Mediterr. J. Math. (2023) 20:264
https://doi.org/10.1007/s00009-023-02465-4
1660-5446/23/050001-16
published online July 10, 2023

Mediterranean Journal of Mathematics

Relations Between the Energy and Topological Indices of a Graph

Akbar Jahanbani, Seyed Mahmoud Sheikholeslami and Slobodan Filipovski

Abstract. In this paper, we give various lower and upper bounds for the energy of graphs in terms of several topological indices of graphs: the first general multiplicative Zagreb index, the general Randić index, the general zeroth-order Randić index, the redefined Zagreb indices, and the atom-bond connectivity index. Moreover, we obtain new bounds for the energy in terms of certain graph invariants as diameter, girth, algebraic connectivity and radius.

Mathematics Subject Classification. 05C50.

Keywords. Energy of graphs, topological indices, Randić index, Zagreb index.

1. Introduction

Let $G = (V, E)$ be a simple undirected graph and let $n = |V(G)|$ and $m = |E(G)|$ be the *order* and the *size* of the graph G, respectively. The *open neighborhood* of vertex v is the set $N_G(v) = \{u \in V(G) \mid uv \in E(G)\}$ and the *degree* of v_i is defined as $d_{v_i} = |N(v_i)|$. Let Δ and δ be the *maximum* and the *minimum degree* of G, respectively. A simple undirected graph in which every pair of distinct vertices is connected by a unique edge, we call *complete graph* and is denoted by K_n.

For a vertex v in a connected nontrivial graph G, with $ecc_G(v) = \max\{d_G(v, u) \mid u \in V(G)\}$ we denote the *eccentricity* of v. The *radius* $r(G)$ of G is defined as $r(G) = \min\{ecc_G(v) \mid v \in V(G)\}$. The *diameter* of a graph G is the maximum distance between two vertices of G; denoted by $D(G)$. A *girth* $g(G)$ of a graph G is the length of the shortest cycle in the graph.

Topological indices represent an important type of molecular descriptors. They have gained considerable popularity and many new topological indices have been proposed and studied in the mathematical chemistry literature in recent years.

Birkhäuser

Various generalizations of the Zagreb indices have been proposed. In [18] a so-called *general zeroth-order Randić index* was introduced. It is defined as

$$^{0}R_{\alpha}(G) = \sum_{v \in V(G)} d_v^{\alpha}$$

where α is a real number. Note that $^{0}R_{-1}$ is the *inverse index* $ID(G)$, $^{0}R_2(G)$ is *the first Zagreb index* $M_1(G)$, $^{0}R_3(G)$ is *the forgotten topological index* $F(G)$.

The *general Randić index*, $R_{\alpha}(G)$, is a generalization of *the second Zagreb index*, reported in [5]. This index is defined as

$$R_{\alpha}(G) = \sum_{uv \in E(G)} (d_u d_v)^{\alpha}.$$

Note that $R_{-1/2}(G)$ is the usual *Randić index* $R(G)$.

The general redefined first Zagreb index is defined as

$$ReZg_{\alpha}(G) = \sum_{uv \in E(G)} \left(\frac{d_u + d_v}{d_u d_v} \right)^{\alpha},$$

for any real number α.

The *first general multiplicative Zagreb index* of a graph G is defined in [27] as

$$P^{\alpha}(G) = \prod_{v \in V(G)} d_v^{\alpha}.$$

These indices are a generalization of the well-known *multiplicative Zagreb indices*. If $\alpha = 1$, then $P^1(G)$ is the *Narumi-Katayama index* NK(G), see [23].

The *atom-bond connectivity index* of G, denoted by $ABC(G)$, is defined in [9] as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

The *Laplacian matrix* L of the graph G is defined as follows: $L_{uv} = 1$ if $(u, v) \in E(G), L_{uv} = 0$ if $(u, v) \notin E(G)$ and $u \neq v$, and $L_{uu} = -d_u$. The *algebraic connectivity* α of a graph G is the second smallest eigenvalue of the Laplacian matrix L.

The *adjacency matrix* $A(G)$ of G is defined by its entries as $a_{ij} = 1$ if $(v_i, v_j) \in E(G)$ and 0 otherwise. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ denote the *eigenvalues* of $A(G)$. The largest eigenvalues of A, λ_1, is called a *spectral radius* of the graph G.

The *energy* of the graph G is defined as

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

where λ_i, $i = 1, 2, \ldots, n$, are the *eigenvalues* of the graph G.
This concept was introduced by *I. Gutman* and is intensively studied in *chemistry*, since it can be used to approximate the total π-*electron* energy

of a *molecule* (see, e.g. [12,13,15]). Since then, numerous bounds for the energy were found (see, e.g. [24,25]).

In the last years, the energy of graphs was related to vertex-degree-based topological indices [3].

Definition 1. The energy of the vertex v_i with respect to G, which is denoted by $\mathcal{E}_G(v_i)$, is given by

$$\mathcal{E}_G(v_i) = |A(G)|_{ii}$$

for $i = 1, \ldots, n$, where $|A| = (AA^*)^{1/2}$ and A is the adjacency matrix of G.

