On Harary energy and Reciprocal distance Laplacian energies

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Abstract. Let $G$ be a simple, undirected, connected and unweighted graphs. The Reciprocal distance energy of a graph $G$ is equal to the sum of the absolute values of the reciprocal distance eigenvalues. In this work, we find a lower bound for the Harary energy, reciprocal distance Laplacian energy and reciprocal distance signless Laplacian energy of a graph. Moreover, we find relationship between the Harary energy and Reciprocal distance Laplacian energies.

1. Introduction and preliminaries

Let $G=(V,E)$ be a connected simple undirected graph with vertex set $V$ and edge set $E$. The distance $d(v_i,v_j)$ between the vertices $v_i$ and $v_j$ of $G$ is equal to the length of (number of edges in) the shortest path that connects $v_i$ and $v_j$. The Harary matrix of graph $G$, which is also called as the Reciprocal Distance matrix, is an $n \times n$ matrix defined as

$$RD_{i,j} = \begin{cases} \frac{1}{d(v_i,v_j)} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

Henceforth, we consider $i \neq j$ for $d(v_i,v_j)$.

The transmission of a vertex $v$, denoted by $Tr_G(v)$ and defined by $Tr_G(v) = \sum_{u \in V(G)} d(u,v)$.

Definition 1 Let $G$ be a simple connected graph with $V(G) = \{v_1,v_2,\ldots,v_n\}$. The reciprocal distance degree of a vertex $v$, denoted by $RTr_G(v)$, is given by

$$RTr_G(v) = \sum_{u \in V(G) \setminus \{v\}} \frac{1}{d(u,v)}.$$

Let $RT_G$ be the $n \times n$ diagonal matrix defined by $RT_{i,i} = RTr_G(v_i)$.

Sometimes we use the notation $RT_i$ instead of $RTr_G(v_i)$ for $i = 1,\ldots,n$.

Definition 2 A connected graph $G$ is called a k-reciprocal distance degree regular graph if $RT_i = k$ for all $i \in \{1,2,\ldots,n\}$.

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The Harary index of a graph \( G \), denoted by \( H(G) \), is defined in [18] as

\[
H(G) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} RD_{i,j} = \frac{1}{2} \sum_{u,v \in V(G)} \frac{1}{d(u,v)}.
\]

Clearly,

\[
H(G) = \frac{1}{2} \sum_{v \in V(G)} RT_{v_G}(v).
\]

We recall that the spectral radius of a matrix \( A \) is \( \rho(A) = \max_{1 \leq i \leq n} \{|\lambda_i(A)|\} \) where, for \( i = 1, \ldots, n \), \( \lambda_i(A) \) are the eigenvalues of the matrix \( A \).

In 2018, Bapat and Panda [3], defined the Reciprocal distance Laplacian matrix as \( RL(G) = RT(G) - RD(G) \) and in 2019, Alhevaz et al. [1], defined the Reciprocal distance signless Laplacian matrix as \( RQ(G) = RT(G) + RD(G) \).

We observe that \( RD(G), RL(G) \) and \( RQ(G) \) are real symmetric matrices, then we can write the eigenvalues in decreasing order, this is

\[
\lambda_1(RD(G)) \geq \lambda_2(RD(G)) \geq \cdots \geq \lambda_n(RD(G)),
\]

\[
\lambda_1(RL(G)) \geq \lambda_2(RL(G)) \geq \cdots \geq \lambda_n(RL(G))
\]

and

\[
\lambda_1(RQ(G)) \geq \lambda_2(RQ(G)) \geq \cdots \geq \lambda_n(RQ(G)).
\]

Moreover, \( RD(G) \) and \( RQ(G) \) are irreducible nonnegative matrices, \( \rho(RD(G)) \) and \( \rho(RQ(G)) \) are a simple eigenvalues of \( RD(G) \) and \( RQ(G) \), respectively. In [14] the authors obtained upper bounds and lower bounds for the spectral radius of Reciprocal distance, Reciprocal distance Laplacian and Reciprocal distance signless Laplacian matrices of a graph, and they characterized the graphs that attained some of the bounds mentioned.

