Laplacian Energy of a Graph with Self-Loops

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Abstract

The purpose of this paper is to extend the concept of Laplacian energy from simple graph to a graph with self-loops. Let G be a simple graph of order n, size m and G_S is the graph obtained from G by adding σ self-loops. We define Laplacian energy of G_S as $LE(G_S) = \sum_{i=1}^{n} |\mu_i(G_S) - \frac{2m+\sigma}{n}|$ where $\mu_1(G_S), \mu_2(G_S), \ldots, \mu_n(G_S)$ are eigenvalues of the Laplacian matrix of G_S . In this paper some basic proprties of Laplacian eigenvalues and bounds for Laplacian energy of G_S are investigated. This paper is limited to bounds in analogy with bounds of E(G) and LE(G) but with some significant differences, more sharper bounds can be found.

1 Introduction

Let G = (V, K) be a simple, undirected graph of order n and size m. In 1978, I. Gutman defined the energy [7] of adjacency matrix A(G) as,

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

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where $\lambda_1, \lambda_2, \ldots, \lambda_n$, are the eigenvalues of adjacency matrix A(G).

The matrix L(G) = D(G) - A(G) is the Laplacian matrix and the Laplacian energy LE(G) of G is defined [10] as,

$$LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| \tag{2}$$

where $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of L(G) and $D(G) = diag(d_1, d_2, \ldots, d_n)$ is the diagonal matrix of vertex degrees of a graph G. For more on terminologies we refer [3,4]

Let $S \subseteq V$ with $|S| = \sigma$. A graph with self-loops G_S with vertex set V and edge set $K(G_S)$ is obtained from simple graph G, by attaching a self-loop to each of its vertices belonging to S.

Since graph with self-loops find its application in Chemistry, [8,9,13,14] Gutman et al. defined adjacency matrix $A(G_S)$ [6] of graph G_S in 2021. The matrix $A(G_S)$ is a symmetric matrix of order n whose $(i, j)^{th}$ element is defined as,

$$A(G_S)_{ij} = \begin{cases} 1 & \text{if the vertices } v_i \sim v_j, \\ 0 & \text{if the vertices } v_i \nsim v_j, \\ 1 & \text{if } i = j \text{ and } v_i \in S, \\ 0 & \text{if } i = j \text{ and } v_i \notin S. \end{cases}$$

Then the energy $E(G_S)$ of graph G_S defined as [6],

$$E(G_S) = \sum_{i=1}^{n} \left| \lambda_i(G_S) - \frac{\sigma}{n} \right|.$$
(3)

where $\lambda_1(G_S), \lambda_2(G_S), \ldots, \lambda_n(G_S)$ are the eigenvalues of $A(G_S)$. For more information on energy, Laplacian energy and energy of graph with self-loops, refer [2, 5, 11, 12, 15].

The Laplacian matrix $L(G_S)$ of a graph G_S was defined by B. Acikmese [1] in 2015 as,

$$L(G_S) = L(G) + \sum_{(i,i) \in K(G_S)} e_i e_i^T$$
(4)

Where $L(G) = \sum_{(i,j)\in K(G_S), i\neq j} (e_i - e_j)(e_i - e_j)^T$ and e_i is a vector with its i^{th} entry +1 and the others zeros.

We now rephrase the Laplacian matrix $L(G_S)$ of the graph G_S as a symmetric matrix $L(G_S)$ of order n, whose $(i, j)^{th}$ element is defined as

$$L(G_S)_{ij} = \begin{cases} -1 & \text{if the vertices } v_i \sim v_j, \\ 0 & \text{if the vertices } v_i \approx v_j, \\ d_i + 1 & \text{if } i = j \text{ and } v_i \in S, \\ d_i & \text{if } i = j \text{ and } v_i \notin S. \end{cases}$$

i.e.,

$$L(G_S) = D(G_S) - A(G_S) \tag{5}$$

where $D(G_S) = diag(d_1(G_S), d_2(G_S), \ldots, d_n(G_S))$ is the diagonal matrix of vertex degrees of G_S .

