MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **62** (2009) 553-560

ISSN 0340 - 6253

NEW UPPER BOUNDS FOR LAPLACIAN ENERGY

Bo Zhou

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

(Received December 30, 2008)

Abstract

We obtain upper bounds and Nordhaus–Gaddum-type results for the Laplacian energy. The bounds in terms of the number of vertices are asymptotically best possible.

1. INTRODUCTION

In this paper we are concerned with simple graphs. Let G be a graph with vertex set $V(G)$. The spectrum of the graph G, consisting of the numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$, is the spectrum of its adjacency matrix $\mathbf{A}(G)$ of G [1]. The Laplacian spectrum of the graph G, consisting of the numbers $\mu_1, \mu_2, \ldots, \mu_n$, is the spectrum of its Laplacian matrix $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$ [2], where $\mathbf{D}(G)$ is the diagonal matrix of vertex degrees of G.

The energy of the graph G is defined as [3–6]

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

Let d_u be the degree of vertex u in the graph G. Let $d(G)$ be the average degree of G, i.e., $d(G) = \frac{1}{n} \sum_{u \in V(G)} d_u = \frac{2m}{n}$, where n and m are respectively the numbers of vertices and edges of G. The Laplacian energy of the graph G is defined as [7]

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

Some recent results on the Laplacian energy were reported in [8, 9]. Nordhaus and Gaddum [10] gave bounds for the sum of the chromatic numbers of a graph G and its complement $\overline{G}$. Nordhaus–Gaddum-type results for energy and Laplacian energy were discussed in [11].

We establish a relation between Laplacian energy, energy and degree sequence of a graph, from which upper bounds for the Laplacian energy in terms of the number of vertices and/or number of edges are deduced and improved Nordhaus–Gaddum-type results for Laplacian energy are given. We find that the bounds in terms of the number of vertices are asymptotically best possible.

2. RESULTS

Let $\mathbf{X}$ be an $n \times n$ complex matrix. The square roots of the eigenvalues of $\mathbf{X}^*\mathbf{X}$ are the singular values of $\mathbf{X}$, denoted by $s_1(\mathbf{X}), s_2(\mathbf{X}), \ldots, s_n(\mathbf{X})$, where $\mathbf{X}^*$ denotes the Hermitian adjoint of $\mathbf{X}$ [13]. The following lemma due to Fan [12] is well-known, see, e.g., [13].

Lemma 1. *Let $\mathbf{X}$ and $\mathbf{Y}$ be $n \times n$ complex matrices. Then*

$$\sum_{i=1}^{n} s_i(\mathbf{X}+\mathbf{Y}) \le \sum_{i=1}^{n} s_i(\mathbf{X}) + \sum_{i=1}^{n} s_i(\mathbf{Y}).$$

For the graph G with n vertices, obviously, $|\lambda_i| = s_i(\mathbf{A}(G))$ and $|\mu_i - d(G)| = s_i\left(\mathbf{L}(G) - d(G)\mathbf{I}_n\right)$ for $i = 1, 2, \ldots, n$, where $\mathbf{I}_n$ is the $n \times n$ identity matrix.

Let K_n be the complete graph with n vertices. Obviously, $\overline{K_n}$ consists of n isolated vertices. The vertex–disjoint union of the graphs G and H is denoted by $G \cup H$.

