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## MISBALANCE DEGREE MATRIX AND RELATED ENERGY OF GRAPHS

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**Abstract.** Given a graph  $G = (V, E)$ , the Misbalance deg (MD) index of  $G$  is defined as

$$MD(G) = \sum_{uv \in E} |d_u - d_v|,$$

where  $E$  is the set of edges of  $G$ , and  $d_u$  be the degree of the vertex  $u \in V$ , set of vertices of  $G$ . A modification of the classical adjacency matrix of a graph is propose based on MD index and its spectra is studied in connection with subdivision, semitotal point graph, semitotal line graph, and total graphs of a regular graph. Analogously two new concepts namely MD energy and MD estrada index are also coined.

**Keywords:** misbalance deg index; graph energy; spectral theory.

**2010 AMS Subject Classification:** 05C50, 05C35.

### 1. INTRODUCTION

The study of topological indices draws considerable attention from the researchers of various disciplines. Topological indices are interesting because they can capture many significant chemical, physical or biological properties of molecules. Over the years loads of topological indices have been proposed and studied, initiated by *Wiener* with his seminal work in 1947 [23].

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Misbalance deg index (MD) is relatively a new addition to this wide list of topological indices. It is a significant predictor of standard enthalpy of vaporization for octane isomers. In fact it was in the list of twenty (20) important topological indices, reported in 2010 [22]. In 2005, *Rodríguez* has started the trend of studying adjacency like matrix based on *Randić* index [18]. Later *Bozkurt et al.*, associated the term *Randić Matrix* for this adjacency like matrix of *Randić* index [4]. Since then various studies of topological indices from an algebraic viewpoint were reported [5, 10, 17, 19, 20], as many interesting properties of graphs are reflected in the study of these matrices. The analogous concepts to graph energy viz., ABC energy [10], geometric-arithmetic energy [20], harmonic energy [13], Zagreb energy [17], ISI energy [3] have also been put forward.

There are several degree-based topological indices, which are introduced and studied over the years [12]. Let us formally define two of such popular indices viz., *second Zagreb index*, *forgotten topological index* which are going to be used in further discussion. The second Zagreb index is defined as

$$M_2(G) = \sum_{uv \in E} d_u d_v,$$

where  $E$  is the set of edges of  $G$ , and  $d_u$  be the degree of the vertex  $u$  of  $G$ .

The forgotten topological index [11],  $F(G)$  is defined as

$$F(G) = \sum_{uv \in E} d_u^2 + d_v^2 = \sum_{u \in V} d_u^3.$$

In this paper we are concerned with the MD index (also known as irregularity [2] of a graph) and the corresponding MD adjacency matrix.

The MD index is defined as

$$MD(G) = \sum_{uv \in E} |d_u - d_v|.$$

Let us now define the MD adjacency matrix or simply MD matrix,  $A_{MD}$  with entries

$$(A_{MD})_{ij} = \begin{cases} |d_i - d_j| & \text{if } ij \in E \\ 0 & \text{otherwise.} \end{cases}$$

The matrix,  $A_{MD}$  is an adjacency like matrix that we can associate with the MD index of a graph. If the eigenvalues of  $A_{MD}$  are  $\xi_1, \xi_2, \dots, \xi_n$ , then the MD energy can be defined as

$$E_{MD} = \sum_{i=1}^n |\xi_i|,$$

which is defined analogous to graph energy [15].

Similarly we can define the MD estrada index as

$$EE_{MD} = \sum_{i=1}^n e^{\xi_i}.$$

Let the characteristic polynomial of classical adjacency matrix be denoted by  $\phi(G; \xi)$ . The characteristic polynomial of  $A_{MD}$  is called the MD characteristic polynomial or simply MD-polynomial, and is denoted by  $\Omega(G; \xi)$ . Thus  $\Omega(G; \xi) = \det(\xi I - A_{MD})$ , where  $I$  is an identity matrix of order  $n$ . Clearly for a regular graph  $G$ ,  $\Omega(G; \xi) = \xi^n$ .

The rest of the paper is organized as follows. In the next section we present some preliminary results on MD matrix and then study the MD spectra of subdivision, semi-total point graph, semi-total line graph, and total graphs of a regular graph. In section 3, we derive some inequalities for MD energy and MD Estrada index. In the section 4, concluding remarks are made.

