Discrete Mathematics Letters
www.dmlett.com

Discrete Math. Lett. **7** (2021) 52–57
DOI: 10.47443/dml.2021.0065

Research Article

Bounds on graph energy and Randić energy

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(Received: 14 June 2021. Received in revised form: 24 June 2021. Accepted: 6 July 2021. Published online: 10 July 2021.)

Abstract

In the present paper, new lower and upper bounds on energy and Randić energy of non-singular (bipartite) graphs are reported. Additionally, it is shown that the obtained lower bounds are stronger than two previously known lower bounds in the literature.

Keywords: graph energy; Randić energy; bound.

2020 Mathematics Subject Classification: 05C50, 05C90.

1. Introduction

Let G be a simple connected graph. Denote by n and m the number of vertices and edges of G, respectively. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ be the set of the vertices of G and d_i be the degree of the vertex $v_i \in V(G)$, $i = 1, 2, \ldots, n$. If v_i and v_j are two adjacent vertices of G, then it is denoted by $i \sim j$. Let Δ and δ be the maximum and minimum vertex degrees of G, respectively.

Let us denote by $\mathbf{A} = \mathbf{A}(G)$ the adjacency matrix of a graph G. The eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ of $\mathbf{A}$ represent the eigenvalues of G [6]. As well known in spectral graph theory, λ_1 is the spectral radius of G and [6]

$$\sum_{i=1}^{n} \lambda_i = 0, \; \sum_{i=1}^{n} \lambda_i^2 = 2m \text{ and } \prod_{i=1}^{n} \lambda_i = \det \mathbf{A}. \tag{1}$$

A graph G is called as non-singular if no eigenvalue of G is equal to zero. For non-singular graphs, it is obvious that $\det \mathbf{A} \neq 0$. A graph G is singular if at least one of its eigenvalue is equal to zero. Then, $\det \mathbf{A} = 0$.

The energy of a graph G was defined in [12] as

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| . \tag{2}$$

This graph invariant is utilized to estimate the total $\pi-$electron energy of a molecule represented by a (molecular) graph. [13, 22]. A vast literature exists on $E(G)$, for survey and comprehensive information, see [2, 11, 14, 19, 23].

Recently, energy of non-singular graphs has also been studied in the literature. In [8], Das et al. obtained a lower bound on energy of non-singular graphs that improves the lower bounds in [3, 22], under certain conditions. Gutman and Das [15] established upper bounds on energy of non-singular (bipartite) molecular graphs. In [15], it was also stated that the upper bound obtained on energy of non-singular molecular graphs improves the upper bound in [3].

The following upper bound on $E(G)$ was found in [11]

$$E(G) \leq \sqrt{2m(n-1) + n\,|\det \mathbf{A}|^{2/n}}. \tag{3}$$

The Randić matrix $\mathbf{R} = \mathbf{R}(G)$ of a graph G is defined so that its $(i, j)-$ th entry is equal to $1/\sqrt{d_i d_j}$ if $i \sim j$ and is equal to 0 otherwise [1]. The eigenvalues $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$ of $\mathbf{R}$ are called as the Randić eigenvalues of G [1]. Some well known results concerning the Randić eigenvalues are [1, 16]

$$\sum_{i=1}^{n} \rho_i = 0\,, \; \sum_{i=1}^{n} \rho_i^2 = 2R_{-1} \text{ and } \prod_{i=1}^{n} \rho_i = \det \mathbf{R} \tag{4}$$

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where

$$R_{-1} = R_{-1}(G) = \sum_{i\sim j} \frac{1}{d_i d_j}$$

is the general Randić index of the graph G [4,18].

In full analogous manner with the graph energy [12], the Randić energy of G was introduced in [1]. It was defined as [1]

$$RE = RE(G) = \sum_{i=1}^{n} |\rho_i| . \tag{5}$$

For details on the properties and bounds of RE, see the recent works [1,9,10,16,17,20,21,23].