In this way, the energy of a graph is given by the sum of the individual energies of the vertices of G,

$$\mathcal{E}(G) = \sum_{i=1}^{n} \mathcal{E}_G(v_i).$$

The energy of a vertex should be understood as the contribution of the vertex to the energy of the graph, in terms of how it interacts with other vertices. It can be seen that the energy of a vertex only depends on the vertices that are in the same component as v. Among graph descriptors used in mathematical chemistry, two of them play a rather important role and have the attention of many researchers around the world: the energy and topological indices of a graph. There are many inequalities for each of these descriptors. However, just a few relationship between them have been established, see in [4]. In this paper, we establish new relations between the energy and some of the topological indices of graphs.

For a graph G with Randić index $R(G)$, Arizmendi et al. [4] recently proved that $\mathcal{E}(G) \geq 2R(G)$, where the equality holds if and only if G is the union of complete bipartite graphs. Yan et al. [28] showed that $\mathcal{E}(G) \leq 2\sqrt{\Delta}R(G)$. Filipovski [10] obtained relations between the energy of graphs and the Randić index. Gutman et al. [14] obtained a relation between a vertex-degree-based topological index and its energy. In this paper, we give various lower and upper bounds for the energy of graphs in terms of some topological indices of graphs as the first general multiplicative Zagreb index, the general Randić index, the general zeroth-order Randić index, the redefined Zagreb index, and the atom-bond connectivity index.

2. Preliminaries and Known Results

In this section, we recall some well-known results from chemical graph theory that will be used in the proofs of the upcoming sections. In [1], the authors established a relation between the Randić index and the diameter of a given graph.

Observation 1. [1] *For any connected graph G on $n \geq 3$ vertices with Randić index $R(G)$ and diameter $D(G)$, it holds*

$$R(G)D(G) \leq \frac{(n-1)(n-3+2\sqrt{2})}{2}.$$

The next result gives a relationship between the Randić index $R(G)$ and the maximum degree $\Delta(G)$ of a given graph. This result is published in [1].

Observation 2. [1] *For any connected graph G on $n \geq 3$ vertices with Randić index $R(G)$ and maximum degree $\Delta(G)$,*

$$R(G)\Delta(G) \leq \frac{n(n-1)}{2}.$$

The following result appears in [1] as well.

Observation 3. [1] *For any connected graph G on $n \geq 3$ vertices with Randić index $R(G)$ and girth $g(G)$,*

$$R(G)g(G) \leq \frac{n^2}{2}.$$

In [21], the authors give a relation between the Randić index and the algebraic connectivity of a given graph.

Observation 4. [21] *For any connected graph G on $n \geq 3$ vertices with Randić index $R(G)$ and algebraic connectivity α,*

$$R(G) \leq \frac{\alpha\left(n-3+2\sqrt{2}\right)}{4\left(1-\cos\frac{\pi}{n}\right)}.$$

The first result concerns the energy of the graph in terms of its order and size. This result is given the following upper bound obtained in 1971 by McClelland [22]:

$$\mathcal{E}(G) \leq \sqrt{2mn}. \tag{2}$$

In [20], the following theorem is proved.

Theorem 1. [20] *Let G be a non-regular n-vertex graph without isolated vertices and $\alpha \neq 0$. Then*

$${}^{0}R_{2\alpha+1}(G) \leq 2R_{\alpha}(G) - \left({}^{0}R_{\alpha}(G)\right)^2 + n\left({}^{0}R_{2\alpha}(G)\right).$$

In this paper, we apply the following two algebraic inequalities.

Lemma 1. [17] *Let a and b $(a \geq b)$ be two non-negative real numbers. Then*

$$\frac{1}{\sqrt{2}}\left(\sqrt{a}+\sqrt{b}\right) \leq \sqrt{a+b} \leq \sqrt{a} + \left(\sqrt{2}-1\right)\sqrt{b}.$$

Lemma 2. [26] *Let a and b be positive numbers. Then*

$$\left(\frac{\sqrt{a}+\sqrt{b}}{2}\right)\left(\sqrt{\frac{a+b}{2}}\right) \leq \sqrt{\frac{a^2+b^2}{2}}.$$

The following lemma plays a key role in this paper.

Lemma 3. [2] *For a graph G and a vertex $v_i \in V(G)$,*

$$\mathcal{E}(G) \leq \sum_{i=1}^{n}\sqrt{d_i}$$

with equality if and only if the connected component containing v_i is isomorphic to S_n and v_i is its center.

Lemma 4. [11] *If G is a non-empty graph with maximum degree Δ, then* $\lambda_1 \geq \sqrt{\Delta}$ *with equality if and only if G is* $\frac{n}{2}K_2$.

3. Main Results

In this section, we establish new relations between the energy of graphs and some well-known topological indices. The first result gives a relation between the energy and the Narumi-Katayama index of graphs.

Theorem 2. *Let G be a connected graph of order n and size m. Then*

$$\mathcal{E}(G) \leq \sqrt{2m(n-1) + n\,(NK(G))^{\frac{1}{n}}}. \tag{3}$$

The equality holds if and only if $G \cong K_2$.