Proposition 1. *Let G be a graph. Then*

$$LE(G) \le E(G) + \sum_{u \in V(G)} |d_u - d(G)| \,.$$

Proof. Let $n = |V(G)|$. Note that

$$\mathbf{L}(G) - d(G)\mathbf{I}_n = \mathbf{D}(G) - \mathbf{A}(G) - d(G)\mathbf{I}_n = -\mathbf{A}(G) + [\mathbf{D}(G) - d(G)\mathbf{I}_n] \,.$$

Applying Lemma 1,

$$\begin{aligned} LE(G) &= \sum_{i=1}^{n} s_i \left(-\mathbf{A}(G) + [\mathbf{D}(G) - d(G)\mathbf{I}_n]\right) \\ &\leq \sum_{i=1}^{n} s_i \left(-\mathbf{A}(G)\right) + \sum_{i=1}^{n} s_i \left([\mathbf{D}(G) - d(G)\mathbf{I}_n]\right) \\ &= \sum_{i=1}^{n} s_i \left(\mathbf{A}(G)\right) + \sum_{i=1}^{n} s_i \left([\mathbf{D}(G) - d(G)\mathbf{I}_n]\right) \\ &= E(G) + \sum_{u\in V(G)} |d_u - d(G)| \,, \end{aligned}$$

as desired. ■

We note that the upper bound in Proposition 1 has been reported in [14], and that it may be attained, e.g., for regular graphs. A proof is included for completeness.

By Proposition 1, we may deduce upper bounds for the Laplacian energy from the upper bounds of energy and the quantity $\sum\limits_{u\in V(G)} |d_u - d(G)|$.

For a graph G with n vertices, it was shown in [15] that

$$E(G) \leq \frac{n^{3/2} + n}{2}$$

with equality if and only if G is a strongly regular graph (regular of degree $\frac{n+\sqrt{n}}{2}$, each pair of adjacent vertices and each pair of non-adjacent vertices have exactly $\frac{n+2\sqrt{n}}{4}$ common neighbors).

Recall that the discrepancy of the graph G with n vertices is defined as

$$\mathrm{disc}(G) = \frac{1}{n} \sum_{u\in V(G)} |d_u - d(G)| \,.$$

Let $a = \min\{d(G), d(\overline{G})\} = \min\{d(G), n-1-d(G)\}$. Then $0 \leq a \leq \frac{n-1}{2}$. Haviland [16] showed that

$$n \cdot \mathrm{disc}(G) \leq a\left(2n - 1 - \sqrt{4na+1}\right),$$

and as a function of a in the range $0 \leq a \leq \frac{n-1}{2}$, the upper bound for $n \cdot \mathrm{disc}(G)$ is maximized at $a = \frac{2n^2-2n-1+(2n-1)\sqrt{n^2-n+1}}{9n}$, and thus

$$n \cdot \mathrm{disc}(G) \leq \frac{2\left[(2n-1)(n+1)(n-2) + 2(n^2-n+1)^{3/2}\right]}{27n}.$$

For a graph G with n vertices, $a\left(2n-1-\sqrt{4na+1}\right)=0$ if and only if $a=0$ for $0\le a\le \frac{n-1}{2}$, i.e., $G=\overline{K_n}$ or $G=K_n$. Applying Proposition 1, and the bounds for $E(G)$ and $n\cdot \mathrm{disc}(G)$ mentioned above, we have

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

$$LE(G) < \frac{n^{3/2}+n}{2} + a\left(2n-1-\sqrt{4na+1}\right)$$

$$LE(G) < \frac{n^{3/2}+n}{2} + \frac{2\left[(2n-1)(n+1)(n-2)+2(n^2-n+1)^{3/2}\right]}{27n}.$$

For a graph G with $n\ge 2$ vertices, our earlier Nordhaus–Gaddum-type result for Laplacian energy [11] says $LE(G)+LE(\overline{G})<n\sqrt{n^2-1}$. This may now be improved as:

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

$$LE(G)+LE(\overline{G}) < n-1+(n-1)\sqrt{n+1}+2a\left(2n-1-\sqrt{4na+1}\right)$$

$$\begin{aligned} LE(G)+LE(\overline{G}) &< n-1+(n-1)\sqrt{n+1} \\ &\quad + \frac{4\left[(2n-1)(n+1)(n-2)+2(n^2-n+1)^{3/2}\right]}{27n}. \end{aligned}$$