Since $L(G_S)$ is a matrix with non-zero diagonal, similarly as in Eq. (2) and Eq. (3) we now define the Laplacian energy of a graph G_S as

$$LE(G_S) = \sum_{i=1}^{n} \left| \mu_i(G_S) - \frac{2m + \sigma}{n} \right|.$$
(6)

where $\mu_1(G_S), \mu_2(G_S), \ldots, \mu_n(G_S)$ are the eigenvalues of $L(G_S)$.

Let $\gamma_i(G_S) = \mu_i(G_S) - \frac{2m+\sigma}{n}$, i = 1, 2, ..., n denote the auxiliary eigenvalues of $L(G_S)$. Then,

$$LE(G_S) = \sum_{i=1}^{n} |\gamma_i(G_S)|.$$
(7)

In the present paper, we discuss the properties of Laplacian eigenvalues, Laplacian energy and its bounds of graph G_S .

2 Laplacian eigenvalues of G_S

The eigenvalues of L(G) and $A(G_S)$ satisfy the following relation [6, 10]:

$$\sum_{i=1}^{n} \mu_i = 2m; \qquad \sum_{i=1}^{n} \mu_i^2 = 2m + \sum_{i=1}^{n} d_i^2. \tag{8}$$

$$\sum_{i=1}^{n} \lambda_i(G_S) = \sigma; \qquad \sum_{i=1}^{n} \lambda_i^2(G_S) = 2m + \sigma.$$
(9)

Lemma 1. Let G(V, K) be a graph with n vertices and m edges. If $S \subseteq V$ with $|S| = \sigma$, then the eigenvalues $\mu_1(G_S), \mu_2(G_S), \ldots, \mu_n(G_S)$ of $L(G_S)$ satisfy,

1.
$$\sum_{i=1}^{n} \mu_i(G_S) = 2m + \sigma$$

2. $\sum_{i=1}^{n} \mu_i^2(G_S) = 2m + \sigma + \sum_{i=1}^{n} d_i^2(G_S) - 2\sum_{v_i \in S} d_i(G_S)$

where $d_i(G_S), i = 1, 2, ..., n$ denote vertex degree of G_S .

Proof. 1. We have,

$$\sum_{i=1}^{n} \mu_i(G_S) = \sum_{i=1}^{n} [L(G_S)]_{ii}$$
$$= \sum_{i=1}^{n} [D(G_S)]_{ii} - \sum_{i=1}^{n} [A(G_S)]_{ii}$$
$$= 2m + \sigma.$$

2. Also,

$$\sum_{i=1}^{n} \mu_i^2(G_S) = \sum_{i=1}^{n} [L(G_S)^2]_{ii}$$
$$= \sum_{i=1}^{n} [D(G_S) - A(G_S)]_{ii}^2$$
$$= \sum_{i=1}^{n} [D(G_S)^2]_{ii} + \sum_{i=1}^{n} [A(G_S)^2]_{ii} - 2\sum_{i=1}^{n} [D(G_S)A(G_S)]_{ii}$$

$$= \sum_{i=1}^{n} d_i^2(G_S) + 2m + \sigma - 2 \sum_{v_i \in S} d_i(G_S).$$

Lemma 2. Let G(V, K) be a graph with n vertices and m edges. If $S \subseteq V$ with $|S| = \sigma$, then the auxiliary eigenvalues $\gamma_1(G_S), \gamma_2(G_S), \ldots, \gamma_n(G_S)$ of $L(G_S)$ satisfy,

1.
$$\sum_{i=1}^{n} \gamma_i(G_S) = 0$$

2.
$$\sum_{i=1}^{n} \gamma_i^2(G_S) = 2M$$

where $M = m + \frac{1}{2} \sum_{i=1}^{n} \left(d_i(G_S) - \frac{2m + \sigma}{n} \right)^2 + \sigma \left(\frac{1}{2} + \frac{2m + \sigma}{n} \right) - \sum_{v_i \in S} d_i(G_S).$

Proof. 1. We have,

$$\sum_{i=1}^{n} \gamma_i(G_S) = \sum_{i=1}^{n} \left(\mu_i(G_S) - \frac{2m + \sigma}{n} \right)$$
$$= \sum_{i=1}^{n} \mu_i(G_S) - \sum_{i=1}^{n} \frac{2m + \sigma}{n}$$
$$= 2m + \sigma - (2m + \sigma)$$
$$= 0.$$

