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Applications of a theorem by Ky Fan in the theory of Laplacian energy of graphs

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Abstract

The Laplacian energy of a graph G is equal to the sum of distances of the Laplacian eigenvalues to their average, which in turn is equal to the sum of singular values of a shift of Laplacian matrix of G. Let X, Y, and Z be matrices, such that Z = X + Y. Ky Fan has established an inequality between the sum of singular values of Z and the sum of the sum of singular values of X and Y respectively. We apply this inequality to obtain new results in the theory of Laplacian energy of a graph.

1 Preliminaries

Let $G = (V, \overline{E})$ be a simple graph, with nonempty vertex set $V = \{v_1, \ldots, v_n\}$ and edge set $\overline{E} = \{e_1, \ldots, e_m\}$. That is to say, G is a simple (n, m)-graph. For any of these graphs $d_1 \ge d_2 \ge \ldots \ge d_n$ corresponds to its vertex degree sequence. In particular $\Delta(G)$ stands for the largest vertex degree of G. The diagonal matrix of order n whose (i, i)-entry is d_i is the diagonal

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vertex degree matrix of G and is denoted by D(G). The (0, 1)-adjacency matrix $A(G) = (a_{ij})$ is defined by $a_{ij} = 1$ if, and only if, vertices *i* and *j* are connected. Its eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ form the spectrum of G. The matrix L(G) = D(G) - A(G) is the Laplacian matrix of G. The Laplacian spectrum of G corresponds to eigenvalues $\mu_1, \mu_2, \ldots, \mu_n$ of L(G). It is well known that for bipartite graphs, Laplacian matrix and the signless Laplacian matrix Q(G) = A(G) + D(G) have equal spectra [2].

The notion of the energy E(G) of an (n, m)-graph G was introduced by Gutman in connection with the π -molecular energy (cf. [8, 9, 11, 14]). It is defined by

$$E\left(G\right) = \sum_{j=1}^{n} \left|\lambda_{j}\right|$$

whereas the Laplacian energy LE(G) of an (n, m)-graph G (cf. [1, 4, 10, 12, 21]) is defined by

$$LE(G) = \sum_{j=1}^{n} \left| \mu_j - (2m/n) \right| .$$
 (1)

The concept of matrix energy [16] was established by analogy with graph energy. For a matrix C, with singular values $s_1(C), s_2(C), \ldots$ its energy $\mathcal{E}(C)$ is equal to $s_1(C) + s_2(C) + \cdots$. Consequently, if $C \in \mathbb{R}^{n \times n}$ is symmetric with eigenvalues $\lambda_1(C), \lambda_2(C), \ldots, \lambda_n(C)$ its energy is given by

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

Let $s \in \mathbb{N}$. Denote by I_s the corresponding identity matrix of order s. Evidently the energy of any graph G is the energy of its adjacency matrix and its Laplacian energy is provided by

$$LE(G) = \mathcal{E}\left(L(G) - \frac{2m}{n}I_n\right).$$
 (2)

The following results are already known.

Theorem 1 Let A and B be two real square matrices of order n and let C = A + B. Then

$$\mathcal{E}(C) \le \mathcal{E}(A) + \mathcal{E}(B).$$
(3)

Moreover equality holds if, and only if, there exists an orthogonal matrix P such that PA and PB are both positive semidefinite matrices.

Lemma 2 ([3]) If $A = (a_{ij})_{i,j=1}^n$ is a positive semidefinite matrix and $a_{ii} = 0$ for some *i*, then $a_{ij} = 0 = a_{ji}, j = 1, 2, ..., n$.

Theorem 1 was obtained by Ky Fan [5] using a variational principle. It also appears in Gohberg and Krein [7] and in Horn and Johnson [13]. No equality case is discussed in these references. Thompson [19, 20] employs polar decomposition theorem and inequalities due to Fan and Hoffman [6] to obtain its equality case. Day and So [3] give the details of a proof for the inequality and the case of equality.

For a matrix A, define $|A| \triangleq (A^T A)^{1/2}$. Here we present the following version of the polar decomposition theorem.

