MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **64** (2010) 75-84

ISSN 0340 - 6253

More on Energy and Laplacian Energy

Bo Zhou

Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China
e-mail: zhoubo@scnu.edu.cn

(Received March 27, 2009)

Abstract

A lot of properties especially bounds for the energy and the Laplacian energy of a graph have been known. We now establish further upper bounds for the energy and upper and lower bounds for the Laplacian energy. An upper bound for the energy of bipartite graphs is given in terms of the Laplacian eigenvalues.

1. INTRODUCTION

Let G be a simple graph with n vertices. The eigenvalues of G are the eigenvalues of its adjacency matrix $\mathbf{A}(G)$, which are denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, arranged in a non-increasing order [1]. The energy of the graph G is defined as [2]

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

It has a long known chemical application with origins in the molecular orbital theory of conjugated π-electron systems and has been studied extensively, see, e.g., [3–5], and for recent results, see, e.g., [6–9]. A lot of bounds for the energy have been known, see, e.g., [4, 6, 8, 9].

Let $\mathbf{D}(\mathrm{G})$ be the diagonal matrix of vertex degrees of the graph G. Then $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$ is the (ordinary) Laplacian matrix of G. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the Laplacian eigenvalues of G, i.e., eigenvalues of $\mathbf{L}(G)$, arranged in a non-increasing order [10]. The Laplacian energy of the graph G is defined as [11]

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

where $d(G) = \frac{2m}{n}$ is the average degree of G and m is the number of edges of G. The basic properties including various upper and lower bounds for Laplacian energy have been established in [11–16], and it has found remarkable chemical applications, beyond the molecular orbital theory of conjugated molecules [17].

We now give upper bounds for the energy and upper and lower bounds for the Laplacian energy. It is of interest to note that an upper bound for the energy of bipartite graphs is given in terms of the Laplacian eigenvalues.

2. PRELIMINARIES

The singular values of a real matrix $\mathbf{X}$ are the square roots of the eigenvalues of the matrix $\mathbf{X}\mathbf{X}^t$, where $\mathbf{X}^t$ denotes the transpose of the matrix $\mathbf{X}$. For an $n \times n$ real matrix $\mathbf{X}$, its singular values are denoted in a non-increasing order by $s_1(\mathbf{X}), s_2(\mathbf{X}), \ldots, s_n(\mathbf{X})$. Thus, with $\mathbf{I}_n$ denoting the $n \times n$ identity matrix, we have

$$E(G) = \sum_{i=1}^{n} s_i(\mathbf{A}(G))$$

$$LE(G) = \sum_{i=1}^{n} s_i\left(\mathbf{L}(G) - d(G)\mathbf{I}_n\right).$$

Note that energy, Laplacian energy and singular values are concerned in [9, 14, 15], and Laplacian energy and singular values are concerned in [16]. We need the following lemmas.

Lemma 1. [18] *Let $\mathbf{M}_1$ and $\mathbf{M}_2$ be $n \times n$ positive semi-definite matrices. Then $s_i(\mathbf{M}_1 - \mathbf{M}_2) \leq s_i(\mathbf{M}_1 \oplus \mathbf{M}_2)$ for $i = 1, 2, \ldots, n$, where $\mathbf{M}_1 \oplus \mathbf{M}_2 = \begin{pmatrix} \mathbf{M}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_2 \end{pmatrix}$.*

Lemma 2. [19] *Let* $\mathbf{M}_1$ *and* $\mathbf{M}_2$ *be* $n \times n$ *real matrices. Then* $\sum_{i=1}^{n} s_i(\mathbf{M}_1 + \mathbf{M}_2) \leq \sum_{i=1}^{n} s_i(\mathbf{M}_1) + \sum_{i=1}^{n} s_i(\mathbf{M}_2)$.

3. ENERGY

For a graph G, $\mathbf{L}^+(G) = \mathbf{D}(G) + \mathbf{A}(G)$ is the signless Laplacian matrix of G [20]. Recall that both the Laplacian matrix and the signless Laplacian matrix are positive semi-definite [10, 20]. Thus, for a graph G, the Laplacian eigenvalues and the signless Laplacian eigenvalues are respectively the singular values of the matrices $\mathbf{L}(G)$ and $\mathbf{L}^+(G)$.