## 2. MD MATRIX

The MD matrix or MD adjacency matrix is a real symmetric matrix with positive entries. Being symmetric, its eigenvalues are real. The diagonal entries of the matrix are all equal to zero. So the trace of the matrix is always zero. The sum of the eigenvalues of the matrix, is also zero. Some of the keys observations about MD matrix are summarize in the following proposition.

**Proposition 2.1.** Let  $G$  be a graph and  $A_{MD}$  be the corresponding MD adjacency matrix. Then

- (i)  $\text{trace}(A_{MD}) = 0$ , and  $A_{MD} = 0$  if  $G$  is regular.
- (ii)  $\text{trace}(A_{MD}^2) = 2F(G) - 4M_2(G)$ .
- (iii) If  $\xi_1, \xi_2, \dots$  be the eigenvalues of  $A_{MD}$ , then  $\sum_{i>j} \xi_i \xi_j = 2M_2(G) - F(G)$ .
- (iv) If  $\xi_1$  is the MD spectral radius, then  $\xi_1 \leq \sqrt{\frac{2(n-1)}{n}(F(G) - 2M_2(G))}$ .

*Proof.* The first statement can be directly obtained from the definition. Let us consider  $A_{MD} = (a_{ij})$ , then the second relation may be obtained from the fact that

$$(A_{MD}^2)_{ii} = \sum_{j=1}^n a_{ij}a_{ji} = \sum_{j=1}^n a_{ij}^2 = \sum_{\substack{j \in \{1,2,\dots,n\} \\ ij \in E}} (|d_i - d_j|)^2,$$

and therefore

$$\text{trace}(A_{MD}^2) = \sum_{i=1}^n \sum_{\substack{j \in \{1,2,\dots,n\} \\ ij \in E}} (|d_i - d_j|)^2 = 2 \sum_{ij \in E} (d_i^2 + d_j^2 - 2d_i d_j) = 2(F(G) - 2M_2(G)).$$

Expression (iii) can easily be obtained from the basic relation  $(\sum_{i=1}^n \xi_i)^2 = \sum_{i=1}^n \xi_i^2 + 2\sum_{i>j} \xi_i \xi_j$ , using the results (i) and (ii).

Squaring the relation  $\xi_1 = -\sum_{i=2}^n \xi_i$  and using Cauchy Schwarz inequality [8] we have

$$(1) \quad \xi_1^2 \leq (n-1) \sum_{i=2}^n \xi_i^2 = (n-1)(\text{trace}(A_{MD}^2) - \xi_1^2).$$

Expression (iv) can obtained using the result (iii) in ( 1). □

**2.1. MD spectra of Subdivision, Semi-total point graph, Semi-total line graph, and Total graphs of a regular graph.**

A subdivision graph of  $G$  is a graph  $S(G)$  obtained from  $G$  by inserting a new vertex on each edge of  $G$ . Thus if the order of  $G$  is  $n$  and its size is  $m$ , then  $|V(S(G))| = m + n$ ,  $|E(S(G))| = 2m$ . If  $u \in V(G)$  then  $d_{S(G)}(u) = d_G(u)$  and if  $v$  is subdivided vertex then  $d_{S(G)}(v) = 2$ . The semi-total vertex graph of  $G$ , denoted by  $R(G)$ , is a graph with vertex set  $V(G) \cup E(G)$  and two vertices in  $R(G)$  are adjacent if they are adjacent vertices in  $G$  or one is a vertex and other is an edge incident to it in  $G$ . Note that if  $u \in V(G)$  then  $d_{R(G)}(u) = 2d_G(u)$  and if  $e \in E(G)$  then  $d_{R(G)}(e) = 2$ . Semi-total line graph of  $G$ , denoted by  $Q(G)$ , is a graph with vertex set  $V(G) \cup E(G)$  and two vertices in  $Q(G)$  are adjacent if one is a vertex and other is an edge incident to it in  $G$  or both are edges adjacent in  $G$ . Note that if  $u \in V(G)$  then  $d_{Q(G)}(u) = d_G(u)$  and if  $e = uv \in E(G)$  then  $d_{Q(G)}(e) = d_G(u) + d_G(v)$ . Total graph of  $G$ , denoted by  $T(G)$ , is a graph with vertex set  $V(G) \cup E(G)$  and two vertices in  $T(G)$  are adjacent if and only if they are adjacent vertices of  $G$  or adjacent edges of  $G$  or one is a vertex and other is an edge incident to it in  $G$ . These four operations and related sums of graphs which are defined based on these operations, popularly known as  $F$ -sums are widely studied for various topological indices [1, 7, 9, 14, 16, 21].

