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Block Sombor index of a graph and its matrix representation

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Abstract: The Sombor index has gained lot of attention in the recent days for its mathematical properties and chemical applicabilities. Here, we initiated the novel block number version of the classical Sombor index and its matrix representation of a graph. The Block Sombor index $BS(G)$ is defined as the sum total of square root of the sum of squares of block numbers of adjacent vertices, where the block number of a vertex is the number of blocks to which that vertex belongs to. The main purpose of this paper is to obtain some bounds and characterizations of $BS(G)$ and its Block Sombor energy E_{BS}. Also, we estimate some properties of spectral radius of Block Sombor matrix $A_{BS}(G)$.

Keywords: Separable graph; Non-separable graph; Sombor Index; Block Sombor Index; Block Sombor Energy.

MSC: 05C09; 05C31; 05C40.

1. Introduction

The graph $G = (V, E)$ considered are simple, finite, non-trivial and undirected with p-vertices in $V(G)$ and q-edges in $E(G)$. The number of vertices adjacent to v is said to be degree of vertex v and is represented as d_v. The minimum and the maximum degrees of vertices are represented as $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. For the graph theoretic terminology not defined here, we refer to [1].

A vertex whose removal results in a trivial or disconnected graph is said to be the cut vertex. A graph that is connected, non-trivial, and has no cut vertices is said to be a non-separable graph. The maximal non-separable subgraph of a graph is said to be the block of that graph. Two blocks are said to be adjacent if they have a cut vertex in common. The block number $b(G)$ represents the total number of blocks in G. The concept of separable graphs play very significant role of Parsimony Haplotyping problem from computational biology, see [2]. For more details, we refer to [3–7].

A graph in which edges represent bonds and vertices represent atoms is said to be a molecular graph. The invariants of the form $\sum f(x,y)$ with the property $f(x,y) = f(y,x)$ are called graphical indices. These are the real numbers derived from the structure of a graph, which are invariant under graph isomorphism. These indices reflect the chemical and physical properties of molecules. Many such invariants have been introduced so far, see [8]. Few of them are as in the Table 1.

Table 1. Graphical indices

Graphical Index	$f(x,y) = f(d_u, d_v)$ or $f(d_u, b_u)$
Sombor Index $[SO(G)]$ (Gutman [9])	$\sqrt{d_u^2 + d_v^2}$
First Zagreb Index $[M_1(G)]$ (Gutman et al. [10])	$d_u + d_v$
Second Zagreb Index $[M_2(G)]$ (Gutman et al. [10])	$d_u . d_v$
Forgotten Index $[F(G)]$ (Furtula and Gutman [11])	$d_u^2 + d_v^2$
First Atom Valency Block Index $[AVB_1(G)]$ (Chaluvaraju and Vyshnavi [12])	$d_u + b_u$
Second Atom Valency Block Index $[AVB_2(G)]$ (Chaluvaraju and Vyshnavi [12])	$d_u . b_u$

2. Discussion and Main Results

In this section, we will discuss the concepts: Block Sombor Index, Matrix representation of Block Sombor index and Block Sombor Energy.

2.1. Block Sombor Index

Recently, many graph theorists showed interest in finding some potential mathematical properties and their chemical applicabilities of the sombor index. Inspired by these aspects, we define the Block Sombor index $BS(G)$ of a graph G as

$$BS(G) = BS = \sum_{uv \in E(G)} \sqrt{b_u^2 + b_v^2}. \tag{1}$$

where b_u represents the number of blocks to which the vertex u belongs to.

