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Research Paper

On Sombor index of extremal graphs

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Abstract. Let G be a finite simple graph. The Sombor index of G is defined as $\sum_{uv\in E(G)}\sqrt{d_u^2+d_v^2}$ where d_u and d_v represent the degrees of vertices u and v in G, respectively. The sum of the absolute values of the adjacency eigenvalues defines the energy of a graph. This paper aims to enhance the current connections between the Sombor index and the energy of graphs. Additionally, we provide some upper bounds for the Sombor index of triangle-free, square-free, K_r-free and tripartite graphs in terms of order, size and minimum degree.

Keywords. C_4-free graph, energy, Sombor index, tripartite graph, triangle-free graph.
Mathematics Subject Classification (2020): 05C07, 05C09, 05C35.

1 Introduction

Let $G=(V(G),E(G))$ be a simple graph (undirected graph with no loop or multiple edge), where $V(G)$ and $E(G)$ denote the set of its vertices and edges, respectively. Throughout this paper, the number of vertices and edges in G are referred to as the order and size of G, respectively. For a vertex $v\in V(G)$, the degree of v, d_v, is the number of edges that are incident to v. The open neighborhood of v is the set $N(v)=\{u\in V(G): uv\in E(G)\}$. Also, Δ and δ denote the maximum and minimum degrees of G, respectively. A path and a complete graph of order n, is denoted by P_n and K_n, respectively. A complete tripartite graph is a tripartite graph (i.e., the set of vertices decomposed into three disjoint sets such that no two vertices within the same set are adjacent) such that every vertex of each set is adjacent

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to every vertex in the other sets. If there are p, q and r vertices in three sets, the complete tripartite graph is denoted by $K_{p,q,r}$.

For an arbitrary graph G, the concept of energy of G was introduced by Gutman [10] in 1978 as the sum of the absolute values of adjacency eigenvalues of G. In this work, the energy of a graph G, is shown by $\mathcal{E}(G)$. Next, in 2021 the Sombor index of G, $SO(G)$, was defined as $\sum_{uv\in E(G)}\sqrt{d_u^2+d_v^2}$ by him [9]. Some results for the Sombor index and the energy of graphs can be found in [1]- [4], [6]- [8], [11]- [21], [23], [25]- [27] and the references therein.

2 Preliminaries

Theorem 2.1. *For an arbitrary graph G with vertices $v_1,\dots,v_n$ we have*

$$\mathcal{E}(G)\le \sum_{i=1}^{n}\sqrt{d_{v_i}}\le\sqrt{2mn}.$$

Moreover, these inequalities become equalities for $G\cong tK_2$ and $\Delta=\delta$, respectively.

Proof. See Theorem 3.1 and Proposition 3.2 of [5]. □

Theorem 2.2. *[9, Thm. 3] For any tree T of order n, $SO(P_n)\le SO(T)\le SO(S_n)$.*

Theorem 2.3. *[25, Thm. 3.1] Let G be a connected graph of order n. If $n\ge 3$, then $\mathcal{E}(G)<SO(G)$.*

Theorem 2.4. *[4, Thm. 3] If G is a connected graph of order n which is not $P_n (n\le 8)$, then $\mathcal{E}(G)\le\dfrac{SO(G)}{2}$.*

Theorem 2.5. *[22] Let G be a C_4-free graph of order $n\ge 4$ and size m. Then $m\le\dfrac{n+n\sqrt{4n-3}}{4}$.*

Theorem 2.6. *[24] Let G be a K_r-free graph of order n and size m. Then $m\le(\dfrac{r-2}{r-1})\dfrac{n^2}{2}$.*

3 Results and Discussion

For a natural number $n\ge 2$, it is well-known that $\mathcal{E}(P_n)=2/(\sin\dfrac{\pi}{2n+2})-2$ for any even number n and $\mathcal{E}(P_n)=2/(\tan\dfrac{\pi}{2n+2})-2$, otherwise. Due to the difficulty of calculating the exact value of $\mathcal{E}(P_n)$ with the stated formula, some upper bounds for $\mathcal{E}(P_n)$ have been introduced in various articles. Clearly by Theorem 2.1, $\mathcal{E}(P_n)\le(n-2)\sqrt{2}+2$. We improve this upper bound. To prove the desired inequality, we first introduce an upper bound for the energy of graphs in terms of Sombor index and minimum degree.