The energy of a graph is a concept originating from theoretical chemistry and in 1978 Ivan Gutman defined the energy of a graph through the eigenvalues of the adjacency matrix of graph [8]. In particular: let \( A(G) \) be the adjacency matrix of a graph \( G \) of order \( n \), then the energy of the graph \( G \) is \( E(G) = \sum_{i=1}^{n} |\lambda_i(A(G))| \).

About the energy of graph, we highlight two classic bounds to a graph on \( n \) vertices and \( m \) edges:

\[
E(G) \leq \sqrt{2mn} \quad \text{and} \quad E(G) \leq \frac{2m}{n} + \sqrt{(n-1) + \left(2m - \left(\frac{2m}{n}\right)^2\right)},
\]

given by McClelland in [13] and given by Koolen and Moulton in [12], respectively.

The energy of a graph has been extensively studied over the years. Although, in some cases it has been possible to determine the energy for certain graphs, but in general it is not possible to determine it exactly. Examples of some works about energy on special graphs, such as bipartite graphs, cyclic and acyclic graphs, regular graph, line graphs, trees with a given diameter [2, 9, 10, 11, 19, 20, 21, 22, 23].

The concept energy of a graph has been extended to different matrices associated with a graph: let \( M \) be a matrix associated with a graph \( G \), then the energy of matrix \( M \) is defined in [4] by

\[
E_M(G) = \sum_{i=1}^{n} |\lambda_i(M(G)) - \bar{\lambda}(M(G))|,
\]

where \( \bar{\lambda}(M) \) is the average of the eigenvalues of matrix \( M \).
where $\bar{\lambda}(M(G))$ is the average of eigenvalues of $M$.

Several authors have defined the energy of different matrices coinciding or using the definition given above.

**Definition 3** [7] The Harary energy of a graph $G$, denoted by $E_H(G)$, is defined as

$$E_H(G) = \sum_{i=1}^{n} |\lambda_i(RD(G))|.$$  

The Harary energy is also called Reciprocal distance energy.

**Definition 4** [1] Let $G$ be a connected graph of order $n$. Then the Reciprocal distance signless Laplacian energy of $G$, denoted by $E_{RQ}(G)$ is defined as

$$E_{RQ}(G) = \sum_{i=1}^{n} \left| \lambda_i(RQ(G)) - \frac{1}{n} \sum_{j=1}^{n} R_{ij} \right|.$$  

**Definition 5** [15] Let $G$ be a connected graph of order $n$. Then the Reciprocal distance Laplacian energy of $G$, denoted by $E_{RL}(G)$ is

$$E_{RL}(G) = \sum_{i=1}^{n} \left| \lambda_i(RL(G)) - \frac{2H(G)}{n} \right|.$$  

In [15], we found bounds on the Reciprocal Distance Energy, Reciprocal Distance Laplacian Energy and Reciprocal Distance signless Laplacian Energy, and we characterized the graphs that attained some of those bounds. Now, in this work we find a new bounds for the Harary energy and reciprocal distance signless Laplacian energy of a graph, and we obtain relationship between the Harary energy and Reciprocal distance Laplacian energies.

On the other hand, in [16] Nikiforov defines the energy of a matrix $M$ as the sum of the singular values of $M$. Let $g = \min\{m,n\}$. Let $s_1(M) \geq s_2(M) \geq \cdots \geq s_g(M)$ be the singular values of matrix $M$. It is well known that if $m > n$ then, for $i = 1, \ldots, n$, $s_i(M) = \sqrt{\lambda_i(M^*M)}$ and if $m \leq n$ then, for $i = 1, 2, \ldots, m$, $s_i(M) = \sqrt{\lambda_i(MM^*)}$. Using the fact that (1) the positive semidefinite matrices $MM^*$ and $M^*M$ have the same nonzero eigenvalues and (2) $RD(G), RL(G)$ and $RQ(G)$ are a symmetric matrix, then Definition 3, Definition 4 and Definition 5 become

$$E_{RD}(G) = \sum_{i=1}^{n} s_i(RD(G)),$$

$$E_{RQ}(G) = \sum_{i=1}^{n} s_i \left( RQ(G) - \frac{2H(G)}{n} I_n \right),$$

and

$$E_{RL}(G) = \sum_{i=1}^{n} s_i \left( RL(G) - \frac{2H(G)}{n} I_n \right),$$

where $\lambda_i(RD(G))$ is the $i$th eigenvalue of $RD(G)$. Several authors have defined the energy of different matrices coinciding or using the definition given above.
respectively, where $I_n$ denote the identity matrix.

