

COMBINED DEGREE SUM ENERGY OF GRAPHS

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ABSTRACT. The combined degree sum matrix of a graph G is defined by $CDS(G) = [c_{ij}]$ where $c_{ij} = d_i + d_j + d_i d_j$ whenever $i \neq j$, and zero otherwise, where d_i is the degree of a vertex v_i in G . The combined degree sum polynomial of G is the characteristic polynomial of $CDS(G)$. The combined degree sum energy of G is equal to the sum of the absolute values of the eigenvalues of $CDS(G)$. The total π -electron energy of different compounds comprising hetero atoms is connected with their $E_{CDS}(G)$ values, and we found a good correlation with the correlation coefficient $r=0.9823$. Combined degree sum polynomial and combined degree sum energy of some graphs are obtained. Further, we establish bounds for the largest CDS eigenvalue and CDS energy of a graphs. Jog et al. [20] gave the expression for degree sum polynomial of semi total line graph $T_1(G)$ of r -regular graph is prone to some error. We give correct expression for it. Finally, we obtain combined degree sum polynomial of graph valued functions and graph operations on regular graphs.

1. INTRODUCTION

A simple, undirected graph is $G = (n, m)$. Let G 's vertex and edge sets be $V(G)$ and $E(G)$, respectively. The number of edges incident to a vertex v in $V(G)$ is the *degree* $deg_G(v)$ (or $d_G(v)$). If the degree of each vertex in G is r , the graph is r -regular.

The combined degree sum matrix of a graph G is an $n \times n$ matrix $CDS(G) = [c_{ij}]$, whose elements are defined as

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

where, d_i is degree of a vertex v_i and d_j is degree of a vertex v_j . Let I be the identity matrix and J be the matrix whose all entries are equal to 1. The *combined degree sum polynomial* of a graph G is defined as

$$P_{CDS(G)}(\eta) = \det(\eta I - CDS(G)).$$

The *eigenvalues* of the matrix $CDS(G)$, denoted by $\eta_1, \eta_2, \dots, \eta_n$ are called the *combined degree sum eigenvalues* of G and their collection is called the *combined*

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degree sum spectra of G . The sum of the absolute values of the combined degree sum eigenvalues of G is called the *combined degree sum energy* of G and is denoted by $E_{CDS}(G)$. Thus

$$E_{CDS}(G) = \sum_{i=1}^n |\eta_i|. \quad (1.1)$$

Example 1.1. Let K_3 be a complete graph. The CDS matrix, CDS polynomial and CDS energy of K_3 are as follows(see Figure 1).

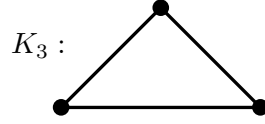


FIGURE 1. Graph K_3 .

$$CDS(K_3) = \begin{pmatrix} 0 & 8 & 8 \\ 8 & 0 & 8 \\ 8 & 8 & 0 \end{pmatrix}$$

$$P_{CDS(K_3)}(\eta) = \eta^3 - 192\eta - 1024.$$

The eigen values of combined degree sum matrix are 16, -8 and -8 . Therefore, $E_{CDS}(K_3) = 32$.

Example 1.2. Consider the graph $G = K_2 \cdot K_3$. The CDS matrix, CDS polynomial and CDS energy of G are as follows(see Figure 2).

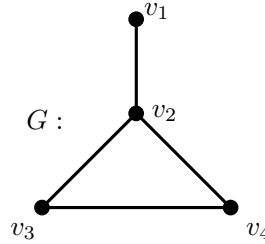


FIGURE 2. Graph $G = K_2 \cdot K_3$.

$$CDS(G) = \begin{pmatrix} 0 & 7 & 5 & 5 \\ 7 & 0 & 11 & 11 \\ 5 & 11 & 0 & 8 \\ 5 & 11 & 8 & 0 \end{pmatrix}$$

$$P_{CDS(G)}(\eta) = -\eta^4 + 405\eta^2 + 3876\eta + 9184.$$

The eigen values of combined degree sum matrix are $\eta_1 = 8$, $\eta_2 \approx -24.11$, $\eta_3 \approx 12.21$ and $\eta_4 \approx 3.89$. Therefore, $E_{CDS}(G) \approx 48.21$.

Graph energy is described by Gutman [17] as the sum of absolute values of the eigenvalues of the associated adjacency matrix of a graph G , which is related to the total π -electron energy in a molecular graph. Several graph polynomials based on different matrices defined on the graph, such as adjacency matrix [12], Laplacian matrix [24], signless Laplacian matrix [13, 28], distance matrix [1], degree sum matrix [20, 29], Seidel matrix [7] are found in the literature of graph theory. [2, 3, 6, 19] for further information. The goal of this research is to look at the characteristic polynomial of the *combined degree sum matrix*, as well as their eigen values and energy.

2. PRELIMINARIES

We require following theorems in order to prove the forthcoming theorems.

Lemma 2.1. [30] *If a, b, c and d are real numbers, then the determinant of the form*

$$\begin{vmatrix} (\eta + a)I_{n_1} - aJ_{n_1} & -cJ_{n_1 \times n_2} \\ -dJ_{n_2 \times n_1} & (\eta + b)I_{n_2} - bJ_{n_2} \end{vmatrix} \quad (2.1)$$

of order $n_1 + n_2$ can be expressed in the simplified form as

$$(\eta + a)^{n_1-1}(\eta + b)^{n_2-1}\{[\eta - (n_1 - 1)a][\eta - (n_2 - 1)b] - n_1 n_2 cd\}.$$

Theorem 2.2. [4] *The Cauchy-Schwarz inequality states that if $(a_1, a_2, \dots, a_n)$ and $(b_1, b_2, \dots, b_n)$ are two real n -vectors, then*

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

Theorem 2.3. [25] *Let a_i and b_i , $1 \leq i \leq n$ are nonnegative real numbers, then*

$$\sum_{i=1}^n a_i^2 \sum_{i=1}^n b_i^2 - \left(\sum_{i=1}^n a_i b_i \right)^2 \leq \frac{n^2}{4} (M_1 M_2 - m_1 m_2)^2,$$

where $M_1 = \max_{1 \leq i \leq n} (a_i)$; $M_2 = \max_{1 \leq i \leq n} (b_i)$; $m_1 = \min_{1 \leq i \leq n} (a_i)$; $m_2 = \min_{1 \leq i \leq n} (b_i)$.