Theorem 3.1. *Let G be a graph of order $n\ge 3$. Then $\mathcal{E}(G)\le\dfrac{SO(G)}{\delta}$.*

Proof. It is sufficient to prove the theorem in the case where G is connected. If G is a tree, then $\delta = 1$ and so $\mathcal{E}(G) < SO(G)$, by Theorem 2.3. Else, G is a graph of size m with $m \geq n$ and hence by Theorem 2.1, we have

$$\frac{SO(G)}{\delta} = \sum_{uv\in E(G)} \sqrt{\frac{d_u^2 + d_v^2}{\delta^2}} \geq \sum_{uv\in E(G)} \sqrt{\frac{\delta^2 + \delta^2}{\delta^2}} = \sqrt{2}m = \sqrt{2m^2} \geq \sqrt{2mn} \geq \mathcal{E}(G),$$

and the proof is complete. □

Theorem 3.2. *For any P_n with $(n \neq 2,4)$, we have $\mathcal{E}(P_n) \leq \sqrt{2}(n-1)$. Moreover, the equality holds if and only if $n = 1,3$.*

Proof. Clearly, the result holds for $n = 1$. Also, $\mathcal{E}(P_3) = 2\sqrt{2} = \sqrt{2}(3-1)$. Further, according to Theorem 2.4, for $n \geq 9$ we have:

$$\mathcal{E}(P_n) \leq \frac{SO(P_n)}{2} = \frac{2(n-3)\sqrt{2} + 2\sqrt{5}}{2} < (n-3)\sqrt{2} + 2\sqrt{2} = \sqrt{2}(n-1).$$

Otherwise, by Table 1 in [4, Theorem 3], we have:

If $n = 5$, then $\mathcal{E}(P_n) \approx \dfrac{SO(P_n)}{2} + 0.4 = 2\sqrt{2} + \sqrt{5} + 0.4 < \sqrt{2}(n-1)$.

If $n = 6$, then $\mathcal{E}(P_n) \approx \dfrac{SO(P_n)}{2} + 0.51 = 3\sqrt{2} + \sqrt{5} + 0.51 < \sqrt{2}(n-1)$.

If $n = 7$, then $\mathcal{E}(P_n) \approx \dfrac{SO(P_n)}{2} + 0.17 = 4\sqrt{2} + \sqrt{5} + 0.17 < \sqrt{2}(n-1)$.

If $n = 8$, then $\mathcal{E}(P_n) \approx \dfrac{SO(P_n)}{2} + 0.22 = 5\sqrt{2} + \sqrt{5} + 0.22 < \sqrt{2}(n-1)$.

Therefore, for any natural number n, $n > 4$, we have $\mathcal{E}(P_n) < \sqrt{2}(n-1)$ and the result follows. □

In [11, Theorem 4] the authors proved that for a bipartite graph G, $\mathcal{E}(G) \leq \sqrt{\frac{2}{\delta^3}}SO(G)$. Next, in [3, Theorem 11] the authors proved this upper bound for arbitrary graphs. In the following, we give another proof.

Theorem 3.3. *Let G be a graph. Then $\mathcal{E}(G) \leq \sqrt{\frac{2}{\delta^3}}SO(G)$. Moreover, the equality holds if and only if $G = tK_2$, for some positive integer t.*

Proof. Let G be a graph of order n and size m. By Theorem 2.1 and the inequality $m \geq \frac{n\delta}{2}$, we have:

$$\begin{aligned}\frac{SO(G)}{\delta} &= \sum_{uv\in E(G)} \sqrt{\frac{d_u^2 + d_v^2}{\delta^2}} \geq \sum_{uv\in E(G)} \sqrt{\frac{\delta^2 + \delta^2}{\delta^2}} = \sqrt{2}m \\ &= \sqrt{2}\sqrt{m^2} \geq \sqrt{\frac{2m\delta n}{2}} = \sqrt{\frac{\delta}{2}}\sqrt{2mn} \geq \sqrt{\frac{\delta}{2}}\mathcal{E}(G).\end{aligned}$$

Also, if the equality holds, then every connected component of G is isomorphic to K_2 and we are done. □

In [25], the authors stated the following lower bound for the Sombor index of connected graphs in terms of their energy and maximum degree.