Now we first present a lemma without proof and then using the lemma we will prove few results on the MD polynomial of the four graph operations discussed above.

**Lemma 2.2.** [6] *If  $M$  is a non-singular matrix, then we have*

$$\begin{vmatrix} M & N \\ P & Q \end{vmatrix} = |M| |Q - PM^{-1}N|.$$

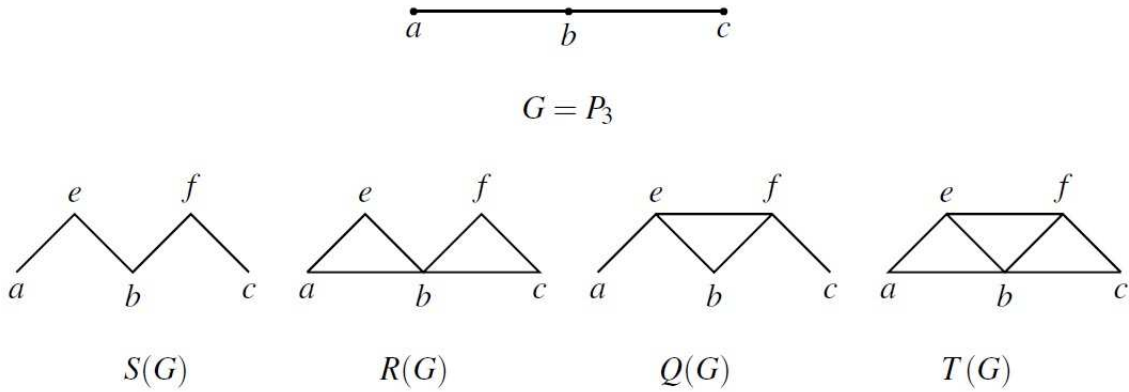


FIGURE 1. Subdivision, Semi-total point, Semi-total line, and Total graphs of a graph

**Theorem 2.3.** *Let  $G$  be an  $r$ -regular graph of  $n$  vertices and  $m$  edges. Then*

$$\Omega(S(G); \xi) = \begin{cases} \xi^{n/2}(\xi^2 - 2)^{n/2}, & \text{if } r = 1 \\ \xi^{2n}, & \text{if } r = 2 \\ \xi^{m-n}(r-2)^{2n} \phi(G; \frac{\xi^2 - r(r-2)^2}{(r-2)^2}), & \text{if } r \geq 3 \end{cases}$$

*Proof.* (i) If  $r = 1$ , then clearly  $G$  will be the union of some  $K_2$  i.e., an edge. Suppose it consists of  $k$  such edges, then  $n = 2k$  and  $m = k$ . The vertices of  $S(G)$  can be labeled in such a way that  $A_{MD}(S(G)) = \begin{bmatrix} 0 & B^T \\ B & 0 \end{bmatrix}$ , where  $B$  is the vertex-edge incidence matrix of

$G$  and  $0$  is zero matrix. Therefore by Lemma 2.2 we have  $\Omega(S(G); \xi) = \begin{vmatrix} \xi I_m & -B^T \\ -B & \xi I_n \end{vmatrix}$ . And using the fact that if  $A$  is the classical adjacency matrix of  $G$  then for an  $r$ -regular graph

$BB^T = A + rI_n$ , we have

$$\begin{aligned} \Omega(S(G); \xi) &= \xi^m \left| \xi I_n - B \frac{I_m}{\xi} B^T \right| \\ &= \xi^{m-n} \left| \xi^2 I_n - BB^T \right| \\ &= \xi^{m-n} \left| \xi^2 I_n - A - rI_n \right| \\ &= \xi^{m-n} \left| (\xi^2 - r) I_n - A \right| \\ &= \xi^{m-n} \phi(G; (\xi^2 - r)). \end{aligned}$$

Now putting  $r = 1$  and using the fact that  $\phi(K_2; \xi) = \xi^2 - 1$ , we get

$$\begin{aligned} \Omega(S(G); \xi) &= \xi^{m-n} ((\xi^2 - 1)^2 - 1)^k \\ &= \xi^{n/2} (\xi^2 - 2)^{n/2}. \end{aligned}$$

(ii) If  $r = 2$  then each component of  $G$  is cycle. Therefore  $S(G)$  is a 2-regular graph with  $2n$  vertices. Hence

$$\Omega(S(G); \xi) = \xi^{2n}.$$

(iii) If  $r \geq 3$ . The vertices of  $S(G)$  can be labeled in such a way that

$$A_{MD}(S(G)) = \begin{bmatrix} 0 & (r-2)B^T \\ (r-2)B & 0 \end{bmatrix},$$

where  $B$  is the vertex-edge incidence matrix of  $G$ ,  $B^T$  is the transpose of  $B$  and  $0$  is zero matrix. Therefore by Lemma 2.2 we have

$$\Omega(S(G); \xi) = \left| \begin{array}{cc} \xi I_m & -(r-2)B^T \\ -(r-2)B & \xi I_n \end{array} \right| = \xi^m \left| \xi I_n - (r-2)^2 B \frac{I_m}{\xi} B^T \right|.$$

On simplification, we get the result.

