



Degree square sum equienergetic and hyperenergetic graphs

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Abstract

Degree square sum matrix $DSS(G)$ of a graph G is a square matrix of order equal to the order of a graph G with its $(i, j)^{th}$ entry as $d_i^2 + d_j^2$ if $i \neq j$ and zero otherwise, where d_i is the degree of the i^{th} vertex of G . In this paper, we study degree square sum hyperenergetic, degree square sum borderenergetic and degree square sum equienergetic graphs.

Keywords

Degree square sum matrix, degree square sum polynomial, degree square sum energy, degree square sum hyperenergetic graphs, degree square sum equienergetic graphs.

AMS Subject Classification

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1. Introduction

Let G be a nontrivial, simple, finite, undirected graph with n vertices and m edges. Let $V(G)$ be the vertex set and $E(G)$ be an edge set of G . The degree $d_G(v)$ of a vertex $v \in V(G)$ is the number of edges incident to it in G . The graph G is r -regular if the degree of each vertex in G is r . Let v_1, v_2, \dots, v_n be the vertices of G and let $d_i = d_G(v_i)$. For undefined graph theoretic terminologies, refer to [17] or [23].

In quantum chemistry the skeleton of certain unsaturated hydrocarbons are represented by graphs. Energy levels of electrons in such a molecule are, infact, the eigenvalues of the corresponding graph. The stability of the molecules as well as other chemically relevant facts are closely connected with graph spectrum and the corresponding eigenvectors. For more information on chemical application of graph theory see [1, 14, 31]. Motivated by this connection of electron energy and eigenvalues of the corresponding graph, in 1978,

Gutman [13] introduced the concept of graph energy as the sum of the absolute values of the eigenvalues of the adjacency matrix of G and the graph spectra as the collection of eigenvalues. The introduction of the graph energy concept resulted in the discovery of numerous novel results, some of which had chemical relevance too.

The adjacency matrix of a graph G is a square matrix $A(G) = [a_{ij}]$ of order n in which $a_{ij} = 1$, if the vertex v_i is adjacent to vertex v_j and $a_{ij} = 0$, otherwise. The characteristic polynomial of $A(G)$ denoted by $\phi(G : \lambda) = \det(\lambda I - A(G))$, where I is an identity matrix of order n . The roots of an equation $\phi(G : \lambda) = 0$ are called the eigenvalues of G and they are labeled as $\lambda_1, \lambda_2, \dots, \lambda_n$. Their collection is called the spectrum of G denoted by $Spec(G)$, refer to [9]. The two nonisomorphic graphs are cospectral if they have the same spectra. The details can be found in [9]. The energy $\varepsilon(G)$ [13] of a graph G with n vertices is defined as $\varepsilon(G) = \sum_{i=1}^n |\lambda_i|$. McClelland [26] showed that for molecular graphs of conjugated hydrocarbons, $\varepsilon(G) \approx a\sqrt{2mn}$, where $a \approx 0.9$. According to this, $\varepsilon(G)$ is monotonically increasing function of m and n . In view of this observation, Gutman [13] conjectured among all graphs with n vertices the complete graph has maximum energy. That is, for any graph G of order n , $\varepsilon(G) \leq \varepsilon(K_n) \leq 2(n-1)$. This conjecture is not true [10]. There are graphs whose energy exceeds the energy of K_n , became motivation for the introduction of concept of hyperenergetic graphs [15]. A graph G is

said to be *hyperenergetic*[15] if $\epsilon(G) > 2(n - 1)$ and is said to be *nonhyperenergetic* if $\epsilon(G) < 2(n - 1)$. A noncomplete graph whose energy is equal to $2(n - 1)$ is called *borderenergetic* [12]. Two graphs G_1 and G_2 are *equienergetic* [1, 4] if $\epsilon(G_1) = \epsilon(G_2)$. One can refer to [4, 5, 11, 14, 16, 18–22, 24, 25, 27–30, 32–35] for more details on the the concept of graph energy.

We have defined a graph matrix called *degree square sum matrix* in [2]. It is an $n \times n$ matrix denoted by $DSS(G) = [dss_{ij}]$ and whose elements are defined as

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

The *degree square sum polynomial* of a graph G is defined as $P_{DSS(G)}(\mu) = \det(\mu I - DSS(G))$, where I is an identity matrix and J is a matrix whose all entries are equal to 1. The *degree square sum eigenvalues* of G are given as $\mu_1, \mu_2, \dots, \mu_n$ and their collection is called the *degree square sum spectra* of G .

The degree square sum energy is given by $E_{DSS}(G) = \sum_{i=1}^n |\mu_i|$.

The details can be found in [2, 3].

