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Laplacian energy and first Zagreb index of Laplacian integral graphs

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Abstract

The set $S_{i,n} = \{0, 1, 2, ..., i-1, i+1, ..., n-1, n\}$, $1 \leqslant i \leqslant n$, is called Laplacian realizable if there exists a simple connected undirected graph whose Laplacian spectrum is $S_{i,n}$. The existence of such graphs was established by S. Fallat et all. In the present paper, we find the Laplacian energy and first Zagreb index of graphs whose Laplacian spectrum is $S_{i,n}$.

1 Introduction

Let $G = (V, E)$ be a simple undirected graph with the vertices set $V(G) = \{v_1, v_2, ..., v_n\}$ and the edge set $E(G)$, where by $m = |E(G)|$ we denote the size of G. If $v_i, v_j \in V(G)$ then we say v_i is adjacent to v_j ($v_i \sim v_j$) if they share a common edge v_iv_j. The *Laplacian matrix* associated with the graph G is the $n \times n$ matrix $L(G) = (a_{ij})$ with entries

$$a_{ij} = \begin{cases} d_{v_i}, & \text{if} \quad i = j, \\ -1, & \text{if} \quad i \neq j \text{ and } v_i \sim v_j, \\ 0, & \text{otherwise.} \end{cases}$$

It is well known (see, e.g., [36]) that $L(G)$ has a zero eigenvalue corresponding to the eigenvector with equal entries, while other eigenvalues are

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non-negative. If $0 = \mu_1 \leqslant \mu_2 \leqslant \cdots \leqslant \mu_n$ are the eigenvalues of the Laplacian matrix of G, then its Laplacian energy is defined as follows

$$LE(G) = \sum_{k=1}^{n} |\mu_k - \overline{a}|, \tag{1}$$

where μ_k are the eigenvalues of the Laplacian matrix (Laplacian eigenvalues) of G and $\overline{a}$ is the average degree of G:

$$\overline{a} = \frac{2m}{n} = \frac{1}{n}\sum_{k=1}^{n} d_{v_k} = \frac{1}{n}\sum_{k=1}^{n} \mu_k. \tag{2}$$

The Laplacian energy was relatively recently introduced by I. Gutman and B. Zhou [29] and subsequently studied by many authors very actively, see, e.g., [1, 12, 13, 19, 25, 39, 43, 45, 49, 52, 53]. The motivation for the Laplacian energy $LE(G)$ comes from ordinary graph energy [4, 5, 23, 24], the Laplacian energy shares many properties (or very similar properties) with the ordinary energy. However, there are many graphs whose Laplacian eigenvalues are integer numbers. Such graphs are called *Laplacian integral* and their Laplacian energy can be found explicitly. A well-known example is the Laplacian energy of the complete graph K_n is $LE(K_n) = 2(n-1)$. In [1], the authors found Laplacian energy of some Laplacian integral graphs. They discussed Laplacian energy for those graphs which is obtained from complete graph K_n according to certain rules.

In this paper, we deal with a certain class of Laplacian integral graphs.

Definition 1.1. If Laplacian eigenvalues of a graph G consist of the set

$$S_{i,n} = \{0, 1, 2, .., i-1, i+1.., n-1, n\} \quad \text{for some } i, 1 \leqslant i \leqslant n, \tag{3}$$

then we say that the graph G realizes $S_{i,n}$. In this case, the set $S_{i,n}$ is called Laplacian realizable.

Such graphs were introduced [17] and their construction was studied in detailed there, see also Section 2 of the present work for some details.

Here we also discuss the first and the second Zagreb indices of the graphs realizing $S_{i,n}$. The *first Zagreb index* $M_1(G)$ of the graph G is equal to the sum of the squares of the degrees of the vertices of graph G:

$$M_1(G) = \sum_{k=1}^{n} d_{v_k}^2. \tag{4}$$

The *second Zagreb index* $M_2(G)$ is the sum of the product of the degrees of adjacent vertices in G. It can be expressed in mathematical form as follows

$$M_2(G) = \sum_{v_i v_j \in E(G)} d_{v_i} d_{v_j} \tag{5}$$

The Zagreb indices M_1 and M_2 were introduced in [28] and elaborated in [27]. The basic properties of M_1 and M_2 up to year 2004 were summarized in [26, 42]. Recently the first Zagreb index was studied in [2, 8, 9, 31, 32, 34, 42, 46, 51], where one can find more references to the previous research in this area. The Zagreb indices reflect the extent of branching of the molecular carbon-atom skeleton, so they can be viewed as molecular structure-descriptors [3, 48].

Thus, in this paper, we investigate the Laplacian energy $LE(G)$ and the first Zagreb index of the graphs whose Laplacian matrices have the set $S_{i,n}$ defined in (3) as its eigenvalues. We derive exact formulas for the Laplacian energy, Theorems 3.5 and 3.7, and for the first Zagreb index, Theorem 4.1. We also find the first Zagreb index for the complements of graphs realizing $S_{i,n}$ and provide lower and upper bounds for the Laplacian energy of such graphs, Theorem 3.9 and Corollary 3.6. In particular, we found out that the Laplacian energy of graphs realizing $S_{i,n}$ does not exceed the first Zagreb index of such graphs, Theorem 4.3. We also list all the L-borderenergetic and L-equienergetic graphs realizing $S_{i,n}$, see Definitions 2.9 and 2.10. As well, we found some graphs in the family of $S_{i,n}$ with same number of spanning trees. Unfortunately, we were not able to find an exact formula for the second Zagreb index of such graphs but we found its values for graphs realizing $S_{i,n}$ up to order $n = 9$, Table 1. We state an open problem to find the exact formula for the second Zagreb index of graphs realizing $S_{i,n}$. It is clear that these formula must be a rational function of i and n.

Finally, we discuss a conjecture from [17] stating that the set $S_{n,n}$ is not Laplacian realizable, see Conjecture 2.6. We list some known results on this conjecture. In particular, we prove that if such graphs exist, then they cannot be the Cartesian product of two graphs. As well, we show for such graphs (if any) the first Zagreb index coincides with the Zagreb of their complements and pose another conjecture on the graphs realizing $S_{n,n}$ (if any).

The results presented in this work may serve as model to compare for studies of the Laplacian energy and Zagreb indices as Laplacian realizable sets $S_{i,n}$ are unique for each n, and possess certain extremal properties. We also believe that use of the Zagreb indices may contribute towards a proof of Conjecture 2.6.

The paper is organized as follows. In Section 2, we give a list of some definitions and known results we use in our work. Section 3 is devoted to the calculation of the Laplacian energy of graphs realizing $S_{i,n}$. Here we provide lower and upper bounds for the Laplacian energy of such graphs. In Section 4, we compute the first Zagreb index $M_1(G)$ of graphs realizing $S_{i,n}$ and show that the Laplacian energy of these graphs does not exceed the first Zagreb index. In Section 5, we discuss Conjecture 2.6. Finally, Section 6 is devoted to some open problems.

