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# Bounds for various graph energies

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**Abstract.** In this paper, we obtain some upper and lower bounds for the spectral radius of some special matrices such as maximum degree, minimum degree, Randic, sum-connectivity, degree sum, degree square sum, first Zagreb and second Zagreb matrices of a simple connected graph $G$ by the help of matrix theory. We also get some upper bounds for the corresponding energies of $G$.

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## 1 Introduction

Erich Hückel used the chemical applications of graph in describing the molecular orbitals and energies of the $\pi$-bonding frameworks. The structure of the simplest hydrocarbon was represented as a graph such that the eigenvalues of the graph is energy levels of electrons. Moreover, the carbon atoms denote the vertices of the graph and chemical bonds between the carbon atoms denote the edges of the graph.

In 1978, inspired by Hückel's study, Ivan Gutman defined the energy of a graph $G$ as

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

where $\lambda_1, \lambda_2, \cdots, \lambda_n$ are the eigenvalues of the adjacency matrix of $G$, [8].

Many authors defined new type energies of a graph by means of different graph matrices and obtained some properties of these energies, see e.g. [1–7, 9, 14–17]. Also, some bounds for various energies of the graphs were investigated in [10–12].

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Now, we give the definitions of various matrices and energies of the graphs which will be used in the following sections:

Let $G$ be a simple connected graph. The matrix $M(G) = [M_{ij}]$ defined as

$$M_{ij} = \begin{cases} \max\{d_i, d_j\}, & \text{if } i \sim j \\ 0, & \text{otherwise} \end{cases}$$

is called the maximum degree matrix of $G$, [1]. The maximum degree energy $E_M$ of $G$ is the sum of the absolute values of the eigenvalues of $M(G)$.

The matrix $m(G) = [m_{ij}]$ defined as

$$m_{ij} = \begin{cases} \min\{d_i, d_j\}, & \text{if } i \sim j \\ 0, & \text{otherwise} \end{cases}$$

is called the minimum degree matrix of $G$, [2]. The minimum degree energy $E_m$ of $G$ is the sum of the absolute values of the eigenvalues of $m(G)$.

The matrix $R(G) = [r_{ij}]$ defined as

$$r_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}}, & \text{if } i \sim j \\ 0, & \text{otherwise} \end{cases}$$

is called the Randic matrix of $G$, [7]. Similarly the Randic energy $E_R$ of $G$ is the sum of the absolute values of the eigenvalues of $R(G)$.

The matrix $SC(G) = [sc_{ij}]$ defined by

$$sc_{ij} = \begin{cases} \frac{1}{\sqrt{d_i + d_j}}, & \text{if } i \sim j \\ 0, & \text{otherwise} \end{cases}$$

is called the sum-connectivity matrix of $G$, [17]. The sum-connectivity energy $E_{SC}$ of $G$ is the sum of the absolute values of the eigenvalues of $SC(G)$.

The matrix $DS(G) = [ds_{ij}]$ defined by

$$ds_{ij} = \begin{cases} d_i + d_j, & \text{if } i \neq j \\ 0, & \text{otherwise} \end{cases}$$

is called the degree sum matrix of $G$, [9]. Then the degree sum energy $E_{DS}$ of $G$ is the sum of the absolute values of the eigenvalues of $DS(G)$.

The matrix $DSS(G) = [dss_{ij}]$ defined as

$$dss_{ij} = \begin{cases} d_i^2 + d_j^2, & \text{if } i \neq j \\ 0, & \text{otherwise} \end{cases}$$

is the degree square sum matrix of $G$, [3]. The degree square sum energy $E_{DSS}$ of $G$ is the sum of the absolute values of the eigenvalues of $DSS(G)$.

The matrix $Z^{(1)}(G) = [z_{ij}^{(1)}]$ defined by

$$z_{ij}^{(1)} = \begin{cases} d_i + d_j, & \text{if } i \sim j \\ 0, & \text{otherwise} \end{cases}$$

is called the first Zagreb matrix of $G$. The first Zagreb energy $ZE_1$ of $G$ is the sum of the absolute values of the eigenvalues of $Z^{(1)}(G)$.

The matrix $Z^{(2)}(G) = [z_{ij}^{(2)}]$ defined by

$$z_{ij}^{(2)} = \begin{cases} d_i d_j, & \text{if } i \sim j \\ 0, & \text{otherwise} \end{cases}$$

is called the second Zagreb matrix of $G$. The second Zagreb energy $ZE_2$ of $G$ is the sum of the absolute values of the eigenvalues of $Z^{(2)}(G)$.