Theorem 1. *Let G be a separable graph with k-cut vertices. Then*

$$BS(G) = \sum_{i=1}^{k} \left[\left(d_{c_i} - \sum_{c_i \sim c_j} 1 \right) \sqrt{1 + b_{c_i}^2} \right] + \sum_{c_i \sim c_j} \sqrt{b_{c_i}^2 + b_{c_j}^2} + \left(q - \sum_{i=1}^{k} d_{c_i} + \sum_{c_i \sim c_j} 1 \right) \sqrt{2}.$$

Proof. Let G be a separable (p,q)-graph and $c_1, c_2, \cdots, c_k$ be the cut vertices of G. Let their degrees be $d_{c_1}, d_{c_2}, \cdots, d_{c_k}$ and block numbers be $b_{c_1}, b_{c_2}, \cdots, b_{c_k}$, respectively. We have the following stages:

Stage 1. Since the cut vertices are adjacent to non-cut vertices and/or cut vertices, number of partitions of the form $(1, b_{c_i})$ is the difference of the degree of the cut vertex and the number of cut vertices adjacent to it.

Stage 2. Since the number of blocks adjacent to each cut vertex varies, number of partitions of the form (b_{c_i}, b_{c_j}) depends on the adjacencies of cut vertices.

Stage 3. For the non-cut vertices which belong to the same block, the number of partitions of the form $(1, 1)$ is difference of total number of edges added to the number of adjacencies of cut vertices and the sum of degrees of all cut vertices.

Formulating these partitions mentioned in three stages, we get the required result. □

Corollary 1. *Let G be a separable graph. Then,*

(i) $BS(G) = (q - d_c)\sqrt{2} + d_c\sqrt{1 + b_c^2}$, *if G has only one cut vertex.*

(ii) $BS(G) = (d_{c_1} - 1)\sqrt{1 + b_{c_1}^2} + (d_{c_2} - 1)\sqrt{1 + b_{c_2}^2} + \sqrt{b_{c_1}^2 + b_{c_2}^2} + (q - d_{c_1} - d_{c_2} + 1)\sqrt{2}$,　*if G has two cut vertices.*

Theorem 2. *Let G be a non-separable graph with $p \geq 2$. Then,*

$$BS(G) = \sqrt{2}q. \tag{2}$$

Proof. Since the block number of each vertex is exactly one in any non-separable graph G. Hence the result follows. □

Corollary 2.

(i) For a complete graph K_p with $p \geq 2$,

$$BS(K_p) = \frac{p(p-1)}{\sqrt{2}}.$$

(ii) For a cycle C_p with $p \geq 3$,

$$BS(C_p) = \sqrt{2}p.$$

(iii) For a complete bipartite graph $K_{m,n}$ with $2 \leq m \leq n$,

$$BS(K_{m,n}) = \sqrt{2}mn.$$

(iv) For a generalized Petersen graph $GP(n,t)$,

$$GP(n,t) = 3\sqrt{2}n,$$

where $GP(n,t)$ is defined to be a graph on $2n$ vertices with $V(GP(n,t)) = \{v_i, u_i : 0 \le i \le n-1\}$ and $E(GP(n,t)) = \{v_i v_{i+1}, v_i u_i, u_i u_{i+t} : 0 \le i \le n-1, \text{subscripts modulo } n\}$.

(v) For a n-hypercube graph Q_n,

$$BS(Q_n) = n\, 2^{n-1/2},$$

where Q_n also called the n-cube graph is a graph whose vertex set V, consists of the 2^n, n-dimensional boolean vectors, i.e., vectors with binary coordinates 0 or 1, where two vertices are adjacent whenever they differ in exactly one coordinate.

(vi) For a $m \times n$ grid graph $L(m,n)$,

$$BS(L(m,n)) = \sqrt{2}(2mn - n - m),$$

where the $m \times n$ grid graph can be represented as a cartesian product of $P_m \,\square\, P_n$ of a path of length $m-1$ and a path of length $n-1$.

2.1.1. Inequalities

Lemma 1. *Let G be a non-trivial connected (p,q)-graph. Then*

(i) $1 \le b_u \le p-1$.

Left inequality holds if and only if u is a non-cut vertex and right inequality holds for a central vertex of a star.

(ii) $b_u \le d_u$.

Equality holds for all vertices in a tree.