Theorem 3 ([15]) Let $A \in \mathbb{R}^{n \times n}$. Then there exist positive semidefinite matrices $X, Y \in \mathbb{R}^{n \times n}$ and orthogonal matrices $P, F \in \mathbb{R}^{n \times n}$ such that A = PX = YF. Moreover, the matrices X, Y are unique, $X = |A|, Y = (AA^T)^{1/2}$. The matrices P and F are uniquely determined if and only if A is nonsingular. The aim of this paper is to study cases of equality.

2 Graphs G for which $LE(G) = E(G) + \mathcal{E}(D(G) - (2m/n)I_n)$

Theorem 4 Let G be a connected (n,m)-graph. Then

$$E(G) + \sum_{i=1}^{n} \left| d_i - \frac{2m}{n} \right| \ge LE(G).$$

$$\tag{4}$$

Moreover equality in (4) holds if, and only if, G is a regular graph.

Proof. The inequality in (4) is proved in [17]. If G is a regular graph then the equality in (4) holds (see [12]). Conversely, suppose the equality in (4) holds. In order to obtain a contradiction, we suppose that G is not regular. Therefore

$$\Delta\left(G\right) = d_1 > \frac{2m}{n} \ . \tag{5}$$

For i = 1, ..., n, let $a_i \triangleq d_i - (2m/n)$. We have $a_1 > 0$, via (5). Bearing in mind that $L(G) - (2m/n)I_n = D(G) - (2m/n)I_n - A(G)$ and the equality in (4), we see that Theorem 1 asserts that there exists an orthogonal matrix P such that $X = P(D - (2m/n)I_n)$ and Y = P(-A(G)) are both positive semidefinite. Hence $P^T X$ and $P^T Y$ are polar decompositions of the matrices $D - \frac{2m}{n}I_n$ and -A(G), respectively. Here, using Theorem 3 we obtain $X = |D - \frac{2m}{n}I_n|$ and Y = |A(G)|. Therefore $X = |D - \frac{2m}{n}I_n|$

 $diag(|a_1|, |a_2|, \ldots, |a_n|)$. Setting

$$P^{T} = \begin{pmatrix} q_{11} & \dots & q_{1n} \\ \vdots & \ddots & \vdots \\ q_{n1} & \dots & q_{nn} \end{pmatrix} \text{ and } A(G) = \begin{pmatrix} 0 & a_{12} & \dots & a_{1n} \\ a_{12} & 0 & \ddots & a_{2n} \\ \vdots & \ddots & \ddots & \vdots \\ a_{1n} & a_{2n} & \dots & 0 \end{pmatrix},$$

 $P^T X = D - (2m/n)I_n$, implies

$$\begin{pmatrix} q_{11} & \dots & q_{1n} \\ \vdots & \ddots & \vdots \\ q_{n1} & \dots & q_{nn} \end{pmatrix} \begin{pmatrix} |a_1| & & \\ & \ddots & \\ & & |a_n| \end{pmatrix} = \begin{pmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{pmatrix}.$$

Then,

$$\begin{pmatrix} |a_1| q_{11} & |a_2| q_{12} & \dots & |a_n| q_{1n} \\ |a_1| q_{21} & |a_2| q_{22} & & |a_n| q_{2n} \\ \vdots & \ddots & \vdots \\ |a_1| q_{n1} & |a_2| q_{n2} & \dots & |a_n| q_{nn} \end{pmatrix} = \begin{pmatrix} a_1 & & & \\ & a_2 & & \\ & & \ddots & \\ & & & a_n \end{pmatrix}$$

Equality at first column imposes $q_{11} = 1$ and, $q_{i1} = 0, i = 2, \dots, n$. It follows that

$$P = \begin{pmatrix} 1 & 0 & \dots & 0 \\ q_{12} & \dots & q_{n2} \\ \vdots & & \ddots & \vdots \\ q_{1n} & \dots & q_{nn} \end{pmatrix}.$$

We must then have

$$Y = -\begin{pmatrix} 1 & 0 & \dots & 0 \\ q_{12} & \dots & q_{n2} \\ \vdots & \ddots & \vdots \\ q_{1n} & \dots & q_{nn} \end{pmatrix} \begin{pmatrix} 0 & a_{12} & \dots & a_{1n} \\ a_{12} & 0 & \ddots & a_{2n} \\ \vdots & \ddots & \ddots & \vdots \\ a_{1n} & a_{2n} & \dots & 0 \end{pmatrix}$$
$$= -\begin{pmatrix} 0 & a_{12} & \dots & a_{1n} \\ * & \dots & * \\ \vdots & \ddots & \vdots \\ * & \dots & * \end{pmatrix}.$$

The previous matrix is positive semidefinite and by Lemma 2, we obtain $a_{1j} = 0, j = 2, ..., n$. This contradicts our assumption that G is a connected graph and the result follows.