To finish this section, we recall that the Frobenius norm of an $n \times n$ matrix $M = (m_{i,j})$ is

$$||M|| = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} |m_{i,j}|^2}.$$  

Moreover, if $M$ is a normal matrix then $||M||^2 = \sum_{i=1}^{n} |\lambda_i(M)|^2$ where $\lambda_1(M), \ldots, \lambda_n(M)$ are the eigenvalues of $M$. In particular, this property is satisfied to $RD(G), RQ(G)$ and $RQ(G)$ matrices.

2. Lower bounds for the Harary energy and Reciprocal distance Laplacian energies

In this section we obtain lower bounds for Harary energy and Reciprocal distance Laplacian energies.

**Lemma 1** [17] Let $n \geq 1$ be an integer and $a_1, a_2, \ldots, a_n$ be some nonnegative real numbers such that $a_1 \geq a_2 \geq \ldots \geq a_n$. Then

$$(a_1 + \cdots + a_n)(a_1 + a_n) \geq a_1^2 + \cdots + a_n^2 + na_1a_n.$$  

Moreover, the equality holds if and only if for some $r \in \{1, \ldots, n\}$, $a_1 = \ldots = a_r$ and $a_{r+1} = \ldots = a_n$.

**Theorem 1** Let $G$ be a graph with $n \geq 2$ vertices and $m \geq 1$ edges. Assume that $\lambda_1(RD(G)), \ldots, \lambda_n(RD(G))$ are all the RD-eigenvalues of $G$ such that $|\lambda_1(RD(G))| \geq \cdots \geq |\lambda_n(RD(G))| \geq 0$. Then

$$E_{RD}(G) \geq \frac{||RD(G)||^2 + n|\lambda_1(RD(G))|\lambda_n(RD(G))}{|\lambda_1(RD(G))| + |\lambda_n(RD(G))|}.$$  

**Proof.** For $i = 1, \ldots, n$ we denote $\lambda_i = \lambda_i(RD(G))$. Using Lemma 1 we obtain that

$$(|\lambda_1| + \cdots + |\lambda_n|)(|\lambda_1||\lambda_n|) \geq |\lambda_1|^2 + \cdots + |\lambda_n|^2 + n|\lambda_1||\lambda_n|.$$  

Since $E_{RD}(G) = \sum |\lambda_i|$, then

$$E_{RD}(G) \geq \frac{|\lambda_1|^2 + \cdots + |\lambda_n|^2 + n|\lambda_1||\lambda_n|}{|\lambda_1| + |\lambda_n|}.$$  

We recall that $RD(G)$ is a normal matrix. Therefore

$$E_{RD}(G) \geq \frac{||RD(G)||^2 + n|\lambda_1||\lambda_n|}{|\lambda_1| + |\lambda_n|}.$$  

**Theorem 2** Let $G$ be a connected graph with $n \geq 2$ vertices. Let $\lambda_p, \lambda_r$ be $RQ$-eigenvalues such that $|\lambda_p(RQ(G)) - \frac{2H(G)}{n}| = \max \left\{ |\lambda_1(RQ(G)) - \frac{2H(G)}{n}|, |\lambda_n(RQ(G)) - \frac{2H(G)}{n}| \right\}$ and $|\lambda_r(RQ(G)) - \frac{2H(G)}{n}| = \min \left\{ |\lambda_1(RQ(G)) - \frac{2H(G)}{n}|, |\lambda_n(RQ(G)) - \frac{2H(G)}{n}| \right\}$. Then

$$E_{RQ}(G) \geq \frac{||RQ(G)||^2 - \frac{(2H(G))^2}{n} + n|\lambda_p(RQ(G)) - \frac{2H(G)}{n}| |\lambda_r(RQ(G)) - \frac{2H(G)}{n}|}{|\lambda_p(RQ(G)) - \frac{2H(G)}{n}| + |\lambda_r(RQ(G)) - \frac{2H(G)}{n}|}.$$  