**Lemma 1.1** *[13] Let A be an $n \times n$ square matrix, then the spectral radius of A satisfies*

$$R_{\min} \leq \rho(A) \leq R_{\max}$$

*where* $R_{\min} = \min_{1 \leq i \leq n} R_i(A)$, $R_{\max} = \max_{1 \leq i \leq n} R_i(A)$, *and* $R_i(A) = \sum_{j=1}^{n} a_{ij}$.

In the following sections, we assume that $G$ is a simple connected graph with $n$ vertices and $m$ edges and the degrees of the vertices of $G$ satisfy $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$.

## 2 The bounds for spectral radius of some matrices of a graph

In this section, we will obtain upper and lower bounds for the spectral radius of maximum degree, minimum degree, Randic, sum-connectivity, degree sum, degree square sum, first Zagreb and second Zagreb matrices of a graph by the help of matrix theory and basic information of graph theory.

**Theorem 2.1** *The bounds for the spectral radius of maximum degree matrix $M$ of $G$ is*

$$\sum_{n \sim j} d_j \leq \rho(M(G)) \leq \Delta^2.$$

*Proof.* By our assumption, $d_n = \delta$ is the minimum degree in $G$, then $R_{\min}(M(G))$ is obtained from the $n$-th row of maximum degree matrix of $G$. For all vertices $j$ which are adjacent to $n$, we have $\max\{d_n, d_j\} = d_j$. Then, by the definition of $M(G)$, we obtain

$$R_{\min}(M(G)) = \sum_{n \sim j} d_j.$$

Also, we assume that $d_1 = \Delta$ is the maximum degree in $G$ implying that $R_{\max}(M(G))$ is obtained from the first row of maximum degree matrix of $G$. The number of the adjacent vertices of 1 is $\Delta$ and for all $k$ which are adjacent to 1, we have $\max\{d_k, d_1\} = d_1 = \Delta$. Then, by the definition of $M(G)$, we obtain

$$R_{\max}(M(G)) = \Delta^2.$$

Hence by using Lemma 1.1, we get

$$\sum_{n \sim j} d_j \leq \rho(M(G)) \leq \Delta^2.$$

**Theorem 2.2** *The bounds for the spectral radius of minimum degree matrix m of G are*

$$\delta^2 \leq \rho(m(G)) \leq \sum_{1\sim j} d_j.$$

*Proof.* Since $d_n = \delta$ is the minimum degree in $G$, $R_{\min}(m(G))$ is obtained from the $n-th$ row of minimum degree matrix of $G$. The number of the adjacent vertices of $n$ is $\delta$, and for all $k$ which are adjacent to $n$, we have $\min\{d_k, d_n\} = d_n = \delta$. Then, by the definition of $m(G)$, we obtain

$$R_{\min}(m(G)) = \delta^2.$$

Moreover, since $d_1 = \Delta$ is the maximum degree in $G$, $R_{\max}(M(G))$ is obtained from the first row of minimum degree matrix of $G$. For all vertices $j$ which are adjacent to 1, we have $\min\{d_1, d_j\} = d_j$. Then, by the definition of $m(G)$, we obtain

$$R_{\max}(m(G)) = \sum_{1\sim j} d_j.$$

Therefore, by using Lemma 1.1, we obtain

$$\delta^2 \leq \rho(m(G)) \leq \sum_{1\sim j} d_j.$$

**Theorem 2.3** *The bounds for the spectral radius of the Randic matrix R of G are*

$$\sum_{n\sim k} \frac{1}{\sqrt{\delta d_k}} \leq \rho(R(G)) \leq \sum_{1\sim j} \frac{1}{\sqrt{\Delta d_j}}.$$

*Proof.* Since $d_n = \delta$ is the minimum degree in $G$, $R_{\min}(R(G))$ is obtained from the $n-th$ row of Randic matrix of $G$. Then, by the definition of $R(G)$, we obtain

$$R_{\min}(R(G)) = \sum_{n\sim k} \frac{1}{\sqrt{\delta d_k}}.$$

Also, since $d_1 = \Delta$ is the maximum degree in $G$, $R_{\max}(R(G))$ is obtained from the first row of randic matrix of $G$. Then, by the definition of $R(G)$, we get

$$R_{\max}(R(G)) = \sum_{1\sim j} \frac{1}{\sqrt{\Delta d_j}}.$$

As a result, by using Lemma 1.1, we have

$$\sum_{n\sim k} \frac{1}{\sqrt{\delta d_k}} \leq \rho(R(G)) \leq \sum_{1\sim j} \frac{1}{\sqrt{\Delta d_j}}.$$

