} LE(G) &= \sum_{i=1}^{n} \mu_i^2(G) = 2m + \sum_{i=1}^{n} d_i^2 = \sum_{i=1}^{n} d_i + \sum_{i=1}^{n} d_i^2 \\ &\geqslant k(k-1) + k(k-1)^2 + 2(n-k) = k^2(k-1) + 2(n-k) > k^2(k-1). \end{aligned}$$

□

3. The Laplacian energy of $L(G)$ and $L(\overline{G})$

We will consider connected graphs with the maximal Laplacian energy in the class of all connected graphs with $n \geqslant 2$ vertices.

Theorem 3.1. *Let $G = (V, E)$ be a connected graph with $|V(G)| = n$ $(n \geqslant 2)$, $|E(G)| = m$ and $\Delta(G) \leqslant d$. Then*

1. *the Laplacian energy of G satisfies*

$$LE(G) \leqslant (2m-n)d + 4m; \tag{3}$$

2. *the equality of (3) holds if and only if*

$$\pi(G) = \{\underbrace{d, \ldots, d}_{s \geqslant 1}, \underbrace{1, \ldots, 1}_{n-s}\}$$

where $\pi(G)$ is the degree sequence of G.

Proof. Considering the inequality

$$(d_i - 1)(d_i - d) \leqslant 0 \quad (1 \leqslant i \leqslant n)$$

we have

$$\begin{aligned} \sum_{i=1}^{n} (d_i - 1)(d_i - d) \leqslant 0 &\implies \sum_{i=1}^{n} d_i^2 \leqslant (d+1) \sum_{i=1}^{n} d_i - dn \\ &\implies \sum_{i=1}^{n} d_i^2 \leqslant 2m(d+1) - dn. \end{aligned} \tag{4}$$

So we have

$$LE(G) = \sum_{i=1}^{n} \mu_i^2(G) = 2m + \sum_{i=1}^{n} d_i^2 \leqslant 2m + 2m(d+1) - dn = (2m-n)d + 4m.$$

Now we discuss how to attain the equality. We know the equality in (4) holds if and only if

$$d_i = 1 \quad \text{or} \quad d_i = d \quad (1 \leqslant i \leqslant n),$$

that is to say,

$$\pi(G) = \{\underbrace{d, \ldots, d}_{s \geqslant 1}, \underbrace{1, \ldots, 1}_{n-s}\},$$

and the proof is completed. □

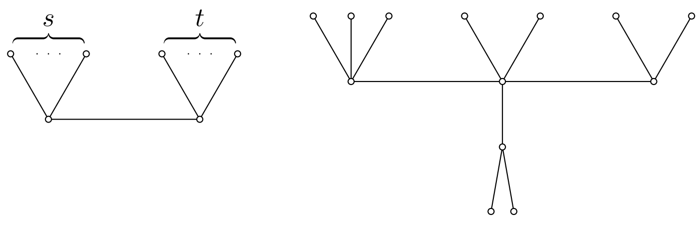
Next, we depict the graphs of $s = 1, 2, 3$ and 4 where s is the number of vertices of degree d. First we give some notation.

Definition 3.1.

(1) Let $T(n_1, \ldots, n_t)$ be the tree of order $t + \sum_{i=1}^{t} n_i$ obtained from $P_t\colon\ v_1v_2\ldots v_t$ by adding n_i new pendant edges at v_i $(1 \leqslant i \leqslant t)$.

(2) Let $T(*, T(a,b), *, \ldots, *)$ be the tree obtained from $P_t\colon\ v_1v_2\ldots v_t$ and $T(a,b)$ by identifying v_2 and v, where v is a vertex of degree $a+1$ in $T(a,b)$, and then attaching some (arbitrary) trees to other vertices.

For example, $T(s,t)$, $T(3, T(2,2), 2)$ in Fig. 1.

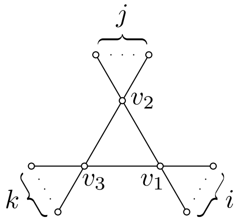


$T(s,t)$ $\qquad$ $T(3, T(2,2), 2)$

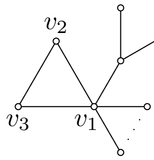
Fig. 1

Definition 3.2.

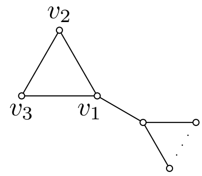
(1) Let $U_3(i,j,k)$ be the unicyclic graph obtained from $C_3\colon\ v_1v_2v_3v_1$ by attaching i, j, k new pendant edges to v_1, v_2 and v_3, respectively (see Fig. 2).