2 Preliminaries

The *complement* of a simple undirected graph G denoted by $\overline{G}$ is a simple graph on the same set of vertices as G in which two vertices are adjacent if and only if they are not adjacent in G. Given two disjoint graphs G_1 and G_2, the *union* of these graphs, $G_1 \cup G_2$, is the graph formed from the unions of the edges and vertices of the graphs G_1 and G_2. The *join* of the graphs G_1 and G_2, $G_1 \vee G_2$, is the graph formed from $G_1 \cup G_2$ by adding all possible edges between vertices in G_1 and vertices in G_2. Clearly, the complement of $G_1 \vee G_2$ is a disconnected graph.

It is easy to see from the form of the Laplacian matrix that the Laplacian spectrum of the union of two graphs is the union of their Laplacian spectra. The Laplacian spectrum $S_L(G)$ of a graph G is the spectrum of the Laplacian matrix of G. The following theorems provide information on the Laplacian spectra of complements and joins of graphs, see e.g. [6, 36].

Theorem 2.1. *Let G be a graph with n vertices with Laplacian eigenvalues*

$$0 = \mu_1 \leqslant \mu_2 \leqslant \mu_3 \leqslant \cdots \leqslant \mu_{n-1} \leqslant \mu_n$$

Then the Laplacian eigenvalues of the complement of G are the following

$$0 \leqslant n - \mu_n \leqslant n - \mu_{n-1} \leqslant \cdots \leqslant n - \mu_3 \leqslant n - \mu_2.$$

It is well known that the Laplacian spectrum of a graph provides some information on the structure of the graph. For example, one can use it to count the number of the spanning trees of the graph.

Definition 2.2. A *spanning tree* is a subgraph of G which includes all of the vertices of G with minimum possible number of edges.

The following theorem in the presented form was proved in [33] (see [40] for more reference).

Theorem 2.3. *Let $\tau(G)$ be the number of spanning trees of a graph G, and μ_k be its Laplacian eigenvalues. Then*

$$\tau(G) = \frac{1}{n} \prod_{k=2}^{n} \mu_k.$$

We note that, in fact, this theorem is an equivalent form of *Kirchhoff's matrix tree theorem*, see, e.g. [36].

2.1 The graphs realizing $S_{i,n}$

As we mentioned in Introduction, the graphs realizing $S_{i,n}$ were described in detail in [17]. The authors of [17] described relations between i and n for $S_{i,n}$ to be Laplacian realizable. Namely, they proved the following two theorems.

Theorem 2.4 ([17]). *Let $n \geqslant 2$ and $1 \leqslant i \leqslant n$. Suppose that $S_{i,n}$ is Laplacian realizable. If $n \equiv 0 \mod 4$ or $n \equiv 3 \mod 4$ then i is even, while if $n \equiv 1 \mod 4$ or $n \equiv 2 \mod 4$, then i is odd.*

The following theorem completely describes the number of all $S_{i,n}$ realizable graphs for $i \neq n$.

Theorem 2.5 ([17]). *Suppose $n \geqslant 2$.*

(i) If $n \equiv 0 \mod 4$, then for each $i = 1, 2, 3, \ldots, \dfrac{n-2}{2}$, $S_{2i,n}$ is Laplacian realizable;

(ii) If $n \equiv 1 \mod 4$, then for each $i = 1, 2, 3, \ldots, \dfrac{n-1}{2}$, $S_{2i-1,n}$ is Laplacian realizable;

(iii) If $n \equiv 2 \mod 4$, then for each $i = 1, 2, 3, \ldots, \dfrac{n}{2}$, $S_{2i-1,n}$ is Laplacian realizable;

(iv) If $n \equiv 3 \mod 4$, then for $i = 1, 2, \ldots, \dfrac{n-1}{2}$, $S_{2i,n}$ is Laplacian realizable.

In [17], the authors also developed an algorithm for constructing the graphs realizing $S_{i,n}$ except the set $S_{n,n}$. On the set $S_{n,n}$ they conjectured the following.

Conjecture 2.6. *The spectrum $S_{n,n}$ is not Laplacian realizable for any $n \geqslant 2$.*

This conjecture was proved to be true for $n \leqslant 11$ in [17] and for $n \geqslant 6,649,688,933$ in [21]. In fact, there exist other sufficient conditions for graphs satisfying this conjecture, see Section 5.

We finish this section with counting the number of spanning trees of graphs realizing $S_{i,n}$. From Theorem 2.3, one immediately obtain the following formula.

Theorem 2.7. *If $S_{i,n}$, $i < n$, is Laplacian realizable, and G is a graph realizing $S_{i,n}$, then*

$$\tau(G) = \frac{(n-1)!}{i} \tag{1}$$

where τ stands for the number of spanning trees. So if $n \geqslant 5$, then $\tau(G)$ is an even number, while it is an odd number whenever $2 \leqslant n \leqslant 4$.

This formula implies the following simple corollary.

Corollary 2.8. *If $n \equiv 2 \mod 4$ and $S_{i,n}$ is realizable for $i < n$, then*

$$\tau(S_{1,n}) = \tau(S_{n,n+1}) = (n-1)!$$

where τ stands for the number of spanning trees.

2.2 The Laplacian Energy

The Laplacian energy of graphs possess many properties similar to the ordinary energy [4, 5, 23, 24] as we mentioned in Introduction. There exist a number of works studying graphs with the same Laplacian energy [14, 18, 35, 44], or with the Laplacian energy equals the one of the complete graph K_n.

Definition 2.9. Two non-isomorphic graphs of same order are called *L-equienergetic* if their Laplacian energies are equal.

A graph G on n vertices is said to be borderenergetic if its ordinary energy equal to the energy of the complete graph K_n . I. Gutman and S. Gong [22] introduced the concept of borderenergetic graphs. F. Tura in [50] developed the concept of *L-borderenergetic* graphs.

Definition 2.10. A graph G is called *L-borderenergetic* if its Laplacian energy equals the Laplacian energy of the complete graph, i.e., $LE(G) = LE(K_n) = 2(n-1)$.

Many authors have presented different families of graphs with same Laplacian energy as that of the complete graph K_n. For recent investigations of this quantity see [15, 16, 47]. In Section 3, we study L-equienergetic and L-borderenergetic graphs realizing $S_{i,n}$.

In the present work, we also find the upper and lower bounds for the Laplacian energy of graphs realizing $S_{i,n}$, see Section 3. There exist bounds for the Laplacian energy of an arbitrary simple connected graph.