Proof. We use the following well-known inequality published in [16]. For non-negative numbers $a_1, a_2, \ldots, a_n$, it holds

$$n\left(\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}\right) \leq n\sum_{i=1}^{n} a_i - \left(\sum_{i=1}^{n}\sqrt{a_i}\right)^2. \tag{4}$$

Setting $a_i = d_i$, the inequality (4) becomes

$$n\left(\frac{1}{n}\sum_{i=1}^{n} d_i - \left(\prod_{i=1}^{n} d_i\right)^{\frac{1}{n}}\right) \leq n\sum_{i=1}^{n} d_i - \left(\sum_{i=1}^{n}\sqrt{d_i}\right)^2.$$

Hence

$$\sum_{i=1}^{n}\sqrt{d_i} \leq \sqrt{2m(n-1) + n\left(\prod_{i=1}^{n} d_i\right)^{\frac{1}{n}}}.$$

Therefore, by Lemma 3 we get

$$\mathcal{E}(G) \leq \sum_{i=1}^{n}\sqrt{d_i} \leq \sqrt{2m(n-1) + n\left(\prod_{i=1}^{n} d_i\right)^{\frac{1}{n}}}.$$

If $G \cong K_2$ it is easy to check that the equality in (3) holds. Conversely, if the equality in (3) holds, according to the above argument, the equality in (4) holds. Thus $d_1 = d_2 = \ldots = d_n$, that is, G is a k-regular graph. In this case $\sum_{i=1}^{n}\sqrt{d_i} = n\sqrt{k} = \sqrt{2mn}$. In order to get an equality in $\mathcal{E}(G) \leq \sum_{i=1}^{n}\sqrt{d_i}$, we consider those regular graphs where the equality between $\mathcal{E}(G)$ and the McClelland bound $\sqrt{2mn}$ holds. It is already known that such graphs are $\frac{n}{2}K_2$. Since G is a connected graph, we get $G \cong K_2$. □

Remark 1. Using the inequality between the arithmetic and geometric means for the numbers $d_1, d_2, \ldots, d_n$ we get

$$\sqrt{2m(n-1) + n\left(\prod_{i=1}^{n} d_i\right)^{\frac{1}{n}}} \leq \sqrt{2m(n-1) + n\left(\frac{d_1 + d_2 + \cdots + d_n}{n}\right)} = \sqrt{2mn}$$

that is, the bound in (3) is better than the bound in (2).

Theorem 1 has the following consequence for $\alpha = \frac{1}{2}$.

Corollary 1. *Let G is a non-regular n-vertex graph without isolated vertices. Then*

$$\mathcal{E}(G) \leq \sqrt{2R_{1/2}(G) - M_1(G) + 2mn}. \tag{5}$$

Remark 2. From $R_{1/2}(G) = \sum_{(u,v)\in E(G)} \sqrt{d_u d_v}$ and from the inequality $2\sqrt{d_u d_v} \leq d_u + d_v$ we get $2R_{1/2}(G) \leq M_1(G)$. Thus

$$2R_{1/2}(G) = \sum_{(u,v)\in E(G)} 2\sqrt{d_u d_v} \leq \sum_{(u,v)\in E(G)} (d_u + d_v) = M_1(G).$$

Hence

$$\mathcal{E}(G) \leq \sqrt{2R_{1/2}(G) - M_1(G) + 2mn} \leq \sqrt{2mn}.$$

Therefore, the bound in (5) is better than the well-known bound $\sqrt{2mn}$.

Proposition 3. *For any graph with $\delta > 1$, we have*

$$\mathcal{E}(G) \leq \frac{2m}{\sqrt{\delta}}.$$

Proof. We have

$$\mathcal{E}(G) \leq \sum_{u\in V(G)} \sqrt{d_u} = \sum_{u\in V(G)} d_u \frac{1}{\sqrt{d_u}} \leq \frac{2m}{\sqrt{\delta}}. \tag{6}$$

That is, for $\delta > 1$, the bound in (6) is better than the well-known upper bound $2m$. □

In the next proposition we reprove the bound $\mathcal{E}(G) \leq 2\sqrt{\Delta}$ proven in [28].

Proposition 4. *Let G be a connected graph with n vertices and maximum degree Δ. Then*

$$\mathcal{E}(G) \leq 2\sqrt{\Delta} R(G).$$

Proof. We have

$$\begin{aligned} 2R(G) &= 2 \sum_{uv\in E(G)} d_u^{-1/2} d_v^{-1/2} \\ &= \sum_{u\in E(G)} d_u^{-1/2} \sum_{v\in N(u)} d_v^{-1/2} \\ &\geq \sum_{u\in E(G)} d_u^{-1/2} \sum_{v\in N(u)} \Delta^{-1/2} = \sum_{u\in E(G)} d_u^{-1/2} d_u \Delta^{-1/2} \\ &= \sum_{u\in E(G)} d_u^{1/2} \Delta^{-1/2} \geq \frac{\mathcal{E}(G)}{\sqrt{\Delta}}. \end{aligned}$$

□

The next theorem reveals a connection between the energy and the redefined first general Zagreb index of graphs.

Theorem 5. *Let G be a connected graph of order $n > 2$. Then*

$$\mathcal{E}(G) \le \sqrt{2} ReZg_{1/2}. \tag{7}$$

The equality is attained if and only if $G \cong K_2$.