Theorem 2.4. [5] *Let a_i and b_i , $1 \leq i \leq n$ are nonnegative real numbers, then*

$$\left| n \sum_{i=1}^n a_i b_i - \left(\sum_{i=1}^n a_i \right) \left(\sum_{i=1}^n b_i \right) \right| \leq \mu(n) (A - a)(B - b),$$

where a, b, A and B are real constants, such that for each i , $1 \leq i \leq n$, $a \leq a_i \leq A$ and $b \leq b_i \leq B$. Further, $\mu(n) = n \lfloor \frac{n}{2} \rfloor \left(1 - \frac{1}{n} \lfloor \frac{n}{2} \rfloor \right)$.

Theorem 2.5. [15] *Let a_i and b_i , $1 \leq i \leq n$ are nonnegative real numbers, then*

$$\sum_{i=1}^n b_i^2 + c_1 c_2 \sum_{i=1}^n a_i^2 \leq (c_1 + c_2) \left(\sum_{i=1}^n a_i b_i \right).$$

where c_1 and c_2 are real constants, such that for each i , $1 \leq i \leq n$ holds, $c_1 a_i \leq b_i \leq c_2 a_i$.

Lemma 2.6. [14] *If a and b are scalars then*

$$\begin{vmatrix} a & b & b & \cdots & b & b \\ b & a & b & \cdots & b & b \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ b & b & b & \cdots & a & b \\ b & b & b & \cdots & b & a \end{vmatrix} = (a - b)^{n-1} [a + (n - 1)b]$$

3. CHEMICAL SIGNIFICANCE OF $E_{CDS}(G)$

We found the close resemblance between total π -electron energy values of hetero atoms and combined degree sum matrix $CDS(G)$ of corresponding molecular graph G . Further, we calculated $E_{CDS}(G)$ with dataset of total π -electron energy values of hetero atoms which are found in [11]. From Fig. 4 we found that $E_{CDS}(G)$ has good correlation hetero atoms (see Fig. 3). The linear regression model for total π -electron energy values of hetero atoms using the data of Tables 1 are obtained using the least squares fitting procedure as implemented in R software [26]. The linear regression analysis gives the following structure property relationship mathematical model for $E_{CDS}(G)$

$$Total\pi - electron\ energy = 0.07(\pm 0.0026)E_{CDS}(G) + 0.3025(\pm 0.4076).$$

$r=0.9823$ (co-efficient of correlation), $r^2(adjusted) = 0.9636$, standard error of estimation=1.107.

From the above data, we can see that $E_{CDS}(G)$ is closely correlated with total π -electron energy of 28 molecules containing hetero atoms.

FIGURE 3. Molecules containing hetero atoms.

Molecule	Code	Total π -electron energy	$E_{CDS}(G)$
Venyl chloride like systems	S_1	2.23	17.46
Butadiene perturbed at $C2$	S_2	5.66	31.61
Acrolein like systems	S_3	5.76	31.61
1, 1-dichloro-ethylene like systems	S_4	6.96	30.97
Glyoxal like and 1, 2-dichloro-ethylene like systems	S_5	6.82	31.61
Pyrrole like systems	S_6	5.23	64
Pyridine like systems	S_7	6.69	80
Pyridazine like systems	S_8	9.06	80
Pyrimidine like systems	S_9	9.10	80
Pyrazine like systems	S_{10}	9.07	80
S-Triazene like systems	S_{11}	9.65	80
Aniline like systems	S_{12}	8.19	97.77
O-phenylene-diamine like systems	S_{13}	12.21	115.76
m-phenylene-diamine like systems	S_{14}	12.22	116.19
p-phenylene-diamine like systems	S_{15}	12.21	117.02
Benzaldehyde like systems	S_{16}	11.00	114.07
Quinoline like systems	S_{17}	14.23	168.08
Iso-quinoline like systems	S_{18}	14.23	168.08
1-Naphthalein like systems	S_{19}	16.15	187.27
2-Naphthalein like systems	S_{20}	16.12	185.20
Iso-indole like systems	S_{21}	13.46	151.68
Indole like systems	S_{22}	13.59	151.68
Benzylidene-aniline like systems	S_{23}	20.10	232.12
Azobenzene like systems	S_{24}	21.02	232.12
Acridine like systems	S_{25}	20.56	258.73
Phenazine like systems	S_{26}	21.62	258.73
9, 10-Anthraquinoline like systems	S_{27}	24.23	298.11
Cabazole like systems	S_{28}	19.39	242.36

TABLE 1. Molecules containing hetero atoms with total π -electron energy and combined degree sum energy.

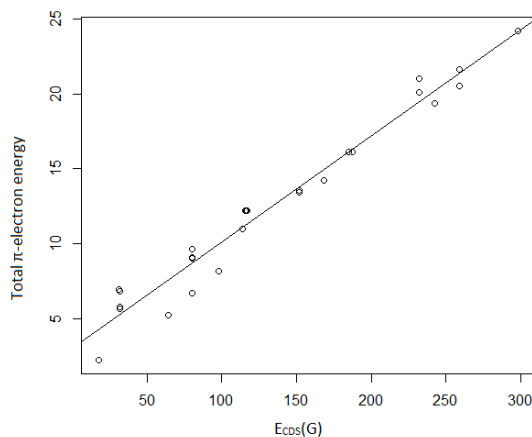


FIGURE 4. Correlation of $E_{CDS}(G)$ with total π -electron energy of molecules containing hetero atoms.