Definition 2.11. The *maximum degree* of G denoted by $\Delta(G)$ is the degree of the vertex with greatest number of edges incident to it, whereas the *minimum degree* denoted by $\delta(G)$ is the degree of the vertex with smallest number of edges incident to it.

The following theorems provide lower and upper bounds for the Laplacian energy of a graph.

Theorem 2.12 ([11]). *Let G be a connected graph of order n with m edges and maximum degree Δ. Then*

$$LE(G) \geqslant 2\Big(\Delta + 1 - \overline{a}\Big),$$

with equality if and only if G is isomorphic to $K_{1,n-1}$. Here $\overline{a}$ is the average degree of the graph G defined in (2).

Theorem 2.13 ([11]). *Let G be a graph of order n and of size m, $m \geqslant \frac{n}{2}$. Then*

$$LE(G) \leqslant 4m - 2\Delta - \frac{4m}{n} + 2.$$

Here the equality holds if and only if G is isomorphic $K_{1,n-1}$ or G is isomorphic $K_{1,\Delta} \cup \overline{K}_{n-\Delta-1}$, $\frac{n}{2} \leqslant \Delta \leqslant n-2$.

2.3 Zagreb indices

As we announced in Introduction, in the present work we deal with the first and second Zagreb indices, see (4)–(5). Note that the Zagreb indices can also be expressed by the following formulæ [28]

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v), \qquad M_2(G) = \frac{1}{2} \sum_{i=1}^{n} d_{v_i}^2 a_i$$

where a_i is the average degree of the vertices adjacent to vertex v_i. We can also represent the first Zagreb index in a similar way.

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

For more detail and applications, we refer the readers to see [7, 8, 30, 34].

The next theorem provides the lower and upper bound for the first Zargeb index of an arbitrary simple graph.

Theorem 2.14 ([31, 32, 46]). *Let G be a simple graph of order n and size m. Then the following hold*

- $$M_1\left(\overline{G}\right) = M_1(G) + n(n-1)^2 - 4m(n-1),$$

  where $\overline{G}$ is the complement of the graph G.

- $$M_1(G) \geqslant \frac{4m^2}{n}.$$
  The equality is attained if and only if the graph G is regular.

- $$M_1(G) \leqslant 2m(\Delta + \delta) - n\Delta\delta,$$
  where Δ and δ is the maximum and minimum degrees of the graph G, respectively.

Moreover, I. Gutman and B. Zhou [29] found upper bounds for the Laplacian energy of an arbitrary graph G with use of the first Zagreb index. As it was shown in [11], the best Gutman-Zhou's estimate is the following.

$$LE(G) \leqslant \frac{2m}{n} + \sqrt{(n-1)\left(2m + M_1(G) - \frac{4m^2}{n} - \frac{4m^2}{n^2}\right)}, \qquad (2)$$

where n and m are the order and the size of the graph G, respectively.

3 Laplacian Energy of graphs realizing $S_{i,n}$

In the present section, we find the Laplacian energy of graphs realizing the sets $S_{i,n}$ and count the number of L-equienergetic graphs realizing these sets.

3.1 Formulas for Laplacian Energy

First, we give a general form for the Laplacian energy of graphs realizing $S_{i,n}$.

Lemma 3.1. *Let $S_{i,n}$ be Laplacian realizable. Suppose that G be a connected graph of order $n \geqslant 2$ realizing $S_{i,n}$, $1 \leqslant i \leqslant n$. Then the Laplacian energy of G has the following form*

$$LE(G) = 2\min\left(T(n,\overline{a}), 0\right) - 2T(\lfloor\overline{a}\rfloor, \overline{a}), \qquad (1)$$

where

$$T(m,\alpha) = \sum_{k=0}^{m}(k-\alpha) = (m+1)\left(\frac{m}{2} - \alpha\right), \qquad m \in \mathbb{N},\ \alpha \in \mathbb{R}, \qquad (2)$$

and $\overline{a}$ is defined in (2).

We remind the reader that the case $i = n$ does not exist conjecturally, see Conjecture 2.6. However, we have to include this case into our study unless the conjecture is proved (if any).

Proof. Let $1 \leqslant i \leqslant n$. By Definition 1.1, we have that the list of eigenvalues of the Laplacian matrix of G is the following

$$\{\mu_1, \dots, \mu_n\} = \{0, 1, 2, \dots, n\} \setminus \{i\}, \quad 1 \leqslant i \leqslant n.$$

Thus, from (2) and (1), we obtain

$$\overline{a} = \frac{1}{n}\left(\sum_{k=1}^{n} k - i\right) = \frac{n+1}{2} - \frac{i}{n}, \tag{3}$$

and

$$LE(G) = \sum_{k=0}^{n} |k - \overline{a}| - |i - \overline{a}|.$$

This formulas imply the following

$$\begin{aligned} LE(G) &= -\sum_{k=0}^{\lfloor \overline{a} \rfloor}(k - \overline{a}) + \sum_{k=\lfloor \overline{a} \rfloor+1}^{n}(k - \overline{a}) - |i - \overline{a}| = -\sum_{k=0}^{\lfloor \overline{a} \rfloor}(k - \overline{a}) + \\ &+ \sum_{k=\lfloor \overline{a} \rfloor+1}^{n}(k - \overline{a}) + \sum_{k=0}^{\lfloor \overline{a} \rfloor}(k - \overline{a}) - \sum_{k=0}^{\lfloor \overline{a} \rfloor}(k - \overline{a}) - |i - \overline{a}| = \\ &= -2T(\lfloor \overline{a} \rfloor, \overline{a}) + T(n, \overline{a}) - |i - \overline{a}|, \end{aligned} \tag{4}$$

where T is defined in (2), and

$$T(n, \overline{a}) = (n+1)\left(\frac{n}{2} - \left(\frac{n+1}{2} - \frac{i}{n}\right)\right) = \frac{(2i - n)(n+1)}{2n}.$$

At the same time,

$$i - \overline{a} = i - \left(\frac{n+1}{2} - \frac{i}{n}\right) = \frac{(2i - n)(n+1)}{2n}.$$

Thus, we have

$$i - \overline{a} = T(n, \overline{a}),$$

so

$$T(n, \overline{a}) - |i - \overline{a}| = T(n, \overline{a}) - |T(n, \overline{a})| = 2\min\left(T(n, \overline{a}), 0\right). \tag{5}$$

Now from (4)–(5), we get (1), as required. □

Note that almost all graphs whose Laplacian spectrum is a set $S_{i,n}$ for some i and n, $i \leqslant n$, have non-integer average degree.

Lemma 3.2. *Let $n \geqslant 2$ be an even number, and let $S_{i,n}$ be Laplacian realizable. Then among graphs realizing $S_{i,n}$ for various i, the only graph having integer average degree is anti-regular graph whose Laplacian spectrum is $S_{\frac{n}{2},n}$.*

We remind the reader that a graph is called *anti-regular* (denoted as A_n) if its vertex degrees attains $(n-1)$ distinct value or if G has exactly two vertices of the same degree. Its Laplacian spectrum is the set $S_{\lfloor \frac{n+1}{2} \rfloor,n}$, see [37, 38].