□

**Theorem 2.4.** *Let  $G$  be an  $r$ -regular graph of  $n$  vertices and  $m$  edges. Then*

$$\Omega(R(G); \xi) = \begin{cases} \xi^{m+n}, & \text{if } r = 1 \\ \xi^{m-n} (2r-2)^{2n} \phi(G; \frac{(\xi-r(2r-2)^2)}{(2r-2)^2}), & \text{if } r \geq 2 \end{cases}$$

*Proof.* (i) If  $r = 1$ . Then  $R(G)$  will be a 2-regular graph with  $m + n$  vertices. Hence

$$\Omega(R(G); \xi) = \xi^{m+n}.$$

(ii) If  $r \geq 2$ . The vertices of  $R(G)$  can be labeled in such a way that

$$A_{MD}(R(G)) = \begin{bmatrix} 0 & (2r-2)B^T \\ (2r-2)B & 0 \end{bmatrix},$$

where  $B$  is the vertex-edge incidence matrix of  $G$ ,  $B^T$  is the transpose of  $B$  and  $0$  is zero matrix. Therefore by Lemma 2.2 we have

$$\Omega(R(G); \xi) = \begin{vmatrix} \xi I_m & -(2r-2)B^T \\ -(2r-2)B & \xi I_n \end{vmatrix} = \xi^m |\xi I_n - (2r-2)^2 B \frac{I_m}{\xi} B^T|.$$

Now using the relation  $BB^T = A + rI_n$ , we get

$$\begin{aligned} \Omega(R(G); \xi) &= \xi^{m-n} |\xi I_n - (2r-2)^2 (A + rI_n)| \\ &= \xi^{m-n} |(\xi - r(2r-2)^2) I_n - (2r-2)^2 A| \\ &= \xi^{m-n} (2r-2)^{2n} \left| \frac{(\xi - r(2r-2)^2)}{(2r-2)^2} I_n - A \right| \\ &= \xi^{m-n} (2r-2)^{2n} \phi\left(G; \frac{(\xi - r(2r-2)^2)}{(2r-2)^2}\right) \end{aligned}$$

□

**Theorem 2.5.** Let  $r \geq 1$  and  $G$  be an  $r$ -regular graph of  $n$  vertices and  $m$  edges. Then

$$\Omega(Q(G); \xi) = r^{2n} \xi^{m-n} \phi\left(G; \frac{\xi^2 - r^3}{r^2}\right).$$

*Proof.* The vertices of  $Q(G)$  can be labeled in such a way that  $A_{MD}(Q(G)) = \begin{bmatrix} 0 & rB^T \\ rB & 0 \end{bmatrix}$ ,

where  $B$  is the vertex-edge incidence matrix of  $G$ ,  $B^T$  is the transpose of  $B$  and  $0$  is zero matrix.

Therefore by Lemma 2.2 we have

$$\Omega(Q(G); \xi) = \begin{vmatrix} \xi I_m & -rB^T \\ -rB & \xi I_n \end{vmatrix} = \xi^m |\xi I_n - r^2 B \frac{I_m}{\xi} B^T|.$$

Again using the relation  $BB^T = A + rI_n$ , we get

$$\begin{aligned} \Omega(R(G); \xi) &= \xi^{m-n} |\xi I_n - r^2(A + rI_n)| \\ &= \xi^{m-n} |(\xi - r^3)I_n - r^2A| \\ &= \xi^{m-n} r^{2n} \left| \frac{\xi - r^3}{r^2} I_n - A \right| \\ &= \xi^{m-n} r^{2n} \phi\left(G; \frac{\xi - r^3}{r^2}\right) \end{aligned}$$