The following upper bound on $RE(G)$ was obtained in [17,21]

$$RE(G) \le 1 + \sqrt{(n-2)(2R_{-1}-1) + (n-1)|\det \mathbf{R}|^{2/(n-1)}}. \tag{6}$$

In the present paper, we find new lower and upper bounds on energy and Randić energy of non-singular (bipartite) graphs. We also show that our lower bounds are stronger than two previously known lower bounds given in [7,9,14,17].

2. Lemmas

We now list some lemmas that will be needed for our main results.

Lemma 2.1. [5] *Let $x_i > -1$ for $1 \le i \le n$. If $\sum_{i=1}^{n} x_i = 0$ and $\sum_{i=1}^{n} x_i^2 \ge a^2(1-n^{-1})$, then*

$$\sum_{i=1}^{n} \ln(1+x_i) \le \ln\left(1+a-an^{-1}\right) + (n-1)\ln\left(1-an^{-1}\right).$$

Lemma 2.2. [6,27] *Let G be a graph with n vertices and maximum vertex degree Δ. Then, for each $i = 1,2,\dots,n$*

$$|\lambda_i| \le \Delta.$$

Lemma 2.3. [10] *Let G be a graph with n vertices and without isolated vertices. Then, for each $i = 1,2,\dots,n$*

$$\delta|\rho_i| \le |\lambda_i| \le \Delta|\rho_i| \tag{7}$$

where Δ and δ denote, respectively, the maximum and minimum vertex degrees of G.

Lemma 2.4. [10] *Let G be a graph with n vertices and without isolated vertices and let λ_1 be its spectral radius. Then*

$$\delta(RE(G)-1) \le E(G) - \lambda_1 \le \Delta(RE(G)-1)$$

where Δ and δ denote, respectively, the maximum and minimum vertex degrees of G.

Lemma 2.5. [6,20] *For a graph G, the Randić spectral radius $\rho_1 = 1$.*

Lemma 2.6. *Let G be a bipartite graph with n vertices and without isolated vertices and let λ_1 be its spectral radius. Then*

$$\delta(RE(G)-2) \le E(G) - 2\lambda_1 \le \Delta(RE(G)-2)$$

where Δ and δ denote, respectively, the maximum and minimum vertex degrees of G.

Proof. Note that $\lambda_1 = -\lambda_n$ and $\rho_1 = -\rho_n$, for bipartite graphs [6]. Then, by taking summation (7) over $i = 2,3,\dots,n-1$ and considering Lemma 2.5 and Equations (2) and (5), one can get the required result. □

Lemma 2.7. [16] *Let G be a graph with n vertices, adjacency matrix $\mathbf{A}$ and Randić matrix $\mathbf{R}$. If $\mathbf{A}$ has n_+, n_0 and n_- positive, zero and negative eigenvalues, respectively $(n_+ + n_0 + n_- = n)$, then $\mathbf{R}$ has n_+, n_0 and n_- positive, zero and negative eigenvalues, respectively.*

For a graph G with n vertices, the following relation between the determinants of its adjacency and Randić matrices was also given in [16].

Lemma 2.8. [16] *If G is a graph with isolated vertices, then $\det \mathbf{R} = \det \mathbf{A} = 0$. If G is a graph without isolated vertices, then*

$$\det \mathbf{R} = \frac{\det \mathbf{A}}{\prod_{i=1}^{n} d_i}.$$

3. Main results

Theorem 3.1. *Let G be a connected non-singular graph with $n \geq 2$ vertices and m edges. Then*

$$E(G) \geq n \left(\frac{|\det \mathbf{A}|}{(1+(n-1)b)(1-b)^{n-1}} \right)^{1/n} \tag{8}$$

where

$$b = \left[\frac{2mn - \left(2m(n-1) + n|\det \mathbf{A}|^{2/n}\right)}{(n-1)\left(2m(n-1) + n|\det \mathbf{A}|^{2/n}\right)} \right]^{1/2}. \tag{9}$$