3 Graphs G for which LE(G) = E(G)

Gutman and Zhou [12] showed that if G is a regular graph then

$$LE(G) = E(G) . (6)$$

In particular, if G is bipartite and regular, then the equality (6) holds. In this section we give conditions for the converse:

Theorem 5 Let G be a bipartite graph. Then the equality (6) holds if, and only if, G is a regular graph.

Proof. Let G be a regular graph. We must then have (6) [12]. Conversely, suppose the equality (6) holds. From definition of Laplacian and signless Laplacian matrices it is clear that

$$\left(Q(G) - \frac{2m}{n}I_n\right) - \left(L(G) - \frac{2m}{n}I_n\right) = 2A(G).$$
⁽⁷⁾

Therefore,

$$\mathcal{E}\left(Q(G) - \frac{2m}{n}I_n - \left(L(G) - \frac{2m}{n}I_n\right)\right) = 2\mathcal{E}\left(A(G)\right)$$
$$= E(G) + E(G)$$
$$= LE(G) + LE(G) .$$

Bearing in mind that G is bipartite we obtain

$$\mathcal{E}\left(Q(G) - \frac{2m}{n}I_n - \left(L(G) - \frac{2m}{n}I_n\right)\right)$$
$$= \mathcal{E}\left(Q(G) - \frac{2m}{n}I_n\right) + \mathcal{E}\left(-\left(L(G) - \frac{2m}{n}I_n\right)\right) . \tag{8}$$

Therefore, Theorem 1 asserts that there exists an orthogonal matrix \boldsymbol{P} , such that

$$X = P\left(Q(G) - \frac{2m}{n}I_n\right) \quad \text{and} \quad Y = P\left(-\left(L(G) - \frac{2m}{n}I_n\right)\right) \tag{9}$$

are both positive semidefinite matrices. Hence $P^T X$ and $P^T Y$ are polar decompositions of

$$Q(G) - \frac{2m}{n}I_n$$
 and $-\left(L(G) - \frac{2m}{n}I_n\right)$

respectively. By Theorem 3 we obtain

$$X = \left| Q(G) - \frac{2m}{n} I_n \right|$$
 and $Y = \left| L(G) - \frac{2m}{n} I_n \right|$.

In view of the fact that G is bipartite, we conclude that X = Y. By using Eq. (9) we arrive at

$$Q(G) + L(G) = \frac{4m}{n} I_n$$

which implies the result. \blacksquare

4 A new upper bound on LE(G)

We shall be considering G with nonempty edge set \overline{E} . Let u, v be two vertices of G. The Laplacian matrix of the graph G(u, v) with n vertices and just one - 544 -

edge between vertices u and v, is determined via

$$L(G(u,v))_{i,j} = \begin{cases} 1 & \text{if } (i,j) = (u,u) \text{ or } (i,j) = (v,v) \\ -1 & \text{if } (i,j) = (u,v) \text{ or } (i,j) = (v,u) \\ 0 & \text{ otherwise.} \end{cases}$$

Spielman [18] expresses the Laplacian matrix of G in terms of L(G(u, v)) by

$$L(G) = \sum_{(u,v)\in\overline{E}} L(G(u,v)) \quad . \tag{10}$$

We consider $\alpha \in \mathbb{R}$. The energy $\mathcal{E}(L(G(u, v)) - \alpha I_n)$ can be computed directly as:

$$\mathcal{E}\left(L\left(G(u,v)\right) - \alpha I_n\right) = (n-1)\left|\alpha\right| + \left|2 - \alpha\right| \quad . \tag{11}$$

On the other hand, for 0 < a < 1, let A, Q, P, and D be the following matrices:

$$A = \begin{bmatrix} a & -1 \\ -1 & a \end{bmatrix}, Q = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}, P = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}, D = \begin{bmatrix} a-1 & 0 \\ 0 & a+1 \end{bmatrix}$$

The proof of the next result is a matter of straightforward computation, and depends on the spectrum of A.