**Example 1** We consider the graphs

\[ G_1, G_2, G_3 \text{ given by Figure 1, } G_4 \text{ is the star on } 7 \text{ vertices, } G_5 \text{ is the path on } 7 \text{ vertices and } G_6 \text{ is the cycle on } 7 \text{ vertices, denoted by } S_7, P_7 \text{ and } C_7 \text{ respectively.} \]

\[ \text{Figure 1.} \]

The following tables show the bounds obtained for the above graphs.
Table 1. Lower bounds for the Harary energy.

|     | $G_1$  | $G_2$  | $G_3$ | $S_7$ | $P_7$  | $C_7$  |
|-----|--------|--------|-------|-------|--------|--------|
| $E_{RD}(G)$ | 12.5568 | 5.5311 | 12 | 8 | 8.3051 | 9.0287 |
| Theorem 1 | 8.718113 | 4.9091 | 7.5 | 7.4444 | 5.0396 | 7.3177 |

Table 2. Lower bounds for the Reciprocal distance signless Laplacian energy.

|     | $G_1$  | $G_2$  | $G_3$ | $S_7$ | $P_7$  | $C_7$  |
|-----|--------|--------|-------|-------|--------|--------|
| $E_{RQ}(G)$ | 12.8889 | 5.6232 | 12 | 9.1845 | 8.5906 | 9.0287 |
| Theorem 2 | 8.1862 | 5.3865 | 7.5 | 7.0861 | 5.2362 | 7.3177 |

Table 3. Lower bounds for the Reciprocal distance Laplacian energy.

|     | $G_1$  | $G_2$  | $G_3$ | $S_7$ | $P_7$  | $C_7$  |
|-----|--------|--------|-------|-------|--------|--------|
| $E_{RL}(G)$ | 13.4953 | 5.5 | 12 | 7.7143 | 9.1142 | 9.0287 |
| Theorem 3 | 9.8525 | 4.5 | 7.5 | 7.1788 | 6.4573 | 7.3177 |

3. Relationship between the Harary energy and Reciprocal distance Laplacian energies

In this section we find relationship between the Harary energy and Reciprocal distance Laplacian energies: first we study two particular cases, when $G$ is a regular graph of diameter 2 and when the graph $G$ is reciprocal distance regular; and finally we give general relations between the Harary energy and Reciprocal distance Laplacian energies.

Theorem 4 [5] Let $G$ be an $r$-regular graph of diameter 2 on $n$ vertices, its adjacency spectrum be $\text{spec}(A(G)) = \{r, \lambda_2, \ldots, \lambda_n\}$. Then the RD-spectrum of $G$ is

$$\text{spec}(RD(G)) = \left\{ \frac{1}{2}(n+r-1), \frac{1}{2}(\lambda_2 - 1), \ldots, \frac{1}{2}(\lambda_n - 1) \right\}.$$ 

Theorem 5 Let $G$ be an $r$-regular graph on $n$ vertices such that $\text{diam}(G) = 2$. Let $r, \lambda_1, \ldots, \lambda_n$ be the adjacency eigenvalues of $G$. Then eigenvalues of the reciprocal distance signless Laplacian matrix of $G$ are

$$n + r - 1 \quad \text{and} \quad \frac{1}{2}(\lambda_i + n + r) - 1, \quad i = 2, \ldots, n$$

Proof. Let $G$ an $r$-regular graph on $n$ vertices. We have $RQ(G) = RT(G) + RD(G)$. Since $\text{diam}(G) = 2$, then

$$RD(G) = \frac{1}{2}(J_n - I_n + A(G)),$$
where $J_n$ denote the all-1 matrix of order $n$ and $I_n$ denote the identity matrix of order $n$.