Proof. Let $n = 2l$, $l \in \mathbb{N}$. Suppose that the Laplacian spectrum of a given graph G is $S_{i,n}$. From (3) it follows that

$$\overline{a} = l + \frac{1}{2} - \frac{i}{2l}. \tag{6}$$

Since $i \leqslant n$, we have

$$\frac{i}{2l} \leqslant 1,$$

so $\overline{a}$ is integer if and only if $\dfrac{i}{2l} = \dfrac{1}{2}$, that is, $i = l = \dfrac{n}{2}$. □

Lemma 3.3. *Let $n \geqslant 1$ be an odd number, and let the set $S_{i,n}$ be Laplacian realizable. Then among graphs realizing $S_{i,n}$ for various i, the only graphs having integer average degree are graphs with Laplacian spectrum $S_{n,n}$.*

We remind the reader that conjecturally the set $S_{n,n}$ is not Laplacian realizable according to Conjecture 2.6.

Proof. Let $n = 2l - 1$, $l \in \mathbb{N}$. Suppose that the Laplacian spectrum of a given graph G is $S_{i,n}$. From (3) it follows that

$$\overline{a} = l - \frac{i}{2l-1}.$$

So, if $1 \leqslant i < n$, we get $\dfrac{i}{2l-1} < 1$, and $\overline{a}$ is non-integer. Thus, it is integer if and only if $i = 2l - 1 = n$. □

Lemmas 3.2–3.3 imply the following simple observation.

Corollary 3.4. *The only graph realizing $S_{i,n}$ with $i = \overline{a}$ is the anti-regular graph with the Laplacian spectrum $S_{\frac{n}{2},n}$ for even n.*

Now we are in a position to find formulas for the Laplacian energy of graphs realizing $S_{i,n}$. We consider the cases of even and odd order of the graph separately.

Theorem 3.5. *Let $n \geqslant 2$ be an even number, and let the set $S_{i,n}$ be Laplacian realizable. If G realizes $S_{i,n}$, then the Laplacian energy of G is given by the following formula.*

$$LE(G) = \begin{cases} \left(\frac{n}{2}\right)^2 + i & \text{for} \quad i \leqslant \frac{n}{2}, \\ \\ \left(\frac{n}{2}\right)^2 + n - i & \text{for} \quad i \geqslant \frac{n}{2}. \end{cases} \tag{7}$$

Proof. Suppose first that G realizes $S_{\frac{n}{2},n}$. By Corollary 3.4, we have $i = \overline{a}$, so from (1)–(2) it follows that

$$LE\,(G) = -2T(\lfloor \overline{a} \rfloor, \overline{a}) = -2(\overline{a}+1)\left(-\frac{\overline{a}}{2}\right) = \frac{n(n+2)}{4} = \left(\frac{n}{2}\right)^2 + \frac{n}{2}, \tag{8}$$

since $\overline{a} = i = \frac{n}{2}$ is integer for even n.

Suppose now that $i > \frac{n}{2}$, and G realizes $S_{i,n}$. Then

$$\frac{1}{2} - \frac{i}{n} < 0,$$

and the formula (6) implies

$$\lfloor \overline{a} \rfloor = \frac{n}{2} - 1.$$

Thus, from (2) and (3) we obtain

$$T(\lfloor \overline{a} \rfloor, \overline{a}) = \frac{n}{2}\left(\frac{n}{4} - \frac{1}{2} - \frac{n+1}{2} + \frac{i}{n}\right) = \frac{n}{2}\left(\frac{i}{n} - \frac{n}{4} - 1\right),$$

and

$$T(n, \overline{a}) = (n+1)\left(\frac{n}{2} - \frac{n+1}{2} + \frac{i}{n}\right) = (n+1)\left(\frac{i}{n} - \frac{1}{2}\right) > 0.$$

By (1) one gets

$$LE(G) = -2T(\lfloor \overline{a} \rfloor, \overline{a}) = -n\left(\frac{i}{n} - \frac{n}{4} - 1\right) = \left(\frac{n}{2}\right)^2 + n - i, \tag{9}$$

whenever $i > \frac{n}{2}$.

Finally, if $i < \frac{n}{2}$ and G realizes $S_{i,n}$, then

$$\frac{1}{2} - \frac{i}{n} > 0,$$

so

$$\lfloor \overline{a} \rfloor = \frac{n}{2},$$

and

$$T(\lfloor \overline{a} \rfloor, \overline{a}) = \left(\frac{n}{2}+1\right)\left(\frac{n}{4} - \frac{n+1}{2} + \frac{i}{n}\right) = \left(\frac{n}{2}+1\right)\left(\frac{i}{n} - \frac{n}{4} - \frac{1}{2}\right),$$

$$T(n, \overline{a}) = (n+1)\left(\frac{i}{n} - \frac{1}{2}\right) < 0.$$

So from (1) it follows that

$$\begin{aligned} LE(G) &= 2T(n,\overline{a}) - 2T(\lfloor \overline{a} \rfloor, \overline{a}) = \\ &= 2(n+1)\left(\frac{i}{n} - \frac{1}{2}\right) - (n+2)\left(\frac{i}{n} - \frac{n}{4} - \frac{1}{2}\right) = \left(\frac{n}{2}\right)^2 + i, \end{aligned} \tag{10}$$

whenever $i < \dfrac{n}{2}$.

Now the formulas (8)–(10) imply (7), as required. □

From (7) it is easy to see that the Laplacian energy $LE(S_{i,n})$ is integer for any even n. Also this formula shows that if G realizes $S_{1,2}$, then $LE(G) = LE(K_2) = 2$, and if G realizes $S_{2,4}$, then $LE(G) = LE(K_4) = 6$.

As well, (7) gives that if G realizes $S_{1,6}$ or $S_{5,6}$, then $LE(G) = LE(K_6) = 10$. It turns out the aforementioned graphs are the only L-borderenergetic graphs among all graphs realizing $S_{i,n}$.

Corollary 3.6. *Let G be a connected graph of order $n = 2l$, $l \in \mathbb{N}$. If G realizes $S_{i,n}$, then its Laplacian energy is an even integer number, and the following inequality holds*

$$LE(K_n) \leqslant LE(G). \tag{11}$$

Here the equality holds if and only if $n \leqslant 6$, and G does not realize $S_{3,6}$. Here K_n is the complete graph of order n.

Proof. From Theorem 2.5 it follows that not every set $S_{i,n}$ is realizable. To study the parity of the Laplacian energy of $S_{i,n}$-realizable graphs, we consider the cases $n = 4m$ and $n = 4m - 2$, $m \in \mathbb{N}$, separately.