4. COMBINED DEGREE SUM POLYNOMIAL OF SOME GRAPHS

In this section, we obtain combined degree sum polynomial of some graphs. It is easy to see that if G is an r -regular graph, then combined degree sum matrix can be expressed as $CDS(G) = r(r+2)J - r(r+2)I$. Therefore, by Lemma 2.1, for an r -regular graph G of order n ,

$$P_{CDS(G)}(\eta) = (\eta + r(r+2))^{n-1}(\eta - r(r+2)(n-1)). \quad (4.1)$$

The complete graph K_n is a regular graph of degree $n-1$ and the cycle C_n is a regular graph of degree 2. Therefore by Eq. 4.1,

$$P_{CDS(K_n)}(\eta) = (\eta + (n+1)(n-1))^{n-1}(\eta - (n+1)(n-1)^2)$$

and

$$P_{CDS(C_n)}(\eta) = (\eta + 8)^{n-1}(\eta - 8(n-1)).$$

Let $V(G)$ be the vertex set of G . The *complement* of a graph G is a graph $\overline{G}$ with vertex set $V(G)$ and two vertices in $\overline{G}$ are adjacent if and only if these are not adjacent in G . If G is an r -regular graph with n vertices then $\overline{G}$ is an $(n-r-1)$ -regular graph on the same number of vertices. Therefore by Eq. 4.1, if G is an r -regular graph with n vertices, then the combined degree sum polynomial of its complement graph is

$$P_{CDS(\overline{G})}(\eta) = (\eta + (n-r-1)(n-r+1))^{n-1}(\eta - (n-r-1)(n-r+1)(n-1)).$$

Definition 4.1. [18] The k^{th} iterated line graph $L^k(G)$ of G is defined as $L^k(G) = L(L^k(G))$, $k = 1, 2, \dots$, where $L^0(G) \cong G$ and $L^1(G) \cong L(G)$.

Corollary 4.2. Let G is an r -regular graph of order n and n_k be the order of $L^k(G)$. The combined degree sum polynomial of k^{th} iterated line graph $L^k(G)$ is $P_{CDS(L^k(G))}(\eta) = (\eta + (2^k r - 2^{k+1} + 2)(2^k r - 2^{k+1} + 4)(n-1))^{n_k-1}(\eta - (2^k r - 2^{k+1} + 2)(2^k r - 2^{k+1} + 4)(n_k - 1)^2)$.

Proof. The k^{th} iterated line graph $L^k(G)$ is a regular graph of degree $2^k r - 2^{k+1} + 2$. Therefore by Eq. 4.1, we get the desired result. $\square$

Definition 4.3. [10] 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 .

Theorem 4.4. If G is an r -regular graph of order n , then

$$P_{CDS(J(G))}(\eta) = \left(\eta + \left(\frac{(n-4)r}{2} + 1 \right) \left(\frac{(n-4)r}{2} + 3 \right) \right)^{\frac{nr}{2}-1} \left(\eta - \left(\frac{(n-4)r}{2} + 1 \right) \left(\frac{(n-4)r}{2} + 3 \right) \left(\frac{nr}{2} - 1 \right) \right).$$

Proof. The jump graph of an r -regular graph is $\left(\frac{(n-4)r}{2} + 1 \right)$ -regular graph with $\frac{nr}{2}$ vertices. Therefore, the result follows from 4.1. $\square$

A graph G is said to be *bipartite* if its vertex set $V(G)$ can be partitioned into two sets V_1 and V_2 such that each edge of G has one end vertex in V_1 and other end vertex in V_2 . A *complete bipartite graph* is a bipartite graph with partite sets V_1 and V_2 in which every vertex of V_1 is adjacent to all vertices of V_2 . The complete bipartite graph is denoted by K_{n_1, n_2} where $|V_1| = n_1$ and $|V_2| = n_2$.

Theorem 4.5. *The combined degree sum polynomial of the complete bipartite graph K_{n_1, n_2} is*

$$P_{CDS(K_{n_1, n_2})}(\eta) = (\eta + 2n_2 + n_2^2)^{n_1-1} (\eta + 2n_1 + n_1^2)^{n_2-1} \{ [\eta - (n_1 - 1)(2n_2 + n_2^2)] [\eta - (n_2 - 1)(2n_1 + n_1^2)] - n_1 n_2 (n_1 + n_2 + n_1 n_2)^2 \}.$$

Proof. The combined degree sum matrix of K_{n_1, n_2} is

$$CDS(K_{n_1, n_2}) = \begin{bmatrix} (2n_2 + n_2^2)(J_{n_1} - I_{n_1}) & (n_1 + n_2 + n_1 n_2)J_{n_1 \times n_2} \\ (n_1 + n_2 + n_1 n_2)J_{n_2 \times n_1} & (2n_1 + n_1^2)(J_{n_2} - I_{n_2}) \end{bmatrix}$$

Therefore,

$$\begin{aligned} P_{CDS(K_{n_1, n_2})}(\eta) &= |\eta I - CDS(K_{n_1, n_2})| \\ &= \begin{vmatrix} (\eta + 2n_2 + n_2^2)I_{n_1} - (2n_2 + n_2^2)J_{n_1} & -(n_1 + n_2 + n_1 n_2)J_{n_1 \times n_2} \\ -(n_1 + n_2 + n_1 n_2)J_{n_2 \times n_1} & (\eta + 2n_1 + n_1^2)I_{n_2} - (2n_1 + n_1^2)J_{n_2} \end{vmatrix} \end{aligned}$$

Using Lemma 2.1, we get the required result. $\square$

Corollary 4.6. *Let $S_n = K_{1, n-1}$ be the star graph with n vertices. Then*

$$P_{CDS(S_n)}(\eta) = (\eta + 3)^{n-2} (6\eta - 2\eta^2 - (n-1)(2n-1)^2).$$

Theorem 4.7. *Let P_n be a path with $n \geq 2$ vertices. Then the combined degree sum polynomial of P_n is*

$$P_{CDS(P_n)}(\eta) = (\eta + 8)^{n-3} (\eta + 3) (\eta^2 + 21\eta - 4(2\eta n + 7) - 26n).$$

Proof. The characteristic polynomial combined degree sum matrix of P_n is

$$\begin{aligned} P_{CDS(P_n)}(\eta) &= |\eta I - CDS(P_n)| \\ &= \begin{vmatrix} \eta & -5 & -5 & \cdots & -5 & -3 \\ -5 & \eta & -8 & \cdots & -8 & -5 \\ -5 & -8 & \eta & \cdots & -8 & -5 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -5 & -8 & -8 & \cdots & \eta & -5 \\ -3 & -5 & -5 & \cdots & -5 & \eta \end{vmatrix} \end{aligned} \quad (4.2)$$

Subtract second column from the columns 3, 4,...,n-1 and subtract first column from the last column of Eq. 4.2 to get Eq. 4.3.

