Iranian Journal of Mathematical Chemistry

IJMC

DOI: 10.22052/IJMC.2024.254674.1850
Vol. 16, No. 1, 2025, pp. 33-38
Research Paper

Lower and Upper Bounds between Energy, Laplacian Energy, and Sombor Index of Some Graphs

Hasan Barzegar[1]*

[1]Department of Mathematics, Tafresh University, Tafresh 39518-79611, Iran

Keywords:
Energy of a graph,
Laplacian energy,
Sombor index

AMS Subject Classification (2020):

05C07; 05C09; 05C50

Article History:

Received: 1 April 2024

Accepted: 14 July 2024

Abstract

Ivan Gutman has introduced two essential indices; the energy of a graph G, and the Sombor index of that. $\varepsilon(G)$, which stands for the first index, is the sum of the absolute values of all eigenvalues related to the adjacency matrix of the graph G. The second, defined as $SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2}$, where d_u and d_v are the degrees of vertices u and v in G, respectively. It was proved that if G is a graph of order at least 3, then $\varepsilon(G) \leq So(G)$ and if G is a connected graph of order n that is not P_n for $n \leq 8$, then $\varepsilon(G) \leq \frac{So(G)}{2}$. In this paper, we have strengthened these results and will obtain several lower and upper bounds between the energy of a graph, Laplacian energy, and the Sombor index.

1 Introduction

Let $G = (V(G), E(G))$ be a simple undirected graph of order n with the set of vertices $V(G)$ and the set of edges $E(G)$ which $\mid E(G) \mid= m$, called the *size* of the graph G. The energy of graphs is highly appealing due to their significance in the field of mathematical chemistry, and many mathematicians have obtained many upper and lower bounds for it in terms of m, n, and some topological indices such as the Randik and the Sombor index. Topological indices on graphs are a group of numerical parameters that predict specific physical and chemical characteristics of molecules, for example, the Winer index is directly related to the boiling point of some materials or the Sombor index is directly related to the Molecular mass of alkanes with a limiting factor 1.009, see [1]. The *Sombor index* is one of the novel topological indices, introduced by Gutman. It's calculated using the formula $SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2 + d_v^2}$. Here d_u and d_v respectively represent the degrees of vertices u and v in the graph G.

The *adjacency matrix* of a graph G, denoted by $A(G)$, is characterized by its elements such that a_{ij} equals 1 if the vertices v_i and v_j are adjacent and equals 0 if they are not. Also, the *degree matrix* of G, represented as $D(G)$, is the matrix whose entries are as $a_{ii} = d_{u_i}$ and 0 otherwise. Let the *Laplacian matrix* of graph$G$ be defined as $L(G) = D(G) - A(G)$. Also,

*Corresponding author
E-mail address: barzegar@tafreshu.ac.ir (H. Barzegar)
Academic Editor: Boris Furtula

assume the eigenvalues of the matrix $A(G)$ are given by the real numbers $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, while the nonnegative real numbers $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n \geq 0$ are the sequence of eigenvalues of $L(G)$. The energy of the graph G is given by the following formula:

$$\varepsilon(G) = \sum_{i=1}^{n} \mid \lambda_i \mid,$$

and the *Laplacian energy* of G is calculated using

$$L\varepsilon(G) = \sum_{i=1}^{n} \mid \mu_i - \frac{2m}{n} \mid .$$

It was proved that if G is a graph of order at least 3 or the minimum degree of vertices are greater than 2, then $\varepsilon(G) \leq So(G)$, see [2, 3].

Theorem 1.1. *([2]). For any graph G where the minimum vertex degree δ is at least 2, it holds that $\varepsilon(G) \leq So(G)$.*

Theorem 1.2. *([3]). Assume that G is a connected graph with n vertices. When n is 3 or more, it holds that $\varepsilon(G) \leq So(G)$.*

Also, if G is a connected graph of order n which is not $P_n(n \leq 8)$, then $\varepsilon(G) \leq \frac{So(G)}{2}$, see [4].