2. Also,
$$\sum_{i=1}^{n} \gamma_i^2(G_S) = \sum_{i=1}^{n} \left(\mu_i(G_S) - \frac{2m+\sigma}{n} \right)^2$$

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

$$= \sum_{i=1}^{n} \left(d_i(G_S) - \frac{2m+\sigma}{n} \right)^2 + 2m + \sigma + 2\sigma \left(\frac{2m+\sigma}{n} \right) - 2 \sum_{v_i \in S} d_i(G_S)$$

$$= 2M.$$

Lemma 3. [4]

- 1. A symmetric diagonally dominant real matrix with non-negative diagonal entries is positive semidefinite.
- 2. Let B be a symmetric real matrix with non-negative row sums and non-positive off-diagonal entries. Define a graph Γ on the index set of the rows of B, where two distinct indices i, j are adjacent when $b_{ij} \neq 0$. The multiplicity of the eigenvalue 0 of B equals the number of connected components C of Γ such that all rows $i \in C$ have zero row sum.

Theorem 1. 1. $L(G_S)$ is positive semidefinite.

- 2. If graph G_S has $p \ge 1$ components such that each of $q \le p$ number of components with at least one self-loop and n Lapalcian eigenvalues are arranged in non-increasing order $\mu_1(G_S) \ge \mu_2(G_S) \ge \cdots \ge \mu_n(G_S)$ then $\mu_{n-i}(G_S) = 0$ for $i = 0, 1, \dots, p q 1$ and $\mu_{n-p+q}(G_S) > 0$.
- *Proof.* 1. By Lemma 3, it follows that $L(G_S)$ being a symmetric diagonally dominant real matrix with non-negative diagonal entries is positive semidefinite.
 - 2. Suppose graph G_S has $p \ge 1$ components. By Lemma 3, obtain the graph Γ which is defined on the index set of the rows of $L(G_S)$. By the definition of Γ it is clear that each connected component of G_S will contribute exactly one connected component C of Γ . Hence Γ has p connected components as G_S has p components. Suppose no self-loop is attached to any of the p components, then $L(G_S) =$ L(G). We know that each row of L(G) will have zero row sum so is each connected components C of Γ . If at least one self-loop is attached to at least one of the component, row corresponding to the added self-loop will have nonzero row sum in $L(G_S)$ which in turn results in corresponding row to have non-zero row sum in connected components C of Γ . Hence that component will not contribute in the multiplicity of eigenvalue 0. Similaryly if G_S has at least one

self-loop in each of q components, then these q components will not contribute in the algebraic multiplicity of eigenvalue 0. Therefore q components will have positive eigenvalues. So multiplicity of 0 is p-q. Also it follows that if the Lapalcian eigenvalues are labeled so that $\mu_1(G_S) \ge \mu_2(G_S) \ge \cdots \ge \mu_n(G_S)$, then $\mu_{n-i}(G_S) = 0$ for $i = 0, 1, \ldots, p-q-1$ and $\mu_{n-p+q}(G_S) > 0$.

3 Laplacian energy of G_S

From literature [10], it is observed that Laplacian energy LE(G) of graph G satisfies $LE(G) \leq \sqrt{2nM}$ and if $2m \geq n$, $2\sqrt{M} \leq LE(G) \leq 2M$, where $M = m + \frac{1}{2} \sum_{i=1}^{n} \left(d_i - \frac{2m}{n} \right)^2$. For Laplacian matrix $L(G_S)$ by Lemma 2, we have $\sum_{i=1}^{n} \gamma_i^2(G_S) = 2M$ where $M = m + \frac{1}{2} \sum_{i=1}^{n} \left(d_i(G_S) - \frac{2m+\sigma}{n} \right)^2 + \sigma \left(\frac{1}{2} + \frac{2m+\sigma}{n} \right) - \sum_{v_i \in S} d_i(G_S)$. Using Cauchy-Schwarz inequality we get,

$$LE(G_S) \le \sqrt{2nM} \tag{10}$$

For $2m \ge n$, Squaring $LE(G_S)$ and using Eq. 10 we get,

$$2\sqrt{M} \le LE(G_S) \le 2M \tag{11}$$

Theorem 2. If graph G_S has p components $(p \ge 1)$ out of which q components $(q \le p)$ have at least one self-loop in each of its component. Then,

$$LE(G_S) \le (p-q)\frac{2m+\sigma}{n} + \sqrt{(n-p+q)(2M-(p-q)(\frac{2m+\sigma}{n})^2)}.$$