$U_3(i, j, k)$



$U_3(T(n-6, 2), 0, 0)$



$U_3(T(0, n-4), 0, 0)$

Fig. 2

Similarly, we introduce $U_4(i, j, k, l)$. Let $U_4(i, j, k, l)$ be the unicyclic graph obtained from C_4: $v_1v_2v_3v_4v_1$ by attaching i, j, k, l new pendant edges to v_1, v_2, v_3 and v_4, respectively.

(2) Let $U_3(T(a, b), *, *)$ be the unicyclic graph obtained from C_3: $v_1v_2v_3v_1$ and $T(a, b)$ by identifying v_1 and v, where v is a vertex of degree $a+1$ in $T(a, b)$, and then attaching some (arbitrary) trees to v_2 and v_3.

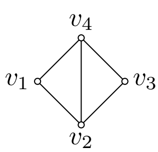
For example, $U_3(T(n-6, 2), 0, 0)$, $U_3(T(0, n-4), 0, 0)$ in Fig. 2.

Definition 3.3.

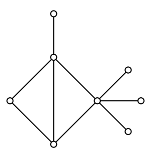
(1) Let $B_4(t_1, \ldots, t_4)$ be the bicyclic graph obtained from B_4: $v_1v_2v_3v_4v_1$ (see Fig. 3) by attaching t_i new pendant edges to v_i ($1 \leqslant i \leqslant 4$), respectively.

(2) Let $B_4(T(a, b), *, \ldots, *)$ be the bicyclic graph obtained from B_4: $v_1v_2v_3v_4v_1$ and $T(a, b)$ by identifying v_1 and v, where v is a vertex of degree $a+1$ in $T(a, b)$, and then attaching some (arbitrary) trees to v_i ($2 \leqslant i \leqslant 4$).

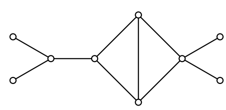
For example, $B_4(0, 0, 3, 1)$ and $B_4(T(0, 2), 0, 2, 0)$ in Fig. 3. Now we depict the extremal graphs with $1 \leqslant s \leqslant 4$ where s is the number of vertices of degree d.



B_4



$B_4(0, 0, 3, 1)$



$B_4(T(0, 2), 0, 2, 0)$

Fig. 3

Theorem 3.2. *If* $\pi(G)=\{\underbrace{d,\ldots,d}_{s\geqslant 1},\underbrace{1,\ldots,1}_{n-s}\}$, *then*

$$G\in\{K_{1,d-1},\ T(d-1,d-1),\, T(d-1,d-2,d-1),\, U_3(d-2,d-2,d-2),\\ T(d-1,d-2,d-2,d-1),\, T(d-1,T(0,d-1),d-1),\, U_3(d-2,d-2,\\ T(d-3,d-1)),\, U_4(d-2,d-2,d-2,d-2),\, B_4(d-2,d-3,d-2,d-3)\},$$

where $1\leqslant s\leqslant 4$.

Proof. We discuss the following cases according to s.

(1) $s=1$. Then
$$\pi(G)=\{d,\underbrace{1,\ldots,1}_{n-1}\},$$
so $G=K_{1,d-1}$.

(2) $s=2$. Then
$$\pi(G)=\{d,d,\underbrace{1,\ldots,1}_{n-2}\},$$
so $G=T(d-1,d-1)$.

(3) $s=3$. Then
$$\pi(G)=\{d,d,d,\underbrace{1,\ldots,1}_{n-3}\},$$
so $G\in\{T(d-1,d-2,d-1),\, U_3(d-2,d-2,d-2)\}$.

(4) $s=4$. Then
$$\pi(G)=\{d,d,d,d,\underbrace{1,\ldots,1}_{n-4}\},$$
so G is one of the graphs $\{T(d-1,d-2,d-2,d-1),\, T(d-1,T(d-3,d-1),d-1),\, U_3(d-2,d-2,T(d-3,d-1)), U_4(d-2,d-2,d-2,d-2),\, B_4(d-2,d-3,d-2,d-3)\}$. □

Next, we give the relation between $L(G)$ and $L(\overline{G})$.

Lemma 3.1. *Let* $L(G)$ *be the Laplacian matrix of a graph* G. *Then there exists a orthogonal matrix* P *such that*

$$P^{-1}LP=\operatorname{diag}(\mu_1,\ldots,\mu_n),\\ P^{-1}JP=\operatorname{diag}(0,\ldots,0,n),$$

where μ_i $(1\leqslant i\leqslant n)$ *are the Laplacian eigenvalues of* G *and* $J=(j_{ik})$ *is a matrix of order* n *with* $j_{ik}=1$ *for* $1\leqslant i,k\leqslant n$.