For a graph G with n vertices, arrange the $2n$ numbers from the union of the Laplacian spectrum and the signless Laplacian spectrum in a non-increasing order, which are denoted by $\gamma_1, \gamma_2, \ldots, \gamma_{2n}$. Let $\mathbf{M}_1 = \mathbf{L}^+(G)$ and $\mathbf{M}_2 = \mathbf{L}(G)$ in Lemma 1, we have

$$2s_i(\mathbf{A}(G)) \leq \gamma_i \quad \text{for } i = 1, 2, \ldots, n$$

and thus we have

Proposition 1. *Let* G *be a graph with* n *vertices. Then*

$$E(G) \leq \frac{1}{2} \sum_{i=1}^{n} \gamma_i \, .$$

Let G be a graph with n vertices and m edges. Recall that $\sum_{i=1}^{n} \mu_i = 2m$ and a similar formula holds also for the signless Laplacian eigenvalues. Thus, $E(G) \leq 2m$ (see [4, 9]).

Let G be a bipartite graph with n vertices. Then the signless Laplacian spectrum of G, i.e., the spectrum of $\mathbf{L}^+(G)$, coincides with the Laplacian spectrum of G, and thus

$$\gamma_1 = \gamma_2 = \mu_1, \ \ldots, \ \gamma_{n-1} = \gamma_n = \mu_{n/2} \quad \text{if } n \text{ is even,}$$

$$\gamma_1 = \gamma_2 = \mu_1, \ \ldots, \ \gamma_{n-2} = \gamma_{n-1} = \mu_{(n-1)/2}, \ \gamma_n = \mu_{(n+1)/2} \quad \text{if } n \text{ is odd.}$$

Therefore, we have

Proposition 2. *Let G be a bipartite graph with n vertices. Then*

$$E(G) \leq \begin{cases} \sum\limits_{i=1}^{n/2} \mu_i & \text{if } n \text{ is even,} \\ \sum\limits_{i=1}^{(n-1)/2} \mu_i + \frac{1}{2}\mu_{(n+1)/2} & \text{if } n \text{ is odd.} \end{cases}$$

Let G be a bipartite graph with n vertices. Then by Proposition 2, $E(G) \leq \sum\limits_{i=1}^{\lceil n/2 \rceil} \mu_i$. Recall that upper bounds for $\sum\limits_{i=1}^{k} \mu_i$ with $k = 1, \ldots, n-2$ have already been discussed in [21, 22].

4. LAPLACIAN ENERGY

Let K_n be the complete graph, and $\overline{K_n}$ the empty graph on n vertices. Let P_n be the path on n vertices. Let $G \cup H$ be vertex–disjoint union of the graphs G and H.

For a graph G with n vertices, let $\mathbf{M}_1 = \mathbf{L}(G)$ and $\mathbf{M}_2 = d(G)\mathbf{I}_n$ in Lemma 1, we have

$$s_i\left(\mathbf{L}(G) - d(G)\mathbf{I}_n\right) \leq \max\{\mu_i, d(G)\} \quad \text{for } i = 1, 2, \ldots, n$$

and thus we have

Proposition 3. *Let G be a graph with n vertices. Then*

$$LE(G) \leq \sum_{i=1}^{n} \max\{\mu_i, d(G)\}\,.$$

Lemma 3. [23] *Let G be a graph with n vertices and minimum degree δ. If $G \neq K_n$, then $\mu_{n-1} \leq \delta$.*

Recall that for a graph with n vertices, $\mu_n = 0$ and the multiplicity of 0 as a Laplacian eigenvalue is equal to the number of connected components of G [10], and that the nonzero Laplacian eigenvalues of K_n are all equal to n for $n \geq 2$. A little more precisely than Proposition 3, we have

Proposition 4. *Let G be a graph with $n \geq 4$ vertices. Then*

$$LE(G) \leq \mu_1 - \mu_{n-1} + d(G) + \sum_{i=2}^{n-2} \max\{\mu_i, d(G)\}\,.$$

Proof. If $G = K_n$ for $n \geq 4$, then $LE(G) = 2n-2 < n^2-2n-1 = \mu_1-\mu_{n-1}+d(G)+\sum_{i=2}^{n-2}\max\{\mu_i, d(G)\}$. Note that $\mu_1 \geq d(G)$, $\mu_n = 0$ and $\mu_i \geq 0$ for $i = 2,\ldots,n-2$. If $G \neq K_n$, then by Lemma 3, $\mu_{n-1} \leq d(G)$, and thus

$$\begin{aligned} LE(G) &= \mu_1 - \mu_{n-1} + d(G) + \sum_{i=2}^{n-2} |\mu_i - d(G)| \\ &\leq \mu_1 - \mu_{n-1} + d(G) + \sum_{i=2}^{n-2} \max\{\mu_i, d(G)\}, \end{aligned}$$

as desired. ■

Proposition 5. *Let G be a graph with $n \geq 3$ vertices and m edges, where $G \neq K_3$. Then*

$$LE(G) \leq 4m - 2\mu_{n-1} - 2d(G) \tag{1}$$

with equality if and only if $G = \overline{K_n}$, $G = K_2 \cup \overline{K_{n-2}}$ or $G = P_3$.