Proof. By using Lemmas 1 and 3, we have

$$\begin{aligned}\mathcal{E}(G) &\le \sum_{u\in V(G)} \sqrt{d_u} = \sum_{uv\in E(G)} \left(\frac{1}{\sqrt{d_u}} + \frac{1}{\sqrt{d_v}}\right) = \sum_{uv\in E(G)} \frac{\sqrt{d_u}+\sqrt{d_v}}{\sqrt{d_u d_v}} \\ &\le \sum_{uv\in E(G)} \frac{\sqrt{2}\sqrt{d_u+d_v}}{\sqrt{d_u d_v}} = \sum_{uv\in E(G)} \sqrt{\frac{2\,(d_u+d_v)}{d_u d_v}}. \end{aligned} \tag{8}$$

This implies the result stated in the theorem. If $G \cong K_2$ it is easy to check that the equality in (7) holds. Conversely, if the equality in (7) holds, then the equality in (8) holds, which is possible only if $d_u = d_v$. Thus G is a regular graph. As before, we proved that the unique regular graph which satisfies the identity $\mathcal{E}(G) = \sum_{v\in V(G)} \sqrt{d_v}$ is K_2. □

Remark 3. By Lemma 1 we have

$$\begin{aligned}\sqrt{2} ReZg_{1/2} &= \sum_{uv\in E(G)} \sqrt{\frac{2\,(d_u+d_v)}{d_u d_v}} \\ &\le \sum_{uv\in E(G)} \frac{\sqrt{2}\left(\sqrt{d_u} + (\sqrt{2}-1)\sqrt{d_v}\right)}{\sqrt{d_u d_v}} \\ &\le \sum_{uv\in E(G)} \frac{\sqrt{2}\left(\sqrt{\Delta} + (\sqrt{2}-1)\sqrt{\Delta}\right)}{\sqrt{d_u d_v}} \\ &= 2\sqrt{\Delta} R(G).\end{aligned}$$

Thus, the bound in (7) is better than the bound in Proposition 5.

The next result concerns the energy of graphs in terms of the Randić index and the maximum and the minimum degree of G.

Theorem 6. *Let G be a connected graph with maximum degree Δ and minimum degree δ. If $|\sqrt{d_v} - \sqrt{d_u}| \ge 1$ for each edge $(u,v) \in E(G)$, then*

$$\mathcal{E}(G) \le (\Delta - \delta)\, R(G). \tag{9}$$

Proof. From $\left(\frac{1}{\sqrt{d_u}} + \frac{1}{\sqrt{d_v}}\right)\left(\frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}}\right) = \frac{1}{d_u} - \frac{1}{d_v}$ we get

$$\frac{1}{\sqrt{d_u}} + \frac{1}{\sqrt{d_v}} = \frac{d_v - d_u}{\left(\sqrt{d_v} - \sqrt{d_u}\right)\sqrt{d_u d_v}}.$$

Since for any edge $uv \in E(G)$ it holds $\frac{1}{\sqrt{d_v}-\sqrt{d_u}} \leq 1$ we get

$$\begin{aligned}
\mathcal{E}(G) &\leq \sum_{u\in V(G)} \sqrt{d_u} \\
&= \sum_{uv\in E(G)} \left(\frac{1}{\sqrt{d_u}} + \frac{1}{\sqrt{d_v}}\right) \\
&= \sum_{uv\in E(G)} \frac{d_v - d_u}{\left(\sqrt{d_v} - \sqrt{d_u}\right)\sqrt{d_u d_v}} \\
&\leq \sum_{uv\in E(G)} \frac{|d_v - d_u|}{\sqrt{d_u d_v}} \\
&\leq (\Delta - \delta)\, R(G).
\end{aligned}$$

This implies the result stated in the theorem. □

The next theorem reveals a connection between the energy and the atom-bond connectivity (ABC) index of graphs.

Theorem 7. *Let G be a graph of order n with no isolated vertices. If $\delta \geq 2$, then*

$$\mathcal{E}(G) \leq 2ABC(G).$$

Proof. By using the definitions and Lemma 3, we have

$$\begin{aligned}
\mathcal{E}(G) &\leq \sum_{v\in V(G)} \sqrt{d_i} \\
&= \sum_{uv\in E(G)} \left(\frac{1}{\sqrt{d_u}} + \frac{1}{\sqrt{d_v}}\right) \quad (as\ d_u, d_v \geq \delta \geq 2) \\
&\leq \sum_{uv\in E(G)} \left(\sqrt{\frac{1}{d_u} + \frac{d_u - 2}{d_u d_v}} + \sqrt{\frac{1}{d_v} + \frac{d_v - 2}{d_u d_v}}\right) \\
&= 2 \sum_{uv\in E(G)} \sqrt{\frac{1}{d_u} + \frac{1}{d_u} - \frac{2}{d_u d_v}} \\
&= 2ABC(G).
\end{aligned}$$

□

In the next theorem, we determine an upper bound for the energy of graphs in terms of the maximum eigenvalues λ_1 and the inverse degree of G.

Theorem 8. *Let G be a non-trivial connected graph of order n and maximum eigenvalue λ_1. Then*

$$\mathcal{E}(G) \leq \lambda_1 \sqrt{nID(G)}. \tag{10}$$

The equality is attained if and only if $G \cong K_2$.