Proof. Since $(D - A)e = 0$, where $e = (1, \dots, 1)^T_{1\times n}$, we assume that $P = (P_1, \dots, P_n)$ where P_i $(1 \leqslant i \leqslant n)$ are mutual orthogonal unit eigenvectors of $L(G)$ and $LP_i = \mu_i P_i$ $(1 \leqslant i \leqslant n)$. Then we have

$$\begin{aligned} P^{-1}LP &= \operatorname{diag}(\mu_1, \dots, \mu_n),\\ P^{-1}JP &= \operatorname{diag}(0, \dots, 0, n). \end{aligned}$$

□

By Lemma 3.1 we obtain immediately the following lemma.

Lemma 3.2. *Let G be a graph and $\overline{G}$ its complement, and let $\mu_1 \geqslant \mu_2 \geqslant \dots \geqslant \mu_n = 0$ be the eigenvalues of $L(G)$. Then*
(1) $L(G) + L(\overline{G}) = L(K_n) = nI - J$;
(2) $\{n - \mu_{n-1}, \dots, n - \mu_1, 0\}$ *are the eigenvalues of* $L(\overline{G})$.

Proof. (1) is obvious. By Lemma 3.1 we have

$$\begin{aligned} P^{-1}L(\overline{G})P &= P^{-1}(nI)P - P^{-1}JP - P^{-1}L(G)P\\ &= \operatorname{diag}(n, \dots, n) - \operatorname{diag}(0, \dots, 0, n) - \operatorname{diag}(\mu_1, \dots, \mu_{n-1}, 0)\\ &= \operatorname{diag}(n - \mu_1, \dots, n - \mu_{n-1}, 0), \end{aligned}$$

and the results follows. □

We consider the relation between $LE(G)$ and $LE(\overline{G})$.

Theorem 3.3. *Let $G = (V, E)$ be a connected graph with $|V(G)| = n$, $|E(G)| = m$ and $\Delta(G) \leqslant d$, and let $\overline{G}$ be the complement of G. Then*
(1) $LE(G) - LE(\overline{G}) = 4mn - n^2(n - 1)$;
(2) $[n(n - 1) - 2m](n - d) \leqslant LE(\overline{G}) \leqslant n(n - 1)^2 - 2m(n - 1)$.

Proof. We assume that $\overline{d}_1, \dots, \overline{d}_n$ and $\overline{\mu}_1 \geqslant \dots \geqslant \overline{\mu}_n$ are the degrees of $\overline{G}$ and its Laplacian eigenvalues, respectively. Since $\overline{G}$ is the complement of G, then Lemma 3.2 yields that

$$\overline{\mu}_{n-i} = n - \mu_i \quad (1 \leqslant i \leqslant n - 1).$$

By (1) and (2) we obtain

$$\begin{aligned} LE(G) &= \sum_{i=1}^{n} \mu_i^2 = \sum_{i=1}^{n-1} \mu_i^2 = \sum_{i=1}^{n-1} [n - \overline{\mu}_{n-i}]^2 = \sum_{i=1}^{n-1} [n^2 - 2n\overline{\mu}_{n-i} + \overline{\mu}_{n-i}^2] \\ &= n^2(n-1) - 2n \sum_{i=1}^{n-1} \overline{\mu}_{n-i} + LE(\overline{G}) \\ &= n^2(n-1) - 2n \sum_{i=1}^{n-1} [n - \mu_i] + LE(\overline{G}) \\ &= LE(\overline{G}) + 4mn - n^2(n-1). \end{aligned}$$

By (1), we have

$$\begin{aligned} LE(\overline{G}) &= \sum_{i=1}^{n} \mu_i^2(\overline{G}) = 2|E(\overline{G})| + \sum_{i=1}^{n} \overline{d}_i^2 \\ &\leqslant 2|E(\overline{G})| + \sum_{i=1}^{n} (n-2)\overline{d}_i \\ &\leqslant 2[C_n^2 - m][n - 2 + 1] = n(n-1)^2 - 2m(n-1). \end{aligned}$$

On the other hand,

$$\begin{aligned} LE(\overline{G}) &= \sum_{i=1}^{n} \mu_i^2(\overline{G}) = 2|E(\overline{G})| + \sum_{i=1}^{n} \overline{d}_i^2 \\ &\geqslant 2|E(\overline{G})| + \sum_{i=1}^{n} (n-d-1)\overline{d}_i \\ &= 2[C_n^2 - m](n - d - 1 + 1) = [n(n-1) - 2m](n-d). \end{aligned}$$

□

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