Theorem 1.3. *([4, Theorem 3]). Assume that G is a connected graph of order n that is not P_n, for $n \leq 8$. Then $\varepsilon(G) \leq \frac{So(G)}{2}$.*

Also, a large number of articles have been written on the topic of energy, Laplacian energy and the Sombor index of graphs, for example see [5–10]. Lately, the energy of a vertex has been developed by Arizmendi and et al. in [11]. In this paper, we have strengthened these results and obtained several lower and upper bounds between the energy of a graph and the Laplacian energy versus the Sombor index.

2 Main results

The objective of this section is to improve the bound on the energy of graph and the Laplacian energy based on its Sombor index.

Denote a complete graph, an edgeless graph, and a path of order n by K_n, $\bar{K_n}$, and P_n, respectively, and put the notation $K_{a,b}$ for a complete bipartite graph of order $n = a+b$. First, the following two lemmas are needed in the sequel.

Lemma 2.1. *([12, Corollary 3.1]). Let G represent a simple graph characterized by $n \geq 2$ vertices and m edges. It follows that $So(G) \geq \frac{2\sqrt{2}m^2}{n}$.*

Lemma 2.2. *([13, Theorem 5.4.1]). For any graph G consisting of n vertices and m edges, it holds that, $\varepsilon(G) \leq \sqrt{2mn}$.*

Now, in the following theorem, we have improved the upper bound of the energy of a graph.

Theorem 2.3. *For any simple graph G consisting of n vertices and m edges, we have:*

$$\varepsilon(G) \leq \frac{So(G)}{2(\frac{m}{n})^{\frac{3}{2}}}.$$

The equality is satisfied if and only if $G = \bar{K_n}$ or $\bigcup_{i=1}^{m} K_2$.

Proof. By McClland bound which is $\varepsilon(G) \leq \sqrt{2mn}$, see [13, Theorem 5.4.1], and Lemma 2.1 we get, $\varepsilon(G) \leq \sqrt{2mn} = \frac{\frac{2\sqrt{2}m^2}{n}}{2(\frac{m}{n})^{\frac{3}{2}}} \leq \frac{So(G)}{2(\frac{m}{n})^{\frac{3}{2}}}$.
For the equality, It is not difficult to check that for graphs $G = \bar{K_n}$ and $G = \bigcup_{i=1}^{m} K_2$, $\varepsilon(G) = \frac{So(G)}{2(\frac{m}{n})^{\frac{3}{2}}} = 2m$ and by Cauchy-Schwarz inequality, $\varepsilon(G) = \sqrt{2mn}$ if and only if for each $1 \leq i \leq n$, $|\lambda_i| = 1$. Thus the equality is satisfied only when $G = \bar{K_n}$ or $G = \bigcup_{i=1}^{m} K_2$. ■

Corollary 2.4. (i) *If a graph G has at least one cyclic, then it follows that $\varepsilon(G) \leq \frac{So(G)}{\frac{2m}{n}}$.*

(ii) *Since $\frac{2m}{n} \geq \delta$, so $2(\frac{m}{n})^{\frac{3}{2}} \geq \frac{\delta^{\frac{3}{2}}}{\sqrt{2}}$ and consequently, for any simple graph G, we have, $\varepsilon(G) \leq \frac{So(G)}{\frac{\delta^{\frac{3}{2}}}{\sqrt{2}}}$.*

The following result is derived as a consequence of Theorem 1.3 and Theorem 2.3.

Theorem 2.5. *If G is a connected graph of order n which is not $P_n (n \leq 8)$, then*

$$\varepsilon(G) \leq \frac{So(G)}{max\{2, 2(\frac{m}{n})^{\frac{3}{2}}\}}.$$

In [2], Ülker and et al. established several lower bounds for the energy of a graph, which are expressed in relation to the Sombor index.

Theorem 2.6. *([2]). Suppose that G is a graph with a maximum degree of $\Delta(G)$. Then we have $\varepsilon(G)\Delta(G)^3 \geq So(G)$.*

Theorem 2.7. *([2]). The inequality $\varepsilon(G)\Delta(G)^2 \geq So(G)$ is valid if G represents a Δ-regular graph.*

In the following, we improve this bound and introduce several new lower bounds on the energy of a graph versus its Sombor index. To do this, we mention that the energy of a graph is the total of its vertex energies, i.e.,

$$\varepsilon(G) = \varepsilon(x_1) + \varepsilon(x_2) \cdots \varepsilon(x_n),$$

where $\varepsilon(x_i)$ is the energy of the vertex x_i, stated in [11].