Proof. For $1 \leq i \leq n$ let a_i and b_i be real numbers. In this proof we use Cauchy-Schwarz inequality (see [16]):

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right). \tag{11}$$

If we take $a_i = d_i$ and $b_i = \frac{1}{\sqrt{d_i}}$ in inequality (11), we have

$$\left(\sum_{i=1}^{n} \sqrt{d_i}\right)^2 \leq \left(\sum_{i=1}^{n} d_i^2\right)\left(\sum_{i=1}^{n} \frac{1}{d_i}\right). \tag{12}$$

In [11], it is proved that

$$\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}}. \tag{13}$$

From the above inequality and (12) we obtain (10).
If $G \cong K_2$ it is easy to check that the equality in (10) holds. Conversely, if the equality in (10) holds, then the equality in Cauchy-Schwarz inequality holds, that is, $\frac{d_i}{\frac{1}{\sqrt{d_i}}} = \frac{d_j}{\frac{1}{\sqrt{d_j}}}$ for each $i \neq j$. Hence $d_i = d_j$, i.e., G is a regular graph. In this case holds equality in (13), since $\lambda_1 = k$. We already prove that the unique regular graph which satisfies $\mathcal{E}(G) = \sum_{i=1}^{n} \sqrt{d_i}$ is the complete graph on two vertices K_2. $\square$

Now we present a relationship between the energy and the general zeroth-order Randić index of graphs.

Theorem 9. *Let G be a graph of order n, maximum degree Δ and minimum degree δ. Then*

$$\mathcal{E}(G) \leq {}^0R_{1/4}(G)[\delta^{1/4} + \Delta^{1/4}] - n\delta^{1/4}\Delta^{1/4}.$$

The equality is attained if and only if $G \cong K_2$.

Proof. Let $a_1, a_2, \ldots, a_n$ be real numbers such that $a \leq a_i \leq A$ for all $1 \leq i \leq n$. Let $\mu = \frac{\sum_{i=1}^{n} a_i}{n}$. Then from [6], the following inequality occurs:

$$\sum_{i=1}^{n} a_i^2 \leq n\left(\mu[A + a] - Aa\right). \tag{14}$$

Let $a_i = d_i^{1/4}$, $\mu = \frac{\sum_{i=1}^{n} d_i^{1/4}}{n}$ and $\delta^{1/4} \leq a_i \leq \Delta^{1/4}$. The inequality (14) is equivalent to

$$\begin{aligned}\sum_{i=1}^{n} \sqrt{d_i} &\leq n\left(\frac{\sum_{i=1}^{n} d_i^{1/4}}{n}[\delta^{1/4} + \Delta^{1/4}] - \delta^{1/4}\Delta^{1/4}\right)\\ &= {}^0R_{1/4}(G)[\delta^{1/4} + \Delta^{1/4}] - n\delta^{1/4}\Delta^{1/4}.\end{aligned}$$

Now Lemma 3 implies the required result. By the same argument as before, we can prove that the equality holds if and only if $G \cong K_2$. $\square$

In the next result, we give a relation between the energy, the inverse degree and the general zeroth-order Randić index of graphs.

Theorem 10. *If G is a graph without isolated vertices, of order n, size m, minimum degree δ and maximum degree Δ, then*

$$\mathcal{E}(G) \leq \sqrt{(2m-n)(n-ID(G))} +^0 R_{-1/2}(G). \tag{15}$$

The equality is attained if and only if $G \cong K_2$.

Proof. Let $w_1, w_2, \ldots, w_n$ be non-negative real numbers (weights). We use the weighted version of the Cauchy-Schwarz inequality

$$\sum_{i=1}^{n} w_i a_i^2 \sum_{i=1}^{n} w_i b_i^2 \geq \left(\sum_{i=1}^{n} w_i a_i b_i \right)^2 .$$

Let $w_i = d_i - 1, a_i = 1$ and $b_i = \frac{1}{\sqrt{d_i}}$, for each $i = 1, 2, \ldots, n$. Thus the above inequality is equivalent to

$$\sum_{i=1}^{n} (d_i - 1) \sum_{i=1}^{n} (d_i - 1) \cdot \frac{1}{d_i} \geq \left(\sum_{i=1}^{n} \frac{d_i - 1}{\sqrt{d_i}} \right)^2$$

and this if and only if

$$(2m-n)(n-ID(G)) \geq \left(\sum_{i=1}^{n} \sqrt{d_i} - {}^0 R_{-1/2}(G) \right)^2 .$$

From $\mathcal{E}(G) \leq \sum_{i=1}^{n} \sqrt{d_i}$ we get

$$\mathcal{E}(G) \leq \sqrt{(2m-n)(n-ID(G))} +^0 R_{-1/2}(G).$$

If $G \cong K_2$ it is easy to check that the equality in (15) holds. On the other hand, since the weighted Cauchy-Schwarz inequality becomes equality when $\frac{a_i}{b_i} = \sqrt{d_i}$ is a constant for each i, we get that $d_1 = d_2 = \cdots = d_n$, that is, G is a regular graph. As before we conclude that $G \cong K_2$. □

The next result gives a relationship between the energy, the general zeroth-order Randić index and the first general multiplicative Zagreb index of graphs.

Theorem 11. *Let G be a graph of order n. Then*

$$\mathcal{E}(G) \leq \left({}^0 R_{1/4}(G) \right)^2 - n(n-1) \left(P_1^{1/2}(G) \right)^{1/n} .$$

The equality is attained if and only if $G \cong K_2$.