**Theorem 2.4** *The bounds for the spectral radius of sum-connectivity matrix SC of G are*

$$\sum_{n\sim k} \frac{1}{\sqrt{\delta + d_k}} \leq \rho(SC(G)) \leq \sum_{1\sim j} \frac{1}{\sqrt{\Delta + d_j}}.$$

*Proof.* Since $d_n = \delta$ is the minimum degree in $G$, $R_{\min}(SC(G))$ is obtained from the $n-th$ row of sum-connectivity matrix of $G$. Then, by the definition of $SC(G)$, we obtain

$$R_{\min}(SC(G)) = \sum_{n\sim k} \frac{1}{\sqrt{\delta + d_k}}.$$

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Also, since $d_1 = \Delta$ is the maximum degree in $G$, $R_{\max}(SC(G))$ is obtained from the first row of sum-connectivity matrix of $G$. Then, by the definition of $SC(G)$, we get

$$R_{\max}(SC(G)) = \sum_{1\sim j} \frac{1}{\sqrt{\Delta + d_j}}.$$

In conclusion, by using Lemma 1.1, we have

$$\sum_{n\sim k} \frac{1}{\sqrt{\delta + d_k}} \leq \rho(SC(G)) \leq \sum_{1\sim j} \frac{1}{\sqrt{\Delta + d_j}}.$$

**Theorem 2.5** *The bounds for the spectral radius of degree sum matrix DS of G is*

$$\delta(n-2) + 2m \leq \rho(DS(G)) \leq \Delta(n-2) + 2m.$$

*Proof.* Since $d_n = \delta$ is the minimum degree in $G$, $R_{\min}(DS(G))$ is obtained from the $n - th$ row of degree sum matrix of $G$. Then, by the definition of $DS(G)$, we have

$$R_{\min}(DS(G)) = \sum_{i=1}^{n-1} \delta + d_i.$$

Since $G$ is a simple connected graph with $n$ vertices and $m$ edges, we have

$$\sum_{i=1}^{n} d_i = 2m. \tag{1}$$

By using (1), we get

$$\begin{aligned} R_{\min}(DS(G)) &= (n-1)\delta + 2m - \delta \\ &= (n-2)\delta + 2m. \end{aligned}$$

Also, since $d_1 = \Delta$ is the maximum degree in $G$, $R_{\max}(DS(G))$ is obtained from the first row of degree sum matrix of $G$. Then, by the definition of $DS(G)$, we get

$$R_{\max}(DS(G)) = \sum_{i=2}^{n} \Delta + d_i.$$

Again, by using (1), we obtain

$$\begin{aligned} R_{\max}(DS(G)) &= (n-1)\Delta + 2m - \Delta \\ &= (n-2)\Delta + 2m. \end{aligned}$$

Hence, by using Lemma 1.1, we have

$$\delta(n-2) + 2m \leq \rho(DS(G)) \leq \Delta(n-2) + 2m.$$

**Theorem 2.6** *The bounds for the spectral radius of degree square sum matrix DSS of G is*

$$\delta^2(n-1) + \sum_{i=1}^{n-1} d_i^2 \leq \rho(DSS(G)) \leq \Delta^2(n-1) + \sum_{i=2}^{n} d_i^2.$$

*Proof.* Since $d_n = \delta$ is the minimum degree in $G$, $R_{\min}(DSS(G))$ is obtained from the $n-th$ row of degree square sum matrix of $G$. Then, by the definition of $DSS(G)$, we have

$$\begin{aligned} R_{\min}(DSS(G)) &= \sum_{i=1}^{n-1} \delta^2 + d_i^2 \\ &= (n-1)\delta^2 + \sum_{i=1}^{n-1} d_i^2. \end{aligned}$$

Also, since $d_1 = \Delta$ is the maximum degree in $G$, $R_{\max}(DSS(G))$ is obtained from the first row of degree square sum matrix of $G$. Then, by the definition of $DSS(G)$, we get

$$\begin{aligned} R_{\max}(DSS(G)) &= \sum_{i=2}^{n} \Delta^2 + d_i^2 \\ &= (n-1)\Delta^2 + \sum_{i=2}^{n} d_i^2. \end{aligned}$$