2. Preliminaries

Lemma 2.1. [2] *If G is an r -regular graph, then*

$$DSS(G) = 2r^2J - 2r^2I.$$

Theorem 2.2. [2] *If G is an r -regular graph of order n , then*

$$P_{DSS(G)}(\mu) = (\mu - 2r^2(n - 1))(\mu + 2r^2)^{n-1}.$$

Theorem 2.3. [2] *If G is an r -regular graph of order n , then $-2r^2$ and $2r^2(n - 1)$ are degree square sum eigenvalues of G with respective multiplicities $(n - 1)$ and 1 and hence $E_{DSS}(G) = 4r^2(n - 1)$.*

Definition 2.4. [17] *The complement \bar{G} of a graph G is a graph with vertex set $V(G)$ and two vertices of \bar{G} are adjacent if and only if they are nonadjacent in G .*

If G is an (n, m) -graph, then \bar{G} is $(n, \binom{n}{2} - m)$ -graph.

Definition 2.5. [17] *The line graph $L(G)$ of a graph G is a graph with vertex set as $E(G)$ where the two vertices of $L(G)$ are adjacent if and only if they correspond to two adjacent edges of G .*

If G is an (n, m) -graph, then $L(G)$ is $(m, -m + \frac{1}{2} \sum_{i=1}^n d_G(v_i)^2)$ -graph.

Theorem 2.6. [2] *Let G be an r -regular graph of order n , then the degree square sum polynomial of $L(G)$ is*

$$P_{DSS(L(G))}(\mu) = (\mu - 4(r - 1)^2(nr - 2))(\mu + 8(r - 1)^2)^{\frac{nr-2}{2}}.$$

Definition 2.7. [6, 7, 17] *The k^{th} iterated line graph of G is defined as $L^k(G) = L(L^{k-1}(G))$, $k = 1, 2, \dots$, where $L^0(G) \cong G$ and $L^1(G) \cong L(G)$.*

Theorem 2.8. [2] *If G is an r -regular graph of order n and n_k be the order of $L^k(G)$, then the degree square sum polynomial of $L^k(G)$, $k = 1, 2, \dots$ is*

$$P_{DSS(L^k(G))}(\mu) = (\mu + 2(2^k r - 2^{k+1} + 2)^2)^{n_k-1} (\mu - 2(n_k - 1)(2^k r - 2^{k+1} + 2)^2),$$

where $n_k = \frac{n}{2^k} \prod_{i=0}^{k-1} (2^i r - 2^{i+1} + 2)$ and $r_k = 2^k r - 2^{k+1} + 2$.

Definition 2.9. [8] *The jump graph $J(G)$ of a graph G is a graph with vertex set as $E(G)$ where the two vertices of $J(G)$ are adjacent if and only if they correspond to two nonadjacent edges of G .*

If G is an (n, m) -graph, then $J(G)$ is

$$\left(m, \frac{m(m+1)}{2} - \frac{1}{2} \sum_{i=1}^n d_G(v_i)^2\right)$$

- graph.

Definition 2.10. [17] *The total graph $T(G)$ of a graph G is the graph whose vertex set is $V(G) \cup E(G)$ and two vertices of $T(G)$ are adjacent if and only if the corresponding elements of G are either adjacent or incident.*

If G is an (n, m) -graph, then $T(G)$ is

$$\left(n + m, 2m + \frac{1}{2} \sum_{i=1}^n d_G(v_i)^2\right)$$

-graph.

We now define following definitions which are key words of this paper.

Definition 2.11. *A graph G of order n is said to be degree square sum hyperenergetic if $E_{DSS}(G) > 4(n - 1)^3$.*

Definition 2.12. *A graph G of order n is said to be degree square sum nonhyperenergetic if $E_{DSS}(G) < 4(n - 1)^3$.*

Definition 2.13. *A noncomplete graph of order n whose energy is equal to $4(n - 1)^3$ is called degree square sum borderenergetic.*

Definition 2.14. *Two graphs G_1 and G_2 are said to be degree square sum equienergetic if they have same degree square sum energy. That is, $E_{DSS}(G_1) = E_{DSS}(G_2)$.*

3. Main results

Theorem 3.1. *If G is an r -regular graph of order n , then \bar{G} is (i) degree square sum borderenergetic for $r = 0$, (ii) degree square sum nonhyperenergetic for $r \geq 1$.*



Proof. The graph \overline{G} is $(n-1-r)$ -regular graph. The degree square sum eigenvalues of \overline{G} are $2(n-1)(n-1-r)^2$, $-2(n-1-r)^2$ ($n-1$ times). Therefore,

$$\begin{aligned} E_{DSS}(\overline{G}) &= \left| 2(n-1)(n-1-r)^2 \right| + \left| -2(n-1-r)^2 \right| (n-1) \\ &= 4(n-1)(n-1-r)^2. \end{aligned}$$

