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ON THE SECOND LAPLACIAN SPECTRAL MOMENT OF A GRAPH

YING LIU, YU QIN SUN, Shanghai

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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 $LE(G) \ge 6n-8$; 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 $V = \{v_1, v_2, \ldots, v_n\}$ 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 $d_1 \ge d_2 \ge \ldots \ge d_n$ and denote by $\pi(G) = (d_1, d_2, \ldots, d_n)$ 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 $D(G) = \text{diag}(d_1, d_2, \ldots, d_n)$ is the diagonal matrix of vertex degrees of G. Denote its Laplacian eigenvalues by $\mu_1(G) \ge \mu_2(G) \ge \ldots \ge \mu_n(G) = 0$ (or $\mu_1 \ge \mu_2 \ge \ldots \ge \mu_n = 0$).

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

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

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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

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

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

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

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 $d_i \ge k - 1$ $(1 \le i \le k)$.

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

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

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

Proof. By (1), (2) and Lemma 2.1, we obtain

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

$$\geqslant k(k-1) + k(k-1)^2 = k^2(k-1).$$

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: $G = K_n$.

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

We prove sufficiency.

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

$$\mu_1(G) \ge \mu_1(P_{2n+1}) \ge \mu_1(P_5) = \frac{5+\sqrt{5}}{2},$$

$$\mu_2(G) \ge \mu_2(P_{2n+1}) \ge \mu_2(P_5) = \frac{3+\sqrt{5}}{2}.$$

So we obtain

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

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 $d_i \ge k - 1$ $(1 \le i \le k)$. So

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

$$\ge k(k-1) + k(k-1)^2 + 2(n-k) = k^2(k-1) + 2(n-k) > k^2(k-1).$$

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 $n \ge 2$ vertices.

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

1. the Laplacian energy of G satisfies

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

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

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

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

Proof. Considering the inequality

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

we have

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

So we have

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

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

$$d_i = 1$$
 or $d_i = d$ $(1 \leq i \leq n),$

that is to say,

$$\pi(G) = \{\underbrace{d, \dots, d}_{s \ge 1}, \underbrace{1, \dots, 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 $P_t: v_1v_2 \ldots v_t$ by adding n_i new pendant edges at v_i $(1 \le i \le t)$.
- (2) Let T(*, T(a, b), *, ..., *) be the tree obtained from $P_t: v_1v_2...v_t$ 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.



Fig. 1

Definition 3.2.

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



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 $(1 \le i \le 4)$, respectively.
- (2) Let $B_4(T(a, b), *, ..., *)$ 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 $(2 \le i \le 4)$.

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 $1 \leq s \leq 4$ where s is the number of vertices of degree d.



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

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

where $1 \leq s \leq 4$.

Proof. We discuss the following cases according to s. (1) s = 1. Then

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

so $G = K_{1,d-1}$. (2) s = 2. Then

$$\pi(G) = \{d, d, \underbrace{1, \dots, 1}_{n-2}\},\$$

so G = T(d - 1, d - 1). (3) s = 3. Then

$$\pi(G) = \{d, d, d, \underbrace{1, \dots, 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, \dots, 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

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

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

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

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

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 $\mu_1 \ge \mu_2 \ge \ldots \ge \mu_n = 0$ 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

$$P^{-1}L(\overline{G})P = P^{-1}(nI)P - P^{-1}JP - P^{-1}L(G)P$$

= diag(n,...,n) - diag(0,...,0,n) - diag(\mu_1,...,\mu_{n-1},0)
= diag(n - \mu_1,...,n - \mu_{n-1},0),

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 $\Delta(G) \leq d$, and let \overline{G} be the complement of G. Then (1) $LE(G) - LE(\overline{G}) = 4mn - n^2(n-1);$ (2) $[n(n-1) - 2m](n-d) \leq LE(\overline{G}) \leq n(n-1)^2 - 2m(n-1).$

Proof. We assume that $\overline{d}_1, \ldots, \overline{d}_n$ and $\overline{\mu}_1 \ge \ldots \ge \overline{\mu}_n$ 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

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

By (1) and (2) we obtain

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

By (1), we have

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

On the other hand,

$$LE(\overline{G}) = \sum_{i=1}^{n} \mu_i^2(\overline{G}) = 2|E(\overline{G})| + \sum_{i=1}^{n} \overline{d}_i^2$$

$$\geq 2|E(\overline{G})| + \sum_{i=1}^{n} (n-d-1)\overline{d}_i$$

$$= 2[C_n^2 - m](n-d-1+1) = [n(n-1) - 2m](n-d).$$

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Authors' addresses: Y. Liu, College of Mathematics and Information, LiXin University of Commerce, Shanghai, 201620, P. R. China, e-mail: lymaths@126.com; Y.Q. Sun, Department of Mathematics and Physics, Shang Hai University of Electric Power, Shanghai, 200090, P. R. China.