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Further Results on L-Borderenergetic Graphs^{*}

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Abstract

If a graph G of order n has the same Laplacian energy as the complete graph K_n does, i.e., if $\mathcal{E}(G) = 2(n-1)$, then G is said to be L-borderenergetic. This is a new concept proposed by F. Tura [25]. Till now there are very few results related to this topic. In this paper, we continue to characterize this kind of graphs and obtain some interesting properties on their structures. First, we use new ways to construct some new L-borderenergetic graphs. Then, we present some asymptotically bounds on the order and size of L-borderenergetic graphs. Finally, we show that all trees, cycles, the complete bipartite graphs, and many 2-connected graphs are not L-borderenergetic.

1 Introduction

All graphs appeared in this paper are simple and undirected. Let G be a graph of order n and size m and $V(G) = \{v_1, v_2, \dots, v_n\}$ be its vertex set with degree sequence d_1, d_2, \dots, d_n . The maximum degree and the minimum degree of G are denoted by Δ and δ , respectively. Denote the complete graph and star of order n by K_n and S_n , respectively. For any subset S of edge-set E(G) of G, i.e., $S \subseteq E(G), G - S$ is the graph obtained by deleting all edges in S from G.

The adjacency matrix of G is denoted by A(G), whose eigenvalues are $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, which consist of the spectrum of G. If D(G) is the diagonal matrix of the vertex degrees of G, L(G) = D(G) - A(G) is defined to be the Laplacian matrix of G. The

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Laplacian spectrum of G is composed of its eigenvalues $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_{n-1} \ge \mu_n = 0$, where the second smallest eigenvalue μ_{n-1} is called the algebraic connectivity. For details on spectral graph theory, see [2].

The energy of a graph G, denoted by $\mathcal{E}(G)$ and proposed by Gutman [10] in 1978, is defined as

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

For more information on graph energy and its applications in chemistry, we refer to [9, 13, 14, 21].

Recently, a new concept of *borderenergetic* graphs [8] was proposed, namely graphs of order n satisfying $\mathcal{E}(G) = 2(n-1)$. The corresponding results on borderenergetic graphs can be seen in [5, 17, 22–24]. Similarly, some related topics on energy of graphs have been studied; see [1, 11, 12, 16, 18–20].

An analogous concept as borderenergetic graphs, called *L*-borderenergetic graphs, was proposed by F. Tura [25]. That is, a graph *G* of order *n* is *L*-borderenergetic if $\mathcal{LE}(G) = \mathcal{LE}(K_n)$, where $\mathcal{LE}(G) = \sum_{i=1}^{n} |\mu_i - \overline{d}|$ and \overline{d} is the average degree of *G*. Bearing in mind that $\mathcal{LE}(K_n) = 2(n-1)$. Some classes of *L*-borderenergetic graphs of order n = 4r + 4 $(r \ge 1)$, are obtained, which are pairwise *L*-noncospectral and *L*-borderenergetic graphs [25]. In [4], a kind of threshold graphs were found to be *L*-borderenergetic, and all the connected non-complete and pairwise non-isomorphic *L*-borderenergetic graphs of small order *n* are depicted for *n* with $4 \le n \le 9$. Meanwhile, we see that these *L*-borderenergetic graphs are rather dense and complicated. But there are very few results on the structures of *L*-borderenergetic graphs [4, 25].

In this paper, we continue to characterize L-borderenergetic graphs and obtain some interesting properties on their structures. First, we use new ways to construct some new L-borderenergetic graphs. Then, we present some asymptotically bounds on the order and size of L-borderenergetic graphs. Finally, we show that all trees, cycles, the complete bipartite graphs, and parts of 2-connected graphs are not L-borderenergetic.

2 Two ways of constructing new *L*-borderenergetic graphs

In this section, we try to construct some L-borderenergetic graphs by deleting some edges in a complete graph K_n . And we use the following two ways in a complete graph K_n . One way is by deleting some independent edges , and the other is by deleting some edges possessing a common vertex. Let M_p be a set of p independent edges in a complete graph K_n , where $0 \le p \le \lfloor n/2 \rfloor$. Let E_q be a set of q edges possessing a common vertex in a complete graph K_n , where $0 \le q \le n - 1$. For the first way, we have

Theorem 1. For any even integer n, the graph $K_n - M_{\frac{n}{2}-1}$ is L-borderenergetic.