Proof. Let m be the number of edges of G. Note that $\sum_{i=1}^{n}\lambda_i^2=2m$ and by the Cauchy–Schwarz inequality, $E(G)\le \lambda_1+\sqrt{(n-1)(2m-\lambda_1^2)}$ with equality if and only if $|\lambda_2|=\cdots=|\lambda_n|$, where λ_1 is the largest eigenvalue of G. Let $\overline{\lambda_1}$ be the largest eigenvalue of $\overline{G}$. Then

$$\begin{aligned} E(G)+E(\overline{G}) &\le \lambda_1+\sqrt{(n-1)(2m-\lambda_1^2)} \\ &\quad +\overline{\lambda_1}+\sqrt{(n-1)\left[n(n-1)-2m-\overline{\lambda_1}^2\right]} \\ &\le \lambda_1+\overline{\lambda_1}+\sqrt{2(n-1)\left[n(n-1)-\left(\lambda_1^2+\overline{\lambda_1}^2\right)\right]} \\ &\le \lambda_1+\overline{\lambda_1}+\sqrt{2(n-1)\left[n(n-1)-\frac{1}{2}\left(\lambda_1+\overline{\lambda_1}\right)^2\right]}. \end{aligned}$$

Note that the function $f(x)=x+\sqrt{2(n-1)\left[n(n-1)-\frac{x^2}{2}\right]}$ is monotonously decreasing for $x\ge\sqrt{2(n-1)}$ and that by Weyl's theorem [13], $\lambda_1+\overline{\lambda_1}$ is no less than the largest eigenvalue $n-1$ of the matrix $\mathbf{A}(G)+\mathbf{A}(\overline{G}) = \mathbf{A}(K_n)$, implying that $\lambda_1+\overline{\lambda_1} \geq n-1 \geq \sqrt{2(n-1)}$ (or from [1], $\lambda_1+\overline{\lambda_1} \geq d(G)+d(\overline{G}) = n-1$). Thus,

$$E(G)+E(\overline{G}) \leq f(n-1) = n-1+(n-1)\sqrt{n+1}\,,$$

and if equality is attained then G is regular, $\lambda_1 = \overline{\lambda_1} = \frac{n-1}{2}$, and thus $\sqrt{\frac{1}{n-1}\left(2m-\lambda_1^2\right)}$ $= \frac{\sqrt{n+1}}{2}$ is an eigenvalue of G with multiplicity $\frac{n-1}{2}\left(1-\frac{1}{\sqrt{n+1}}\right)$, which can not be an integer for $n \geq 3$. Then the above bound for $E(G)+E(\overline{G})$ can not be attained. Now the result follows from the bounds for $n \cdot \mathrm{disc}(G)$. ■

Let $G = K_q \cup \overline{K_{n-q}}$. Then $d(G) = \frac{q(q-1)}{n}$. The Laplacian spectrum of G consists of q ($q-1$ times) and 0 ($n-q+1$ times). It follows that

$$LE(G) = \frac{nq-q(q-1)}{n}(q-1)+\frac{q(q-1)}{n}(n-q+1) = \frac{2q(q-1)(n-q+1)}{n}.$$

Let $q = \frac{2n}{3}$. Then

$$LE(G) = \frac{4(2n-3)(n+3)}{27}.$$

Note that $d(\overline{G}) = \frac{n(n-1)-q(q-1)}{n}$ and the Laplacian spectrum of $\overline{G}$ consists of n ($n-q$ times), $n-q$ ($q-1$ times) and 0 (1 times). We have

$$\begin{aligned} LE(\overline{G}) &= \frac{n+q(q-1)}{n}(n-q)+\frac{nq-n-q(q-1)}{n}(q-1) \\ &\quad +\frac{n^2-n-q(q-1)}{n} \\ &= \frac{2(n-q)\left[n+q(q-1)\right]}{n} = \frac{2n(4n+3)}{27}. \end{aligned}$$