Proof. Consider a graph G_S with p components $(p \ge 1)$. Let each of $q \le p$ components has at least one self-loop. Then by Theorem 1, $\gamma_{n-i}(G_S) = -\frac{2m+\sigma}{n}$ for $i = 0, 1, \ldots, p-q-1$.

Consider,

$$\sum_{i=1}^{n-p+q} \sum_{j=1}^{n-p+q} (|\gamma_i(G_S)| - |\gamma_j(G_S)|)^2 \ge 0$$

$$\sum_{i=1}^{n-p+q} \left(\sum_{j=1}^{n-p+q} |\gamma_i(G_S)|^2 + \sum_{j=1}^{n-p+q} |\gamma_j(G_S)|^2 - 2 \sum_{j=1}^{n-p+q} |\gamma_i(G_S)| |\gamma_j(G_S)| \right) \ge 0$$

$$2(n-p+q) \left(2M - (p-q) \left(\frac{2m+\sigma}{n} \right)^2 \right) \ge 2 \left(LE(G_S) - (p-q) \left(\frac{2m+\sigma}{n} \right) \right)^2$$

Thus,

$$(p-q)\left(\frac{2m+\sigma}{n}\right) + \sqrt{(n-p+q)\left(2M-(p-q)\left(\frac{2m+\sigma}{n}\right)^2\right)} \ge LE(G_S).$$

Theorem 3. For complete graph K_n with σ self-loops,

$$LE(G_S) = \frac{(n^2 - 3n + 2\sigma)}{n} + \sqrt{(n+1)^2 - 4\sigma}.$$

Proof. Let $(K_n)_S$ be a complete graph with self-loops so that $|S| = \sigma$. Since all vertices are adjacent, position of self-loop will not change the Laplacian energy. Then,

$$L(K_n)_S = \begin{bmatrix} ((n+1)I - J)_{\sigma \times \sigma} & -J_{\sigma \times (n-\sigma)} \\ -J_{(n-\sigma) \times \sigma} & (nI - J)_{(n-\sigma) \times (n-\sigma)} \end{bmatrix}$$

Let $W = \begin{bmatrix} X \\ Y \end{bmatrix}$ be an eigenvector such that X consists of σ components
and Y is of $(n - \sigma)$ tupled vector. Let $\mu(G_S)$ be a eigenvalue of $L(G_S)$.
Then,

$$[\mu(G_S)I - L(G_S)] \begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} [(\mu(G_S) - n - 1)I + J] X_{\sigma \times 1} + JY_{\sigma \times 1} \\ JX_{(n-\sigma)\times 1} + [(\mu(G_S) - n)I + J]Y_{(n-\sigma)\times 1} \end{bmatrix}$$
(12)

Case 1: Let $X = X_j = e_1 - e_j, j = 2, 3, ..., \sigma$. and $Y = O_{n-\sigma \times 1}$

From expression 12,

$$(\mu(G_S) - n - 1)X_j + JX_j + JO_{n-\sigma} = (\mu(G_S) - (n+1))X_j$$

It implies that, $\mu(G_S) = (n+1)$ is an eigenvalue with multiplicity of at least $(\sigma - 1)$ since there are $(\sigma - 1)$ linearly independent eigenvectors of the form X_i .

Case 2: Suppose X is a zero vector of order σ and $Y = Y_j = e_1 - e_j$, $j = 2, 3, \ldots, n - \sigma$ Then from expression 12,

$$JO_{\sigma} + (\mu(G_S) - n)Y_j + JY_j = (\mu(G_S) - n)Y_j$$

So, $\mu(G_S) = n$ is an eigenvalue with multiplicity at least $(n - \sigma - 1)$ since there are $n - \sigma - 1$ linearly independent eigenvectors of the form Y_j .