Hence, by using Lemma 1.1, we obtain

$$\delta^2(n-1) + \sum_{i=1}^{n-1} d_i^2 \leq \rho(DSS(G)) \leq \Delta^2(n-1) + \sum_{i=2}^{n} d_i^2.$$

**Theorem 2.7** *The bounds for the spectral radius of first zagreb matrix $Z^{(1)}$ of G is*

$$\delta^2 + \sum_{n\sim k} d_k \leq \rho(Z^{(1)}(G)) \leq \Delta^2 + \sum_{1\sim j} d_j.$$

*Proof.* Since $d_n = \delta$ is the minimum degree in $G$, $R_{\min}(Z^{(1)}(G))$ is obtained from the $n-th$ row of first zagreb matrix of $G$. Then, by the definition of $Z^{(1)}(G)$, we have

$$R_{\min}(Z^{(1)}(G)) = \sum_{n\sim k} \delta + d_k.$$

Since the number of the adjacent vertices of $n$ is $\delta$, we have

$$R_{\min}(Z^{(1)}(G)) = \delta^2 + \sum_{n\sim k} d_k.$$

Moreover, since $d_1 = \Delta$ is the maximum degree in $G$, $R_{\max}(Z^{(1)}(G))$ is obtained from the first row of first zagreb matrix of $G$. Then, by the definition of $Z^{(1)}(G)$, we get

$$R_{\max}(Z^{(1)}(G)) = \sum_{1\sim j} \Delta + d_j.$$

Since the number of the adjacent vertices of 1 is $\Delta$, we have

$$R_{\max}(Z^{(1)}(G)) = \Delta^2 + \sum_{1\sim j} d_j.$$

Therefore, by using Lemma 1.1, we have

$$\delta^2 + \sum_{n\sim k} d_k \leq \rho(Z^{(1)}(G)) \leq \Delta^2 + \sum_{1\sim j} d_j.$$

**Theorem 2.8** *The bounds for the spectral radius of second zagreb matrix $Z^{(2)}$ of G is*

$$\delta\sum_{n\sim k} d_k \leq \rho(Z^{(2)}(G)) \leq \Delta\sum_{1\sim j} d_j.$$

*Proof.* Since $d_n = \delta$ is the minimum degree in $G$, $R_{\min}(Z^{(2)}(G))$ is obtained from the $n-th$ row of second zagreb matrix of $G$. Then, by the definition of $^{(2)}(G)$, we have

$$R_{\min}(Z^{(2)}(G)) = \delta\sum_{n\sim k} d_k.$$

Moreover, since $d_1 = \Delta$ is the maximum degree in $G$, $R_{\max}(Z^{(2)}(G))$ is obtained from the first row of second zagreb matrix of $G$. Then, by the definition of $^{(2)}(G)$, we get

$$R_{\max}(Z^{(2)}(G)) = \Delta\sum_{1\sim j} d_j.$$

As a result, by using Lemma 1.1, we have

$$\delta\sum_{n\sim k} d_k \leq \rho(Z^{(2)}(G)) \leq \Delta\sum_{1\sim j} d_j.$$

## 3 Some upper bounds for some energies of graphs

In this section, we will obtain upper bounds for maximum degree, minimum degree, Randic, sum-connectivity, degree sum, degree square sum, first Zagreb and second Zagreb energies of a graph.

**Theorem 3.1** *An upper bound for the maximum degree energy $E_M$ of G is*

$$E_M(G) \leq n\Delta^2.$$

*Proof.* Since $G$ is a graph with $n$ vertices, maximum degree matrix of $G$ has $n$ eigenvalues. By Theorem 2.1, we know that $\rho(M(G))$ can be at most $\Delta^2$. Then, an upper bound for all eigenvalues is $\Delta^2$. Hence, we obtain

$$E_M(G) \leq n\Delta^2.$$

**Theorem 3.2** *An upper bound for the minimum degree energy $E_m$ of G is*

$$E_m(G) \leq n\sum_{1\sim j} d_j.$$

*Proof.* Since $G$ is a graph with $n$ vertices, minimum degree matrix of $G$ has $n$ eigenvalues. By Theorem 2.2, we know that $\rho(m(G))$ can be at most $\sum_{1\sim j} d_j$. Then, an upper bound for all eigenvalues is $\sum_{1\sim j} d_j$. Hence, we obtain