$$= \begin{vmatrix} \eta & -5 & 0 & \cdots & 0 & -3-\eta \\ -5 & \eta & -8-\eta & \cdots & -8-\eta & 0 \\ -5 & -8 & \eta+8 & \cdots & -8 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -5 & -8 & 0 & \cdots & \eta+8 & 0 \\ -3 & -5 & 0 & \cdots & 0 & \eta+3 \end{vmatrix} \quad (4.3)$$

Adding last row to the first row and then adding rows 3, 4,...,n-1 to the second row of Eq. 4.3, we get Eq. 4.4.

$$= \begin{vmatrix} \eta-3 & -10 & 0 & \cdots & 0 & 0 \\ -5(n-2) & \eta-8(n-3) & 0 & \cdots & 0 & 0 \\ -5 & -8 & \eta+8 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -5 & -8 & 0 & \cdots & \eta+8 & 0 \\ -3 & -5 & 0 & \cdots & 0 & \eta+3 \end{vmatrix} \quad (4.4)$$

Eq. 4.4 can be reduced to

$$P_{CDS(P_n)}(\eta) = (\eta+8)^{n-3}(\eta+3) \begin{vmatrix} \eta-3 & -10 \\ -5(n-2) & \eta-8(n-3) \end{vmatrix}$$

$$P_{CDS(P_n)}(\eta) = (\eta+8)^{n-3}(\eta+3) (\eta^2 + 21\eta - 4(2\eta n + 7) - 26n).$$

□

Definition 4.8. [18] The graph $W_n = K_1 + C_{n-1}$ ($n \geq 4$) is called a wheel graph.

Theorem 4.9. The combined degree sum polynomial of the wheel graph W_n is

$$P_{CDS(W_n)}(\eta) = (\eta+15)^{n-2} \{ \eta[\eta - (n-2)15] - (n-1)(4n-1)^2 \}.$$

Proof. The combined degree sum matrix of W_n is

$$CDS(W_n) = \begin{bmatrix} 0(J_1 - I_1) & (4n-1)J_{1 \times n-1} \\ (4n-1)J_{n-1 \times 1} & 15(J_{n-1} - I_{n-1}) \end{bmatrix}$$

Therefore,

$$P_{CDS(W_n)}(\eta) = |\eta I - CDS(W_n)|$$

$$= \begin{vmatrix} (\eta+0)I_1 - 0J_1 & -(4n-1)J_{1 \times n-1} \\ -(4n-1)J_{n-1 \times 1} & (\eta+15)I_{n-1} - (15)J_{n-1} \end{vmatrix}$$

Using Lemma 2.1, we get the required result.

□

5. COMBINED DEGREE SUM ENERGY

The result of this section are straightforward by using the results of section 4 via Eq. (1.1). By Eq. (2.1), the combined degree sum eigen values of an r -regular graph G are $-r(r+2)(n-1)$ times and $r(r+2)(n-1)$. Therefore, for an r -regular graph G on n vertices, $E_{CDS}(G) = 2r(r+2)(n-1)$. Hence, $E_{CDS}(K_n) = 2(n+1)(n-1)^2$ and $E_{CDS}(C_n) = 16(n-1)$. If G is an r -regular graph on n vertices then $E_{CDS}(\overline{G}) = 2(n-r-1)(n-r+1)(n-1)$ and $E_{CDS}(L^k(G)) = 2(2^k r - 2^{k+1} + 2)(2^k r - 2^{k+1} + 4)(n-1)$.

From Theorem 4.5, $E_{CDS}(K_{n_1, n_2}) = (n_2 - 1)(2n_1 + n_1^2) + (n_1 - 1)(2n_2 + n_2^2) + \sqrt{((n_2 - 1)(2n_1 + n_1^2) + (n_1 - 1)(2n_2 + n_2^2))^2 - 4((n_2 - 1)(2n_1 + n_1^2)(n_1 - 1)(2n_2 + n_2^2) - n_1 n_2 (n_1 + n_2 + n_1 n_2)^2)}$. By Theorem 4.7, $E_{CDS}(P_n) = 8n - 21 + \sqrt{64n^2 - 232n + 553}$. By Theorem 4.9, $E_{CDS}(W_n) = 15(n-2) + \sqrt{225(n-2)^2 + 4(n-1)(4n-1)^2}$.

6. BOUNDS FOR THE LARGEST CDS EIGENVALUES AND CDS ENERGY

Theorem 6.1. *The eigen values of $CDS(G)$ satisfies the relations*

1. $\sum_{i=1}^n \eta_i = 0$.
2. $\sum_{i=1}^n \eta_i^2 = 2S$, where $S = \sum_{i < j} (d_i + d_j + d_i d_j)^2$.

Proof. By the definition of $CDS(G)$, $\sum_{i=1}^n \eta_i = 0$
Next,

$$\begin{aligned}
 \sum_{i=1}^n \eta_i^2 &= \text{trace}((CDS(G))^2) \\
 &= \sum_{i=1}^n \sum_{j=1}^n c_{ij} c_{ji} \\
 &= \sum_{i=1}^n \sum_{j=1}^n c_{ij}^2 \\
 &= 2 \sum_{i < j} (d_i + d_j + d_i d_j)^2 \\
 &= 2S, \text{ where } S = \sum_{i < j} (d_i + d_j + d_i d_j)^2.
 \end{aligned}$$

□

Theorem 6.2. *If G is a connected graph with n vertices, then*

$$\eta_1 \leq \sqrt{\frac{2S(n-1)}{n}}.$$

Proof. Let $a_i = 1$ and $b_i = \eta_i$ for $i = 2, 3, \dots, n$ in Theorem 2.2. Therefore

$$\left(\sum_{i=2}^n \eta_i \right)^2 \leq (n-1) \left(\sum_{i=2}^n \eta_i^2 \right) \quad (6.1)$$

From Theorem 6.1, we have $\sum_{i=2}^n \eta_i = -\eta_1$ and $\sum_{i=2}^n \eta_i^2 = 2S - \eta_1^2$. Therefore Eq. 6.1 becomes

$$(-\eta_1)^2 \leq (n-1)(2S - \eta_1^2)$$

which gives

$$\eta_1 \leq \sqrt{\frac{2S(n-1)}{n}}.$$

□

Equality holds for η_1 if G is regular graph.