Proof. We first recall that $|\lambda_i| > 0$, $1 \leq i \leq n$, for a non-singular graph G. Let $r = \frac{E(G)}{n}$ and $x_i = \frac{|\lambda_i|}{r} - 1$, for $1 \leq i \leq n$. Observe that $x_i > -1$. By means of Equations (1)–(3), we also have

$$\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} \left(\frac{|\lambda_i|}{r} - 1 \right) = \frac{\sum_{i=1}^{n} |\lambda_i|}{r} - n = 0$$

and

$$\begin{aligned}
\sum_{i=1}^{n} x_i^2 &= \sum_{i=1}^{n} \left(\frac{|\lambda_i|}{r} - 1 \right)^2 = \frac{\sum_{i=1}^{n} \lambda_i^2}{r^2} - \frac{2\sum_{i=1}^{n} |\lambda_i|}{r} + n \\
&= \frac{2mn^2}{(E(G))^2} - n \\
&\geq \frac{2mn^2}{2m(n-1) + n|\det \mathbf{A}|^{2/n}} - n \\
&= \left(\frac{2mn^3}{(n-1)\left(2m(n-1) + n|\det \mathbf{A}|^{2/n}\right)} - \frac{n^2}{n-1} \right) \left(1 - \frac{1}{n}\right) \\
&= \left(n^2 \left[\frac{2mn - \left(2m(n-1) + n|\det \mathbf{A}|^{2/n}\right)}{(n-1)\left(2m(n-1) + n|\det \mathbf{A}|^{2/n}\right)} \right] \right) \left(1 - \frac{1}{n}\right) \\
&= (nb)^2 \left(1 - \frac{1}{n}\right).
\end{aligned}$$

From Lemma 2.1, we get that

$$\sum_{i=1}^{n} \ln \left(\frac{|\lambda_i|}{r} \right) \leq \ln(1+(n-1)b) + (n-1)\ln(1-b).$$

Hence,

$$\prod_{i=1}^{n} |\lambda_i| \leq r^n (1+(n-1)b)(1-b)^{n-1}$$

that is,

$$|\det \mathbf{A}| \leq \left(\frac{E(G)}{n} \right)^n (1+(n-1)b)(1-b)^{n-1}.$$

This leads to the lower bound (8). □

For a non-singular graph G of order n, the following lower bound on $E(G)$ was found in [7, 14]

$$E(G) \geq n (|\det \mathbf{A}|)^{1/n}. \tag{10}$$

Remark 3.1. *Let b be given by Equation (9). Note that $0 \leq b < 1$, since G is connected non-singular graph with $n \geq 2$ vertices and the fact that [11, 22]*

$$E(G) \leq \sqrt{2m(n-1) + n|\det \mathbf{A}|^{2/n}} \leq \sqrt{2mn}.$$

Let

$$f(x) = (1+(n-1)x)(1-x)^{n-1}.$$

Note that f is decreasing for $0 \leq x < 1$ [25]. Thus, $f(b) \leq f(0) = 1$, this implies that the lower bound (8) is stronger than the lower bound (10) for connected non-singular graphs. Further, if G is the graph K_2, then the equality in (8) holds.

Theorem 3.2. *Let G be a connected non-singular graph with $n \geq 2$ vertices, m edges and maximum vertex degree Δ. Then*

$$E(G) \leq \frac{2m}{n} + n - 1 + \Delta \ln\left(\frac{n\,|\det \mathbf{A}|}{2m}\right). \tag{11}$$

The equality in (11) is achieved for $G \cong K_n$.