Theorem 3. *Let G be a non-trivial connected graph. Then*

$$\sqrt{2}q \le BS(G) \le \sqrt{2}q(p-1).$$

Left inequality holds if and only if G is non-separable.

Proof. Let G be a non-trivial connected graph. By Lemma 1(i), we have $1 \le b_u \le p-1$. Therefore squaring up and adding the block numbers of two vertices, we have $2 \le b_u^2 + b_v^2 \le 2(p-1)^2$. Also, taking square root of this inequality and adding up them over the number of edges, we have the required inequality.

Now, we prove the second part.

If the graph G has no cut vertices, then each vertex has block number $b_u = 1$ as they belong to exactly one block, which leads to the partition $(1,1)$ for each edge $uv \in E(G)$. Thus we obtain the left equality. $\square$

For existence of right equality of the above theorem, we pose the following open problem.

Open Problem. Characterize when $BS(G) = \sqrt{2}q(p-1)$?

Theorem 4. *Let G be a non-trivial connected graph. Then*

$$BS(G) \le SO(G).$$

Equality holds if and only if G is a non-trivial tree.

Proof. Let G be a simple connected graph. By Lemma 1(ii), we have

$$BS(G) = \sum_{uv \in E(G)} \sqrt{b_u^2 + b_v^2} \le \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} = SO(G).$$

Now, we prove the second part.

Since each vertex in a non-trivial tree, apart from the pendant vertices is a cut vertex, the block number of each vertex is same as the degree of that vertex. Hence the equality holds.

Conversely, suppose $BS(G) = SO(G)$ holds for a graph which is not a tree. Then there exist at least three vertices such that every pair of vertices are adjacent forming a complete graph. This is a contradiction to our assumption as $BS(K_p) = \dfrac{p(p-1)}{\sqrt{2}}$ and $SO(K_p) = \dfrac{p(p-1)^2}{\sqrt{2}}$. Hence $BS(G) < SO(G)$ if G is not a tree. $\square$

In [13], it was proven for a non-trivial connected graph that,

$$SO(G) \le \frac{1}{\sqrt{2}}(M_1(G) + q(\Delta - \delta)).$$

From the above and Theorem 4, we obtain the following result:

Corollary 3. *Let G be a simple connected graph with $p \ge 2$. Then*

$$BS(G) \le \frac{1}{\sqrt{2}}(M_1(G) + q(\Delta - \delta)).$$

Theorem 5. *Let G be a non-trivial connected graph. Then*

$$BS(G) \le \frac{\sqrt{2}M_2(G)}{\delta(G)}.$$

Proof. Let G be a non-trivial connected graph. Then

$$
\begin{aligned}
BS(G) = \sum_{uv \in E(G)} \sqrt{b_u^2 + b_v^2} &= \sum_{uv \in E(G)} b_u b_v \sqrt{\frac{1}{b_u^2} + \frac{1}{b_v^2}} \\
&\le \sum_{uv \in E(G)} d_u d_v \sqrt{\frac{1}{\delta^2} + \frac{1}{\delta^2}} \\
&= \frac{\sqrt{2}M_2(G)}{\delta(G)}.
\end{aligned}
$$

$\square$

Theorem 6. *Let G be a non-trivial connected graph. Then*

$$BS(G) \le \sqrt{qF(G)}.$$

Proof. Let G be a non-trivial connected graph. Then

$$
\begin{aligned}
BS(G) = \sum_{uv \in E(G)} \sqrt{b_u^2 + b_v^2} &= \sum_{uv \in E(G)} 1.\sqrt{b_u^2 + b_v^2} \\
&\le \sqrt{\sum_{uv \in E(G)} 1^2 . \sum_{uv \in E(G)} (d_u^2 + d_v^2)} = \sqrt{qF(G)}.
\end{aligned}
$$

$\square$

In [14], it was proven for a non-trivial connected graph that,

$$F(G) \le (\Delta + \delta)M_1(G) - 2q\Delta\delta.$$

From the above and Theorem 6, we obtain the following result:

Corollary 4. *Let G be a simple connected graph with $p \ge 2$. Then*

$$BS(G) \le \sqrt{q[(\Delta + \delta)M_1(G) - 2q\Delta\delta]}.$$

In [15], it was proven for a non-trivial connected graph that,

$$F(G) \le \Delta M_1(G) - \frac{(2q\Delta - M_1(G))^2}{n\Delta - 2q}.$$

From the above and Theorem 6, we obtain the following result:

Corollary 5. *Let G be a simple connected graph. Then*

$$BS(G) \leq \sqrt{q\left[\Delta M_1(G) - \frac{(2q\Delta - M_1(G))^2}{n\Delta - 2q}\right]}.$$

Theorem 7. *Let G be a connected regular graph with $p \geq 2$. Then*

$$BS(G) \leq \frac{\sqrt{2}\, AVB_2(G)}{\delta(G)}.$$

Proof. Let G be a (p, q)-regular graph with $p \geq 2$. Then

$$BS(G) = \sum_{uv \in E(G)} \sqrt{b_u^2 + b_v^2} = \sum_{uv \in E(G)} b_u b_v \sqrt{\frac{1}{b_u^2} + \frac{1}{b_v^2}}$$

$$\leq \sum_{uv \in E(G)} b_u d_u \sqrt{\frac{1}{\delta^2} + \frac{1}{\delta^2}}$$

$$= \frac{\sqrt{2} AVB_2(G)}{\delta(G)}. \qquad \qquad \square$$

In [12], it was proven for a non-trivial connected graph that,

$$AVB_2(G) \leq \frac{1}{4} AVB_1(G)^2.$$

From the above and Theorem 7, we obtain the following result:

Corollary 6. *Let G be a simple connected graph with $p \geq 2$. Then*

$$BS(G) \leq \frac{AVB_1(G)^2}{2\sqrt{2}\delta(G)}.$$

2.2. Matrix representation of Block Sombor index

The spectral graph theory including the concept of graph energy plays a good role in analyzing the matrices. For more details we refer to [16–26]. The Adjacency matrix $A(G) = A = [a_{ij}]_{p \times p}$ of a graph G with vertex set $V(G) = \{v_1, v_2, \cdots, v_p\}$ is the symmetric matrix whose elements are,

$$a_{ij} = \begin{cases} 1, & if\ v_i v_j \in E(G) \\ 0, & otherwise. \end{cases}$$

The energy $E_A(G) = E_A$ of a graph G is the sum of all absolute eigen values of the adjacency matrix A. Anologously, we define the Block Sombor Matrix $A_{BS}(G) = A_{BS} = [bs_{ij}]_{p \times p}$ of the graph G as the symmetric matrix of order p, whose elements are

$$bs_{ij} = \begin{cases} \sqrt{b_{v_i}^2 + b_{v_j}^2}, & v_i v_j \in E(G) \\ 0, & otherwise. \end{cases}$$

The characteristic polynomial is influential aspect of spectral graph theory, due to its algebraic construction, which has massive graphical information. For this purpose, we define the following:
The Block Sombor polynomial of a graph G is defined as $P_{BS}(G, \lambda) = det(\lambda I - A_{BS})$, where I is a $p \times p$ unit matrix.

As A_{BS} is a real symmetric matrix, all roots of $\phi_{BS}(G, \lambda) = 0$ are real. Therefore, they can be arranged in order as $\lambda_1 \geq \lambda_2 \geq \lambda_3 \cdots \geq \lambda_p$, where λ_1 is said to be spectral radius of A_{BS}.

Lemma 2. *Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$ be the eigen values of A_{BS}. Then*

(i) $\sum_{i=1}^{p} \lambda_i = 0.$

(ii) $\sum_{i=1}^{p} \lambda_i^2 \leq 2F(G).$
   Equality holds if and only if G is a non-trivial tree.