Theorem 6.3. *If G is a graph with n vertices, then*

$$\sqrt{2S} \leq E_{CDS}(G) \leq \sqrt{2nS}.$$

Proof. For $a_i = 1$ and $b_i = \eta_i$ in Theorem 2.2 we obtain,

$$\left(\sum_{i=1}^n \eta_i\right)^2 \leq n \left(\sum_{i=1}^n |\eta_i|^2\right)$$

Now

$$\begin{aligned} (E_{CDS}(G))^2 &\leq 2nS \\ E_{CDS}(G) &\leq \sqrt{2nS} \end{aligned} \tag{6.2}$$

This is an upper bound. Now

$$(E_{CDS}(G))^2 = \left(\sum_{i=1}^n \eta_i\right)^2 \geq \sum_{i=1}^n |\eta_i|^2 = 2S,$$

which gives a lower bound

$$E_{CDS}(G) \geq \sqrt{2S}. \tag{6.3}$$

Combining Eq. 6.2 and Eq. 6.3 we get

$$\sqrt{2S} \leq E_{CDS}(G) \leq \sqrt{2nS}.$$

□

Theorem 6.4. *If G is a graph with n vertices, then*

$$E_{CDS}(G) \geq \sqrt{2nS - \frac{n^2}{4}(|\eta_1| - |\eta_n|)^2}.$$

Proof. For $a_i = 1$ and $b_i = \eta_i$ in Theorem 2.3 we get,

$$\sum_{i=1}^n 1^2 \sum_{i=1}^n |\eta_i|^2 - \left(\sum_{i=1}^n |\eta_i|\right)^2 \leq \frac{n^2}{4}(|\eta_1| - |\eta_n|)^2$$

$$2nS - (E_{CDS}(G))^2 \leq \frac{n^2}{4}(|\eta_1| - |\eta_n|)^2$$

$$E_{CDS}(G) \geq \sqrt{2nS - \frac{n^2}{4}(|\eta_1| - |\eta_n|)^2}.$$

□

Theorem 6.5. *If G is an (n, m) graph, then*

$$E_{CDS}(G) \geq \sqrt{2nS - \mu(n)(|\eta_1| - |\eta_n|)^2},$$

where $\mu(n) = n \lfloor \frac{n}{2} \rfloor \left(1 - \frac{1}{n} \lfloor \frac{n}{2} \rfloor\right)$.

Proof. Let $a_i = |\eta_i| = b_i$, $A = \eta_1 = B$ and $a = |\eta_n| = b$ in Theorem 2.4 then

$$\left| n \sum_{i=1}^n |\eta_i|^2 - \left(\sum_{i=1}^n |\eta_i| \right)^2 \right| \leq \mu(n) \left(|\eta_1| - |\eta_n| \right)^2 \quad (6.4)$$

Since, $E_{CDS}(G) = \sum_{i=1}^n |\eta_i|$ and $\left(\sum_{i=1}^n |\eta_i| \right)^2$
Inequality 6.4 gives

$$2nQ - (E_{CDS}(G))^2 \leq \mu(n)(|\eta_1| - |\eta_n|)^2$$

$$E_{CDS}(G) \geq \sqrt{2nS - \mu(n)(|\eta_1| - |\eta_n|)^2}.$$

□

Theorem 6.6. *If G is a graph with n vertices, then*

$$E_{CDS}(G) \geq \frac{2S + n|\eta_1||\eta_n|}{|\eta_1| + |\eta_n|},$$

where $|\eta_1|$ is maximum and $|\eta_n|$ is minimum absolute value of η_i 's.

Proof. Let $a_i = 1$ and $b_i = \eta_i$, $c_1 = |\eta_n|$ and $c_2 = |\eta_1|$ in Theorem 2.5 then

$$\sum_{i=1}^n |\eta_i|^2 + |\eta_1||\eta_n| \sum_{i=1}^n 1^2 \leq (|\eta_1| + |\eta_n|) \left(\sum_{i=1}^n |\eta_i| \right)$$

Since $E_{CDS}(G) = \sum_{i=1}^n |\eta_i|$ and $\sum_{i=1}^n |\eta_i|^2 = 2S$.

On simplification,

$$2S + |\eta_1||\eta_n| \leq (|\eta_1| + |\eta_n|)E_{CDS}(G) \quad (6.5)$$

simple calculation of inequality 6.5 yields the required result. □

7. DEGREE SUM POLYNOMIAL OF SEMITOTAL LINE GRAPH OF r -REGULAR GRAPH

Definition 7.1. [31] The semitotal line graph $T_1(G)$ is a graph obtained from G by adding a new vertex corresponding to each edge of G and by joining those pairs of these new vertices which lie on adjacent edges of G .

The concept of degree sum matrix $DS(G)$ introduced by Ramane et al. [29]. The degree sum matrix of a graph [29] G is an $n \times n$ matrix $DS(G) = [d_{ij}]$, whose elements are defined as

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

The degree sum polynomial of a graph G is defined as

$$P_{DS(G)}(\gamma) = \det(\gamma I - DS(G)).$$

The *eigenvalues* of the matrix $DS(G)$, denoted by $\gamma_1, \gamma_2, \dots, \gamma_n$ are called the *degree sum eigenvalues* of G and their collection is called the *combined degree sum spectra* of G . Jog et al. [20] obtained the degree sum polynomial of graph valued functions on regular graphs. The expression for degree sum polynomial of semi total line graph $T_1(G)$ of r -regular graph is prone to some error. We give correct expression for it.

Theorem 7.2. [20] *The degree sum polynomial of semi-total line graph of r -regular graph of G is given by*

$$P_{DS(T_1(G))}(\gamma) = [\gamma + 2r]^{n-1}[\gamma + 4r]^{\frac{nr}{2}-1} \left[\gamma^2 - 2\gamma r(nr + n - 3) + 4r^2(n-1)(nr-2) - 2n^2r(r+1)^2 \right].$$

The correct version of Theorem 7.2 is as follows.