Proof. At first, recall that the following inequality

$$x \leq 1 + x \ln x\,,$$

for $x > 0$ [24]. Obviously, $|\lambda_i| > 0$, $1 \leq i \leq n$, for a non-singular graph G. Considering these facts with Equation (2), we have

$$\begin{aligned} E(G) &= \lambda_1 + \sum_{i=2}^{n} |\lambda_i| \\ &\leq \lambda_1 + \sum_{i=2}^{n} (1 + |\lambda_i| \ln |\lambda_i|) \\ &\leq \lambda_1 + n - 1 + \Delta \sum_{i=2}^{n} \ln |\lambda_i|\,, \text{ by Lemma 2.2} \\ &= \lambda_1 + n - 1 + \Delta \ln |\det \mathbf{A}| - \Delta \ln \lambda_1. \end{aligned} \tag{12}$$

Let us consider the function $f(x)$, defined by

$$f(x) = x - \Delta \ln x.$$

It is not difficult to see that f is a decreasing function in the interval $1 \leq x \leq \Delta$. Notice that $\lambda_1 \geq \frac{2m}{n}$ [6] and $\frac{2m}{n}$ is the average of the vertex degrees that is inevitably greater than unity for connected (molecular) graphs [15]. These together with Lemma 2.2 imply that $1 \leq \frac{2m}{n} \leq \lambda_1 \leq \Delta$. Therefore, we have

$$f(\lambda_1) \leq f\left(\frac{2m}{n}\right) = \frac{2m}{n} - \Delta \ln\left(\frac{2m}{n}\right).$$

Based on this inequality and Equation (12), we obtain the upper bound in (11). Moreover, one can readily check that the equality in (11) is achieved for $G \cong K_n$. □

Theorem 3.3. *Let G be a connected non-singular bipartite graph with $n \geq 2$ vertices, m edges and maximum vertex degree Δ. Then*

$$E(G) \leq \frac{4m}{n} + n - 2 + \Delta \ln\left(\frac{n^2\,|\det \mathbf{A}|}{4m^2}\right). \tag{13}$$

Proof. Notice that $x \leq 1 + x \ln x$, for $x > 0$ [24]. Further, $|\lambda_i| > 0$, $1 \leq i \leq n$, for non-singular graphs and $\lambda_1 = -\lambda_n$, for bipartite graphs [6]. Taking into account these with Equation (2), we obtain

$$\begin{aligned} E(G) &= 2\lambda_1 + \sum_{i=2}^{n-1} |\lambda_i| \\ &\leq 2\lambda_1 + \sum_{i=2}^{n-1} (1 + |\lambda_i| \ln |\lambda_i|) \\ &\leq 2\lambda_1 + n - 2 + \Delta \sum_{i=2}^{n-1} \ln |\lambda_i|\,, \text{ by Lemma 2.2} \\ &= 2\lambda_1 + n - 2 + \Delta \ln |\det \mathbf{A}| - \Delta \ln \lambda_1^2. \end{aligned} \tag{14}$$

Let

$$f(x) = 2x - \Delta \ln x^2.$$

It can be readily seen that f is a decreasing function in the interval $1 \leq x \leq \Delta$. Recall from Theorem 3.2 that both $\frac{2m}{n}$ and λ_1 belong to this interval and $\lambda_1 \geq \frac{2m}{n}$ [6]. Thus,

$$f(\lambda_1) \leq f\left(\frac{2m}{n}\right) = \frac{4m}{n} - \Delta \ln\left(\frac{4m^2}{n^2}\right).$$

Combining this with Equation (14), we get the required result in (13). □

In the next theorem, we give a lower bound on Randić energy of non-singular graphs considering the similar techniques in Theorem 3.1 together with Equations (4)–(6) and Lemmas 2.1, 2.5 and 2.7. Therefore, its proof is omitted.

Theorem 3.4. *Let G be a connected non-singular graph with $n \geq 3$ vertices. Then*

$$RE(G) \geq 1 + (n-1)\left(\frac{|\det \mathbf{R}|}{(1+(n-2)c)(1-c)^{n-2}}\right)^{1/(n-1)} \tag{15}$$

where

$$c = \left[\frac{(n-1)(2R_{-1}-1) - \left((n-2)(2R_{-1}-1) + (n-1)(|\det \mathbf{R}|)^{2/(n-1)}\right)}{(n-2)\left((n-2)(2R_{-1}-1) + (n-1)(|\det \mathbf{R}|)^{2/(n-1)}\right)}\right]^{1/2}. \tag{16}$$