From Definition 2.11, the graph \overline{G} is degree square sum hyperenergetic if $E(\overline{G}) > 4(n-1)^3$. That is, if $4(n-1)(n-1-r)^2 > 4(n-1)^3$. This inequality does not hold for any value of r , whereas the two quantities are equal when $r=0$. Hence, \overline{G} is degree square sum borderenergetic for $r=0$ and degree square sum nonhyperenergetic for $r \geq 1$. \square

Theorem 3.2. *The graph $L(K_n)$ is degree square sum borderenergetic for $n=2, 3$, and degree square sum nonhyperenergetic for $n \geq 4$.*

Proof. The graph K_n is $(n-1)$ -regular graph of order n . By Theorem 2.2, the degree square sum polynomial of K_n is given by, $P_{DSS(K_n)}(\mu) = (\mu - 2(n-1)^3) (\mu + 2(n-1)^2)^{n-1}$.

By Theorem 2.6,

$$P_{DSS(L(K_n))}(\mu) = \left(\mu - 4(n-2)^2(n(n-1)-2) \right) \left(\mu + 8(n-2)^2 \right)^{\frac{n(n-1)-2}{2}}.$$

The degree square sum eigenvalues of $L(K_n)$ are

$$\mu = \begin{cases} 4(n-2)^2(n(n-1)-2), & 1 \text{ time,} \\ -2(n-2)^2, & \binom{n}{2} - 1 \text{ times.} \end{cases}$$

Therefore,

$$\begin{aligned} E_{DSS}(L(K_n)) &= \left| 4(n-2)^2(n(n-1)-2) \right| \\ &\quad + \left| -2(n-2)^2 \right| \left(\binom{n}{2} - 1 \right) \\ &= 8(n-2)^2(n(n-1)-2). \end{aligned}$$

This is clearly equal to and less than

$$E_{DSS}(K_n) = 4 \left(\frac{n(n-1)-2}{2} \right)^3 \text{ for } n=2, 3 \text{ and } n \geq 4 \text{ respectively. Hence, } L(K_2) \text{ and } L(K_3) \text{ are degree square sum borderenergetic and } G \cong L(K_n) \text{ (} n \geq 4 \text{) is degree square sum nonhyperenergetic. } \square$$

Theorem 3.3. *If $G(\cong K_2, K_3)$ is an r -regular graph of order n , then $L(G)$ is degree square sum nonhyperenergetic.*

Proof. From Theorem 2.3, the degree square sum eigenvalues of r -regular graph G of order n are $2r^2(n-1)$, $-2r^2(n-1)$ times). The line graph $L(G)$ is $(2r-2)$ -regular

graph. Hence, the degree square sum eigenvalues of $L(G)$ are $4(r-1)^2(nr-2)$, $-8(r-1)^2$ ($\frac{nr}{2}-1$ times). Therefore,

$$\begin{aligned} E_{DSS}(L(G)) &= \left| 4(r-1)^2(nr-2) \right| \\ &\quad + \left| -8(r-1)^2 \right| \left(\frac{nr}{2} - 1 \right) \\ &= 8(r-1)^2(nr-2). \end{aligned}$$

From Definition 2.11, the graph $L(G)$ is degree square sum hyperenergetic if $E_{DSS}(L(G)) > 4(m-1)^3$. That is, if $8(r-1)^2(nr-2) > 4(\frac{nr}{2}-1)^3$. This inequality does not hold for any value of r . Hence, $L(G)$ is degree square sum nonhyperenergetic. \square

Theorem 3.4. *If G is an r -regular graph of order n , then*

$$E_{DSS}(L^2(G)) = 8nr(r-1)(2r-3)^2.$$

Proof. From Theorem 2.3, the degree square sum eigenvalues of r -regular graph G of order n are $2r^2(n-1)$, $-2r^2(n-1)$ times). Hence, the degree square sum eigenvalues of $L^2(G)$ are $4nr(r-1)(2r-3)^2$, $-8(2r-3)^2$ ($\frac{nr}{2}(r-1)$ times). Therefore,

$$\begin{aligned} E_{DSS}(L^2(G)) &= \left| 4nr(r-1)(2r-3)^2 \right| \\ &\quad + \left| -8(2r-3)^2 \right| \left(\frac{nr}{2}(r-1) \right) \\ &= 8nr(r-1)(2r-3)^2. \end{aligned}$$

\square

From the Theorem 3.4, we have the following results.