Case 3: Let $X = 1_{\sigma}$ and $Y = \frac{-\sigma}{(\mu(G_S) - \sigma)} \mathbf{1}_{n-\sigma}$ where, $\mu(G_S)$ is root of the equation $\mu(G_S)^2 - (n+1)\mu(G_S) + \sigma = 0$ From Eq. 12, $((\mu(G_S) - n - 1)I + J)\mathbf{1}_{\sigma} + J\left(\frac{-\sigma}{n-\sigma}\right)\mathbf{1}_{n-\sigma}$

$$= \left(\left(\mu(G_S) - n - 1\right) + \sigma + \left(n - \sigma\right) \left(\frac{-\sigma}{\mu(G_S) - \sigma}\right) \right) \mathbf{1}_{\sigma}$$
$$= \left(\frac{(\mu(G_S) - n - 1)(\mu(G_S) - \sigma) + \sigma(\mu(G_S) - \sigma) - \sigma(\mu(G_S) - \sigma)}{\mu(G_S) - \sigma} \right) \mathbf{1}_{\sigma}$$
$$= \left(\frac{\mu(G_S)^2 - (n + 1)\mu(G_S) + \sigma}{\mu(G_S) - \sigma} \right) \mathbf{1}_{\sigma}$$

Thus, $\mu(G_S) = \frac{(n+1)+\sqrt{(n+1)^2-4\sigma}}{2}$ and $\mu(G_S) = \frac{(n+1)-\sqrt{(n+1)^2-4\sigma}}{2}$ are the eigenvalues with multiplicity of at least one. Therefore Laplacian spectrum of complete graph with self-loops is given by,

$$\begin{cases} n & n+1 & \frac{n+1+\sqrt{(n+1)^2-4\sigma}}{2} & \frac{(n+1)-\sqrt{(n+1)^2-4\sigma}}{2} \\ n-1-\sigma & \sigma-1 & 1 & 1 \end{cases} \}.$$

The Lapalcian energy of complete graph with self-loops is given by,

$$LE((K_n)_S) = (n-1-\sigma) \left| n - \frac{n^2 - n + \sigma}{n} \right| + (\sigma-1) \left| (n+1) - \frac{n^2 - n + \sigma}{n} \right|$$
$$+ \left| \frac{(n+1) + \sqrt{(n+1)^2 - 4\sigma}}{2} - \frac{n^2 - n + \sigma}{n} \right|$$
$$+ \left| \frac{(n+1) - \sqrt{(n+1)^2 - 4\sigma}}{2} - \frac{n^2 - n + \sigma}{n} \right|$$
$$= (n-1-\sigma) \left(\frac{n-\sigma}{n} \right) + (\sigma-1) \left(\frac{2n-\sigma}{n} \right) + \sqrt{(n+1)^2 - 4\sigma}$$

Further simplification will result in,

$$LE((K_n)_S) = \frac{(n^2 - 3n + 2\sigma)}{n} + \sqrt{(n+1)^2 - 4\sigma}.$$

Theorem 4. For complete bipartite graph $K_{m,n}$ with number of self-loops s and k in the partite m and n respectively. Then the characteristic polynomial P(x) is $P(\mu(K_{(m,n)_S})) = (\mu(K_{(m,n)_S}) - (n+1))^{s-1} (\mu(K_{(m,n)_S}))^{s-1} (\mu(K_{(m,n)_S}))^{s-1} (\mu(K_{(m,n)_S}) - (m+1))^{k-1} (\mu(K_{(m,n)_S}) - n)^{m-s-1} (\mu(K_{(m,n)_S}) - m)^{n-k-1} Q(\mu(K_{(m,n)_S}))), where <math>Q(\mu(K_{(m,n)_S})) = \mu^4 (K_{(m,n)_S}) - 2(m+n+1)\mu^3 (K_{(m,n)_S}) + (m(m+3) + n(n+3) + 3mn + 1)\mu^2 (K_{(m,n)_S}) - (m(n^2 + k+1) + n(m^2 + s + 1) + (m+n)^2)\mu (K_{(m,n)_S}) + km(1+n) + ns(m+1) - ks.$