Proof. Let I_n be a unit matrix of order n. Though deleting M_p from the complete graph K_n , we get the graph $K_n - M_p$ and the corresponding Laplacian matrix is as follows:

$$L(K_n - M_p) =$$

$$\begin{pmatrix} n-2 & 0 & -1 & \cdots & & & -1 \\ 0 & n-2 & -1 & \cdots & & & -1 \\ -1 & -1 & n-2 & \cdots & & & -1 \\ \vdots & \vdots & \vdots & \ddots & & & \vdots \\ & & & n-2 & & & \\ & & & & n-1 & & \\ & & & & & \ddots & \\ -1 & -1 & -1 & \cdots & & & n-1 \end{pmatrix}$$

By some simplifications for the determinant $\det(\mu I_n - L(K_n - M_p))$, we finally obtain $\det(\mu I_n - L(K_n - M_p)) =$

$ \mu $		μ	μ	• • •				μ
0	$\mu-n+2$	0	0	• • •				0
0	0	$\mu-n+1$	-1					0
0	0	-1	$\mu-n+1$					0
			÷	·				
					$\mu-n+1$			
						$\mu - n$		
							·	:
0								$\mu - n$
1								1

$$= \mu(\mu - n)^{n-p-1}(\mu - n + 2)^p.$$

Thus, the eigenvalues of $L(K_n - M_p)$ are n, n-2, 0 with multiplicities n - p - 1, p, 1, respectively. Note that the average degree of $K_n - M_p$ is $n - 1 - \frac{2p}{n}$. Then from the definition of Laplacian energy, we obtain

$$\mathcal{L}\mathcal{E}(K_n - M_p) = \frac{(-2)[2p^2 - (n-2)p - n^2 + n]}{n}.$$
(1)

When $p = \frac{n}{2} - 1$, we can check that $\mathcal{L}\mathcal{E}(K_n - M_{\frac{n}{2}-1}) = 2(n-1)$ by (1).

Different from the case in Theorem 1, we obtain the graph $K_n - E_l$ by another way. With similar calculation as Theorem 1, we get

$$\mathcal{L}\mathcal{E}(K_n - E_l) = \frac{(2n-8)l + 2n^2 - 2n}{n}.$$
(2)

Note that (2) implies that $\mathcal{LE}(K_n - E_l)$ does not depend on l in the case of n = 4. So it means that the graphs $K_4 - E_1$, $K_4 - E_2$ and $K_4 - E_3$ are all L-borderenergetic. But for n > 4, any L-borderenergetic graph can not be found by this way.

3 Bounds on the order and size of *L*-borderenergetic graphs

In this section, we present an upper bound on the size and an lower bound on the order of *L*-borderenergetic graphs, respectively.

Lemma 2. [15] Let G be a connected graph with order n and size m. Then

$$\mathcal{L}\mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2M - \left(\frac{2m}{n}\right)^2\right]},$$

where $M = m + \frac{1}{2} \sum_{i=1}^{n} (d_i - \frac{2m}{n})^2$.

Theorem 3. If G is an L-border energetic graph of order n and size m, then

$$m \le \frac{1}{2(2\overline{d}-1)} \left[Z_g(G) + (n-1)\overline{d}^2 - \frac{(2n-2-\overline{d})^2}{n-1} \right],\tag{3}$$

where $Z_g(G) = \sum_{i=1}^n d_i^2$, called the first Zagreb index of G. When G is 4-regular, the bound in (3) is asymptotically tight.

Proof. By Lemma 2, we have

$$2(n-1) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2M - \left(\frac{2m}{n}\right)^2\right]}$$

= $\frac{2m}{n} + \sqrt{(n-1)\left[2m + \sum_{i=1}^n (d_i - \frac{2m}{n})^2 - \left(\frac{2m}{n}\right)^2\right]}$
= $\overline{d} + \sqrt{(n-1)\left[2m + \sum_{i=1}^n d_i^2 + n\overline{d}^2 - 4m\overline{d} - \overline{d}^2\right]}$
= $\overline{d} + \sqrt{(n-1)\left[2m + Z_g(G) + n\overline{d}^2 - 4m\overline{d} - \overline{d}^2\right]}.$

From above inequality, we can easily get

$$(2n-2-\overline{d})^2 \le (n-1)\left[(2-4\overline{d})m + (n-1)\overline{d}^2 + Z_g(G)\right].$$
(4)

Through some simplification for (4), we can arrive at

$$m \le \frac{1}{2(2\overline{d}-1)} \left[Z_g(G) + (n-1)\overline{d}^2 - \frac{(2n-2-\overline{d})^2}{n-1} \right]$$

When G is 4-regular, we have m = 2n, $\overline{d} = 4$ and $Z_g(G) = 16n$. Then by above inequality, we get

$$m \le \frac{2(7n^2 - 6n - 5)}{7(n - 1)}.$$

Since

$$\lim_{n \to \infty} \frac{\frac{2(7n^2 - 6n - 5)}{7(n-1)}}{2n} = 1,$$

the bound in (3) is asymptotically tight when G is 4-regular.