Suppose first that $n = 4m$. Then by Theorem 2.5, the set $S_{i,4m}$ is realizable if and only if i is an even number. Now if $i = 2l$, then from (7) for any graph G realizing $S_{2l,4m}$ we obtain

$$LE(G) = \begin{cases} (2m)^2 + 2l & \text{for} \quad 1 \leqslant l \leqslant m, \\ \\ (2m+1)^2 - (2l+1) & \text{for} \quad m \leqslant l \leqslant 2m. \end{cases} \tag{12}$$

Analogously, if $n = 4m-2$, then by Theorem 2.5, the set $S_{i,4m-2}$ is realizable if and only if i is an odd number. If $i = 2l-1$, then from (7) for any graph G realizing $S_{2l-1,4m-2}$ one gets

$$LE(G) = \begin{cases} (2m-1)^2 + 2l - 1 & \text{for} \quad 1 \leqslant l \leqslant m, \\ \\ (2m)^2 - 2l & \text{for} \quad m \leqslant l \leqslant 2m-1. \end{cases} \tag{13}$$

From the formulas (12)–(13) it follows that if n is even, then the Laplacian energy of any graph realizing $S_{i,n}$ is even.

Before proving inequality (11), we note that

$$LE(K_n) = 2(n-1). \tag{14}$$

This formula follows immediately from the fact that the Laplacian spectrum of the complete graph K_n is $\{0, \underbrace{n, \ldots, n}_{n-1}\}$ and from the formulas (1)–(2).

We also note that it is sufficient to prove the inequality (11) only for $i \leqslant \frac{n}{2}$, since the Laplacian energy of any graph realizing $S_{i,n}$ equals the Laplacian energy of any graph realizing $S_{n-i,n}$ by (7). So let $i \leqslant \frac{n}{2}$, then according to (7), if G realizes $S_{i,n}$, then the following holds

$$LE(G) - LE(K_n) = \frac{n^2}{4} + i - 2(n-1) = \left(\frac{n}{2} - 2\right)^2 + i - 2.$$

This formula shows that in (11) the strict inequality holds for any $n \geqslant 8$ and for $n = 6$ and $i = 3$. By Theorem 2.5, we have that for $n \leqslant 5$ and for $n = 6, i \neq 3$ the only Laplacian realizable sets are $S_{1,2}$, $S_{2,4}$, $S_{1,6}$, and $S_{5,6}$. It is easy to see that for all graphs realizing these sets, there is equality in (11), as required. $\square$

Now we are in a position to find the Laplacian energy of graphs realizing $S_{i,n}$ with odd n. The case $n = 1$ is trivial. So we omit it from our consideration.

Theorem 3.7. *Let $n \geqslant 3$ be an odd number. Then the Laplacian energy of any graph G realizing $S_{i,n}$ is given by the following formula.*

$$LE(G) = \begin{cases} (n+1)\left(\dfrac{n-1}{4} + \dfrac{i}{n}\right) & \text{for} \quad i \leqslant \dfrac{n-1}{2}, \\ \\ (n+1)\left(\dfrac{n+3}{4} - \dfrac{i}{n}\right) & \text{for} \quad i \geqslant \dfrac{n+1}{2}. \end{cases} \tag{15}$$

Proof. Indeed, from (2) and (3) it follows that

$$\begin{aligned} T(n,\overline{a}) < 0 \quad &\text{if} \quad i < \frac{n+1}{2}, \\ T(n,\overline{a}) > 0 \quad &\text{if} \quad i \geqslant \frac{n+1}{2}. \end{aligned} \tag{16}$$

Moreover, since n is odd, the formula (3) implies

$$\lfloor \overline{a} \rfloor = \frac{n+1}{2} - 1 = \frac{n-1}{2}$$

for any i, $1 \leqslant i \leqslant n$.

Let $i \geqslant \dfrac{n+1}{2}$. Then for any graph G realizing $S_{i,n}$ we have

$$LE(G) = -2T(\lfloor \overline{a} \rfloor, \overline{a}) = (2\overline{a} - \lfloor \overline{a} \rfloor)(\lfloor \overline{a} \rfloor + 1) =$$

$$= \frac{n+1}{2}\left(n+1-\frac{2i}{n}-\frac{n-1}{2}\right) = (n+1)\left(\frac{n+3}{4}-\frac{i}{n}\right).$$

If $i < \dfrac{n+1}{2}$, so, in fact, $i \leqslant \dfrac{n-1}{2}$, then by (1) and (16),for any graph G realizing $S_{i,n}$ one obtains

$$LE(G) = 2T(n,\overline{a}) - 2T(\lfloor \overline{a} \rfloor, \overline{a}) =$$

$$= (n+1)(n-2\overline{a}) + (n+1)\left(\frac{n+3}{4}-\frac{i}{n}\right) = (n+1)\left(\frac{n-1}{4}+\frac{i}{n}\right).$$

□

Remark 3.8. Theorem 3.7 shows that the Laplacian energy of any graph realizing $S_{i,n}$ is non-integer rational number whenever n is odd.

Thus, Theorem 3.5 and 3.7, and Corollary 3.6 imply the following general fact.

Theorem 3.9. *Let G realize $S_{i,n}$, $n \geqslant 2$. If $S_{i,n}$ is not $S_{2,3}$ or $S_{1,5}$, then the following inequalities are fulfilled.*

$$2(n-1) \leqslant LE(G) \leqslant \frac{n(n+2)}{4}. \tag{17}$$

Here the lower bound is achieved if G realizes $S_{1,2}$, $S_{2,4}$, $S_{1,6}$, or $S_{5,6}$ only, while the upper bound is achieved if G is the anti-regular graph A_n.

Proof. If n is even, the statement of the theorem follows from Theorem 3.5, Corollary 3.6, and identity (14), since for the anti-regular graph A_n whose spectrum is $S_{\lfloor \frac{n+1}{2} \rfloor, n}$, one has

$$LE(A_n) = \frac{n(n+2)}{4}$$

by (7), and for any graph G realizing $S_{i,n}$, the following inequality holds

$$LE\,(G) \leqslant LE(A_n)$$

for $1 \leqslant i \leqslant n$.

Let now n be an odd number. From (15) it follows that if a graph G_1 realizes $S_{\frac{n-1}{2},n}$ and a graph G_2 realizes $S_{\frac{n+1}{2},n}$, then

$$LE(G_1) = LE(G_2) = \frac{(n^2-1)(n+2)}{4n} < \frac{n^2(n+2)}{4n} = \frac{n(n+2)}{4},$$

and $LE(G) \leqslant LE(G_1)$ for any graph G realizing $S_{i,n}$ with $1 \leqslant i \leqslant n$. Thus, the upper bound in (17) for odd n is established completely, as well.

