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Communications in Mathematical and in Computer Chemistry

ISSN 0340 - 6253

(Laplacian) Borderenergetic Graphs and Bipartite Graphs^{*}

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(Received February 22, 2019)

Abstract

A graph G of order n and size m is (Laplacian) borderenergetic if it has the same (Laplacian) energy as the complete graph K_n does. In this paper, we prove that when $m < \frac{2(n-1)^2}{n}$, a borderenergetic graph is not bipartite. Moreover, for a borderenergetic bipartite graph, we present a lower bound of its largest eigenvalue and an upper bound of its middle eigenvalue, respectively. Analogously, Laplacian borderenergetic bipartite graphs is observed and some asymptotically tight bounds on their first Zagreb indices are shown.

1 Introduction

All graphs considered in this paper are simple and undirected. Let G be a graph with order n and size m. The complete graph of order n is denoted by K_n . The degree of vertex v_i in the graph G is denoted by d_i . The first Zagreb index [12, 16] of the graph Gis defined as

$$M_1 = M_1(G) = \sum_{i=1}^n d_i^2$$
.

^{*}Supported by the NSFQH No.2018-ZJ-925Q, 2017-ZJ-790; NSFC No.11701311; NSFGD No. 2016A030310307

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For terminology and notation not given here, we refer to [1].

Let A(G) be an adjacency matrix of G and set $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of the adjacency matrix A(G). The nullity $\eta(G)$ of the graph G is the multiplicity of the eigenvalue zero in its adjacency spectrum. If D(G) is the diagonal matrix of the vertex degrees of G, L(G) = D(G) - A(G) is the Laplacian matrix of G. Let $\mu_1 \geq \mu_2 \geq \cdots \geq$ $\mu_n = 0$ be the eigenvalues of L(G). The energy of a graph G [13,14], denoted by $\mathcal{E}(G)$, is defined as

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

For additional information on graph energy and its applications in chemistry, we refer to [14, 15, 18].

Recently, Gong et al. [10] proposed the concept of *borderenergetic* graphs, namely graphs of order *n* satisfying $\mathcal{E}(G) = 2(n-1)$. The corresponding results on borderenergetic graphs can be seen in [6, 17, 19, 20, 23].

Analogously, F. Tura [25] proposed the concept of Laplacian borderenergetic, i.e., Lborderenergetic graphs. That is, a graph G of order n is L-borderenergetic if $LE(G) = LE(K_n)$, where $LE(G) = \sum_{i=1}^{n} |\mu_i - \overline{d}|$ and \overline{d} is the average degree of G. More results on L-borderenergetic graphs, we can refer to [7–9, 21, 24–26].

Through the computer, the borderenergetic graphs with order $7 \le n \le 11$ have been found [10, 19, 23], we see that all these graphs are not bipartite. But until now the properties between a borderenergetic graph and a bipartite graph are not be surveyed. In this paper we prove that when $m < \frac{2(n-1)^2}{n}$, a borderenergetic graph is not bipartite. Moreover, for a borderenergetic bipartite graph, we present a lower bound of its largest eigenvalue and an upper bound of its middle eigenvalue, respectively. Analogously, Laplacian borderenergetic bipartite graphs are observed and some asymptotically tight bounds on their first Zagreb indices are given.

2 Borderenergetic bipartite graphs

In this section, some properties between a borderenergetic graph and a bipartite graph are surveyed.

Lemma 1. [2, 3] The graph G is bipartite if and only if its eigenvalues are symmetric with respect to the origin, i.e., if $\lambda_i = -\lambda_{n+1-i}$ holds for $i = 1, 2, \dots n$.

Theorem 2. Let G be a borderenergetic graph and suppose $m < \frac{2(n-1)^2}{n}$. Then G is not bipartite.

Proof. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_s > 0 > \lambda'_1 \geq \lambda'_2 \geq \cdots \geq \lambda'_t$ be the eigenvalues of A(G). Note that s and t are the numbers of positive eigenvalues and negative eigenvalues, respectively. Then

$$\sum_{i=1}^{s} \lambda_i + \sum_{j=1}^{t} \lambda'_j = 0 .$$
 (1)

And we have

$$\sum_{i=1}^{s} \lambda_i^2 + \sum_{j=1}^{t} (\lambda_j')^2 = 2m .$$
 (2)

Since G is borderenergetic, we obtain

$$\sum_{i=1}^{s} \lambda_i + \sum_{j=1}^{t} (-\lambda'_j) = 2(n-1) .$$
(3)

Hence, by (1) and (3), we get

$$\sum_{i=1}^{s} \lambda_i = \sum_{j=1}^{t} (-\lambda'_j) = n - 1 .$$
(4)