Theorem 3.4. *[25, Theorem 3.2] If G is a connected graph of order $n \geq 3$, then*

$$SO(G) \geq \begin{cases} \frac{\delta}{\sqrt{2}}(\mathcal{E}(G)^2 - n(n-1)\Delta) & if\ \delta \geq 2, \\ \frac{\sqrt{5}}{2}(\mathcal{E}(G)^2 - n(n-1)\Delta) & if\ \delta = 1. \end{cases}$$

In the following, we improve and simplify the lower bound obtained in Theorem 3.4 as follows:

Theorem 3.5. *Let G be a connected graph of order $n \geq 3$ which is not P_n $(n \leq 6)$. Then*

$$SO(G) \geq \begin{cases} \frac{n\delta^2}{\sqrt{2}} \geq \sqrt{8}n & if\ \delta \geq 2, \\ \sqrt{5}n & if\ \delta = 1. \end{cases}$$

Proof. Let $|E(G)| = m$. First assume that $\delta = 1$. So $2m = \sum_{i=1}^{n} d(v_i) \leq (n-1)\Delta + 1$ and consequently $2mn \leq n(n-1)\Delta + n$. Therefore, $2mn - n(n-1)\Delta \leq n$ and hence according to Theorems 2.1 and 3.4, we have

$$\frac{\sqrt{5}}{2}(\mathcal{E}(G)^2 - n(n-1)\Delta) \leq \frac{\sqrt{5}}{2}(2mn - n(n-1)\Delta) < \sqrt{5}n.$$

Next, we prove that $SO(G) \geq \sqrt{5}n$. To show this, we consider the following three cases:
Case 1. G is not a tree. Thus, $m \geq n$. Also, the weight of each edge is at least $\sqrt{5}$. This implies that $SO(G) \geq \sqrt{5}n$.
Case 2. G is a tree of order $n \geq 7$. Since, P_n has the minimum Sombor index among all trees of order n by Theorem 2.2, we have

$$SO(G) \geq SO(P_n) = (n-3)\sqrt{8} + 2\sqrt{5} \geq \sqrt{5}n.$$

Case 3. G is a tree of order $3 \leq n \leq 6$. By an easy computation one can see that the inequality holds except for $P_r, r = 3, \ldots, 6$.
Now, we assume that $\delta \geq 2$. Obviously, $2m \leq (n-1)\Delta + \delta$ and so $2mn \leq n(n-1)\Delta + n\delta$. Therefore, $2mn - n(n-1)\Delta \leq n\delta$ and hence by Theorems 2.1 and 3.4, we have

$$\frac{\delta}{\sqrt{2}}(\mathcal{E}(G)^2 - n(n-1)\Delta) \leq \frac{\delta}{\sqrt{2}}(2mn - n(n-1)\Delta) \leq \frac{n\delta^2}{\sqrt{2}}.$$

But, $SO(G) \geq \frac{n\delta}{2}\sqrt{\delta^2 + \delta^2} = \frac{\sqrt{2}n\delta^2}{2} = \frac{n\delta^2}{\sqrt{2}}$ and the proof is complete. □

Theorem 3.6. *Let G be a C_4-free graph of order n and size m. Then $SO(G) \leq m\sqrt{\delta^2 + (n-\delta+1)^2}$.*

Proof. First note that if u and v are two adjacent vertices of $V(G)$, then $|N(u) \cap N(v)| \leq 1$. To see this, let x and y be two common neighbors of both u and v. Then $u - x - v - y - u$ is a cycle of length 4, a contradiction. So $|N(v)| - 1 \leq (n-2) - (|N(u)| - 1) + 1$ and this implies that $d_u + d_v \leq (n-1) + 2 = n+1$. Therefore, we have:

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \leq \sum_{uv \in E(G)} \sqrt{d_u^2 + (n+1-d_u)^2}.$$

Now, we consider the function $f(x) = x^2 + (n+1-x)^2$ on $\delta \leq x \leq \Delta$. By a simple calculation, it can be seen that $f(x)$ has a unique minimum at $x = \frac{n+1}{2}$. Also $\delta \leq \frac{n+1}{2}$, since for any two adjacent vertices u and v we have $2\delta \leq d_u + d_v \leq n+1$. Now, we consider two following cases:
Case 1. If $\delta \leq \Delta \leq \frac{n+1}{2}$, then $f(x)$ is a decreasing function on $[\delta, \Delta]$ and hence $f(\delta) = \delta^2 + (n+1-\delta)^2$ is the maximum value of $f(x)$ on $[\delta, \Delta]$.
Case 2. If $\delta \leq \frac{n+1}{2} \leq \Delta$, then $f(x)$ is a decreasing function on $\delta \leq x \leq \frac{n+1}{2}$ and an increasing function on $\frac{n+1}{2} \leq x \leq \Delta$. Hence the maximum value of $f(x)$ on $[\delta, \Delta]$ occurs in δ or Δ. We claim that $f(\delta) \geq f(\Delta)$. For proving the claim, let uv be an edge in $E(G)$ with $d_u = \Delta$. Since $d_v \geq \delta$, we have $\Delta + \delta \leq d_u + d_v \leq n+1$. Therefore, $\delta^2 - \Delta^2 \geq (n+1)(\delta - \Delta)$ and hence $2\delta^2 - 2(n+1)\delta \geq 2\Delta^2 - 2(n+1)\Delta$. Thus $2\delta^2 - 2(n+1)\delta + (n+1)^2 \geq 2\Delta^2 - 2(n+1)\Delta + (n+1)^2$ and consequently $\delta^2 + (n+1-\delta)^2 \geq \Delta^2 + (n+1-\Delta)^2$. So $f(\delta) \geq f(\Delta)$ and the claim is proven.
Now, we have

$$SO(G) \leq \sum_{uv \in E(G)} \sqrt{d_u^2 + (n+1-d_u)^2} \leq m\sqrt{\delta^2 + (n+1-\delta)^2}$$

and the proof is complete. □

Corollary 3.7. *Let G be a C_4-free graph of order n. Then*

$$SO(G) \leq \frac{n + n\sqrt{4n-3}}{4} \sqrt{\delta^2 + (n-\delta+1)^2}.$$

Proof. The proof is clear by Theorems 2.5 and 3.6. □

Theorem 3.8. *Let G be a triangle-free graph of order n and size m. Then $SO(G) \leq m\sqrt{\delta^2 + (n-\delta)^2}$.*

Proof. The proof is similar to the method used in the proof of Theorem 3.6. □

Corollary 3.9. *Let G be a triangle-free graph of order n. Then $SO(G) \leq \frac{n^2}{4}\sqrt{\delta^2 + (n-\delta)^2}$.*

Proof. The proof is clear by Theorems 2.6 and 3.8. □

Remark 3.10. *As we showed in the proof of Theorem 3.6, for C_4-free graphs of order n, we have $\Delta + \delta \leq n+1$. It can be proved similarly that $\Delta + \delta \leq n$ for triangle-free graphs of order n. Therefore, all the upper bounds stated for Sombor index, Reduced Sombor index, and Sombor coindex in [7, Theorem 2], [18, Theorem 2.14] and [21, Theorem 1] should be modified.*

In [7] the authors proved the following upper bound for the Sombor index of bipartite graphs.

Theorem 3.11. *[7, Theorem 3] Let G be a bipartite graph of order n. Then*

$$SO(G) \leq \begin{cases} \dfrac{n^3}{4\sqrt{2}} & if\, n \equiv 0 \pmod 2, \\ \dfrac{(n^2-1)\sqrt{n^2+1}}{4\sqrt{2}} & if\, n \equiv 1 \pmod 2. \end{cases}$$

Now, we introduce an upper bound for the Sombor index of tripartite graphs. Clearly, $K_{2,1,1}$ is the only tripartite graph of order 4 and by an easy computation we have $SO(K_{2,1,1}) = 4\sqrt{13} + 3\sqrt{2}$. For the other tripartite graphs we state the following.