This example and the previous two propositions imply

Proposition 4. *Let $\mathbb{G}_n$ be the class of graphs with n vertices. Let*

$$LE(n) = \max\{LE(G) : G \in \mathbb{G}_n\}$$

$$NGLE(n) = \max\{LE(G)+LE(\overline{G}) : G \in \mathbb{G}_n\}.$$

Then

$$\lim_{n\to\infty} \frac{LE(n)}{n^2} = \frac{8}{27}$$

$$\lim_{n\to\infty} \frac{NGLE(n)}{n^2} = \frac{16}{27}.$$

Recall that the first Zagreb index [17, 18] of the graph G is $Zg(G) = \sum_{u \in V(G)} d_u^2$. Let G be a graph with n vertices and m edges. By the Cauchy–Schwarz inequality,

$$\sum_{u \in V(G)} |d_u - d(G)| \le \sqrt{n \sum_{u \in V(G)} [d_u - d(G)]^2} = \sqrt{nZg(G) - 4m^2}$$

with equality if and only if $|d_u - d(G)|$ is a constant for each $u \in V(G)$. We note that $\frac{1}{n} \sum_{u \in V(G)} [d_u - d(G)]^2$ was called the variance of G, e.g., in [19]. Thus, by Proposition 1, we have

$$LE(G) \le E(G) + \sqrt{nZg(G) - 4m^2}\,.$$

Remark 1. We may give somewhat finer upper bounds for the Laplacian energy by applying Proposition 1. We give an example. Let G be a graph with $n \ge 2$ vertices, m edges and the first Zagreb index Zg, then [20]

$$E(G) \le \sqrt{\frac{Zg}{n}} + \sqrt{(n-1)\left(2m - \frac{Zg}{n}\right)}$$

with equality if and only if G is K_n, $\overline{K_n}$, mK_2 (m copies of vertex–disjoint K_2), or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{2m-(2m/n)^2}{n-1}}$. Thus,

$$LE(G) \le \sqrt{\frac{Zg}{n}} + \sqrt{(n-1)\left(2m - \frac{Zg}{n}\right)} + \sqrt{nZg(G) - 4m^2}$$

with equality if and only if G is K_n, $\overline{K_n}$, mK_2, or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{2m-(2m/n)^2}{n-1}}$; and

$$LE(G) \le \sqrt{\frac{Zg}{n}} + \sqrt{(n-1)\left(2m - \frac{Zg}{n}\right)} + a\left(2n - 1 - \sqrt{4na+1}\right)$$

with equality if and only if $G = K_n$ or $G = \overline{K_n}$.

Remark 2. Let G be a graph with $n \ge 3$ vertices and $m > 0$ edges. If G is K_{r+1}-free with $2 \le r \le n-1$, then [21]

$$Zg(G) \le \frac{2r-2}{r} nm$$

with equality for $r = 2$ if and only if G is a complete bipartite graph, and thus

$$LE(G) \le E(G) + \sqrt{\frac{2r-2}{r} n^2 m - 4m^2}\,.$$

In particular, if G is bipartite ($r = 2$), then [22]

$$E(G) \leq \frac{n(\sqrt{n}+\sqrt{2})}{\sqrt{8}},$$

and thus

$$\begin{aligned} LE(G) &\leq E(G) + \sqrt{n^2m - 4m^2} \\ &< \frac{n(\sqrt{n}+\sqrt{2})}{\sqrt{8}} + \frac{n^2}{4}. \end{aligned}$$