We observe that, in this case, $RT(G) = \frac{1}{2} (n + r - 1) I_n$. Thus

$$RQ(G) = \frac{1}{2} (J_n + (n + r - 2) I_n + A(G))$$

Note that eigenvectors of $A(G)$ are also eigenvectors of matrix $J_n$ and $\text{spec}(J_n) = \{n, 0, \ldots, 0\}$. Therefore,

$$\text{spec}(RQ(G)) = \left\{n + r - 1, \frac{1}{2}(\lambda_2 + n + r) - 1, \ldots, \frac{1}{2}(\lambda_n + n + r) - 1\right\}.$$  

\[\square\]

**Theorem 6** Let $G$ be an $r$-regular graph on $n$ vertices such that $\text{diam}(G) = 2$. Let $r, \lambda_1, \ldots, \lambda_n$ be the adjacency eigenvalues of $G$. Then eigenvalues of the reciprocal Laplacian matrix of $G$ are $0$ and $\frac{1}{2}(n + r - \lambda_i), i = 2, \ldots, n$

**Proof.** Analogously to Theorem 5, if $G$ is an $r$-regular graph on $n$ vertices such that $\text{diam}(G) = 2$, then

$$RL(G) = RT(G) - RD(G) = \frac{1}{2}(n + r - 1) I_n - RD(G).$$

Therefore, for $i = 1, 2, \ldots, n - 1$, $\lambda_i(RL(G)) = \frac{1}{2}(n + r - \lambda_i)$ and $\lambda_n(RL(G)) = 0$. \[\square\]

**Theorem 7** Let $G$ be a $r$-regular graph of diameter 2 on order $n$. Then

$$E_{RQ}(G) = E_{RD}(G) = E_{RL}(G).$$

**Proof.** Note that

$$E_{RD}(G) = \frac{1}{2}(n + r - 1) + \frac{1}{2} \sum_{i=2}^{n} |\lambda_i - 1|,$$

$$E_{RL}(G) = \left|0 - \frac{1}{2}(n + r - 1)\right| + \sum_{i=2}^{n} \left|\frac{1}{2}(n + r - \lambda_i) - \frac{1}{2}(n + r - 1)\right|$$

$$= \frac{1}{2}(n + r - 1) + \frac{1}{2} \sum_{i=2}^{n} |\lambda_i + 1|$$

$$= E_{RD}(G)$$

and

$$E_{RQ}(G) = \left|(n + r - 1) - \frac{1}{2}(n + r - 1)\right| + \sum_{i=2}^{n} \left|\frac{1}{2}(\lambda_i + n + r) - 1 - \frac{1}{2}(n + r - 1)\right|$$

$$= \frac{1}{2}(n + r - 1) + \frac{1}{2} \sum_{i=2}^{n} |\lambda_i - 1|$$

$$= E_{RD}(G).$$

Thus, the result is obtained. \[\square\]
**Theorem 8** Let $G$ be a $k$-reciprocal distance regular graph of order $n$. Then

$$E_{RQ}(G) = E_{RD}(G) = E_{RL}(G).$$

**Proof.** If $G$ is a $k$-reciprocal distance regular graph then

$$RQ(G) = kI_n + RD(G)$$

and

$$RL(G) = kI_n - RD(G).$$

Thus

$$\lambda_i(RQ(G)) = k + \lambda_i(RD(G))$$

and

$$\lambda_i(RL(G)) = k - \lambda_i(RD(G)).$$

Then

$$E_{RQ}(G) = \sum_{i=1}^{n} |\lambda_i(RQ(G)) - k| = \sum_{i=1}^{n} |k + \lambda_i(RD(G)) - k| = E_{RD}(G),$$

and

$$E_{RL}(G) = \sum_{i=1}^{n} |\lambda_i(RL(G)) - k| = \sum_{i=1}^{n} |k - \lambda_i(RD(G)) - k| = E_{RD}(G).$$

Therefore, the result is obtained. 

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**Lemma 2** [6] Let $X$, $Y$ and $Z$ be square matrices of order $n$, such that $Z = X + Y$. Then

$$\sum_{i=1}^{n} s_i(Z) \leq \sum_{i=1}^{n} s_i(X) + \sum_{i=1}^{n} s_i(Y).$$

Equality holds if and only if there exists an orthogonal matrix $P$, such that $PX$ and $PY$ are both positive semidefinite matrix.