By contradiction, if G is bipartite, then by Lemma 1 the eigenvalues of A(G) are symmetric about the origin. Thus, by (2), it arrives that

$$\sum_{i=1}^{s} \lambda_i^2 = \sum_{j=1}^{t} (\lambda_j')^2 = m .$$
 (5)

Bearing in mind that $s = t \leq \lfloor \frac{n}{2} \rfloor$ when G is bipartite. As $f(x) = x^2$ is a convex function on $x \in R$, we use the Jensen inequality to obtain the inequality below.

$$\left(\frac{\lambda_1 + \lambda_2 + \dots + \lambda_s}{s}\right)^2 \leq \frac{\lambda_1^2 + \lambda_2^2 + \dots + \lambda_s^2}{s},$$
$$\left(\frac{n-1}{s}\right)^2 \leq \frac{m}{s}.$$

By above inequality, we get

$$\frac{(n-1)^2}{m} \le s. \tag{6}$$

Due to $m < \frac{2(n-1)^2}{n}$, we have $\frac{(n-1)^2}{m} > \frac{n}{2}$. So we see that $s > \frac{n}{2}$, which contracts with $s \leq \lfloor \frac{n}{2} \rfloor$ and means that G is not bipartite.

Obviously, from Theorem 2, we can see that, if G is borderenergetic and bipartite, then the numbers of positive eigenvalues and negative eigenvalues of A(G) are not less than $\frac{(n-1)^2}{m}$, respectively.

Theorem 3. Let G be a borderenergetic graph. If G is bipartite, then the numbers of positive eigenvalues and negative eigenvalues of A(G) are not less than $\frac{(n-1)^2}{m}$, respectively.

Proof. Let s and t be the numbers of positive eigenvalues and negative eigenvalues of A(G), respectively. Since G is bipartite, we have s = t. From (6) in the proof of Theorem 2, we see that

$$\frac{(n-1)^2}{m} \le s = t \ .$$

When G is a connected k-cyclic graph, we know that m = n + k - 1. Then using Theorem 2, we can get Corollary 4.

Corollary 4. Let G be a connected borderenergetic graph. If G is a k-cyclic graph with $k \leq n-3$, then G is not bipartite.

Proof. By $k \leq n-3$, we get

$$k < n - 3 + \frac{2}{n} = \frac{2(n-1)^2}{n} - n + 1.$$

Then

$$n+k-1 < \frac{2(n-1)^2}{n}.$$

Since G is a k-cyclic graph, we see that m = n + k - 1 and

$$m < \frac{2(n-1)^2}{n}.$$

As G is a borderenergetic graph, by Theorem 2, the result holds.

Note that the order n is not less than 7 for any connected borderenergetic graph G [10]. From Corollary 4, if n = 7, there are no k-cyclic ($0 \le k \le 4$) bipartite graphs as borderenergetic graphs. If n = 8, there are no k-cyclic ($0 \le k \le 5$) bipartite graphs as borderenergetic graphs. We have the similar results for the cases $n = 9, 10, 11, \cdots$.

It is well known that, for almost all graphs, their nullities are 0. Now we consider such borderenergetic bipartite graphs satisfying their nullities are 0, and we survey their largest eigenvalues and middle eigenvalues. Gutman [11] in 1974 given the following lower and upper bounds on the energy of a bipartite graph G.

$$\mathcal{E}(G) \ge \sqrt{4m + n(n-2)(\det A(G))^{2/n}}.$$
(7)

$$\mathcal{E}(G) \le \sqrt{2mn - 4m + 2n(\det A(G))^{2/n}}.$$
(8)

Theorem 5. Let G be a borderenergetic bipartite graph with $\eta(G) = 0$. Then

$$\lambda_1 \ge \sqrt{\frac{2(n-1)^2 - mn + 2m}{n}}$$

Proof. By Lemma 1 and $\eta(G) = 0$, we see that the order n of G is even and

$$det A(G) = (-1)^{n/2} \lambda_1^2 \lambda_2^2 \cdots \lambda_{n/2}^2.$$

Since G is borderenergetic, by (8), we have

$$\begin{array}{rcl} 2(n-1) & \leq & \sqrt{2mn - 4m + 2n(detA(G))^{2/n}} \,, \\ 4(n-1)^2 & \leq & 2mn - 4m + 2n((-1)^{n/2}\lambda_1^2\lambda_2^2\cdots\lambda_{n/2}^2)^{2/n} \,, \\ & \leq & 2mn - 4m + 2n(\lambda_1^{2\cdot\frac{n}{2}})^{2/n} \,, \\ & = & 2mn - 4m + 2n\lambda_1^2 \,. \end{array}$$

From above, we obtain

$$\lambda_1 \ge \sqrt{\frac{2(n-1)^2 - mn + 2m}{n}} \ .$$

Theorem 6. Let G be a borderenergetic bipartite graph with $\eta(G) = 0$. Then

$$\lambda_{n/2} \le \sqrt{\frac{4(n-1)^2 - 4m}{n(n-2)}}$$
.