Proof. Let $(K_{m,n})_S$ be complete bipartite graph with s, k number of selfloops in the two partites of order m and n respectively. Then the Laplacian matrix $L(K_{(m,n)_S}) =$

$$\begin{pmatrix} (n+1)I_{s\times s} & 0_{s\times (m-s)} & -1_{s\times k} & -1_{s\times (n-k)} \\ 0_{(m-s)\times s} & nI_{(m-s)\times (m-s)} & -1_{(m-s)\times k} & -1_{(m-s)\times (n-k)} \\ -1_{k\times k} & -1_{k\times (m-s)} & (m+1)I_{k\times k} & 0_{k\times (n-k)} \\ -1_{(n-k)\times k} & -1_{(n-k)\times (m-s)} & 0_{(n-k)\times k} & mI_{(n-k)\times (n-k)} \end{bmatrix}$$
asider det (\$\mu(K_{(m,n)_S}) I - L(K_{(m,n)_S})\$), where \$\mu(K_{(m,n)_S})\$ is an eigen-

Consider det $(\mu(K_{(m,n)S})I - L(K_{(m,n)S}))$, where $\mu(K_{(m,n)S})$ is an eigenvalue of $L(K_{(m,n)S})$.

Step 1: Replace R_i by $R'_i = R_i - R_{i-1}$, where $i = n, n - 1, \dots, k + 3, k+2, k, k-1, \dots, m+3, m+2, m, m-1, \dots, s+3, s+2, s, s-1, \dots, 3, 2$.

Then det $(\mu(K_{(m,n)S})I - L(K_{(m,n)S}))$ will get reduced to new determinant say det(A).

Step 2: Replace C_i of det(A) by $C'_i = C_i + C_{i+1}$, where i = n - 1, n - 2, ..., k + 1, k - 1, k - 2, ..., m + 1, m - 1, ..., s + 1, s - 1, ..., 2, 1. Let the new determinant be det(B).

 $\begin{array}{c} \text{Step 3: Expanding det}(B) \text{ successively along the rows } i, i = 2, 3, \dots, s, \\ s+2, \dots, m, m+2, \dots, k, k+2, \dots, n-1, n. \text{ Then, det}(B) = (\mu\left(K_{(m,n)_S}\right) - (n+1))^{s-1}(\mu\left(K_{(m,n)_S}\right) - (m+1))^{k-1}(\mu\left(K_{(m,n)_S}\right) - n)^{m-s-1}(\mu\left(K_{(m,n)_S}\right) - m)^{n-k-1} \det(C), \text{ where det}(C) = \\ \\ \mu\left(K_{(m,n)_S}\right) - n - 1 & 0 & k & n-k \\ 0 & \mu\left(K_{(m,n)_S}\right) - n & k & n-k \\ s & m-s & \mu\left(K_{(m,n)_S}\right) - m - 1 & 0 \\ s & m-s & 0 & \mu\left(K_{(m,n)_S}\right) - m \end{array} \right|.$

Further simplifying the determinant we get, $\det(C) = \mu^4 (K_{(m,n)S}) - 2(m+n+1)\mu^3 (K_{(m,n)S}) + (m(m+3)+n(n+3)+3mn+1)\mu^2 (K_{(m,n)S}) - (m(n^2+k+1)+n(m^2+s+1)+(m+n)^2)\mu (K_{(m,n)S}) + km(1+n)+ns(m+1) - ks$. Then the Laplacian characteristic polynomial of $(K_{m,n})_S$ is given by $P(\mu(K_{(m,n)S})) = (\mu(K_{(m,n)S}) - (n+1))^{s-1} (\mu(K_{(m,n)S}) - (m+1))^{k-1} (\mu(K_{(m,n)S}) - n)^{m-s-1} (\mu(K_{(m,n)S}) - m)^{n-k-1} Q(\mu(K_{(m,n)S})), where <math>Q(\mu(K_{(m,n)S})) = \mu^4 (K_{(m,n)S}) - 2(m+n+1)\mu^3 (K_{(m,n)S}) + (m(m+3)+n(n+3)+3mn+1)\mu^2 (K_{(m,n)S}) - (m(n^2+k+1)+n(m^2+s+1)+(m+n)^2)\mu (K_{(m,n)S}) + km(1+n)+ns(m+1)-ks.$

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