Proof. Let $a_1, a_2, \ldots, a_n$ be positive real numbers. We apply the next inequality proved in [19]

$$\left(\sum_{i=1}^{n} \sqrt{a_i} \right)^2 \geq \sum_{i=1}^{n} a_i + n(n-1) \left(\prod_{i=1}^{n} a_i \right)^{1/n} . \tag{16}$$

Setting $a_i = \sqrt{d_i}$ for $i = 1, \ldots, n$, the inequality (16) becomes

$$\left(\sum_{i=1}^{n} d_i^{1/4} \right)^2 \geq \sum_{i=1}^{n} \sqrt{d_i} + n(n-1) \left(\prod_{i=1}^{n} \sqrt{d_i} \right)^{1/n}$$

that is

$$\sum_{i=1}^{n} \sqrt{d_i} \leq \left({}^{0}R_{1/4}(G)\right)^2 - n(n-1)\left(P_1^{1/2}(G)\right)^{1/n}.$$

Lemma 3 implies the result stated in the theorem. By the same argument as before, we can prove that equality holds if and only if $G \cong K_2$. $\square$

Let G be a graph without isolated vertices. In the next theorem, we determine an upper bound on the energy of a graph in terms of its size, minimum degree, maximum degree, and general Randić index.

Theorem 12. *Let G be a graph of size m, with no isolated vertices, maximum degree Δ and minimum degree δ. Then*

$$\mathcal{E}(G) \leq m\left(\frac{1}{\sqrt[4]{\delta}} - \frac{1}{\sqrt[4]{\Delta}}\right)^2 + 2R_{-1/4}(G). \tag{17}$$

The equality is attained if and only if $G \cong K_2$.

Proof. For $e = (u, v) \in E(G)$ we use the following identity

$$\left(\frac{1}{\sqrt{d_u}} + \frac{1}{\sqrt{d_v}}\right) = \left(\frac{1}{\sqrt[4]{d_u}} - \frac{1}{\sqrt[4]{d_v}}\right)^2 + \frac{2}{\sqrt[4]{d_u d_v}}. \tag{18}$$

Hence, by the definitions, we get

$$\begin{aligned}
\mathcal{E}(G) &\leq \sum_{uv\in E(G)} \left(\frac{1}{\sqrt{d_u}} + \frac{1}{\sqrt{d_v}}\right) \\
&= \sum_{uv\in E(G)} \left(\frac{1}{\sqrt[4]{d_u}} - \frac{1}{\sqrt[4]{d_v}}\right)^2 + \sum_{uv\in E(G)} \frac{2}{\sqrt[4]{d_u d_v}} \qquad (19)\\
&\leq \sum_{uv\in E(G)} \left(\frac{1}{\sqrt[4]{\delta}} - \frac{1}{\sqrt[4]{\Delta}}\right)^2 + \sum_{uv\in E(G)} \frac{2}{\sqrt[4]{d_u d_v}} \qquad (20)\\
&= m\left(\frac{1}{\sqrt[4]{\delta}} - \frac{1}{\sqrt[4]{\Delta}}\right)^2 + 2R_{-1/4}(G).
\end{aligned}$$

$\square$

Note that $\left(\frac{1}{\sqrt{d_u}} + \frac{1}{\sqrt{d_v}}\right) = \left(\frac{1}{\sqrt[4]{d_u}} + \frac{1}{\sqrt[4]{d_v}}\right)^2 - \frac{2}{\sqrt[4]{d_u d_v}}$. By this identity we get the following result.

Corollary 2. *Let G be a graph of size m with no isolated vertices and minimum degree δ. Then*

$$\mathcal{E}(G) \leq \frac{4m}{\sqrt{\delta}} - 2R_{-1/4}(G).$$

In the next two theorems, we provide a relationship between the energy and the general zeroth-order Randić index of graphs.

Theorem 13. *If G is a non-trivial graph of size m, then*

$$\mathcal{E}(G) \leq \frac{2m\,{}^0R_{3/4}(G) + {}^0R_{1/4}(G)F(G)}{2M_1(G)}.$$

The equality is attained if and only if $G \cong K_2$.

Proof. If a_i and b_i are nonnegative real numbers, then the following inequality holds ([8], p. 4).

$$\frac{1}{2}\left[\sum_{i=1}^{n} a_i^3 \sum_{i=1}^{n} b_i + \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i^3\right] \geq \sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2. \tag{21}$$

For $a_i = d_i^{1/4}$ and $b_i = d_i$, the inequality (21) becomes

$$\frac{1}{2}\left[\sum_{i=1}^{n} d_i^{3/4} \sum_{i=1}^{n} d_i + \sum_{i=1}^{n} d_i^{1/4} \sum_{i=1}^{n} d_i^3\right] \geq \sum_{i=1}^{n} \sqrt{d_i} \sum_{i=1}^{n} d_i^2$$

from where we get

$$\sum_{i=1}^{n} \sqrt{d_i} \leq \frac{2m\,{}^0R_{3/4}(G) + {}^0R_{1/4}(G)F(G)}{2M_1(G)}.$$

Lemma 3 leads to the desired bound. By the same argument as before, we can prove that equality holds if and only if $G \cong K_2$. □

Theorem 14. *Let G be a graph without isolated vertices, of order n, minimum degree δ and maximum degree Δ. Then*

$$\mathcal{E}(G) \leq (\sqrt[4]{\delta} + \sqrt[4]{\Delta})\,{}^0R_{1/4}(G) - n\sqrt[4]{\delta\Delta}. \tag{22}$$

The equality is attained if and only if $G \cong K_2$.