The second inequality is strict because the bound for $E(G)$ can not be attained for the complete bipartite graph, which is equal to $2\sqrt{s(n-s)} \leq n$ for some $1 \leq s \leq \lfloor \frac{n}{2} \rfloor$. Note that for rational number α with $0 < \alpha \leq \frac{1}{2}$, $LE\left(K_{\alpha n,(1-\alpha)n}\right) = 2\alpha n + 2\alpha(1-\alpha)(1-2\alpha)n^2$. Let $LE_{bip}(n)$ be the maximum Laplacian energy of n-vertex bipartite graphs. Then $2\alpha(1-\alpha)(1-2\alpha) < \lim\limits_{n\to\infty} \frac{LE_{bip}(n)}{n^2} \leq 0.25$. For real x with $0 < x \leq \frac{1}{2}$, $x(1-x)(1-2x)$ is maximum if and only if $x = \frac{3-\sqrt{3}}{6}$. Let $\alpha = 0.211 < \frac{3-\sqrt{3}}{6}$, we have $0.19 < \lim\limits_{n\to\infty} \frac{LE_{bip}(n)}{n^2} \leq 0.25$. If G is a tree, then $Zg(G) \leq n(n-1)$, and thus

$$LE(G) \leq E(G) + \sqrt{n-1}(n-2).$$

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

References

[1] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, 3rd ed., Johann Ambrosius Barth, Heidelberg, 1995.

[2] R. Grone, R. Merris, The Laplacian spectrum of a graph II, *SIAM J. Discrete Math.* **7** (1994) 221–229.

[3] I. Gutman, The energy of a graph, *Ber. Math.–Statist. Sekt. Forschungszentrum Graz* **103** (1978) 1–22.

[4] I. Gutman, Total π-electrom energy of benzenoid hydrocarbons, *Topics Curr. Chem.* **162** (1992) 29–63.

[5] I. Gutman, The energy of a graph: old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer-Verlag, Berlin, 2001, pp. 196–211.

[6] I. Gutman, Topology and stability of conjugated hydrocarbons. The dependence of total π-electron energy on molecular topology, *J. Serb. Chem. Soc.* **70** (2005) 441–456.

[7] I. Gutman, B. Zhou, Laplacian energy of a graph, *Lin. Algebra Appl.* **414** (2006) 29–37.

[8] B. Zhou, I. Gutman, On Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 211–220.

[9] B. Zhou, I. Gutman, T. Aleksić, A note on Laplacian energy of graphs, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 441–446.

[10] E. A. Nordhaus, J. W. Gaddum, On complementary graphs, *Amer. Math. Monthly* **63** (1956) 175–177.

[11] B. Zhou, I. Gutman, Nordhaus–Gaddum-type relations for the energy and Laplacian energy of graphs, *Bull. Acad. Serbe Sci. Arts* (*Cl. Math. Natur.*) **134** (2007) 1–11.

[12] K. Fan, Maximum properties and inequalities for the eigenvalues of completely continuous operators, *Proc. Nat. Acad. Sci. U.S.A.* **37** (1951) 760–766.

[13] R. A. Horn, C. R. Johnson, *Matrix Analysis*, Cambridge Univ. Press, Cambridge, 1989.

[14] W. So, M. Robbiano, N. M. M. de Abreu, I. Gutman, Applications of a theorem by Ky Fan in the theory of graph energy, *Lin. Algebra Appl.*, in press.

[15] J. H. Koolen, V. Moulton, Maximal energy graphs, *Adv. Appl. Math.* **26** (2001) 47–52.

[16] J. Haviland, On irregularity in graphs, *Ars Combin.* **78** (2006) 283–288.

[17] I. Gutman, B. Ruščić, N. Trinajstic, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Phys. Chem.* **62** (1975) 3399–3405.

[18] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[19] F. K. Bell, A note on the irregularity of graphs, *Lin. Algebra Appl.* **161** (1992) 45–54.

[20] B. Zhou, Energy of a graph, *MATCH Commun. Math. Comput. Chem.* **51** (2004) 111–118.

[21] B. Zhou, Remarks on Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 591–596.

[22] J. H. Koolen, V. Moulton, Maximal energy bipartite graphs, *Graphs Combin.* **19** (2003) 131–135.