Theorem 7.3. *The degree sum polynomial of semi-total line graph of r -regular graph of G is given by*

$$P_{DS(T_1(G))}(\gamma) = [\gamma + 2r]^{n-1}[\gamma + 4r]^{\frac{nr}{2}-1} \left[\gamma^2 - 2\gamma r(nr + n - 3) + 4r^2(n-1)(nr-2) - \frac{9n^2r^3}{2} \right].$$

Proof. The characteristic polynomial degree sum matrix of $T_1(G)$ is

$$DS(T_1(G)) = \begin{vmatrix} 0 & 2r & \cdots & 2r & 3r & 3r & \cdots & 3r \\ 2r & 0 & \cdots & 2r & 3r & 3r & \cdots & 3r \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 2r & 2r & \cdots & 0 & 3r & 3r & \cdots & 3r \\ 3r & 3r & \cdots & 3r & 0 & 4r & \cdots & 4r \\ 3r & 3r & \cdots & 3r & 4r & 0 & \cdots & 4r \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 3r & 3r & \cdots & 3r & 4r & 4r & \cdots & 0 \end{vmatrix}$$

$$P_{DS(T_1(G))}(\gamma) = |\gamma I - DS(T_1(G))|$$

$$= \begin{vmatrix} \gamma & -2r & \cdots & -2r & -3r & -3r & \cdots & -3r \\ -2r & \gamma & \cdots & -2r & -3r & -3r & \cdots & -3r \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -2r & -2r & \cdots & \gamma & -3r & -3r & \cdots & -3r \\ -3r & -3r & \cdots & -3r & \gamma & -4r & \cdots & -4r \\ -3r & -3r & \cdots & -3r & -4r & \gamma & \cdots & -4r \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -3r & -3r & \cdots & -3r & -4r & -4r & \cdots & \gamma \end{vmatrix} \quad (7.1)$$

To reduce the lower block containing all $-(3r)$ to zero in Eq. 7.1 we perform, $R_i \rightarrow R_i + \frac{3r}{\gamma-2r(n-1)} \sum_{j=1}^n R_j$. Then Eq. 7.1 reduces to,

$$= \begin{vmatrix} \gamma & -2r & \cdots & -2r & & -3r & & -3r & \cdots & -3r \\ -2r & \gamma & \cdots & -2r & & -3r & & -3r & \cdots & -3r \\ \vdots & \vdots & \ddots & \vdots & & \vdots & & \vdots & \ddots & \vdots \\ -2r & -2r & \cdots & \gamma & & -3r & & -3r & \cdots & -3r \\ 0 & 0 & \cdots & 0 & \gamma - \frac{n(3r)^2}{\gamma-2r(n-1)} & -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} & \cdots & -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} & & \\ 0 & 0 & \cdots & 0 & -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} & \gamma - \frac{n(3r)^2}{\gamma-2r(n-1)} & \cdots & -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} & & \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & & \\ 0 & 0 & \cdots & 0 & -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} & -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} & \cdots & \gamma - \frac{n(3r)^2}{\gamma-2r(n-1)} & & \end{vmatrix}$$

which gives,

$$= \begin{vmatrix} \gamma & -2r & \cdots & -2r \\ -2r & \gamma & \cdots & -2r \\ \vdots & \vdots & \ddots & \vdots \\ -2r & -2r & \cdots & \gamma \end{vmatrix} \times \begin{vmatrix} \gamma - \frac{n(3r)^2}{\gamma-2r(n-1)} & -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} & \cdots & -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} \\ -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} & \gamma - \frac{n(3r)^2}{\gamma-2r(n-1)} & \cdots & -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} \\ \vdots & \vdots & \ddots & \vdots \\ -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} & -4r - \frac{n(3r)^2}{\gamma-2r(n-1)} & \cdots & \gamma - \frac{n(3r)^2}{\gamma-2r(n-1)} \end{vmatrix}$$

On applying lemma 2.6, we get the desired result. $\square$

8. COMBINED DEGREE SUM POLYNOMIAL OF GRAPH VALUED FUNCTIONS OF R-REGULAR GRAPHS

In this section, we obtain combined degree sum polynomial of some graph valued functions of r-regular graphs.

Definition 8.1. [18] The subdivision graph $S(G)$ of a graph G is the graph obtained by inserting a vertex into every edge of G .

Theorem 8.2. *The combined degree sum polynomial of subdivision graph of r -regular graph G is given by*

$$P_{CDS(S(G))}(\eta) = [\eta + r(r+2)]^{n-1} [\eta + 8]^{\frac{nr}{2}-1} \left[\eta^2 - \eta(r^2(n-1) + 6nr - 2(r+4)) - \frac{n^2r}{2}(3r+2)^2 + 4r(n-1)(r+2)(nr-2) \right].$$

Proof. The characteristic polynomial combined degree sum matrix of $S(G)$ is

$$CDS(S(G)) = \begin{vmatrix} 0 & r(r+2) & \cdots & r(r+2) & 3r+2 & 3r+2 & \cdots & 3r+2 \\ r(r+2) & 0 & \cdots & r(r+2) & 3r+2 & 3r+2 & \cdots & 3r+2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ r(r+2) & r(r+2) & \cdots & 0 & 3r+2 & 3r+2 & \cdots & 3r+2 \\ 3r+2 & 3r+2 & \cdots & 3r+2 & 0 & 8 & \cdots & 8 \\ 3r+2 & 3r+2 & \cdots & 3r+2 & 8 & 0 & \cdots & 8 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 3r+2 & 3r+2 & \cdots & 3r+2 & 8 & 8 & \cdots & 0 \end{vmatrix} \quad (8.1)$$

$$P_{CDS(S(G))}(\eta) = |\eta I - CDS(S(G))|$$

$$= \begin{vmatrix} \eta & -r(r+2) & \cdots & -r(r+2) & -(3r+2) & -(3r+2) & \cdots & -(3r+2) \\ -r(r+2) & \eta & \cdots & -r(r+2) & -(3r+2) & -(3r+2) & \cdots & -(3r+2) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -r(r+2) & -r(r+2) & \cdots & \eta & -(3r+2) & -(3r+2) & \cdots & -(3r+2) \\ -(3r+2) & -(3r+2) & \cdots & -(3r+2) & \eta & -8 & \cdots & -8 \\ -(3r+2) & -(3r+2) & \cdots & -(3r+2) & -8 & \eta & \cdots & -8 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -(3r+2) & -(3r+2) & \cdots & -(3r+2) & -8 & -8 & \cdots & \eta \end{vmatrix} \quad (8.2)$$