$$E_m(G) \leq n\sum_{1\sim j} d_j.$$

**Theorem 3.3** *An upper bound for the Randic energy $E_R$ of G is*

$$E_R(G) \leq n\sum_{1\sim j}\frac{1}{\sqrt{\Delta d_j}}.$$

*Proof.* Since $G$ is a graph with $n$ vertices, Randic matrix of $G$ has $n$ eigenvalues. By Theorem 2.3, we know that $\rho(R(G))$ can be at most $\sum_{1\sim j} \frac{1}{\sqrt{\Delta d_j}}$. Then, an upper bound for all eigenvalues is $\sum_{1\sim j} \frac{1}{\sqrt{\Delta d_j}}$. Hence, we obtain

$$E_R(G) \leq n \sum_{1\sim j} \frac{1}{\sqrt{\Delta d_j}}.$$

**Theorem 3.4** *An upper bound for the sum-connectivity energy $E_{SC}$ of $G$ is*

$$E_{SC}(G) \leq n \sum_{1\sim j} \frac{1}{\sqrt{\Delta + d_j}}.$$

*Proof.* Since $G$ is a graph with $n$ vertices, sum-connectivity matrix of $G$ has $n$ eigenvalues. By Theorem 2.4, we know that $\rho(SC(G))$ can be at most $\sum_{1\sim j} \frac{1}{\sqrt{\Delta+d_j}}$. Then, an upper bound for all eigenvalues is $\sum_{1\sim j} \frac{1}{\sqrt{\Delta+d_j}}$. Hence, we obtain

$$E_{SC}(G) \leq n \sum_{1\sim j} \frac{1}{\sqrt{\Delta + d_j}}.$$

**Theorem 3.5** *An upper bound for the degree sum energy $E_{DS}$ of $G$ is*

$$E_{DS}(G) \leq n\left[\Delta(n-2) + 2m\right].$$

*Proof.* Since $G$ is a graph with $n$ vertices, degree sum matrix of $G$ has $n$ eigenvalues. By Theorem 2.5, we know that $\rho(DS(G))$ can be at most $\Delta(n-2) + 2m$. Then, an upper bound for all eigenvalues is $\Delta(n-2) + 2m$. Hence, we obtain

$$E_{DS}(G) \leq n\left[\Delta(n-2) + 2m\right].$$

**Theorem 3.6** *An upper bound for the degree square sum energy $E_{DSS}$ of $G$ is*

$$E_{DSS}(G) \leq \Delta^2 n(n-1) + n \sum_{i=2}^{n} d_i^2.$$

*Proof.* Since $G$ is a graph with $n$ vertices, degree square sum matrix of $G$ has $n$ eigenvalues. By Theorem 2.6, we know that $\rho(DSS(G))$ can be at most $\Delta^2(n-1) + \sum_{i=2}^{n} d_i^2$. Then, an upper bound for all eigenvalues is $\Delta^2(n-1) + \sum_{i=2}^{n} d_i^2$. Hence, we obtain

$$E_{DSS}(G) \leq \Delta^2 n(n-1) + n \sum_{i=2}^{n} d_i^2.$$

**Theorem 3.7** *An upper bound for the first Zagreb energy $ZE_1$ of $G$ is*

$$ZE_1(G) \leq n\Delta^2 + n \sum_{1\sim j} d_j.$$

*Proof.* Since $G$ is a graph with $n$ vertices, first Zagreb matrix of $G$ has $n$ eigenvalues. By Theorem 2.7, we know that $\rho(ZE_1(G))$ can be at most $\Delta^2 + \sum_{1\sim j} d_j$. Then, an upper bound for all eigenvalues is $\Delta^2 + \sum_{1\sim j} d_j$. Hence, we obtain

$$ZE_1(G) \leq n\Delta^2 + n\sum_{1\sim j} d_j.$$

**Theorem 3.8** *An upper bound for the second Zagreb energy $ZE_2$ of $G$ is*

$$ZE_2(G) \leq n\Delta\sum_{1\sim j} d_j.$$

*Proof.* Since $G$ is a graph with $n$ vertices, second Zagreb matrix of $G$ has $n$ eigenvalues. By Theorem 2.8, we know that $\rho(ZE_2(G))$ can be at most $\Delta\sum_{1\sim j} d_j$. Then, the upper bound for all eigenvalues is $\Delta\sum_{1\sim j} d_j$. Hence, we obtain

$$ZE_2(G) \leq n\Delta\sum_{1\sim j} d_j.$$

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