If G is r-regular, then from Theorem 3 we can directly have

Corollary 4. If G is an L-borderenergetic r-regular graph of order n and size m, then

$$m \le \frac{1}{2(2r-1)} \left[(2n-1)r^2 - \frac{(2n-2-r)^2}{n-1} \right].$$
 (5)

Due to regularity, the bound in (5) is also fit for borderenergetic graphs. Next we show an lower bound on the order of borderenergetic graphs.

Lemma 5. [7] For a graph G, let $\kappa(G)$ be its vertex connectivity. Then $\mu_{n-1} \leq \kappa(G)$.

Theorem 6. If G is an L-border energetic graph of order n and size m, then

$$n \ge 2\overline{d} - \delta + 1. \tag{6}$$

Proof. Let σ be the largest integer such that $\mu_{\sigma} \geq \overline{d}$. Since G is L-borderenergetic,

$$2(n-1) = \sum_{i=1}^{n} |\mu_i - \overline{d}| = \sum_{i=1}^{\sigma} (\mu_i - \overline{d}) + \sum_{j=\sigma+1}^{n} (\overline{d} - \mu_j)$$

$$= \sum_{i=1}^{\sigma} \mu_i - \sigma \overline{d} + (n-\sigma)\overline{d} - \sum_{j=\sigma+1}^{n} \mu_j$$

$$= \sum_{i=1}^{\sigma} \mu_i - \sigma \overline{d} + (n-\sigma)\overline{d} - \left(2m - \sum_{i=1}^{\sigma} \mu_i\right)$$

$$= 2\sum_{i=1}^{\sigma} \mu_i - 2\sigma \overline{d}.$$

By the definition of σ , we have

$$2\sum_{i=1}^{\sigma} \mu_{i} - 2\sigma \overline{d} = \max_{1 \le i \le n-1} \left\{ 2\sum_{j=1}^{i} \mu_{j} - 2i\overline{d} \right\}$$
$$= 2\max_{1 \le i \le n-1} \left\{ 2m - \sum_{j=i+1}^{n} \mu_{j} - i\overline{d} \right\}$$
$$\geq 2[2m - (n-2)\overline{d} - \mu_{n-1}]$$
$$= 4m - 2(n-2)\overline{d} - 2\mu_{n-1}$$
$$= 2n\overline{d} - 2(n-2)\overline{d} - 2\mu_{n-1}$$
$$= 2(2\overline{d} - \mu_{n-1}).$$

Thus,

$$2(n-1) \ge 2(2\overline{d} - \mu_{n-1}). \tag{7}$$

By the definition of the vertex connectivity and Lemma 5, we have $\mu_{n-1} \leq \kappa(G) \leq \delta$. Then we obtain $n \geq 2\overline{d} - \delta + 1$ from (7).

The authors in [4] found a kind of L-borderenergetic graphs denoted by S_n^1 , that is the graph with *m* edges obtained from an *n*-order star S_n by adding an edge. Note that the graph S_n^1 has a vertex of degree 1, which implies that there exit some Lborderenergetic graphs with the minimum degree $\delta = 1$. So we pay attention to this kind of L-borderenergetic graphs. By Theorem 6 and $\overline{d} = 2m/n$, we can deduce

Corollary 7. If G is an L-border energetic graph of order n and size m with $\delta = 1$, then

$$n \ge 2\sqrt{m}.\tag{8}$$

In fact, when n = 4, 6, 8, we can find the corresponding *L*-borderenergetic graphs $L_4^1, L_6^1, L_8^1 \in \mathcal{L}_n^1$ (see Figure 1.), which attain the bound in (8), where \mathcal{L}_n^1 be the set of *L*-borderenergetic graphs of order *n* with $n = 2\sqrt{m}$ and $\delta = 1$.



Figure 1. The L-border energetic graphs $L_4^1, L_6^1, L_8^1 \in \mathcal{L}_n^1$

4 Non-L-borderenergetic graphs

In this section, we show that all trees, cycles, the complete bipartite graphs, and many 2connected graphs are not L-borderenergetic. First, we present that the complete bipartite graphs are not L-borderenergetic.