Proof. It may be easily checked that for $G = \overline{K_3}$, $K_2 \cup K_1$ or P_3, (1) is an equality.

Suppose that $n \geq 4$. By Proposition 4 and using the fact that $\sum_{i=1}^{n-1}\mu_i = 2m$, we have

$$\begin{aligned} LE(G) &\leq \mu_1 - \mu_{n-1} + d(G) + \sum_{i=2}^{n-2} \max\{\mu_i, d(G)\} \\ &\leq \mu_1 - \mu_{n-1} + d(G) + \sum_{i=2}^{n-2} \mu_i + (n-3)d(G) \\ &= 2m - 2\mu_{n-1} + (n-2)d(G) = 4m - 2\mu_{n-1} - 2d(G). \end{aligned}$$

This proves (1). Equality holds in (1) if and only if $d(G) = 0$ (i.e., $G = \overline{K_n}$) or $d(G) > 0$ and $\mu_2 = \cdots = \mu_{n-2} = 0$ (i.e., $G = K_2 \cup \overline{K_{n-2}}$). ■

If G is a graph with n vertices and m edges, then by Proposition 5, $LE(G) \leq 4m\left(1 - \frac{1}{n}\right)$ with equality if and only if $m = 0, 1$. This was recently reported by Robbiano and Jiménez [15].

Consider the graph G consisting of a graph H (not necessarily connected) with n_1 vertices and m edges and of additional n_2 isolated vertices. For sufficiently large n_2, $LE(G) = \frac{4m(n_2+p)}{n_1+n_2}$ where p is the number of components of H (see [11]). This example shows that the upper bound $4m$ for $LE(G)$ may be arbitrarily approached.

Proposition 6. *Let G be a graph with $n \geq 2$ vertices and at least one edge. Then for any edge e of G,*

$$LE(G) \leq LE(G-e) + 4\left(1 - \frac{1}{n}\right).$$

Proof. Relabel the vertices of G such that $\mathbf{L}(G) = \mathbf{L}(G-e) + \mathbf{C}$ where $\mathbf{C} = \begin{pmatrix} \mathbf{L}(K_2) & \mathbf{O}_{2,n-2} \\ \mathbf{O}_{n-2,2} & \mathbf{O}_{n-2,n-2} \end{pmatrix}$ with $\mathbf{O}_{r,s}$ denoting the $r \times s$ zero matrix. Then

$$\mathbf{L}(G) - d(G)\mathbf{I}_n = \mathbf{L}(G-e) - d(G-e)\mathbf{I}_n + \mathbf{C} - \frac{2}{n}\mathbf{I}_n.$$

Note that the spectrum of $\mathbf{C} - \frac{2}{n}\mathbf{I}_n$ consists of $2 - \frac{2}{n}$ with multiplicity one and $-\frac{2}{n}$ with multiplicity $n-1$. Let $\mathbf{M_1} = \mathbf{L}(G-e) - d(G-e)\mathbf{I}_n$ and $\mathbf{M}_2 = \mathbf{C} - \frac{2}{n}\mathbf{I}_n$ in Lemma 2, we have

$$LE(G) \leq LE(G-e) + 2 - \frac{2}{n} + \frac{2}{n}(n-1),$$

from which the result follows. ■

Note that $G \cup \overline{K_r}$ denotes the graph obtained from G by adding r isolated vertices with $G \cup \overline{K_0} = G$.

Let G be a graph with n vertices and m edges. Note that for $n \geq 3$, $LE(P_3 \cup \overline{K_{n-3}}) - LE(K_2 \cup \overline{K_{n-2}}) = \left[3 - \frac{4}{n} + |1 - \frac{4}{n}| + \frac{4}{n} \cdot (n-2)\right] - 4\left(1 - \frac{1}{n}\right) < 4\left(1 - \frac{1}{n}\right)$, and for $n \geq 4$, $LE(K_2 \cup K_2 \cup \overline{K_{n-4}}) - LE(K_2 \cup \overline{K_{n-2}}) = \left[\left(2 - \frac{4}{n}\right) \cdot 2 + \frac{4}{n} \cdot (n-2)\right] - 4\left(1 - \frac{1}{n}\right) = 8\left(1 - \frac{2}{n}\right) - 4\left(1 - \frac{1}{n}\right) < 4\left(1 - \frac{1}{n}\right)$. Then by Proposition 6, $LE(G) \leq 4m\left(1 - \frac{1}{n}\right)$ with equality if and only if $m = 0, 1$. Again, we have the result in [15] mentioned above.