Theorem 3.12. *Let $G \neq K_{2,1,1}$ be a tripartite graph of order n. Then*

$$SO(G) \leq \begin{cases} 6\sqrt{2}k^3 & n = 3k, \\ 4(k+1)^2[\frac{1}{\sqrt{2}}k + (k-1)\sqrt{1+(\frac{k}{k+1})^2}] & n = 3k+1, \\ 4(k+1)^2[\frac{1}{\sqrt{2}}(k+\frac{1}{2}) + k\sqrt{1+(\frac{2k+1}{2k+2})^2}] & n = 3k+2. \end{cases}$$

Proof. Suppose that $G = G(X,Y,Z)$ is a tripartite graph with $|X| = p$, $|Y| = q$, $|Z| = r$, $n = p+q+r \neq 4$ and $p \geq q \geq r$. Clearly, $SO(G) \leq SO(K_{p,q,r})$ and equality holds if and only if $G \cong K_{p,q,r}$. Therefore,

$$SO(G) \leq SO(K_{p,q,r}) = pq\sqrt{(n-p)^2+(n-q)^2} + p(n-p-q)\sqrt{(n-p)^2+(p+q)^2} + q(n-p-q)\sqrt{(n-q)^2+(p+q)^2}.$$

Let us consider the function

$$f(x,y) = xy\sqrt{(n-x)^2+(n-y)^2} + x(n-x-y)\sqrt{(n-x)^2+(x+y)^2} + y(n-x-y)\sqrt{(n-y)^2+(x+y)^2},$$

where $\lceil\frac{n}{3}\rceil \leq x \leq n-2$ and $1 \leq y \leq x$. In order to have a better vision of this function, its graph is displayed for different values of parameter n in Fig. 1.

The maximum value of $f(x,y)$ is determined from the common solutions of equations $f_x = 0$ and $f_y = 0$. On the other hand, $f(x,y)$ is symmetric (i.e. $f(x,y) = f(y,x)$). Therefore, we should obtain the maximum points of the function $f(x,x)$. Consider