**Theorem 9** Let $G$ be a graph of order $n$. Then

$$E_{RQ}(G) - E_{RL}(G) \leq 2E_{RD}(G) \leq E_{RQ}(G) + E_{RL}(G).$$

**Proof.** We observe that $RQ(G) - RL(G) = 2RD(G)$, then

$$\left( RQ(G) - \frac{2H(G)}{n}I \right) - \left( RL(G) - \frac{2H(G)}{n}I \right) = 2RD(G).$$

By the Lemma 2 we get the left inequality. Now, apply the same Lemma 2 on

$$\left( RQ(G) - \frac{2H(G)}{n}I \right) = \left( RL(G) - \frac{2H(G)}{n}I \right) + 2RD(G),$$

we get the right inequality. 

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**Theorem 10** If $G$ is a connected graph of order $n$. Then

$$E_{RQ}(G) \leq E_{RD}(G) + \sum_{i=1}^{n} \left| RT_i - \frac{2H(G)}{n} \right|. $$
**Proof.** Applying Lemma 2 to
\[ RQ(G) - \frac{2H(G)}{n} I_n = RT(G) - \frac{2H(G)}{n} I_n + RD(G) \]
we obtain
\[ \sum_{i=1}^{n} s_i \left( RQ(G) - \frac{2H(G)}{n} I_n \right) \leq \sum_{i=1}^{n} s_i \left( RT(G) - \frac{2H(G)}{n} I_n \right) + \sum_{i=1}^{n} s_i (RD(G)) \]
\[ E_{RQ}(G) \leq \sum_{i=1}^{n} \left| RT_i(G) - \frac{2H(G)}{n} \right| + \sum_{i=1}^{n} |\lambda_i RD(G)| \]
\[ E_{RQ}(G) \leq \sum_{i=1}^{n} \left| RT_i(G) - \frac{2H(G)}{n} \right| + E_{RD}(G). \]

**Corollary 1** If \( G \) is a connected graph, then
\[ E_{RQ}(G) \leq E_{RD}(G) + \sqrt{n \sum_{i=1}^{n} RT_i^2 - (2H(G))^2}. \]

**Proof.** By Cauchy-Schwarz inequality, we get
\[ \sum_{i=1}^{n} \left| RT_i(G) - \frac{2H(G)}{n} \right| \leq \sqrt{n \sum_{i=1}^{n} \left( RT_i(G) - \frac{2H(G)}{n} \right)^2} = \sqrt{n \sum_{i=1}^{n} RT_i^2 - (2H(G))^2}. \]
Now, replacing in Theorem 10 the result is obtained.

**Theorem 11** Let \( G \) be a graph of order \( n \). Then
\[ E_{RL}(G) \leq E_{RD}(G) + \sum_{i=1}^{n} \left| RT_i - \frac{2H(G)}{n} \right|. \]

**Proof.** Applying Lemma 2 to
\[ RL(G) - \frac{2H(G)}{n} I_n = \left( RT(G) - \frac{2H(G)}{n} I_n \right) + (-RD(G)) \]
we obtain
\[ \sum_{i=1}^{n} s_i \left( RL(G) - \frac{2H(G)}{n} I_n \right) \leq \sum_{i=1}^{n} s_i \left( RT(G) - \frac{2H(G)}{n} I_n \right) + \sum_{i=1}^{n} s_i (-RD(G)) \]
\[ E_{RL}(G) \leq \sum_{i=1}^{n} \left| RT_i(G) - \frac{2H(G)}{n} \right| + \sum_{i=1}^{n} |\lambda_i (-RD(G))| \]
\[ E_{RL}(G) \leq \sum_{i=1}^{n} \left| RT_i(G) - \frac{2H(G)}{n} \right| + E_{RD}(G). \]
Corollary 2 If $G$ is a connected graph, then

$$E_{RL}(G) \leq E_{RD}(G) + \sqrt{n \sum_{i=1}^{n} RT_i^2 - (2H(G))^2}.$$  

Proof. The prove is similar to Corollary 1.

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