□

**Theorem 2.6.** *Let  $G$  be an  $r$ -regular graph of  $n$  vertices and  $m$  edges. Then*

$$\Omega(T(G); \xi) = \xi^{m+n}.$$

*Proof.* We know that if  $G$  is a regular graph of  $n$  vertices and  $m$  edges, then the total graph,  $T(G)$  of  $G$  is also a regular graph of  $m + n$  vertices. So,  $\Omega(T(G); \xi) = \xi^{m+n}$ . □

### 3. MD ENERGY AND MD ESTRADA INDEX

#### 3.1. Bounds of MD Energy.

**Theorem 3.1.** *Let  $G$  be a graph with second Zagreb, forgotten topological index  $M_2(G)$  and  $F(G)$  respectively. Then*

$$\sqrt{2F(G) - 4M_2(G)} \leq E_{MD} \leq \sqrt{2nF(G) - 4nM_2(G)}.$$

*Proof.* Let  $\xi_1, \xi_2, \dots, \xi_n$  be the eigenvalues of  $A_{MD}$ . Using Cauchy-Schwarz inequality, we have

$$\sum_{i=1}^n |\xi_i| \sum_{i=1}^n |\xi_i| \leq n \sum_{i=1}^n |\xi_i|^2,$$

which implies  $E_{MD}^2 \leq n \text{trace}(A_{MD}^2) = 2nF(G) - 4nM_2(G)$ . And hence the upper bound.

The lower bound can be obtained from the fact that  $(\sum_{i=1}^n |\xi_i|)^2 \geq \sum_{i=1}^n |\xi_i|^2$ . □

The lower bound can be improved using the fact that determinant of a matrix is the product of its eigenvalues.



**Theorem 3.2.** Let  $G$  be a graph with second Zagreb, forgotten topological index  $M_2(G)$  and  $F(G)$  respectively. Then

$$E_{MD}(G) \geq \sqrt{2nF(G) - 4nM_2(G) + n(n-1)|\det(A_{MD})|^{2/n}},$$

where  $A_{MD}$  is the MD adjacency matrix of  $G$  and  $|V(G)| = n$ .

*Proof.* Let  $\xi_1, \xi_2, \dots, \xi_n$  be the eigenvalues of  $A_{MD}$ .

$$(2) \quad E_{MD}^2(G) = \left( \sum_{i=1}^n |\xi_i| \right)^2 = \sum_{i=1}^n |\xi_i|^2 + \sum_{i \neq j} |\xi_i \xi_j|.$$

Again using AM-GM inequality we have

$$(3) \quad \frac{\sum_{i \neq j} |\xi_i \xi_j|}{n(n-1)} \geq \left( \prod_{i=1}^n |\xi_i|^{2(n-1)} \right)^{1/n(n-1)} = \left( \prod_{i=1}^n |\xi_i| \right)^{2/n}.$$

Using (3) in (2), we get

$$E_{MD}^2(G) \geq \text{trace}(A_{MD}^2) + n(n-1)|\det(A_{MD})|^{2/n}.$$

The results follows immediately. □

**3.2. Bounds of MD Estrada Index.** Now we first present a popular inequality without proof, using which we obtain bounds of  $EE_{MD}$ .

**Lemma 3.3.** For non-negative  $x_1, x_2, \dots, x_n$  and  $k \geq 2$ ,

$$\sum_{i=1}^n (x_i)^k \leq \left( \sum_{i=1}^n (x_i)^2 \right)^{k/2}.$$

**Theorem 3.4.** Let  $G$  be a graph with second Zagreb, forgotten topological index  $M_2(G)$  and  $F(G)$  respectively. Then

$$EE_{MD}(G) \leq e^{\sqrt{2F(G) - 4M_2(G)}}$$

*Proof.* Let  $\xi_1, \xi_2, \dots, \xi_n$  be the eigenvalues of  $A_{MD}$ . Then

$$\begin{aligned} EE_{MD}(G) &= \sum_{i=1}^n e^{\xi_i} = \sum_{i=1}^n \sum_{k \geq 0} \frac{\xi_i^k}{k!} = \sum_{k \geq 0} \sum_{i=1}^n \frac{\xi_i^k}{k!} \\ &\leq \sum_{k \geq 0} \frac{1}{k!} \left( \sum_{i=1}^n \xi_i^2 \right)^{k/2} = \sum_{k \geq 0} \frac{1}{k!} (2F(G) - 4M_2(G))^{k/2} \quad (\text{Using lemma 3.3}), \\ &= \sum_{k \geq 0} \frac{1}{k!} (\sqrt{2F(G) - 4M_2(G)})^k = e^{\sqrt{2F(G) - 4M_2(G)}}. \end{aligned}$$

□

**Theorem 3.5.** *Let  $G$  be a connected graph with order  $n > 2$ . Then*

$$EE_{MD}(G) \leq (n - 1) + e^{\sqrt{2F(G) - 4M_2(G) - 1}},$$

where  $F(G)$  and  $M_2(G)$  are the forgotten topological index and second Zagreb index of  $G$  respectively.