Theorem 2.8. *([11]). Let G be a graph that contains at least one edge. For every vertex $x_i \in V(G)$, we have $\varepsilon(x_i) \geq \frac{d_i}{\Delta_G}$. Equality is established if and only if $G \cong K_{d,d}$.*

The subsequent lemma directly follows from the aforementioned theorem.

Lemma 2.9. *Assume that G is a graph whose maximum degree is denoted by Δ. Then*

$$\varepsilon(G) \geq \frac{2m}{\Delta},$$

where equality is achieved if and only if $G \cong K_{d,d}$.

Proof. Using Theorem 2.8, $\varepsilon(G) = \Sigma_{i=1}^{n}\varepsilon(x_i) \geq \Sigma_{i=1}^{n}\frac{d_i}{\Delta} = \frac{2m}{\Delta}$. ■

Now, we are ready to improve the upper bound on the energy of a graph versus its Sombor index.

Theorem 2.10. *Assume that G is a graph whose maximum degree is denoted by Δ. Then*

$$\varepsilon(G) \geq \frac{So(G)}{\frac{\Delta^2}{\sqrt{2}}}.$$

Here, equality is achieved if and only if G is a regular complete bipartite graph.

Proof. Since $So(G) = \Sigma_{uv\in V(G)}\sqrt{d_u^2 + d_v^2} \leq \Sigma_{uv\in V(G)}\sqrt{\Delta^2 + \Delta^2} = \sqrt{2}m\Delta$, by Lemma 2.9 we get,

$$\varepsilon(G) \geq \frac{2m}{\Delta} = \sqrt{2}m\Delta\frac{\sqrt{2}}{\Delta^2} \geq \frac{So(G)}{\frac{\Delta^2}{\sqrt{2}}}.$$

It is easily demonstrable that the equation $So(G) = \sqrt{2}m\Delta$ holds true if and only if the graph G is a Δ-regular graph. According to Lemma 2.9, equality is satisfied if and only if $G \cong K_{d,d}$. ■

Theorem 2.11. *For every simple graph G with n vertices and m edges,*

$$\varepsilon(G) \geq \frac{So(G)}{\frac{\sqrt{m}\Delta}{\sqrt{2}}}.$$

Here, a necessary and sufficient condition for equality is that G must be a regular complete bipartite graph.

Proof. By [14], $2\sqrt{m} \leq \varepsilon(G)$ and the equality is satisfied if and only if G is a complete bipartite graph plus arbitrarily many isolated vertices. Also, it is not difficult to check that $So(G) \leq \sqrt{2}m\Delta$ with equality if and only if G is a regular graph. So $So(G) \leq \sqrt{2}m\Delta = (2\sqrt{m})\frac{\sqrt{m}\Delta}{\sqrt{2}} \leq \frac{\sqrt{m}\Delta}{\sqrt{2}}\varepsilon(G)$ with equality if and only if G is a regular complete bipartite graph. ■

In the sequel, we present an upper bound and a lower bound for Laplacian energy in terms of the Sombor index.

Theorem 2.12. *For any simple graph G characterized by n vertices and m edges, we have, $L\varepsilon(G) \leq \frac{So(G)}{\frac{\sqrt{2}m}{n}}$.*

Proof. By [13, Theorem 5.7.3], $L\varepsilon(G) \leq \sqrt{nM_1(G) + 2mn - 4m^2}$ where $M_1(G)$ is the first zagreb index. It is not difficult to check that $2mn - 4m^2 \leq 0$. So $L\varepsilon(G) \leq \sqrt{nM_1(G)}$. By [12, Theorem 3.1], $M_1(G) \leq \sqrt{2}So(G)$ and by Lemma 2.1, $\sqrt{2}n \leq \frac{n^2 So(G)}{2m^2}$. Thus $L\varepsilon(G) \leq \sqrt{nM_1(G)} \leq \sqrt{\sqrt{2}nSo(G)} \leq \sqrt{\frac{n^2 So(G)}{2m^2}.So(G)} = \frac{So(G)}{\frac{\sqrt{2}m}{n}}$. ■

Corollary 2.13. *For any simple graph G consisting of n vertices and m edges, we have:*