To reduce the lower block containing all $-(3r+2)$ to zero in Eq. 8.2 we perform, $R_i \rightarrow R_i + \frac{3r+2}{\eta-r(r+2)(n-1)} \sum_{j=1}^n R_j$. Then Eq. 8.2 reduces to,

$$= \begin{vmatrix} \eta & -r(r+2) & \cdots & -r(r+2) & -(3r+2) & -(3r+2) & \cdots & -(3r+2) \\ -r(r+2) & \eta & \cdots & -r(r+2) & -(3r+2) & -(3r+2) & \cdots & -(3r+2) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -r(r+2) & -r(r+2) & \cdots & \eta & -(3r+2) & -(3r+2) & \cdots & -(3r+2) \\ 0 & 0 & \cdots & 0 & \eta - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & \cdots & -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} \\ 0 & 0 & \cdots & 0 & -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & \eta & \cdots & -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & \cdots & \eta - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} \end{vmatrix}$$

which gives,

$$= \begin{vmatrix} \eta & -r(r+2) & \cdots & -r(r+2) \\ -r(r+2) & \eta & \cdots & -r(r+2) \\ \vdots & \vdots & \ddots & \vdots \\ -r(r+2) & -r(r+2) & \cdots & \eta \end{vmatrix} \times \begin{vmatrix} -\eta - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & \cdots & -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} \\ -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & \eta - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & \cdots & -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} \\ \vdots & \vdots & \ddots & \vdots \\ -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & -8 - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} & \cdots & \eta - \frac{n(3r+2)^2}{\eta-r(r+2)(n-1)} \end{vmatrix}$$

On applying lemma 2.6, we get the desired result. $\square$

Definition 8.3. [31] The semitotal point graph $T_2(G)$ is a graph obtained from G by inserting a new vertex into every edge of G and by joining each new vertex to the end points of the edge corresponding to it.

Theorem 8.4. The combined degree sum polynomial of semi-total point graph of r -regular graph G is given by

$$\begin{aligned} P_{CDS(T_2(G))}(\eta) &= [\eta + 4r(r+1)]^{n-1} [\eta + 8]^{\frac{nr}{2}-1} \left[\eta^2 - 4\eta(r^2(n-1) - r + 2) \right. \\ &\quad \left. - \frac{n^2 r}{2} (2 + 6r)^2 + 16r(n-1)(r+1)(nr-2) \right]. \end{aligned}$$

Proof. The characteristic polynomial combined degree sum matrix of $T_2(G)$ is

$$CDS(T_2(G)) = \begin{vmatrix} 0 & 4r(r+1) & \cdots & 4r(r+1) & 2+6r & 2+6r & \cdots & 2+6r \\ 4r(r+1) & 0 & \cdots & 4r(r+1) & 2+6r & 2+6r & \cdots & 2+6r \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 4r(r+1) & 4r(r+1) & \cdots & 0 & 2+6r & 2+6r & \cdots & 2+6r \\ 2+6r & 2+6r & \cdots & 2+6r & 0 & 8 & \cdots & 8 \\ 2+6r & 2+6r & \cdots & 2+6r & 8 & 0 & \cdots & 8 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 2+6r & 2+6r & \cdots & 2+6r & 8 & 8 & \cdots & 0 \end{vmatrix} \quad (8.3)$$

$$P_{CDS(T_2(G))}(\eta) = |\eta I - CDS(T_2(G))|$$

$$= \begin{vmatrix} \eta & -4r(r+1) & \cdots & -4r(r+1) & -(2+6r) & -(2+6r) & \cdots & -(2+6r) \\ -4r(r+1) & \eta & \cdots & -4r(r+1) & -(2+6r) & -(2+6r) & \cdots & -(2+6r) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -4r(r+1) & -4r(r+1) & \cdots & \eta & -(2+6r) & -(2+6r) & \cdots & -(2+6r) \\ -(2+6r) & -(2+6r) & \cdots & -(2+6r) & \eta & -8 & \cdots & -8 \\ -(2+6r) & -(2+6r) & \cdots & -(2+6r) & -8 & \eta & \cdots & -8 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -(2+6r) & -(2+6r) & \cdots & -(2+6r) & -8 & -8 & \cdots & \eta \end{vmatrix} \quad (8.4)$$

To reduce the lower block containing all $-(2+6r)$ to zero in Eq. 8.4 we perform, $R_i \rightarrow R_i + \frac{2+6r}{\eta-4r(r+1)(n-1)} \sum_{j=1}^n R_j$. Then Eq. 8.4 reduces to,

$$= \begin{vmatrix} \eta & -4r(r+1) & \cdots & -4r(r+1) & -(2+6r) & -(2+6r) & \cdots & -(2+6r) \\ -4r(r+1) & \eta & \cdots & -4r(r+1) & -(2+6r) & -(2+6r) & \cdots & -(2+6r) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -4r(r+1) & -4r(r+1) & \cdots & \eta & -(2+6r) & -(2+6r) & \cdots & -(2+6r) \\ 0 & 0 & \cdots & 0 & \eta - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & \cdots & -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} \\ 0 & 0 & \cdots & 0 & -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & \eta & \cdots & -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & \cdots & \eta - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} \end{vmatrix}$$

which gives,

$$= \begin{vmatrix} \eta & -4r(r+1) & \cdots & -4r(r+1) \\ -4r(r+1) & \eta & \cdots & -4r(r+1) \\ \vdots & \vdots & \ddots & \vdots \\ -4r(r+1) & -4r(r+1) & \cdots & \eta \end{vmatrix} \times \begin{vmatrix} -\eta - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & \cdots & -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} \\ -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & \eta - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & \cdots & -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} \\ \vdots & \vdots & \ddots & \vdots \\ -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & -8 - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} & \cdots & \eta - \frac{n(2+6r)^2}{\eta-4r(r+1)(n-1)} \end{vmatrix}$$

On applying lemma 2.6, we get the desired result. $\square$

Theorem 8.5. *The combined degree sum polynomial of semi-total line graph of r -regular graph G is given by*

$$P_{CDS(T_1(G))}(\eta) = [\eta + r(r+2)]^{n-1} [\eta + 4r(r+1)]^{\frac{nr}{2}-1} \left[\eta^2 + \eta(2nr^3 + 3nr^2 - 10r - r^2 + 2nr) + 2r^2(r+1)(r+2)(n-1)(nr-2) \right].$$