Proof. Let $x_1, x_2, \ldots, x_n$ and $y_1, y_2, \ldots, y_n$ be real numbers such that there exist real constants a and A so that for each $i = 1, 2, \ldots, n$ holds $ax_i \leq y_i \leq Ax_i$. Then the following inequality is valid (see [7])

$$\sum_{i=1}^{n} y_i^2 + Aa \sum_{i=1}^{n} x_i^2 \leq (a + A) \sum_{i=1}^{n} x_i y_i. \tag{23}$$

For $y_i = d_i^{1/4}, x_i = 1, a = \sqrt[4]{\delta}$ and $A = \sqrt[4]{\Delta}, i = 1, 2, \ldots, n$ the inequality (23) becomes

$$\sum_{i=1}^{n} \sqrt{d_i} + \sqrt[4]{\delta\Delta} \sum_{i=1}^{n} 1 \leq (\sqrt[4]{\delta} + \sqrt[4]{\Delta}) \sum_{i=1}^{n} d_i^{1/4},$$

that is,

$$\sum_{i=1}^{n} \sqrt{d_i} \leq (\sqrt[4]{\delta} + \sqrt[4]{\Delta})\,{}^0R_{1/4}(G) - n\sqrt[4]{\delta\Delta}.$$

The last inequality leads to the desired bound. By the same argument as before, we can prove that the equality holds if and only if $G \cong K_2$.

□

The following result gives a relation between the energy, the first Zagreb index and the maximum degree of G.

Theorem 15. *Let G be a non-trivial connected graph of order n and maximum degree Δ. Then*

$$\mathcal{E}(G) \leq M_1(G) + \sqrt{\Delta} - \Delta^2 - \ln\left(\frac{NK(G)}{\Delta}\right).$$

The equality is attained if and only if $G \cong K_2$.

Proof. We consider the following function for $x > 0$

$$g(x) = x^2 - \sqrt{x} - \ln(x).$$

The first derivative of $g(x)$ is $g'(x) = 2x - \frac{1}{2\sqrt{x}} - \frac{1}{x}$. It is easy to note that for $x \geq 1$, $g(x)$ is increasing, thus $g(x) = x^2 - \sqrt{x} - \ln(x) \geq 1^2 - \sqrt{1} - \ln(1) = 0$. Hence $\sqrt{x} \leq x^2 - \ln(x)$. Using this result and Lemma 3, we get

$$\begin{aligned}
\mathcal{E}(G) &\leq \sum_{i=1}^{n} \sqrt{d_i} \\
&= \sqrt{d_1} + \sum_{i=2}^{n} \sqrt{d_i} \leq \sqrt{d_1} + \sum_{i=2}^{n} \left(d_i^2 - \ln(d_i)\right) \\
&= M_1(G) + \sqrt{\Delta} - \Delta^2 - \ln\left(\prod_{i=2}^{n} d_i\right) \\
&= M_1(G) + \sqrt{\Delta} - \Delta^2 - \ln\left(\frac{NK(G)}{\Delta}\right).
\end{aligned}$$

This completes the proof of the theorem. By the same argument as before, we can prove that equality holds if and only if $G \cong K_2$. □

4. Applications

In this section, we present several results which relate the energy of the graph and its diameter, girth, algebraic connectivity and its radius. The results are based on Observation 1–4.

By $\mathcal{E}(G) \leq 2\sqrt{\Delta}R(G)$ and Observation 1, we obtain a relation between the energy and the diameter of the graph.

Lemma 5. *Let G be a connected graph of order $n \geq 3$, maximum degree Δ and diameter D. Then*

$$\mathcal{E}(G) \leq \frac{\sqrt{\Delta}(n-1)(n-3+2\sqrt{2})}{D(G)}.$$

Based on Observation 2, we obtain a result that gives a relation between the energy, the maximum and the minimum degree of graphs.

Lemma 6. *Let G be a connected graph of order $n \geq 3$, maximum degree Δ and minimum degree δ. Then*

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

By Observation 3 we obtain a relation between the energy and the girth of a given graph.

Lemma 7. *Let G be a connected graph of order $n \geq 3$, maximum degree Δ and girth g. Then*

$$\mathcal{E}(G) \leq \frac{\sqrt{\Delta} n^2}{g(G)}.$$

By Observation 4, we obtain a relation between the energy and the algebraic connectivity of a graph.

Lemma 8. *Let G be a connected graph of order $n \geq 3$, maximum degree Δ and algebraic connectivity α. Then*

$$\mathcal{E}(G) \leq \frac{\sqrt{\Delta}\alpha\left(n-3+2\sqrt{2}\right)}{2\left(1-\cos\frac{\pi}{n}\right)}.$$

Lemma 9. *Let G be a non-trivial connected graph of order n. Then*

$$\mathcal{E}(G) \leq n\sqrt{n-r}.$$

Proof. For each vertex $v \in V(G)$, we have $d_v \leq n - ecc_G(v)$. According to the definition of the energy, we obtain

$$\mathcal{E}(G) \leq \sum_{v \in V(G)} \sqrt{d_v} \leq \sum_{v \in V(G)} \sqrt{n - ecc_G(v)} \leq n\sqrt{n-r}.$$

□

Funding SF is supported by the Slovenian Research Agency through the Grants P1-0285, J1-3001, J1-3003, J1-4008, J1-4414 and N1-0210.

Data Availability Statement My manuscript has no associate data or the data will not be deposited.