*Proof.* Let  $\xi_1, \xi_2, \dots, \xi_p$  be the positive eigenvalues and  $\xi_{p+1}, \xi_{p+2}, \dots, \xi_n$  be the non positive eigenvalues of  $A_{MD}$ . Then

$$\begin{aligned} EE_{MD}(G) &= \sum_{i=1}^n e^{\xi_i} \leq (n - p) + \sum_{i=1}^p e^{\xi_i} \\ &= (n - p) + \sum_{k=0}^{\infty} \sum_{i=1}^p \frac{\xi_i^k}{k!} = n + \sum_{k \geq 1} \sum_{i=1}^p \frac{\xi_i^k}{k!} \\ &\leq n + \sum_{k \geq 1} \frac{(\sum_{i=1}^p \xi_i^2)^{k/2}}{k!} \quad (\text{Using lemma 3.3}) \\ &= n + \sum_{k \geq 1} \frac{\text{trace}(A_{MD}^2) - (\sum_{i=p+1}^n \xi_i^2)^{k/2}}{k!} \\ &\leq n + \sum_{k \geq 1} \frac{2F(G) - 4M_2(G) - (\sum_{i=p+1}^n \xi_i^2)^{k/2}}{k!} \end{aligned}$$

Since  $G$  has atleast one edge, so  $K_2$  will be an induced subgraph of  $G$ . We know that eigenvalues of  $K_2$  are -1 and 1. Hence by interlacing property  $\xi_i \leq -1$ , for  $p + 1 \leq i \leq n$ , which implies  $\sum_{i=p+1}^n \xi_i^2 \geq 1$ . Hence the result. □

**Lemma 3.6.** *Let  $u$  and  $v$  be two non adjacent vertices of  $G$ . Then*

$$EE_{MD}(G + uv) \geq EE_{MD}(G),$$

where  $G + uv$  is the graph obtained from  $G$  by joining the vertices  $u$  and  $v$  by an edge.

*Proof.* Let  $\vartheta_k(G)$  denotes the number of paths of length  $k$  in  $G$ . Then clearly  $\vartheta_k(G + uv) = \vartheta_k(G) + \vartheta_k(G; uv)$ , where  $\vartheta_k(G; uv)$  is the number of paths of length  $k$  passing through the edge  $uv$ . Hence

$$\sum_{i=1}^n \left( \sum_{k=0}^{\infty} \frac{\vartheta_k(G + uv)}{k!} \right)_{ii} \geq \sum_{i=1}^n \left( \sum_{k=0}^{\infty} \frac{\vartheta_k(G)}{k!} \right)_{ii} \Rightarrow \text{Trace}(e^{A_{MD}(G+uv)}) \geq \text{Trace}(e^{A_{MD}(G)}),$$

which immediately implies the desired result.  $\square$

The above expression says that the addition of a new edge to the graph increases the MD estrada index. So if we keep on adding the edges to  $G$  it will finally become  $K_n$  and  $EE_{MD}(G) \leq EE_{MD}(K_n)$ . Hence we can propose the following result.

**Theorem 3.7.** *For any graph  $G$ ,  $EE_{MD}(G) \leq n$ , equality holds iff  $G \cong K_n$ .*

*Proof.* The result follows from the fact that for any graph  $G$ ,  $EE_{MD}(G) \leq EE_{MD}(K_n)$ . And the MD spectrum of  $K_n$  is 0 with multiplicity  $n$ . So  $EE_{MD}(K_n) = n$ . Hence the result follows immediately. For equality clearly we must have  $G \cong K_n$ .  $\square$

#### 4. CONCLUDING REMARKS

In this paper, the spectral properties of a modified classical adjacency matrix, called MD matrix, corresponding to Misbalance degree index of a graph are discussed. Based on the eigenvalues of the newly proposed MD matrix, the concepts MD energy and MD estrada index are introduced. We also obtain some bounds of these new graph invariants. The Laplacian like matrix related to MD index can be an interesting topic for future study.

#### CONFLICT OF INTERESTS

The author(s) declare that there is no conflict of interests.

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