Proof. Let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \cdots \geq \lambda_p$ be the eigen values of A_{BS}.

(i) If the sum of all the eigen values counted with multiplicities is the trace of the matrix, then the principal diagonal elements of A_{BS} are all zeroes. Hence the trace is zero. Thus the result.

(ii) If $\{v_1, v_2, \cdots, v_p\}$ is the set of vertices of G, then

$$\sum_{i=1}^{p} \lambda_i^2 = tr(A_{BS}^2) = \sum_{i=1}^{p}\sum_{j=1}^{p} A_{BS}(v_i, v_j) A_{BS}(v_j, v_i)$$

$$= 2 \sum_{v_i v_j \in E(G)} A_{BS}(v_i, v_j) A_{BS}(v_j, v_i)$$

$$= 2 \sum_{v_i v_j \in E(G)} b_{v_i}^2 + b_{v_j}^2$$

$$\leq 2 \sum_{v_i v_j \in E(G)} d_{v_i}^2 + d_{v_j}^2 = 2F(G).$$

Now, we prove the second part of (ii).

Since each vertex in a non-trivial tree, other than the pendant vertices is a cut vertex, the block number of each vertex is same as the degree of that vertex. Hence the equality holds.

Conversely, suppose G is not a tree but $\sum_{i=1}^{p} \lambda_i^2 = 2F(G)$ holds. Then there exist at least three vertices such that every pair of vertices are adjacent forming a complete graph. This is a contradiction to our assumption because in a complete graph, $\sum_{i=1}^{p} \lambda_i^2 = 2p(p-1)$ and $F(K_p) = 2q(p-1)^2$. Hence $\sum_{i=1}^{p} \lambda_i^2 < 2F(G)$ if G is not a tree.

Hence the proof. $\square$

Theorem 8. *Let G be any non-trivial connected (p,q)-graph. Then,*

$$\lambda_1 \leq \sqrt{\frac{2(p-1)}{(p-2)} F(G)}.$$

Proof. Let G be non-trivial connected (p,q)-graph. Then, taking $a_i = \lambda_i$ and $b_i = 1$ for $i = 1,2,\cdots,p$ in Cauchy-Schwarz inequality, we get,

$$\left(\sum_{i=2}^{p} \lambda_i\right)^2 \leq (p-1)\sum_{i=2}^{p} \lambda_i^2.$$

$$\implies \left(\sum_{i=2}^{p} \lambda_i\right)^2 - \lambda_1^2 \leq (p-1)\left[\sum_{i=2}^{p} \lambda_i^2 - \lambda_1^2\right].$$

Solving this, we get the required inequality. $\square$

2.3. Block Sombor Energy

The Block Sombor Energy of a graph G is defined as,

$$E_{BS} = \sum_{i=1}^{p} |\lambda_i| = \sum_{i=1}^{p} \sigma_i,$$

where $\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \cdots \geq \sigma_p$ are the absolute values of λ_i.

Lemma 3. *[27] Consider a class of real polynomials* $\mathcal{P}(a_1, a_2)$*, of the form*

$$P_n(x) = x^n + a_1 x^{n-1} + a_2 x^{n-2} + b_3 x^{n-3} + \cdots + b_n,$$

where a_1 and a_2 are given real numbers. Let $x_1 \geq x_2 \geq \cdots \geq x_n$ be roots of $P_n(x) \in \mathcal{P}(a_1, a_2)$. Then,

$$\overline{x} + \frac{1}{n}\sqrt{\frac{\theta}{n-1}} \leq x_1 \leq \overline{x} + \frac{1}{n}\sqrt{\theta(n-1)}, \tag{3}$$

$$\overline{x} + \frac{1}{n}\sqrt{\frac{\theta(i-1)}{n-i+1}} \leq x_i \leq \overline{x} + \frac{1}{n}\sqrt{\frac{\theta(n-i)}{i}}; \quad i = 2, 3, \cdots, n-1, \tag{4}$$

$$\overline{x} - \frac{1}{n}\sqrt{\theta(n-1)} \leq x_n \leq \overline{x} - \frac{1}{n}\sqrt{\frac{\theta}{n-1}}, \tag{5}$$

where $\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ *and* $\theta = n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2$.