Proof. Similar to the proof of Theorem 5, we note that the order n of G is even and

$$det A(G) = (-1)^{n/2} \lambda_1^2 \lambda_2^2 \cdots \lambda_{n/2}^2 .$$

Since G is borderenergetic, by (7), we get

$$2(n-1) \geq \sqrt{4m + n(n-2)(det A(G))^{2/n}},$$

$$\begin{array}{rcl} 4(n-1)^2 & \geq & 4m+n(n-2)((-1)^{n/2}\lambda_1^2\lambda_2^2\cdots\lambda_{n/2}^2)^{2/n} \,, \\ \\ & \geq & 4m+n(n-2)(\lambda_{n/2}^{2(\frac{n}{2})})^{2/n} \,, \\ \\ & = & 4m+n(n-2)\lambda_{n/2}^2 \,\,. \end{array}$$

Thus, we have

$$\lambda_{n/2} \le \sqrt{\frac{4(n-1)^2 - 4m}{n(n-2)}}$$

3 Laplacian borderenergetic bipartite graphs

When a graph is bipartite, the Laplacian spectrum and signless Laplacian spectrum are the same. So here we only discuss the former case. In this section, some asymptotically tight bounds on the first Zagreb index of a Laplacian borderenergetic bipartite graph are shown.

Lemma 7. [4] Let G be a bipartite graph of order n with m edges. Then

$$LE(G) \le \frac{4m}{n} + \sqrt{(n-2)\left(2M - \frac{8m^2}{n^2}\right)},$$
(9)

where

$$M = m + \frac{M_1}{2} - \frac{2m^2}{n}$$

Lemma 8. [5] Let G be a bipartite graph of order n with m edges and the first Zagreb index M_1 . Then

$$LE(G) \ge \frac{2m}{n} + \sqrt{2M_1 + 4m - \frac{8m^2}{n} - \frac{12m^2}{n^2}} .$$
 (10)

Through applying Lemma 7 and Lemma 8, we obtain the following results.

Theorem 9. Let G be a L-borderenergetic bipartite graph. Then

$$M_1 \ge \frac{(2(n-1) - 4m/n)^2}{n-2} + \frac{8m^2}{n^2} + \frac{4m^2}{n} - 2m.$$

If G is $\sqrt{4k_1^2 - 2k_1 + 4}$ - regular, and $m = k_1n + k_2$, where $k_1 > 0$ and $k_2 \ge 0$, then the lower bound above is asymptotically tight.

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Proof. Since G is a L-borderenergetic bipartite graph, by Lemma 7, we have

$$2(n-1) \le \frac{4m}{n} + \sqrt{(n-2)\left(2M - \frac{8m^2}{n^2}\right)}.$$
(11)

From (11), it arrives at

$$M \ge \frac{(2(n-1) - 4m/n)^2}{2(n-2)} + \frac{4m^2}{n^2}.$$
(12)

Due to $M = m + \frac{M_1}{2} - \frac{2m^2}{n}$, we obtain

$$M_1 \ge \frac{(2(n-1) - 4m/n)^2}{n-2} + \frac{8m^2}{n^2} + \frac{4m^2}{n} - 2m.$$
(13)

When $m = k_1 n + k_2$, by the right hand of (13), we get

$$\frac{(2(n-1)-4m/n)^2}{n-2} + \frac{8m^2}{n^2} + \frac{4m^2}{n} - 2m$$

= $\frac{4n(k_1n+k_2)^2 + 4n(n-1)^2 - 2(k_1n+k_2)(n^2+6n-8)}{n(n-2)}$. (14)

If G is $\sqrt{4k_1^2 - 2k_1 + 4}$ -regular, then

$$M_1 = n(4k_1^2 - 2k_1 + 4). (15)$$

Using (15) to divide (14) and computing the limit as n tends to infinity, we have

$$\lim_{n \to \infty} \frac{\frac{4n(k_1n + k_2)^2 + 4n(n-1)^2 - 2(k_1n + k_2)(n^2 + 6n - 8)}{n(n-2)}}{n(4k_1^2 - 2k_1 + 4)} = 1$$

Thus, it means that the lower bound of (13) is asymptotically tight when G is $\sqrt{4k_1^2 - 2k_1 + 4}$ -regular, and $m = k_1 n + k_2$, where $k_1 > 0$ and $k_2 \ge 0$.

Contrarily, an upper bound, in terms of its order and size, on the first Zagreb index of a Laplacian borderenergetic bipartite graph is given below.