Let now n be odd and $n \geqslant 7$. From (15), it follows that the Laplacian energy of graphs realizing $S_{i,n}$ increases as i increases for $1 \leqslant i \leqslant \dfrac{n-1}{2}$, and decreases as i increases for $\dfrac{n-1}{2} \leqslant i \leqslant n$. Since the Laplacian energy of a graph realizing $S_{1,n}$ is greater than the Laplacian energy of a graph realizing $S_{n,n}$, we obtain that for any graph G realizing $S_{i,n}$ with odd $n \geqslant 7$, the following holds

$$LE(G) \geqslant \frac{(n+1)(n-1)}{4} \geqslant \frac{8(n-1)}{4} = 2(n-1)$$

where $\dfrac{(n+1)(n-1)}{4}$ is the Laplacian energy of a graph realizing $S_{n,n}$. Here the lower bound can be achieved only if $n = 7$, that is, if G realizes $S_{7,7}$ that is impossible since $S_{7,7}$ is not Laplacian realizable, see Section 5 for references and explanations. Consequently, the lower bound in (17) is is not achieved for odd $n \geqslant 7$.

If $n \leqslant 5$ is odd, then the only Laplacian realizable sets are the exceptional ones $S_{2,3}$, $S_{3,3}$, $S_{1,5}$, or $S_{5,5}$, according to Theorem 2.5. However, some known results [17] on Conjecture 2.6 give us that $S_{3,3}$ and $S_{5,5}$ are not Laplacian realizable, see Proposition 2.5.

Now (15) shows that if G realizes $S_{2,3}$, then

$$LE(G) = \frac{10}{3} < 4 = LE\left(K_3\right),$$

and if G realizes $S_{1,5}$, then

$$LE(G) = \frac{36}{5} < 8 = LE(K_5).$$

Therefore, for graphs realizing $S_{2,3}$ and $S_{1,5}$ the lower bound in (17) does not hold. □

3.2 L-equienergetic graphs realizing $S_{i,n}$

In the present section, we count the number of L-equienergetic graphs realizing $S_{i,n}$ (see Definition 2.9). From Theorems 2.5, 3.5, and 3.7, for odd n there are no L-equienergetic graphs realizing $S_{i,n}$, so in this section, we set n to be *even*.

Theorem 3.10. *Let n be an even number. There exist exactly $\left\lfloor \frac{n-2}{4} \right\rfloor$ pairs of L-equienergetic graphs realizing $S_{i,n}$.*

Proof. Let $n = 4m$. Then from (12) it follows that if G_1 and G_2 realize the sets $S_{2l,4m}$ and $S_{4m-2l,4m}$, respectively, then $LE(G_1) = LE(G_2)$ for $l = 1, \dots, m-1$.

Analogously, if $n = 4m-2$, and if G_1 and G_2 realize the sets $S_{2l-1,4m-2}$ and $S_{4m-2l-1,4m-2}$, respectively, then $LE(G_1) = LE(G_2)$ for $l = 1, \dots, m-1$.

Thus, we get that if n is even ($4m$ or $4m-2$), then there are exactly

$$m - 1 = \left\lfloor \frac{n-2}{4} \right\rfloor$$

pairs of L-equienergetic graphs realizing $S_{i,n}$, as required. □

Remark 3.11. Note that if n is even, and if graphs G_1 and G_2 realize $S_{i,n}$ and $S_{k,n}$, respectively, then G_1 and G_2 are L-equienergetic if and only if $i+k = n$. Additionally, (3) implies that in this case

$$\overline{a}(G_1) + \overline{a}(G_2) = \frac{n+1}{2} - \frac{i}{n} + \frac{n+1}{2} - \frac{n-i}{n} = n.$$

4 The first Zagreb index for $S_{i,n}$ realizable graph

In this section, we find the first Zagreb index $M_1(G)$ for graphs realizing $S_{i,n}$. We remind the reader that the first Zagreb index is defined by the formula (4).

$$M_1(G) = \sum_{k=1}^{n} d_{v_k}^2 \tag{1}$$

At first, we establish the general form for $M_1(G)$ of graphs realizing $S_{i,n}$.

Theorem 4.1. *Suppose $n \geqslant 2$. If G is a graph of order n realizing $S_{i,n}$ for certain i, $1 \leqslant i \leqslant n$, then*

$$M_1(G) = \frac{n(n-1)(n+1)}{3} - i(i-1). \tag{2}$$

Before proving this theorem, we remind the reader that the case $i = n$ conjecturally does not exist.

Proof. Given a graph G, its Laplacian eigenvalues satisfy the following well-known relation [36]

$$\mathrm{Tr}(L) = \sum_{k=1}^{n} \mu_k = \sum_{k=1}^{n} d_{v_k} = 2m, \tag{3}$$

where $m = |E(G)|$ is the number of edges (size of G) and $\mathrm{Tr}(L)$ denotes trace of $L(G)$. So we have

$$\mathrm{Tr}\left(L^2\right) = \mathrm{Tr}\left[(D-A)^2\right] = \mathrm{Tr}\left(D^2\right) + \mathrm{Tr}\left(A^2\right) - 2\mathrm{Tr}(DA),$$

where D is the vertex degree diagonal matrix of the graph G, and A is its adjacency matrix. Since $\mathrm{Tr(DA)} = 0$, by (3) we obtain

$$\mathrm{Tr}\left(L^2\right) = \sum_{k=1}^{n} d_{v_k}^2 + 2m = \sum_{k=1}^{n} d_{v_k}^2 + \sum_{k=1}^{n} \mu_k, \tag{4}$$

where m is the size of the graph, and μ_k, $k = 1, \ldots, n$, are the eigenvalues of L. Thus, formulas (1) and (4) imply

$$M_1(G) = \sum_{k=1}^{n} d_{v_k}^2 = \mathrm{Tr}\left(L^2\right) - \sum_{k=1}^{n} \mu_k. \tag{5}$$

If G realizes $S_{i,n}$, than for the trace of the square of the Laplacian matrix of G, we get

$$\operatorname{Tr}\left(L^2\right) = \sum_{k=1}^{n} \mu_k^2 = \sum_{k=0}^{n} k^2 - i^2 = \frac{n(n+1)(2n+1)}{6} - i^2, \tag{6}$$

while the sum of its eigenvalues of $L(G)$ is given by the following formula

$$\sum_{k=1}^{n} \mu_k = \sum_{k=1}^{n} k - i = \frac{n(n+1)}{2} - i. \tag{7}$$

Now from (4)–(7), we obtain (2) for any i, $1 \leqslant i \leqslant n$. $\square$

Remark 4.2. From (2) it is easy to see if G realizes $S_{i,n}$, then its first Zagreb index is an even integer number. Moreover, formula (2) shows that the first Zagreb index of $S_{i,n}$-realizable graphs is a decreasing function of i for a fixed n.