Lemma 4. *The following inequalities hold for* $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p$

$$\frac{E_{BS}}{p} + \frac{1}{p}\sqrt{\frac{p\,tr(A_{BS}^2) - E_{BS}^2}{p-1}} \leq \sigma_1 \leq \frac{E_{BS}}{p} + \frac{1}{p}\sqrt{(p-1)(p\,tr(A_{BS}^2) - E_{BS}^2)},$$

$$\frac{E_{BS}}{p} + \frac{1}{p}\sqrt{\frac{(i-1)\left[p\,tr(A_{BS}^2) - E_{BS}^2\right]}{p-i+1}} \leq \sigma_i \leq \frac{E_{BS}}{p} + \frac{1}{p}\sqrt{\frac{(p-i)\left[p\,tr(A_{BS}^2) - E_{BS}^2\right]}{i}}; \quad i = 2, 3, \cdots, p-1,$$

$$\frac{E_{BS}}{p} - \frac{1}{p}\sqrt{(p-1)(p\,tr(A_{BS}^2) - E_{BS}^2)} \leq \sigma_p \leq \frac{E_{BS}}{p} - \frac{1}{p}\sqrt{\frac{p\,tr(A_{BS}^2) - E_{BS}^2}{p-1}}.$$

Proof. Consider the polynomial,

$$P_p(x) = \prod_{i=1}^{p}(x - \sigma_i) = x^p + a_1 x^{p-1} + a_2 x^{p-2} + b_3 x^{p-3} + \cdots + b_p.$$

Since $a_1 = -\sum_{i=1}^{p}\sigma_i = -E_{BS}$ and $a_2 = \frac{1}{2}\left(\left(\sum_{i=1}^{p}\sigma_i\right)^2 - \sum_{i=1}^{p}\sigma_i^2\right) = \frac{1}{2}\left[E_{BS}^2 - tr(A_{BS})^2\right]$, polynomial $P_p(x)$ belongs to the class of real polynomials of the form $\mathcal{P}(-E_{BS}, \frac{1}{2}E_{BS}^2 - \frac{1}{2}tr(A_{BS})^2)$.
By Lemma 3, we have,

$$\overline{x} = \frac{1}{p}\sum_{i=1}^{p}\sigma_i = \frac{E_{BS}}{p}.$$

$$\theta = p\sum_{i=1}^{p}\sigma_i^2 - \left(\sum_{i=1}^{p}\sigma_i\right)^2 = p\,tr(A_{BS}^2) - E_{BS}^2.$$

Substituting these in inequalities (3), (4) and (5), we get the required results. $\qquad\square$

Theorem 9. *Let G be a connected* (p, q)*-graph with* $p \geq 2$*. Then*

$$E_{BS} \leq k + \sqrt{(p-1)(tr(A_{BS}^2) - k^2)}, \tag{6}$$

for any real number k with the property $\sigma_1 \geq k \geq \sigma_p$.

Proof. By Lemma 4, we have

$$k \le \sigma_1 \le \frac{E_{BS}}{p} + \frac{1}{p}\sqrt{(p-1)(p\,tr(A_{BS}^2) - E_{BS}^2)}$$

$$\implies (pk - E_{BS})^2 \le (p-1)p\,tr(A_{BS}^2) - pE_{BS}^2 + E_{BS}^2$$

$$\implies p^2k^2 + E_{BS}^2 - 2pkE_{BS} + pE_{BS}^2 - E_{BS}^2 \le (p-1)p\,tr(A_{BS}^2)$$

$$\implies (E_{BS} - k)^2 \le (p-1)tr(A_{BS}^2) - (p-1)k^2$$

$$\implies E_{BS} \le k + \sqrt{(p-1)(tr(A_{BS}^2) - k^2)}. \qquad \square$$

By Lemma 4 and Theorem 9, we have the following result:

Corollary 7. *Let G be a (p,q)-graph with $p \ge 2$. Then,*

$$E_{BS} \le min\left\{\sigma_1 + \sqrt{(p-1)tr(A_{BS}^2) - \sigma_1^2}, \sigma_p + \sqrt{(p-1)tr(A_{BS}^2) - \sigma_p^2}\right\}.$$

Corollary 8. *Let G be a (p,q)-graph with $p \ge 2$. Then,*

$$E_{BS} \le \sqrt{2pF(G)}.$$

Proof. For $k = \sqrt{\dfrac{tr(A_{BS}^2)}{p}}, \sigma_1 \ge \sqrt{\dfrac{tr(A_{BS}^2)}{p}} \ge \sigma_p$, by Theorem 9, we have,

$$E_{BS} \le \sqrt{\frac{tr(A_{BS}^2)}{p}} + \sqrt{(p-1)\left[tr(A_{BS}^2) - \frac{tr(A_{BS}^2)}{p}\right]}$$

$$= \sqrt{\frac{tr(A_{BS}^2)}{p}} + \sqrt{\frac{(p-1)^2}{p}tr(A_{BS}^2)}$$

$$= p\sqrt{\frac{tr(A_{BS}^2)}{p}} \le \sqrt{2pF(G)}. \qquad \square$$

Lemma 5. *[28] For a sequence of non-negative real numbers $b_1 \ge b_2 \ge \cdots \ge b_n \ge 0$,*

$$\sum_{i=1}^{n} b_i + n(n-1)\left(\prod_{i=1}^{n} b_i\right)^{\frac{1}{n}} \le \left(\sum_{i=1}^{n} \sqrt{b_i}\right)^2 \le (n-1)\sum_{i=1}^{n} b_i + n\left(\prod_{i=1}^{n} b_i\right)^{\frac{1}{n}}. \qquad (7)$$

Theorem 10. *Let G be a (p,q)-graph with $p \ge 2$. Then*

$$\sqrt{tr(A_{BS}^2) + p(p-1)(|det A|)^{\frac{2}{p}}} \le E_{BS} \le \sqrt{(p-1)tr(A_{BS}^2) + p(|det A|)^{\frac{2}{p}}}.$$

Proof. Substituting $b_i = \sigma_i^2 (i = 1, 2, \cdots, p)$, in equation 7 of Lemma 5, we obtain

$$\sum_{i=1}^{p} \sigma_i^2 + p(p-1)\left(\prod_{i=1}^{p} \sigma i^2\right)^{\frac{1}{p}} \le \left(\sum_{i=1}^{p} \sqrt{\sigma i^2}\right)^2 \le (p-1)\sum_{i=1}^{p} \sigma i^2 + p\left(\prod_{i=1}^{p} \sigma i^2\right)^{\frac{1}{p}}.$$

$$\implies tr(A_{BS}^2) + p(p-1)(|det A|)^{\frac{2}{p}} \le E_{BS}^2 \le (p-1)tr(A_{BS}^2) + p(|det A|)^{\frac{2}{p}}.$$

Thus, we obtain the above inequality. $\qquad \square$

Theorem 11. *Let G be a (p,q)-graph with $p \ge 2$. Then*

$$\sqrt{2tr(A_{BS}^2)} \le E_{BS} \le \sqrt{p\,tr(A_{BS}^2)}.$$

Left equality holds if and only if $\lambda_1 = -\lambda_p$, $\lambda_2 = \lambda_3 = \cdots = \lambda_{p-1} = 0$. Right equality holds if and only if $\sigma_1 = \sigma_2 = \cdots = \sigma_p$.