References

[1] Aouchiche, M., Hansen, P., Zheng, M.: Variable neighborhood search for extremal graphs. 19. Further conjectures and results about the Randic index. MATCH Commun. Math. Comput. Chem. **58**, 83–102 (2007)

[2] Arizmendi, O., Hidalgo, J.F., Juarez-Romero, O.: Energy of a vertex. Linear Algebra Appl. **557**, 464–495 (2018)

[3] Arizmendi, O., Juarez-Romero, O.: On bounds for the energy of graphs and digraphs. In: Contributions of Mexican Mathematicians Abroad in Pure and Applied Mathematics., vol. 709, pp. 1–19. American Mathematical Society, Providence (2018)

[4] Arizmendi, G., Arizmendi, O.: Energy of a graph and Randić index. Linear Algebra Appl. **609**, 332–338 (2021)

[5] Bollobaś, B., Erdös, P.: Graphs of extremal weights. Ars Combin. **50**, 225–233 (1998)

[6] Che, Z., Chen, Z.: Lower and upper bounds of the forgotten topological index. MATCH Commun. Math. Comput. Chem. **76**, 635–648 (2016)

[7] Diaz, J.B., Metcalf, F.T.: Stronger forms of a class of inequalities of G. Pólya - G. Szego and L. V. Kantorovich. Bull. Am. Math. Soc. **69**, 415–418 (1963)

[8] Dragomir, S.S.: On some inequalities (Romanian), Caiete Metodico Stiin, tifice, No. 13, pp. 20. Faculty of Mathematics, Timi Soara University, Romania (1984)

[9] Estrada, E., Torres, L., Rodríguez, L., Gutman, I.: An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes. Indian J. Chem. A **37**, 849–855 (1998)

[10] Filipovski, S.: Relations between the energy of graphs and other graph parameters. MATCH Commun. Math. Comput. Chem. **87**, 661–672 (2022)

[11] Favaron, O., Mahéo, M., Saclé, J.F.: Some eigenvalue properties in graphs (conjectures of Graffiti-II). Discrete Math. **111**, 197–220 (1993)

[12] Gutman, I., Trinajstić, N.: Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons. Chem. Phys. Lett. **17**, 535–538 (1972)

[13] Gutman, I., Polansky, O.E.: Mathematical Concepts in Organic Chemistry. Springer, Berlin (1986)

[14] Gutman, I., Monsalve, J., Rada, J.: A relation between a vertex-degree-based topological index and its energy. Linear Algebra Appl. **636**, 134–142 (2022)

[15] Gutman, I.: The energy of a graph: old and new results. In: Betten, A., Kohnert, A., Laue, R., Wassermann, A. (eds.) Algebraic Combinatorics and Applications, pp. 196–211. Springer, Berlin (2001)

[16] Hardy, G.H., Littlewood, J.E., Pólya, G.: Inequalities. Cambridge University Press, Cambridge (1988)

[17] Hua, H., Das, KCh., Wang, H.: On atom-bond connectivity index of graphs. J. Math. Anal. Appl. **479**, 1099–1114 (2019)

[18] Hu, Y., Li, X., Shi, Y., Xu, T., Gutman, I.: On molecular graphs with smallest and greatest zeroth-order general Randić index. MATCH Commun. Math. Comput. Chem. **54**, 425–434 (2005)

[19] Kober, H.: On the arithmetic and geometric means and on Hölders inequality. Proc. Am. Math. Soc. **9**, 452–459 (1958)

[20] Lu, M., Liu, H., Tian, F.: The connectivity index. MATCH Commun. Math. Comput. Chem. **51**, 149–154 (2004)

[21] Li, X., Shi, Y., Wang, L.: On a relation between Randic index and algebraic connectivity. MATCH Commun. Math. Comput. Chem. **68**, 843–849 (2012)

[22] McClelland, B.: Properties of the latent roots of a matrix: the estimation of π-electron energies. J. Chem. Phys. **54**, 640–643 (1971)

[23] Narumi, H., Katayama, H.: Simple topological index-A newly devised index characterizing the topological nature of structural isomers of saturated hydrocarbons. Mem. Fac. Eng. Hokkaido Univ. **16**, 209–214 (1984)

[24] Ramanna, R.B.: On Zagreb energy and edge-Zagreb energy. Commun. Comb. Optim. **6**, 155–169 (2021)

[25] Shooshtary, H., Rodríguez, J.: New bounds on the energy of a graph. Commun. Comb. Optim. **7**, 81–90 (2022)

[26] Taneja, I.J.: Refinement of inequalities among means. J. Comb. Inf. Syst. Sci. **31**, 343–364 (2006)

[27] Vetrlk, T., Balachandran, S.: General multiplicative Zagreb indices of trees. Discrete Appl. Math. **247**, 341–351 (2018)

[28] Yan, Z., Liu, C., Pan, Y., Li, J.: Energy, Randić index and maximum degree of graphs. MATCH Commun. Math. Comput. Chem. **86**, 539–542 (2021)

Akbar Jahanbani and Seyed Mahmoud Sheikholeslami
Azarbaijan Shahid Madani University
Tabriz
Iran
e-mail: akbarjahanbani92@gmail.com

Seyed Mahmoud Sheikholeslami
e-mail: s.m.sheikholeslami@azaruniv.ac.ir

Slobodan Filipovski
University of Primorska
Koper
Slovenia
e-mail: slobodan.filipovski@famnit.upr.si

Received: February 22, 2022.
Revised: June 8, 2023.
Accepted: June 19, 2023.