Lemma 6 Let A, Q, P and D be as above. Then $A = QDQ^{-1}$. Moreover A = P |A|.

As an immediate consequence we have $|A| = Q |D| Q^{-1}$.

Theorem 7 Let G be an (n,m)-graph. Then

$$LE(G) \le 4m\left(1 - \frac{1}{n}\right). \tag{12}$$

Equality holds if, and only if, $\overline{E} = \emptyset$ or G is the union of one edge and n-2 isolated vertices.

Proof. The description of L(G) in (10) makes the next equality evident, that is:

$$L(G) - \frac{2m}{n} I_n = \sum_{(u,v)\in\overline{E}(G)} \left(L(G(u,v)) - \frac{2}{n} I_n \right).$$
(13)

The inequality in (12) is a consequence of Eqs. (2), (13), Theorem 1 and Eq. (11), by changing α to 2/n. On the equality case in (12), it is easily checked that (12) is an equality in the cases considered in the statement. Conversely, suppose that we have equality in (12), $\overline{E} \neq \emptyset$ and $m \geq 2$. Consider $\overline{E} = \{e_1, e_2, \ldots e_m\}$ where $e_i = \{u_i, v_i\}, i = 1, \ldots, m$. Thus, the next equality is implied by equality in (12), (13) and (11).

$$\mathcal{E}\left(L\left(G\right) - \frac{2m}{n}I_{n}\right) = \sum_{i=1}^{m} \mathcal{E}\left(L\left(G(e_{i})\right) - \frac{2}{n}I_{n}\right).$$
 (14)

Using (13) and Theorem 1 we obtain

$$\mathcal{\mathcal{E}}\left(L\left(G\right) - \frac{2m}{n}I_{n}\right) \leq \mathcal{\mathcal{E}}\left(L\left(G(e_{1})\right) - \frac{2}{n}I_{n}\right) + \mathcal{\mathcal{E}}\left(\sum_{i=2}^{m}\left(L\left(G(e_{i})\right) - \frac{2}{n}I_{n}\right)\right).$$
 (15)

Replacing (14) into (15) and apply Theorem 1 to obtain

$$\mathcal{E}\left(\sum_{i=2}^{m} \left(L\left(G(e_i)\right) - \frac{2}{n}I_n\right)\right) = \sum_{i=2}^{m} \mathcal{E}\left(L\left(G(e_i)\right) - \frac{2}{n}I_n\right).$$
 (16)

By the same kind of reasoning, but this time considering (16) rather than (14), we obtain

$$\mathcal{E}\left(\sum_{i=3}^{m} \left(L\left(G(e_i)\right) - \frac{2}{n}I_n\right)\right) = \sum_{i=3}^{m} \mathcal{E}\left(L\left(G(e_i)\right) - \frac{2}{n}I_n\right).$$

Using a reasoning analogous to that above, we arrive at

$$\mathcal{E}\left(\left(L\left(G(e_m)\right) - \frac{2}{n}I_n\right) + \left(L\left(G(e_{m-1})\right) - \frac{2}{n}I_n\right)\right)$$
$$= \mathcal{E}\left(L\left(G(e_m)\right) - \frac{2}{n}I_n\right) + \mathcal{E}\left(L\left(G(e_{m-1})\right) - \frac{2}{n}I_n\right).$$
(17)

Invoking again Theorem 1, there exists an orthogonal matrix P such that

$$X = P\left(L\left(G(e_m)\right) - \frac{2}{n}I_n\right) \quad \text{and} \quad Y = P\left(L\left(G(e_{m-1})\right) - \frac{2}{n}I_n\right) \quad (18)$$

are positive semidefinite matrices. Hence $P^T X$ and $P^T Y$ are polar decompositions of nonsingular matrices $L(G(e_m)) - \frac{2}{n}I_n$ and $L(G(e_{m-1})) - \frac{2}{n}I_n$ respectively. By Theorem 3 we conclude that

$$X = \left| L\left(G(e_m)\right) - \frac{2}{n} I_n \right| \qquad \text{and} \qquad Y = \left| L\left(G(e_{m-1})\right) - \frac{2}{n} I_n \right| \ .$$