$$g(x) = f(x,x) = \sqrt{2}x^2(n-x) + 2x(n-2x)\sqrt{(n-x)^2+4x^2}$$

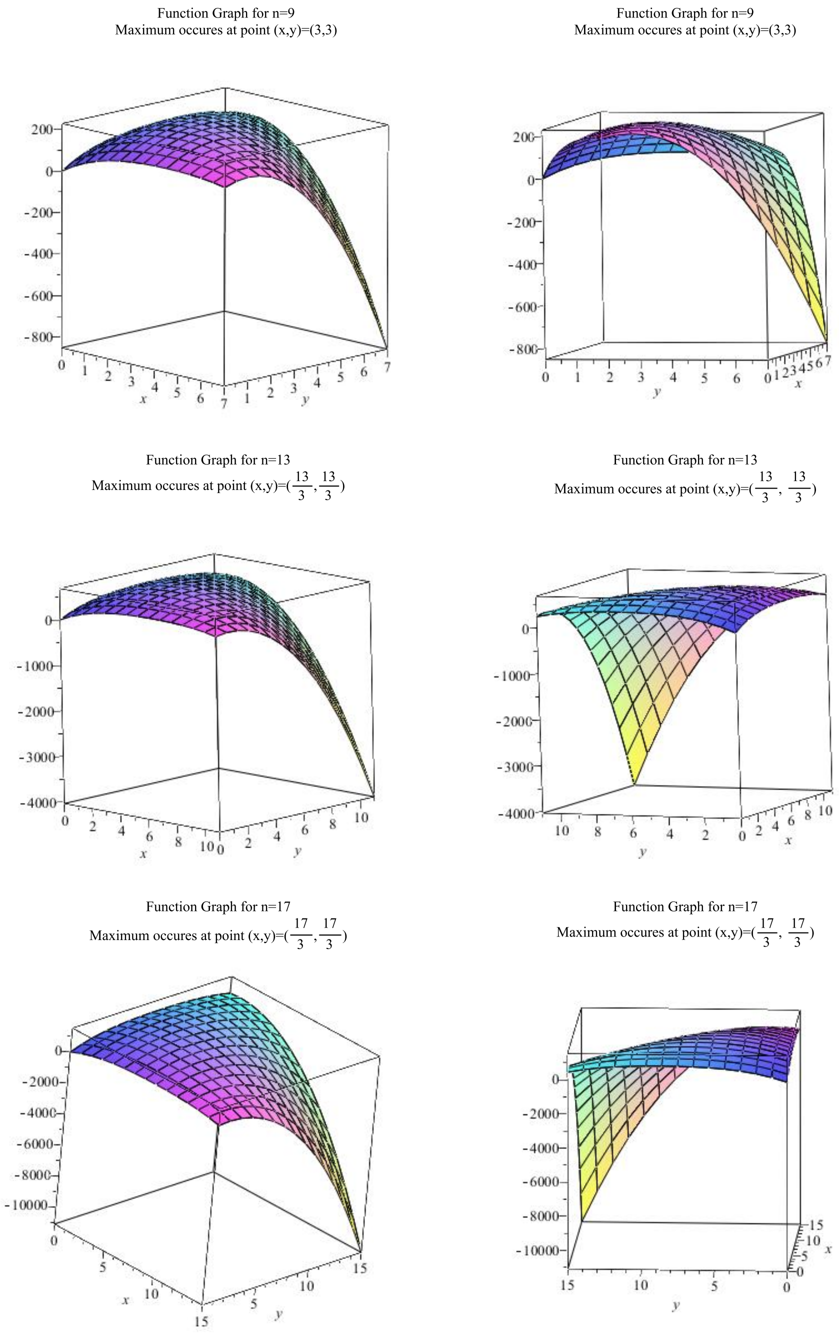

Figure 1. graph of function f for $n = 9, 13, 17$.

for $\lceil \frac{n}{3} \rceil \leq x \leq \frac{n-1}{2}$. By performing calculations, it is shown that $g'(x) \leq 0$ on $[\lceil \frac{n}{3} \rceil, \frac{n-1}{2}]$. Therefore, $g(x)$ is a decreasing function and consequently, $f(x,y)$ obtains its maximum value at $x = y = \lceil \frac{n}{3} \rceil$. Hence

$$SO(G) \leq \sqrt{2}\lceil \frac{n}{3} \rceil^2 (n - \lceil \frac{n}{3} \rceil) + 2\lceil \frac{n}{3} \rceil (n - 2\lceil \frac{n}{3} \rceil) \sqrt{(n - \lceil \frac{n}{3} \rceil)^2 + 4\lceil \frac{n}{3} \rceil^2}$$

and the result follows. □

Theorem 3.13. *Let G be a K_r-free graph of order n. Then $SO(G) \leq (\frac{r-2}{r-1})\frac{n^2(n-1)}{\sqrt{2}}$.*

Proof. The degree of each vertex of G is at most $n-1$. Therefore, for any $uv \in E(G)$, we have $\sqrt{d_u^2 + d_v^2} \leq \sqrt{2}(n-1)$ and so by Theorem 2.6

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \leq (\frac{r-2}{r-1})\frac{n^2}{2}(\sqrt{2}(n-1))$$

and we are done. □

4 Conclusion

The concept of graph energy was introduced by Gutman in 1978, originating from theoretical chemistry. It is defined as the sum of the absolute values of all eigenvalues of the graph's adjacency matrix. This concept is related to the total π-electron energy in a molecule, represented by a molecular graph.

Degree-based and distance-based indices are two essential types of indices in chemical graph theory. These indices are graph invariants used in quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies. Numerous indices defined to date have been proven to be valuable for modeling various physical, chemical, pharmaceutical, and other molecular properties.

In this paper, we investigated the Somber index as a degree-based index in mathematical chemistry. We also enhanced the current connections between the Sombor index and the energy of graphs. Additionally, we provided upper bounds for the Sombor indices of C_3, C_4 and K_r-free tripartite graphs in terms of order, size, and minimum degree.

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