For a (connected) graph G of order n, the authors derived that [9, 17]

$$RE(G) \geq 1 + (n-1)(|\det \mathbf{R}|)^{1/(n-1)} = 1 + (n-1)\left(\frac{|\det \mathbf{A}|}{\prod_{i=1}^{n} d_i}\right)^{1/(n-1)}. \tag{17}$$

Remark 3.2. *Let c be defined by Equation (16). Observe that $0 \leq c < 1$, since G is connected non-singular graph with $n \geq 3$ vertices and the fact that [17, 20, 21]*

$$\begin{aligned} RE(G) &\leq 1 + \sqrt{(n-2)(2R_{-1}-1) + (n-1)|\det \mathbf{R}|^{2/(n-1)}} \\ &\leq 1 + \sqrt{(n-1)(2R_{-1}-1)}. \end{aligned}$$

Consider the function $f(x)$ defined as follows

$$f(x) = (1+(n-2)x)(1-x)^{n-2}.$$

Notice that f is decreasing for $0 \leq x < 1$ [26]. Then $f(c) \leq f(0) = 1$. Combining this with Lemma 2.8, we deduce that the lower bound (15) is stronger than the lower bound (17) for connected non-singular graphs. Furthermore, if G is the complete graph K_n, then the equality in (15) is attained.

Theorem 3.5. *Let G be a connected non-singular graph with $n \geq 2$ vertices, m edges, maximum vertex degree Δ and minimum vertex degree δ. Then*

$$RE(G) \leq 1 + \frac{n-1+\Delta \ln\left(\frac{n|\det \mathbf{A}|}{2m}\right)}{\delta}. \tag{18}$$

The equality in (18) is achieved for $G \cong K_n$.

Proof. According to Lemma 2.4 and Equation (12), we have

$$\begin{aligned} RE(G) &\leq 1 + \frac{E(G) - \lambda_1}{\delta} \\ &\leq 1 + \frac{n-1+\Delta(\ln|\det \mathbf{A}| - \ln \lambda_1)}{\delta}. \end{aligned}$$

From the above and the fact that $\lambda_1 \geq \frac{2m}{n}$ [6], we arrive at

$$RE(G) \leq 1 + \frac{n-1+\Delta\left(\ln|\det \mathbf{A}| - \ln \frac{2m}{n}\right)}{\delta}.$$

Hence the upper bound in (18) holds. Moreover, it is elementary to check that the equality in (18) is achieved for $G \cong K_n$. □

Theorem 3.6. *Let G be a connected non-singular bipartite graph with $n \geq 2$ vertices, m edges, maximum vertex degree Δ and minimum vertex degree δ. Then*

$$RE(G) \leq 2 + \frac{n-2+\Delta \ln\left(\frac{n^2|\det \mathbf{A}|}{4m^2}\right)}{\delta}. \tag{19}$$

Proof. From Lemma 2.6 and Equation (14), we directly get

$$RE(G) \leq 2 + \frac{E(G) - 2\lambda_1}{\delta}$$

$$\leq \quad 2+\frac{n-2+\Delta\left(\ln|\det \mathbf{A}|-\ln\lambda_1^2\right)}{\delta}.$$

Considering this with the lower bound $\lambda_1 \geq \frac{2m}{n}$ [6], we obtain

$$RE\,(G) \leq 2+\frac{n-2+\Delta\left(\ln|\det \mathbf{A}|-\ln\frac{4m^2}{n^2}\right)}{\delta}$$

which is the upper bound in (19). □

Remark 3.3. *We finally note that the upper bounds in Equations* (11)*,* (13)*,* (18) *and* (19) *can be improved using a lower bound such that* $\lambda_1 \geq \gamma \geq \frac{2m}{n}$ *in Theorems 3.2, 3.3, 3.5 and 3.6, respectively.*

Acknowledgment

The author would like to thank the two anonymous referees for their valuable comments and suggestions.

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