As

$$L(G(e_m)) - \frac{2}{n}I_n$$
 and $L(G(e_{m-1})) - \frac{2}{n}I_n$

are invertible matrices, P is the unique orthogonal matrix for which (18) is true. Let b = 1 - 2/n. Then the matrix $L(G(e_m)) - \frac{2}{n}I_n$ can be expressed as

$$\begin{pmatrix} -\frac{2}{n} & 0 & \dots & & 0 \\ & \ddots & & & & \\ 0 & b & \dots & 0 & -1 & \vdots \\ \vdots & 0 & -\frac{2}{n} & \vdots & & \\ & \vdots & \ddots & 0 & & \\ 0 & -1 & 0 & \dots & b & & \\ & & & & \ddots & \\ 0 & \dots & 0 & & -\frac{2}{n} \end{pmatrix}$$

By relatively straightforward means one can show that

$$L\left(G(e_m)\right) - \frac{2}{n}I_n = F_m B F_m^T \tag{19}$$

with F_m denoting a particular permutation matrix and B is the nonsingular matrix

$$\begin{pmatrix} b & -1 & \dots & & 0 \\ -1 & b & \dots & & \vdots \\ \vdots & 0 & -\frac{2}{n} & \vdots & \\ \vdots & & \ddots & 0 \\ & & & \dots \\ 0 & \dots & & 0 & -\frac{2}{n} \end{pmatrix}$$

Now let Q be the matrix

By Lemma 6 and Theorem 3 we conclude that Q is the unique orthogonal matrix for which

$$B = Q |B| \quad . \tag{20}$$

Therefore, Eq. (19) implies

$$\left| L\left(G(e_m)\right) - \frac{2}{n} I_n \right| = F_m \left| B \right| F_m^T = F_m Q^{-1} B F_m^T .$$
(21)

Now we can replace (19) and (21) in

$$L(G(e_m)) - \frac{2}{n}I_n = P^T \left| L(G(e_m)) - \frac{2}{n}I_n \right|$$

to obtain

$$F_m Q F_m^T = P^T \; .$$

Then $P = F_m Q F_m^T$ is the unique orthogonal matrix such that

$$P\left(L\left(G(e_m)\right) - \frac{2}{n}I_n\right)$$

is positive definite and it is depending of edge e_m . We see that this contradicts to the requirement that

$$Y = P\left(L\left(G(e_{m-1})\right) - \frac{2}{n}I_n\right)$$

is a positive definite matrix. This proves the assertion. \blacksquare

5 An upper bound on the Laplacian energy for the union of graphs

Here and throughout this section, \bigoplus denotes the block matrix direct sum [13].

Theorem 8 Let $k \in \mathbb{N}$. Let $\{G_i\}_{i=1}^k$ be a collection of $k, (n_i, m_i)$ -graphs, $i = 1, \ldots, k$. Consider $G = G_1 \cup G_2 \cup \ldots \cup G_k$ so that $n = \sum_{i=1}^k n_i$ is the order of G and $m = \sum_{i=1}^k m_i$ is the size of G. Then

$$LE(G) \le \sum_{i=1}^{k} LE(G_i) + \sum_{i=1}^{k} \left| \frac{2m_i}{n_i} - \frac{2m}{n} \right| n_i.$$
 (22)

Equality holds if, and only if, $2m_i/n_i = 2m/n$ for all $i = 1, \ldots, k$.

Proof. The following equality follows immediately from the statement,

$$\frac{2m}{n} = \left(1/\sum_{j=1}^{k} n_j\right) \left(\sum_{i=1}^{k} 2m_i\right) = \sum_{i=1}^{k} \frac{2m_i}{n_i} \left(n_i/\sum_{j=1}^{k} n_j\right) .$$
(23)

In other words 2m/n is a convex combination of $2m_i/n_i$, i = 1, ..., k.