As in [9], by Proposition 6, we also have

Corollary 1. (*i*) *Let G be a connected graph with n vertices and m edges, and T its spanning tree. Then*

$$LE(G) \leq 4(m - n + 1)\left(1 - \frac{1}{n}\right) + LE(T).$$

(*ii*) *Let G be a Hamiltonian graph with n vertices and m edges. Then*

$$LE(G) \leq 4(m - n)\left(1 - \frac{1}{n}\right) + LE(C_n)$$

where C_n stands for the n-vertex cycle.

Let G be a graph with vertex set $V(G)$. For $u \in V(G)$, d_u denotes the degree of u in G. Define $\alpha(G) = \sum_{u \in V(G)} |d_u - d(G)|$. Using Lemma 2, the following lemma was proved in [9, 15].

Lemma 4. [9, 15] *Let G be a graph. Then*

$$LE(G) \leq E(G) + \alpha(G)$$

with equality if and only if G is regular.

Proposition 7. *(i) Let G be a tree with n vertices, of which p are pendent vertices, where $2 \leq p \leq n-1$. Then*

$$LE(G) < E(G) + 2p\left(1 - \frac{2}{n}\right).$$

(ii) Let G be a unicyclic graph with n vertices, of which p are pendent vertices, where $0 \leq p \leq n-3$. Then

$$LE(G) \leq E(G) + 2p$$

with equality if and only if $p = 0$.

Proof. If G is a tree with n vertices, of which p are pendent vertices, then

$$\begin{aligned} \alpha(G) &= \sum_{u \in V(G)} \left| d_u - \frac{2(n-1)}{n} \right| \\ &= \left[\frac{2(n-1)}{n} - 1 \right] \cdot p + \sum_{\substack{u \in V(G) \\ d_u \geq 2}} \left[d_u - \frac{2(n-1)}{n} \right] \\ &= \sum_{u \in V(G)} d_u - 2p - \frac{2(n-1)}{n}(n-2p) \\ &= \frac{2p(n-2)}{n}. \end{aligned}$$

Thus the result in (i) follows easily from Lemma 4.

If G is a unicyclic graph with n vertices, of which p are pendent vertices, then

$$\begin{aligned} \alpha(G) &= \sum_{u \in V(G)} |d_u - 2| = p + \sum_{\substack{u \in V(G) \\ d_u \geq 2}} (d_u - 2) \\ &= \sum_{u \in V(G)} d_u - 2(n-p) = 2p. \end{aligned}$$

Thus the result in (ii) follows easily from Lemma 4. ■

By Corollary 1 (i) and Proposition 7 (i), we have:

Corollary 2. *Let G be a connected graph with n vertices and m edges, and T its spanning tree with p pendent vertices, where $n \geq 3$. Then*

$$LE(G) < E(T) + 4(m-n+1)\left(1-\frac{1}{n}\right) + 2p\left(1-\frac{2}{n}\right).$$

In the following, we give a lower bound for the Laplacian energy.

Proposition 8. *Let G be a graph with $n \geq 3$ vertices. Then*

$$LE(G) \geq 2d(G) \tag{2}$$

with equality if and only if G is a regular complete k-partite graph for $1 \leq k \leq n$.

Proof. Note that $LE(K_n) = 2(n-1) = 2d(K_n)$. If $G \neq K_n$, then by Lemma 3, $\mu_{n-1} \leq d(G)$ and thus

$$\begin{aligned}
LE(G) &= \mu_1 - \mu_{n-1} + d(G) + \sum_{i=2}^{n-2} |\mu_i - d(G)| \\
&\geq \mu_1 - \mu_{n-1} + d(G) + \left|\sum_{i=2}^{n-2} [\mu_i - d(G)]\right| \\
&= \mu_1 - \mu_{n-1} + d(G) + |2m - (\mu_1 + \mu_{n-1}) - (n-3)d(G)| \\
&= \mu_1 - \mu_{n-1} + d(G) + |3d(G) - \mu_1 - \mu_{n-1}| \\
&\geq \mu_1 - \mu_{n-1} + d(G) + 3d(G) - \mu_1 - \mu_{n-1} \\
&= 4d(G) - 2\mu_{n-1} \geq 2d(G).
\end{aligned}$$

This proves (2). The equality case in (2) has already been proven in [12]. ■

Acknowledgement. This work was supported by the Guangdong Provincial Natural Science Foundation of China (no. 8151063101000026).

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