Proof. We have,

$$\left(\sum_{i=1}^{p} \lambda i\right)^2 = 0 = \sum_{i=1}^{p} \lambda i^2 + 2\sum_{i<j} \lambda_i \lambda_j.$$

Thus,

$$\sum_{i=1}^{p} \lambda_i^2 = -2\sum_{i<j} \lambda_i \lambda_j = 2\left|\sum_{i<j} \lambda_i \lambda_j\right|.$$

Therefore,

$$E_{BS}^2 = \left(\sum_{i=1}^{p} |\lambda i|\right)^2 = \sum_{i=1}^{p} |\lambda i|^2 + 2\sum_{i<j} |\lambda_i||\lambda_j|$$

$$\geq \sum_{i=1}^{p} |\lambda i|^2 + 2\left|\sum_{i<j} \lambda_i \lambda_j\right| = 2\sum_{i=1}^{p} |\lambda i|^2 = 2tr(A_{BS}^2).$$

Thus the left inequality is proved.

The equality holds if and only if $\sum_{i<j} |\lambda_i||\lambda_j| = |\sum_{i<j} \lambda_i \lambda_j|$, that is when $\lambda_1 = -\lambda_p$, $\lambda_2 = \lambda_3 = \cdots = \lambda_{p-1} = 0$.

The Lagrange's identity says, for $(a) = (a_1, a_2, \cdots, a_n)$ and $(b) = (b_1, b_2, \cdots, b_n)$, the two sets of real numbers,

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \left(\sum_{i=1}^{n} a_i b_i\right)^2 = \sum_{1 \leq i < j \leq n} (a_i b_j - a_j b_i)^2.$$

Substituting $a_i = \sigma i, b_i = 1, (i = 1, 2, \cdots, p)$ in the above identity, we get,

$$p\sum_{i=1}^{p} \sigma_i^2 - \left(\sum_{i=1}^{p} \sigma i\right)^2 = \sum_{1 \leq i < j \leq p} (\sigma_i - \sigma_j)^2.$$

$\sum_{1 \leq i < j \leq p} (\sigma_i - \sigma_j)^2 \geq 0$ with equality if and only if $\sigma_1 = \sigma_2 = \cdots = \sigma_p$. Thus we have,

$$p\sum_{i=1}^{p} \sigma_i^2 - \left(\sum_{i=1}^{p} \sigma i\right)^2 \geq 0 \implies p\, tr(A_{BS}^2) \geq E_{BS}^2.$$

Thus the right inequality is obtained.   □

Corollary 9. *Let G be a (p,q)-graph with $p \geq 2$. If $\sqrt{b_u^2 + b_v^2} \geq c > 0$, then*

$$2c\sqrt{q} \leq 2\sqrt{cBS(G)} \leq E_{BS}.$$

Theorem 12. *For any connected (p,q)-graph with $p \geq 2$,*

$$\frac{\sqrt{2}}{(p-1)} BS(G) \leq E_A(G) \leq \left(\sqrt{2}pBS(G)\right)^{\frac{1}{2}}.$$

Proof. Let G be a connected (p,q)-graph with $p \geq 2$.
By Theorem 3, we have

$$q \leq \frac{BS(G)}{\sqrt{2}} \qquad and \qquad q \geq \frac{BS(G)}{\sqrt{2}(p-1)}. \tag{8}$$

McClelland inequality is $E_A(G) \leq \sqrt{2pq}$. Thus from first inequality of (8) and McClelland inequality, we have the required left inequality. Also, the required right inequality follows from the second inequality of (8).   □

3. Conclusion

Spectral graph theory has a wide variety of applications in many computational sciences. In view of the above fact, here, we discussed the properties, bounds and characterizations of the newly introduced Block Sombor Index and its Matrix representation along with Block Sombor Energy and Spectral radius of a graph.

Author Contributions: All authors contributed equally to the writing of this paper. All authors read and approved the final manuscript.

Conflicts of Interest: The authors declare no conflict of interest.

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