Note that if G realizes $S_{i,n}$ then its Laplacian energy does not exceed its first Zagreb index.

Theorem 4.3. *Let $n \geqslant 2$, and let a graph G of order n realizes $S_{i,n}$. Then the following inequality is true.*

$$LE(G) \leqslant M_1(G). \tag{8}$$

Here the equality holds if and only if $n = 2$ and $i = 1$ (the complete graph K_2).

Proof. Suppose first that n is an even number. Graphs realizing the sets $S_{i,n}$ and $S_{n-i,n}$ are L-equienergetic by (7). Moreover, for graphs realizing $S_{i,n}$ the first Zagreb index is a decreasing function of i for a fixed n whenever $1 \leqslant i \leqslant n$, see Remark 4.2. Consequently, it is sufficient to prove inequality (8) for $i \geqslant \dfrac{n}{2}$.

So, let G realize $S_{i,n}$ for some $i \geqslant \dfrac{n}{2}$. Then according to (7) and (2), we have

$$M_1(G) - LE(G) = \frac{n(n^2-1)}{3} - i(i-1) - \frac{n^2}{4} - n + i =$$

$$= \frac{n(n^2-1)}{3} - \frac{n^2}{4} - n - i^2 + 2i \geqslant$$

$$\geqslant \frac{n(n^2-1)}{3} - \frac{n^2}{4} - n - n^2 + 2n = \frac{n}{12}(4n^2 - 15n + 8) > 0$$

for any $n \geqslant 4$. Thus, we have

$$M_1(G) - LE(G) > 0$$

whenever $n \geqslant 4$ and $i \geqslant \dfrac{n}{2}$, if G realizes $S_{i,n}$. So, strict inequality (8) holds for even $n \geqslant 4$.

If $n = 2$, then by Theorem 2.5 the only graph realizing $S_{i,2}$ is K_2 realizing $S_{1,2}$, and from (7) and (2) we have

$$LE(K_2) = M_1(K_2) = 2,$$

as required.

Assume now that n is odd. We remind the reader that sets $S_{i,n}$ are Laplacian realizable not for all i, $1 \leqslant i \leqslant n$, according to Theorem 2.5. However, we prove that inequality (8) is true for any i, even if $S_{i,n}$ is not Laplacian realizable.

From (15) it follows that graphs realizing $S_{i,n}$ and $S_{n-i,n}$ are L-equienergetic. Moreover, the first Zagreb index of graphs realizing $S_{i,n}$ is a decreasing function of i whenever $1 \leqslant i \leqslant n$. Thus, it is enough to consider $\dfrac{n+1}{2} \leqslant i \leqslant n$.

So for a graph G realizing $S_{i,n}$, we have

$$M_1(G) - LE(G) = \frac{n(n^2-1)}{3} - i(i-1) - (n+1)\left(\frac{n+3}{4} - \frac{i}{n}\right) =$$

$$= \frac{(n+1)(4n^2-7n+9)}{12} - i^2 + \left(2 + \frac{1}{n}\right) i \geqslant$$

$$\geqslant \frac{(n+1)(4n^2-7n+9)}{12} - n^2 + 2n + 1 = \frac{(n-1)(n-3)(4n+1)}{12} > 0$$

for any odd $n \geqslant 5$. Thus, we have

$$M_1(G) - LE(G) > 0.$$

whenever $n \geqslant 5$ and $i \geqslant \dfrac{n+1}{2}$ if G realizes $S_{i,n}$. Consequently, strict inequality (8) holds for odd $n \geqslant 5$.

If now $n = 3$, then Theorem 2.5 states that the only graph realizing $S_{i,3}$ is $K_{1,2}$ (complete bipartite graph) which realizes $S_{2,3}$, and from (15) and (2) we have

$$\frac{10}{3} = LE(K_{1,2}) < M_1(K_{1,2}) = 6.$$

Thus, in (8) equality holds if and only if $n = 2$ and $i = 1$. $\square$

Remark 4.4. It is interesting to compare the upper bound (2) with (8) which does not depend on the number of edges. We postpone such a comparison for another project.

Finally, we find first Zagreb index for the complements of graphs realizing $S_{i,n}$.

Theorem 4.5. *Let a graph G realize $S_{i,n}$, $n \geqslant 2$. Then the first Zagreb index of its complement $\overline{G}$ is given by the following formula.*

$$M_1\left(\overline{G}\right) = \frac{n(n-1)(n-5)}{3} + i(2n-i-1). \tag{9}$$

Proof. Indeed, from Theorem 2.14, it follows that

$$M_1(\overline{G}) = M_1(G) + n(n-1)^2 - 4m(n-1),$$

where m is the size of the graph G. Now (3) and (7) imply

$$2m = \frac{n(n+1)}{2} - i,$$

so from (2) one has

$$\begin{aligned} M_1\left(\overline{G}\right) = \frac{n(n-1)(n+1)}{3} - i(i-1) + \\ + n(n-1)^2 - 2(n-1)\left(\frac{n(n+1)}{2} - i\right). \end{aligned} \tag{10}$$

Simplifying (10) we get (9), as required. □

Remark 4.6. From (9) it is easy to see that the first Zagreb index of the complement of the graph G realizing $S_{i,n}$ is even integer. Moreover, Theorem 4.5 shows that the first Zagreb index of the complement of graphs realizing $S_{i,n}$ is an increasing function of i for a fixed n whenever $i = 1, \ldots, n$.

5 The $S_{n,n}$-conjecture and properties of graphs realizing $S_{n,n}$

In the present section, we briefly survey known necessary conditions for graphs to realize the set $S_{n,n}$ and provide a couple of new observation on the graph realizing $S_{n,n}$.

As we mentioned in Section 2, in the work [17] it was conjectured that the spectrum $S_{n,n}$ is not Laplacian realizable for any $n \geqslant 2$. In that paper the authors observed a few simple facts.

Proposition 5.1 ([17]). *If G realizes $S_{n,n}$, then the following conditions hold.*

- *The number of edges of G and $\overline{G}$ equals*

$$m = \frac{n(n-1)}{4}; \tag{1}$$

- $n \equiv 0, 1 \mod 4$;
- *n is not a prime number.*

All these facts can be easily established, and we provide their proofs here for completeness. Indeed, (1) follows immediately from the formula (3). Since m must be integer, one gets that if a graph G of order n realizes $S_{n,n}$, then $n = 0$ or $1 \mod 4$.

Additionally, from (1) we have that the number of spanning trees of a graph realizing $S_{n,n}$ is given by the following formula

$$\frac{(n-1)!}{n}.$$

Since this number must be integer, we obtain that n cannot be prime whenever the given graph realizes $S_{n,n}$.