Theorem 8. If G is a complete bipartite graph $K_{a,b}$ $(1 \le a \le b)$, then G is not Lborderenergetic.

Proof. Note that the Laplacian eigenvalues of $K_{a,b}$ are a + b, a, b, 0 with multiplicities 1, b-1, a-1, 1 respectively, and the average degree of $K_{a,b}$ is $\frac{2ab}{a+b}$. Then from the definition of Laplacian energy, we obtain

$$\mathcal{L}\mathcal{E}(K_{a,b}) = 2a + \frac{2ab(b-a)}{a+b}.$$
(9)

Suppose $K_{a,b}$ is L-borderenergetic. Then by (9), we have

$$2a + \frac{2ab(b-a)}{a+b} = 2(a+b-1)$$

$$ab(b-a) = ab+b^2 - a - b$$

$$b-a-1 = \frac{b(b-1)-a}{ab}.$$
(10)

By (10), it is easy to see that the quality $\frac{b(b-1)-a}{ab}$ is an integer. Then let $k = \frac{b(b-1)-a}{ab}$, and we obtain b(b-1) - a = kab and

$$b - 1 - ak = \frac{a}{b}.\tag{11}$$

Thus, it is obvious that the quality $\frac{a}{b}$ is an integer from (11), which is a contradiction in the case a < b. For the case a = b and a > 2, from (11), we get $k = 1 - \frac{2}{a}$, which is also a contradiction. But for the cases a = b = 1 and a = b = 2, it is not hard to verify that both graphs $K_{1,1}$ and $K_{2,2}$ are not *L*-borderenergetic. Therefore, all complete bipartite graphs are not *L*-borderenergetic.

Then for trees, we will use the above theorem and a lemma below.

Lemma 9. [6] For any tree T of order n, $\mathcal{LE}(T) < \mathcal{LE}(S_n)$ holds.

Theorem 10. For any tree T of order n, T is not L-borderenergetic.

Proof. Since the star S_n is the complete bipartite $K_{1,n-1}$, by using the formula (9), we have $\mathcal{L}\mathcal{E}(S_n) = 2 + \frac{2(n-1)(n-2)}{n} = 2(n-2+\frac{2}{n}) < 2(n-1)$. Thus, by Lemma 9, we know that, for any tree of order n, its Laplacian energy is less than 2(n-1).

For 2-connected graphs, we can easily confirm that cycles are not L-borderenergetic. This is because the energy and Laplacian energy are the same when graphs are regular by Theorem 11, and the authors in [23] proved that there are no borderenergetic graphs in the case of $\Delta \leq 3$.

Theorem 11. [4] If G is a d-regular graph, then $\mathcal{LE}(G) = \mathcal{E}(G)$.

Moreover, we find another kind of 2-connected graphs that are also not L-borderenergetic. Denote by t(G) the number of vertices of degree 3 in G.

Theorem 12. If G is a 2-connected graph with maximum degree $\Delta = 3$ and $t(G) \ge 7$, then G is not L-borderenergetic.

Proof. As graph G is 2-connected, there are no vertices of degree 1 in G. So the number of vertices of degree 2 is n - t(G). By Lemma 2, we know

$$\mathcal{L}\mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2M - \left(\frac{2m}{n}\right)^2\right]},$$

where $M = m + \frac{1}{2} \sum_{i=1}^{n} (d_i - \frac{2m}{n})^2$. Let $f(x) = \frac{2x}{n} + \sqrt{(n-1) \left[2 \left(x + \frac{1}{2} \sum_{i=1}^{n} \left(d_i - \frac{2x}{n} \right)^2 \right) - \left(\frac{2x}{n} \right)^2 \right]}$. Then we see that the function f(x) is increasing as $x \in [0, \frac{3n}{2}]$. Due to $m \leq \frac{3n}{2}$, we have $f(m) \leq f(\frac{3n}{2})$. Hence,

$$\mathcal{LE}(G) \leq 3 + \sqrt{(n-1) \left[3n + \sum_{i=1}^{n} (d_i - 3)^2 - 9 \right]} \\ \leq 3 + \sqrt{(n-1)(3n + n - t(G) - 9)} \\ \leq 3 + \sqrt{(n-1)(4n - t(G) - 9)}.$$
(12)

 $t(G) + 16 > 0. \text{ From } (t(G) - 7)n - t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (n - 1)(4n - t(G) - 9), \text{ it follows for a started of } t(G) + 16 = (2n - 5)^2 - (2n$ that $2n-5 > \sqrt{(n-1)(4n-t(G)-9)}$ and $2(n-1) > 3 + \sqrt{(n-1)(4n-t(G)-9)}$. In other words, G is not L-borderenergetic.