Theorem 10. Let G be a L-borderenergetic bipartite graph. Then

$$M_1 \le \frac{(2(n-1) - 2m/n)^2}{2} + \frac{4m^2}{n} + \frac{6m^2}{n^2} - 2m$$

Proof. As G is a L-borderenergetic bipartite graph, by Lemma 8, we get

$$2(n-1) \le \frac{2m}{n} + \sqrt{2M_1 + 4m - \frac{8m^2}{n} - \frac{12m^2}{n^2}} .$$
(16)

Obviously, by (16), we have

$$M_1 \le \frac{(2(n-1)-2m/n)^2}{2} + \frac{4m^2}{n} + \frac{6m^2}{n^2} - 2m.$$

References

- [1] J. A. Bondy, U. S. R. Murty, Graph Theory, Springer, New York, 2008.
- [2] D. Cvetković, M. Doob, H. Sachs, Spectra of Graphs Theory and Application, Academic Press, New York, 1980.
- [3] D. Cvetković, P. Rowlinson, S. K. Simić, An Introduction to the Theory of Graph Spectra, Cambridge Univ. Press, Cambridge, 2010.
- [4] K. C. Das, S. Mojallal, I. Gutman, On energy and Laplacian energy of bipartite graphs, Appl. Math. Comput. 273 (2016) 759–766.
- [5] K. C. Das, S. Mojallal, I. Gutman, On Laplacian energy in terms of graph invariants, *Appl. Math. Comput.* 268 (2015) 83–92.
- [6] B. Deng, X. Li, I. Gutman, More on borderenergetic graphs, *Lin. Algebra Appl.* 497 (2016) 199–208.
- [7] B. Deng, X. Li, More on L-borderenergetic graphs, MATCH Commun. Math. Comput. Chem. 77 (2017) 115–127.
- [8] B. Deng, X. Li, J. Wang, Further results on L-borderenergetic graphs, MATCH Commun. Math. Comput. Chem. 77 (2017) 607–616.
- [9] B. Deng, X. Li, Y. Li, (Signless) Laplacian borderenergetic graphs and the join of graphs, MATCH Commun. Math. Comput. Chem. 80 (2018) 449–457.
- [10] S. Gong, X. Li, G. Xu, I. Gutman, B. Furtula, Borderenergetic graphs, MATCH Commun. Math. Comput. Chem. 74 (2015) 321–332.
- [11] I. Gutman, Bounds for total π -electron energy, Chem. Phys. Lett. 24 (1974) 283–283.
- [12] I. Gutman, Degree-based topological indices, Croat. Chem. Acta 86 (2013) 351–361.
- [13] I. Gutman, Acylclic systems with extremal Hückel π-electron energy, Theor. Chim. Acta. 45 (1977) 79–87.
- [14] I. Gutman, The energy of a graph, Ber. Math. Statist. Sekt. Forschungsz. Graz 103 (1978) 1–22.
- [15] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.
- [16] S.M. Hosamani, I. Gutman, Zagreb indices of transformation graphs and total transformation graphs, *Appl. Math. Comput.* 247 (2014) 1156–1160.

- [17] Y. Hou, Q. Tao, Borderenergetic threshold graphs, MATCH Commun. Math. Comput. Chem. 75 (2016) 253–262.
- [18] X. Li, Y. Shi, I. Gutman, Graph Energy, Springer, New York, 2012.
- [19] X. Li, M. Wei, S. Gong, A computer search for the borderenergetic graphs of order 10, MATCH Commun. Math. Comput. Chem. 74 (2015) 333–342.
- [20] X. Li, M. Wei, X. Zhu, Borderenergetic graphs with small maximum or large minimum degrees, MATCH Commun. Math. Comput. Chem. 77 (2017) 25–36.
- [21] L. Lu, Q. Huang, On the existence of non-complete L-borderenergetic graphs, MATCH Commun. Math. Comput. Chem. 77 (2017) 625–634.
- [22] I. Milovanović, E. Milovanović, I. Gutman, Upper bounds for some graph energies, *Appl. Math. Comput.* 289 (2016) 435–443.
- [23] Z. Shao, F. Deng, Correcting the number of borderenergetic graphs of order 10, MATCH Commun. Math. Comput. Chem. 75 (2016) 263–266.
- [24] Q. Tao, Y. Hou, A computer search for the L-borderenergetic graphs, MATCH Commun. Math. Comput. Chem. 77 (2017) 595–606.
- [25] F. Tura, L-borderenergetic graphs, MATCH Commun. Math. Comput. Chem. 77 (2017) 37–44.
- [26] F. Tura, L-borderenergetic graphs and normalized Laplacian energy, MATCH Commun. Math. Comput. Chem. 77 (2017) 617–624.