In order to simplify the writing and omit some subscripts, we take $I_{n_i}\equiv I_i$ and $2m_i/n_i-2m/n\equiv b_i$. It is clear that

$$L(G) - \frac{2m}{n} I_n = \bigoplus_{i=1}^k \left(L(G_i) - \frac{2m}{n} I_i \right)$$
$$= \bigoplus_{i=1}^k \left(L(G_i) - \frac{2m_i}{n_i} I_i \right) + \bigoplus_{i=1}^k b_i I_i$$

Therefore, as a consequence of Eq. (2) and Theorem 1, the inequality in (22) follows. On the equality case, the condition is sufficient [12]. Conversely we suppose the equality in (22) is true and suppose that, the equalities $2m_i/n_i = 2m/n$ for all i = 1, ..., k, fail. Therefore, by (23) there exists ℓ such that $2m_\ell/n_\ell > 2m/n$. We can assume that $\ell = 1$. As a consequence of Theorem 1 and equality in (22), there exists an orthogonal matrix P such that

$$X = P \bigoplus_{i=1}^{k} \left(L(G_i) - \frac{2m_i}{n_i} I_i \right) \quad \text{and} \quad Y = P \bigoplus_{i=1}^{k} b_i I_i$$

are both positive semidefinite. Hence $P^T X$ and $P^T Y$ are polar decompositions of the matrices

$$\bigoplus_{i=1}^{k} \left(L(G_i) - \frac{2m_i}{n_i} I_i \right) \quad \text{and} \quad \bigoplus_{i=1}^{k} b_i I_i$$

respectively. By Theorem 3, we arrive at $Y = \bigoplus_{i=1}^{k} |b_i| I_i$. Thus

$$\bigoplus_{i=1}^{k} |b_i| I_i = P \bigoplus_{i=1}^{k} b_i I_i .$$

$$(24)$$

We can write the orthogonal matrix P as

$$P = \begin{pmatrix} P_{11} & P_{12} & \dots & P_{1k} \\ P_{21} & P_{22} & \dots & P_{2k} \\ \vdots & & \ddots & \vdots \\ P_{k1} & \dots & & P_{kk} \end{pmatrix},$$
(25)

with the diagonal matrices P_{jj} , j = 1, ..., k, of order n_j respectively. From (24) we have

$$\begin{pmatrix} |b_1| I_1 & 0 & \dots & 0 \\ 0 & |b_2| I_2 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \dots & 0 & |b_k| I_k \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & \dots & P_{1k} \\ P_{21} & P_{22} & \dots & P_{2k} \\ \vdots & & \ddots & \vdots \\ P_{k1} & \dots & P_{kk} \end{pmatrix} \begin{pmatrix} b_1 I_1 & 0 & \dots & 0 \\ 0 & b_2 I_2 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \dots & 0 & b_k I_k \end{pmatrix}$$

and then

$$\begin{pmatrix} |b_1| I_1 & 0 & \dots & 0\\ 0 & |b_2| I_2 & \dots & 0\\ \vdots & & \ddots & \vdots\\ 0 & \dots & 0 & |b_k| I_k \end{pmatrix} = \begin{pmatrix} b_1 P_{11} & P_{12} & \dots & P_{1k}\\ b_1 P_{21} & P_{22} & \dots & P_{2k}\\ \vdots & & \ddots & \vdots\\ b_1 P_{k1} & \dots & P_{kk} \end{pmatrix}.$$
 (26)

As $b_1 = 2m_1/n_1 - 2m/n > 0$, via (26) we obtain $P_{11} = I_1$ and $P_{j1} = 0$, j = 2, ..., k. Substituting these P_{j1} into (25) and then replacing the matrix P in the equality $X = P \bigoplus_{i=1}^{k} (L(G_i) - (2m_i/n_i)I_i)$, we conclude that $L(G_1) - (2m_1/n_1)I_1$ is a positive semidefinite matrix. Now we have the required contradiction since

$$-\frac{2m_1}{n_1} \in \sigma\left(L(G_1) - \frac{2m_1}{n_1} I_1\right) \;.$$

Hence the assertion follows. \blacksquare

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