Remark. Theorem 12 only considers 2-connected graphs with maximum degree 3 and the number t(G) of vertices of degree 3 satisfying $t(G) \ge 7$. But, the other cases, such as the 2-connected graphs with $1 \le t \le 6$ and the graphs with $\Delta \le 4$, need to be further studied.

References

- S. Akbari, F. Moazami, S. Zare, Kneser graphs and their complements are hyperenergetic, MATCH Commun. Math. Comput. Chem. 61 (2009) 361–368.
- [2] D. Cvetković, P. Rowlinson, S. Simić, An Introduction to the Theory of Graph Spectra, Cambridge Univ. Press, Cambridge, 2009.
- [3] K. C. Das, S. A. Mojallal, I. Gutman, On Laplacian energy in terms of graph invariants, Appl. Math. Comput. 259 (2015) 470–479.
- [4] B. Deng, X. Li, More on L-borderenergetic graphs, MATCH Commun. Math. Comput. Chem. 77 (2017) 115–127.
- [5] B. Deng, X. Li, I. Gutman, More on borderenergetic graphs, *Lin. Algebra Appl.* 497 (2016) 199–208.
- [6] E. Fritscher, C. Hoppen, I. Rocha, V. Trevisan, On the sum of the Laplacian eigenvalues of a tree, *Lin. Algebra Appl.* 435 (2011) 371–399.
- [7] A. Ghosh, S. Boyd, Upper bounds on algebraic connectivity via convex optimization, *Lin. Algebra Appl.* 418 (2006) 693–707.
- [8] S. C. Gong, X. Li, G. H. Xu, I. Gutman, B. Furtula, Borderenergetic graphs, MATCH Commun. Math. Comput. Chem. 74 (2015) 321–332.
- [9] I. Gutman, Acylclic systems with extremal Hückel π-electron energy, Theor. Chim. Acta. 45 (1977) 79–87.
- [10] I. Gutman, The energy of a graph, Ber. Math. Stat. Sekt. Forschungsz. Graz 103 (1978) 1–22.
- [11] I. Gutman, Hyperenergetic and hypoenergetic graphs, in: D. Cvetković, I. Gutman (Eds.), Selected Topics on Applications of Graph Spectra, Math. Inst., Belgrade, 2011, pp. 113–135.
- [12] I. Gutman, X. Li, Y. Shi, J. Zhang, Hypoenergetic trees, MATCH Commun. Math. Comput. Chem. 60 (2009) 415–426.
- [13] I. Gutman, X. Li, J. Zhang, Graph energy, in: M. Dehmer, F. Emmert–Streib (Eds.), Analysis of Complex Networks – From Biology to Linguistics, Wiley–VCH, Weinheim, 2009, pp. 145–174.
- [14] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.

- [15] I. Gutman, B. Zhou, Laplacian energy of a graph, Lin. Algebra Appl. 414 (2006) 29–37.
- [16] Y. Hou, I. Gutman, Hyperenergetic line graphs, MATCH Commun. Math. Comput. Chem. 43 (2001) 29–39.
- [17] Y. Hou, Q. Tao, Borderenergetic threshold graphs, MATCH Commun. Math. Comput. Chem. 75 (2016) 253–262.
- [18] X. Li, H. Ma, All hypoenergetic graphs with maximum degree at most 3, *Lin. Algebra Appl.* **431** (2009) 2127–2133.
- [19] X. Li, H. Ma, All connected graphs with maximum degree at most 3 whose energies are equal to the number of vertices, MATCH Commun. Math. Comput. Chem. 64 (2010) 7–24.
- [20] X. Li, H. Ma, Hypoenergetic and strongly hypoenergetic k-cyclic graphs, MATCH Commun. Math. Comput. Chem. 64 (2010) 41–60.
- [21] X. Li, Y. Shi, I. Gutman, Graph Energy, Springer, New York, 2012.
- [22] 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.
- [23] X. Li, M. Wei, X. Zhu, Borderenergetic graphs with small maximum or large minimum degrees, MATCH Commun. Math. Comput. Chem. 77 (2016) 25–36.
- [24] Z. Shao, F. Deng, Correcting the number of borderenergetic graphs of order 10, MATCH Commun. Math. Comput. Chem. 75 (2016) 263–266.
- [25] F. Tura, L-borderenergetic graphs, MATCH Commun. Math. Comput. Chem. 77 (2017) 37–44.