In [41], the authors proved that if graph realizing $S_{n,n}$ exists it must have diameter at most 6. Recently, this result was improved by K.C. Das, S.G. Lee, and G.S. Cheon [10] who showed that if G realizes $S_{n,n}$, then both graphs G and $\overline{G}$ must have diameter 3.

Additionally, in [17] and [21] the following facts were established.

Proposition 5.2. *If a graph G of order n realizes $S_{n,n}$, then*

- $2 \leqslant \delta \leqslant \Delta \leqslant n-3$, *where δ and Δ are the minimum and maximum vertex degree of the graph G, respectively;*
- $12 \leqslant n \leqslant 6,649,688,932$.

Moreover, Theorem 2.1 implies the following.

Proposition 5.3. *A graph G of order n realizes $S_{n,n}$ if and only if its complement $\overline{G}$ realizes $S_{n,n}$.*

From (2) and (9) it follows that if a graph G realizes $S_{n,n}$, then

$$M_1(G) = M_1\left(\overline{G}\right) = \frac{n(n-1)(n-2)}{3}.$$

In fact, the formula for $M_1(G)$ was found in [17], as well, but the authors did not mention Zagreb indices in that paper.

At the same time, in [2] it was proved that $M_1(G)$ and $M_1(\overline{G})$ are equal if and only if G and $\overline{G}$ have the same number of edges, so we have

$$e\left(\overline{G}\right) = e(K_n) - e(G) = \frac{n(n-1)}{4},$$

where

$$e(K_n) = \frac{n(n-1)}{2}.$$

is the number of edges of the complete graph K_n.

It is clear [20, p. 107] that the necessary condition for a graph G to be self-complementary, i.e., $G \cong \overline{G}$ (G is isomorphic to $\overline{G}$), is that the number of edges of the graph G is equal the half of the edges of the complete graph K_n. This fact suggests considering the self-complement graphs as potential candidates to realize $S_{n,n}$. However, calculations show that self-complementary graphs of order up to 12 (inclusive) do not realize $S_{n,n}$. On the base of these calculations we conjecture the following.

Conjecture 5.4. *Any Laplacian integral self-complementary graph has at least one multiple eigenvalue.*

In other word, we conjecture that $S_{n,n}$-realizable graph are *not* self-complementary (if exist).

At the end of this section, we establish one more simple fact about graphs that can potentially realize $S_{n,n}$. This fact is related to one more operation on graphs called the Cartesian product (see, e.g., [36] and references there).

Definition 5.5. The *Cartesian product* of the graphs G_1 and G_2 denoted by $G_1 \times G_2$ having vertex set is the cartesian product $V(G_1) \times V(G_2)$. Suppose $v_1, v_2 \in V(G_1)$ and $u_1, u_2 \in V(G_2)$, then the vertices (v_1, u_1) and (v_2, u_2) of $G_1 \times G_2$ are adjacent if and only if one of the following conditions holds

- $v_1 = v_2$ and $u_1 u_2 \in E(G_2)$;
- $u_1 = u_2$ and $v_1 v_2 \in E(G_1)$.

The Laplacian spectrum of graph Cartesian product is given by the following theorem, see, e.g., [36].

Theorem 5.6. *Let G_1 and G_2 be graphs with Laplacian spectra $S_L(G_1) = \{\lambda_1, \lambda_2, \ldots, \lambda_{n-1}, \lambda_n\}$ and $S_L(G_2) = \{\mu_1, \mu_2, \ldots, \mu_{m-1}, \mu_m\}$. Then*

$$S_L(G_1 \times G_2) = \{\lambda_i + \mu_k, 1 \leqslant i \leqslant n, 1 \leqslant k \leqslant m\}.$$

Now for graphs realizing the set $S_{n,n}$ we have the following fact.

Proposition 5.7. *If G realizes $S_{n,n}$, then G is not a Cartesian product of graphs.*

Proof. If $G = G_1 \times G_2$ and G realizes $S_{n,n}$, then the Laplacian spectra of graphs G_1 and G_2 do not contain multiple eigenvalues, since the set $S_{n,n}$ does not contain repeated numbers, and since the Laplacian eigenvalues of both graphs G_1 and G_2 belong to the Laplacian spectrum of G according to Theorem 5.6.

So, if $G = G_1 \times G_2$ and G realizes $S_{n,n}$, then G_1 realizes some set

$$S_{l,m} = \{0, 1, 2, \ldots, l-1, l+1, \ldots, m-1, m\},$$

and G_2 realizes some set

$$S_{p,q} = \{0, 1, 2, \ldots, p-1, p+1, \ldots, q-1, q\}.$$

By Theorem 5.6, the Laplacian spectrum contains the eigenvalue $(l-1)+(p+1) = p+l$ and the eigenvalue $(l+1)+(p-1) = p+l$, that is, the eigenvalue $p+l$ is of multiplicity at least 2. We get a contradiction, since the set $S_{n,n}$ does not contain repeated numbers. □

6 Conclusion and open problems

In this work, we found the Laplacian energy and the first Zagreb index for the graphs whose Laplacian spectrum is of the form $\{0, 1, \ldots, i-1, i+1, \ldots, n\}$ for some i, $1 \leqslant i \leqslant n-1$. We also gave lower and upper bounds for the Laplacian energy and a relation between the first Zagreb index and the Laplacian energy of graphs realizing $S_{i,n}$. Additionally, we discuss some aspects of the $S_{n,n}$-conjecture, Conjecture 2.6, stating that graphs realizing $S_{n,n}$ do not exist. Finally, we proved that if a graph realizes $S_{n,n}$, then it is not a Cartesian product of two graphs.

Together with the first Zagreb index of graphs realizing $S_{i,n}$ we tried to find the second Zagreb index. Unfortunately, we were unable to find an explicit formula for the second Zagreb index of graphs realizing $S_{i,n}$. We suppose that it should be a rational function of i and n. Some values of the second Zagreb index of graphs realizing $S_{i,n}$ are represented in Table 1.

Table 1. Second Zagreb index of graphs realizing $S_{i,n}$

Second Zagreb index $M_2(G)$									
$i\backslash n$	1	2	3	4	5	6	7	8	9
1		1			57	120			623
2			4	19			224	389	
3					44	106			619
4							192	354	
5						71			560
6							141	290	
7									474
8									
9									

Thus, we would like to pose the following problem.

Problem 1. Find the formula for the second Zagreb index of graphs realizing $S_{i,n}$.

One more problem we are interesting in is stated in Conjecture 5.4. If this conjecture is true, then graphs realizing $S_{n,n}$ are not self-complementary. However, if such graphs do not exist, then Conjecture 5.4 is true. For instance, it is true for $n < 12$ and $n > 6,649,688,932$ according to Proposition 5.2.

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