(i) *If G is a tree, then $\frac{\sqrt{2}m}{n} \geq 1$ and hence $L\varepsilon(G) \leq So(G)$.*

(ii) *If G is not a tree, then $m \geq n$ and hence $L\varepsilon(G) \leq \frac{So(G)}{\sqrt{2}}$.*

(iii) *Since $2m \geq n\delta$, then $L\varepsilon(G) \leq \frac{So(G)}{\frac{\delta}{\sqrt{2}}}$.*

Proof. In the case (i), note that for $n \leq 2$, the result is obtained by direct calculation. ■

Theorem 2.14. *For any simple graph G consisting of n vertices and m edges we have, $L\varepsilon(G) \geq \frac{So(G)}{\frac{m}{\sqrt{2}n}}$.*

Proof. By [13, Theorem 5.7.3],

$$\begin{aligned} L\varepsilon(G) &\geq 2\sqrt{M_1(G) + 2m - \frac{4m^2}{n}} \geq 2\sqrt{M_1(G)} \\ &\geq 2\sqrt{\frac{4m^2}{n}} = \frac{4m}{\sqrt{n}} = \frac{2\sqrt{2}m^2}{n} \times \frac{\sqrt{2n}}{m} \\ &\geq \frac{So(G)}{\frac{m}{\sqrt{2n}}}. \end{aligned}$$

■

Conflicts of Interest. The author declares that he has no conflicts of interest regarding the publication of this article.

References

[1] M. Mohammadi, H. Barzegar and A. R. Ashrafi, Comparisons of the Sombor index of Alkane, Alkyl, and Annulene series with their molecular mass, *J. Chem.* **2022** (2022) #8348525, https://doi.org/10.1155/2022/8348525.

[2] A. Ülker, A. Gürsoy and N. K. Gürsoy, The energy and Sombor index of graphs, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 51–58, https://doi.org/10.46793/match.87-1.051U.

[3] A. Ülker, A. Gürsoy, N. K. Gürsoy and I. Gutman, Relating graph energy and Sombor index, *Discrete Math. Lett.* **8** (2022) 6–9, https://doi.org/10.47443/dml.2021.0085.

[4] S. Akbari, M. Habibi and S. Rouhani, A note on an equality between energy and Sombor index of a graph, *MATCH Commun. Math. Comput. Chem.* **90** (2023) 765–771, https://doi.org/10.46793/match.90-3.765A.

[5] J. Guerrero, Laplacian energies of vertices, *arxiv:2201.01252v1 [math.CO]* (2022).

[6] I. Gutman, Geometric approach to degree based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11–16.

[7] I. Gutman, N. M. M. de Abreu, C. T. M. Vinagre, A. S. Bonifásio and S. Radenković, Relation between energy and Laplacian energy, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 343–354.

[8] H. Liu, L. You and Y. Huang, Ordering chemical graphs by Sombor indices and its applications, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 5–22, https://doi.org/10.46793/match.87-1.005L.

[9] M. S. Reja and S. M. A. Nayeem, On Sombor index and graph energy, *MATCH Commun. Math. Comput. Chem.* **89** (2023) 451–466, https://doi.org/10.46793/match.89-2.451R.

[10] H. Shoshtari and J. Rodríguez., New bounds on the energy of a graph, *Commun. Comb. Optim.* **7** (2022) 81–90, https://doi.org/10.22049/CCO.2021.26999.1179.

[11] O. Arizmendi, J. F. Hidalgo and O. Juarez-Romero, Energy of vertex, *Linear Algebra Appl.* **557** (2018) 464–495, https://doi.org/10.1016/j.laa.2018.08.014.

[12] I. Milovanović, E. Milovanović and M. Matejić, On some mathematical properties of Sombor indices, *Bull. Int. Math. Virtual Inst.* **11** (2021) 341–353.

[13] S. Wagner and H. Wang, *Introduction to Chemical Graph Theory*, Taylor and Francis Group, LLC, 2019.

[14] G. Caporossi, D. Cvetković, I. Gutman and P. Hansen, Variable neighborhood search for extremal graphs. 2. Finding graphs with extremal energy, *J. Chem. Inf. Comput. Sci.* **39** (1999) 984–996, https://doi.org/10.1021/ci9801419.