Corollary 3.5. *If G_1 and G_2 are two regular graphs on n vertices and of regularity r , then $L^2(G_1)$ and $L^2(G_2)$ are degree square sum equienergetic.*

Corollary 3.6. *If G_1 and G_2 are two regular graphs on n vertices and of regularity r , then $L^k(G_1)$ and $L^k(G_2)$ (for $k \geq 1$) are degree square sum equienergetic.*

Theorem 3.7. *If G is an r -regular graph of order n , then $J(G)$ is (i) degree square sum borderenergetic for $r=1$, (ii) degree square sum nonhyperenergetic for $r \geq 2$.*

Proof. The jump graph $J(G)$ is $\left(\frac{r(n-4)+2}{2}\right)$ -regular graph. The degree square sum eigenvalues of $J(G)$ are $\frac{1}{4}(r(n-4)+2)^2(nr-2)$, $-\frac{1}{2}(r(n-4)+2)^2$ ($\frac{nr}{2}-1$ times). Therefore,

$$\begin{aligned} E_{DSS}(J(G)) &= \left| \frac{1}{4}(r(n-4)+2)^2(nr-2) \right| \\ &\quad + \left| -\frac{1}{2}(r(n-4)+2)^2 \right| \left(\frac{nr}{2} - 1 \right) \\ &= \frac{1}{2} \left(r(n-4)+2 \right)^2 (nr-2). \end{aligned}$$

From Definition 2.11, the graph $J(G)$ is degree square sum hyperenergetic if $E(J(G)) > 4(m-1)^3$. That is, if



$\frac{1}{2} \left(r(n-4) + 2 \right)^2 (nr-2) > 4 \left(\frac{nr}{2} - 1 \right)^3$. This inequality does not hold for any value of r , whereas the two quantities are equal when $r = 1$. Hence, $J(G)$ is degree square sum borderenergetic for $r = 1$ and degree square sum nonhyperenergetic for $r \geq 2$. \square

Theorem 3.8. *If G is an r -regular graph of order n , then $T(G)$ is degree square sum nonhyperenergetic.*

Proof. The total graph $T(G)$ is $2r$ -regular graph. The degree square sum eigenvalues of $T(G)$ are $4r^2(n(r+2)-2)$, $-8r^2 \left(\frac{n(r+2)-2}{2} \right)$ times). Therefore,

$$\begin{aligned} E_{DSS}(T(G)) &= |4r^2(n(r+2)-2)| \\ &\quad + |-8r^2| \left(\frac{n(r+2)-2}{2} \right) \\ &= 8r^2 \left(n(r+2)-2 \right). \end{aligned}$$

The graph $T(G)$ is degree square sum hyperenergetic if $E_{DSS}(T(G)) > 4(n+m-1)^3$, from Definition 2.11. That is, if $8r^2 \left(n(r+2)-2 \right) > \frac{1}{2} \left(n(r+2)-2 \right)^3$. This inequality does not hold for any value of r . Hence, $T(G)$ is degree square sum nonhyperenergetic. \square

Theorem 3.9. *If G is an r -regular graph of order n , then $\overline{T(G)}$ is*

- (i) *degree square sum hyperenergetic for $G \cong \overline{K_2}$,*
- (ii) *degree square sum nonhyperenergetic for $G \not\cong \overline{K_2}$.*

Proof. The graph $\overline{T(G)}$ is $\left(n + \frac{nr}{2} - 2r - 1 \right)$ -regular graph.

The degree square sum eigenvalues of $\overline{T(G)}$ are

$$\begin{aligned} &2 \left(n + \frac{nr}{2} - 2r - 1 \right) \left(n + \frac{nr}{2} - 1 \right), \\ &-2 \left(n + \frac{nr}{2} - 2r - 1 \right) \left(n + \frac{nr}{2} - 1 \right) \text{ times).} \end{aligned}$$

Therefore,

$$\begin{aligned} E_{DSS}(\overline{T(G)}) &= \left| 2 \left(n + \frac{nr}{2} - 2r - 1 \right) \left(n + \frac{nr}{2} - 1 \right) \right| \\ &\quad + \left| -2 \left(n + \frac{nr}{2} - 2r - 1 \right) \right| \left(n + \frac{nr}{2} - 1 \right) \\ &= 4 \left(n \left(\frac{r}{2} + 1 \right) - 1 \right) \left(n \left(\frac{r}{2} + 1 \right) - 2r - 1 \right). \end{aligned}$$

From Definition 2.11, the graph $\overline{T(G)}$ is degree square sum hyperenergetic if $E(\overline{T(G)}) > 4 \left(n + \frac{nr}{2} - 1 \right)^3$. That is, if

$4 \left(n \left(\frac{r}{2} + 1 \right) - 1 \right) \left(n \left(\frac{r}{2} + 1 \right) - 2r - 1 \right) > 4 \left(n + \frac{nr}{2} - 1 \right)^3$. This inequality holds for $G \cong \overline{K_2}$. Hence, $\overline{T(G)}$ is degree square sum hyperenergetic for $G \cong \overline{K_2}$ and degree square sum nonhyperenergetic, otherwise. \square

4. Conclusion

In this paper, we have characterized degree square sum hyperenergetic, borderenergetic and equienergetic transformation graphs.

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