Proof. For any regular graph G of order n regularity r , the combined degree sum matrix of $T_1(G)$ is

$$CDS(T_1(G)) = \begin{vmatrix} 0 & r(r+2) & \cdots & r(r+2) & r(3+2r) & r(3+2r) & \cdots & r(3+2r) \\ r(r+2) & 0 & \cdots & r(r+2) & r(3+2r) & r(3+2r) & \cdots & r(3+2r) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ r(r+2) & r(r+2) & \cdots & 0 & r(3+2r) & r(3+2r) & \cdots & r(3+2r) \\ r(3+2r) & r(3+2r) & \cdots & 4r(r+1) & 0 & 4r(r+1) & \cdots & 4r(r+1) \\ r(3+2r) & r(3+2r) & \cdots & 4r(r+1) & 4r(r+1) & 0 & \cdots & 4r(r+1) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ r(3+2r) & r(3+2r) & \cdots & 4r(r+1) & 4r(r+1) & 4r(r+1) & \cdots & 0 \end{vmatrix}$$

The characteristic polynomial is,

$$P_{CDS(T_1(G))}(\eta) = |\eta I - CDS(T_1(G))|$$

$$= \begin{vmatrix} \eta & -r(r+2) & \cdots & -r(r+2) & -r(3+2r) & -r(3+2r) & \cdots & -r(3+2r) \\ -r(r+2) & \eta & \cdots & -r(r+2) & -r(3+2r) & -r(3+2r) & \cdots & -r(3+2r) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -r(r+2) & -r(r+2) & \cdots & \eta & -r(3+2r) & -r(3+2r) & \cdots & -r(3+2r) \\ -r(3+2r) & -r(3+2r) & \cdots & -r(3+2r) & \eta & -4r(r+1) & \cdots & -4r(r+1) \\ -r(3+2r) & -r(3+2r) & \cdots & -r(3+2r) & -4r(r+1) & \eta & \cdots & -4r(r+1) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -r(3+2r) & -r(3+2r) & \cdots & -r(3+2r) & -4r(r+1) & -4r(r+1) & \cdots & \eta \end{vmatrix} \quad (8.5)$$

To reduce the lower block containing all $-(2+6r)$ to zero in Eq. 8.5 we perform, $R_i \rightarrow R_i + \frac{r(3+2r)}{\eta-r(r+2)(n-1)} \sum_{j=1}^n R_j$. On applying lemma 2.6, we get the desired result. $\square$

Definition 8.6. [18] 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 if the corresponding elements of G are adjacent or incident.

Theorem 8.7. For any regular graph of order n regularity r , the combined degree sum polynomial of total graph $T(G)$ is

$$P_{CDS(T(G))}(\eta) = (\eta + 4r(r+1))^{n+m-1} (\eta - 4r(r+1)(n+m-1)).$$

Proof. Since total graph of a r -regular graph is $2r$ -regular, result follows from Theorem 4.1. $\square$

Definition 8.8. [32] The vertex splitting graph $S'(G)$ of a graph G is obtained from G by adding for each vertex v of G a new vertex v' so that v' is adjacent to every vertex that is adjacent to v . We denote $V'(G) = \{v' : v \in V(G)\}$.

Theorem 8.9. Let G be an r -regular graph of order n . The combined degree sum polynomial of the splitting graph $S'(G)$ is

$$P_{CDS(S'(G))}(\eta) = [\eta + r(r+2)]^{n-1} [\eta + 4r(1+r)]^{n-1} \left[(\eta - r(r+2)(n-1)) (\eta - 4r(1+r)(n-1)) - n^2 r^2 (3+2r)^2 \right].$$

Proof. The splitting graph $S'(G)$ of a r -regular graph G has two types of vertices. The n vertices with degree r and n vertices are of degree $2r$. The combined degree sum matrix of $S'(G)$ is

$$CDS(S'(G)) = \begin{bmatrix} r(r+2)(J_n - I_n) & r(3+2r)J_n \\ r(3+2r)J_n & 4r(1+r)(J_n - I_n) \end{bmatrix}$$

Therefore,

$$\begin{aligned} P_{CDS(S'(G))}(\eta) &= |\eta I - CDS(S'(G))| \\ &= \begin{vmatrix} (\eta + r(r+2))I_n - r(r+2)J_n & -r(3+2r)J_{n \times n} \\ -r(3+2r)J_{n \times n} & (\eta + 4r(1+r))I_n - 4r(1+r)J_n \end{vmatrix} \end{aligned}$$

Using Lemma 2.1, we get the required result. $\square$

Definition 8.10. [21] The edge splitting graph $L_S(G)$ of a graph G is a graph with vertex set $E(G) \cup E_1(G)$ with two vertices adjacent if they correspond to adjacent edges of G or one corresponds to an element e'_i of $E_1(G)$ and the other to an element e_j of $E(G)$ where $e_j \in N(e_i)$.

Theorem 8.11. Let G be an r -regular graph of order n and size m . The combined degree sum polynomial of the edge splitting graph $L_S(G)$ is

$$\begin{aligned} P_{CDS(L_S(G))}(\eta) &= [\eta + 4r(r-1)]^{m-1} [\eta + 8(r-1)(2r-1)]^{m-1} \left[(\eta - 4r(r-1)(n-1))(\eta \right. \\ &\quad \left. - 8(r-1)(2r-1)(n-1)) - 4m^2(r-1)^2(4r-1)^2 \right]. \end{aligned}$$

Proof. The edge splitting graph $L_S(G)$ of a r -regular graph G has two types of vertices. The m vertices with degree $2(r-1)$ and m vertices are of degree $4(r-1)$. The combined degree sum matrix of $L_S(G)$ is

$$CDS(L_S(G)) = \begin{bmatrix} 4r(r-1)(J_m - I_m) & 2(r-1)(4r-1)J_m \\ 2(r-1)(4r-1)J_m & 8(r-1)(2r-1)(J_m - I_m) \end{bmatrix}$$

Therefore,

$$\begin{aligned} P_{CDS(L_S(G))}(\eta) &= |\eta I - CDS(L_S(G))| \\ &= \begin{vmatrix} (\eta + 4r(r-1))I_m - 4r(r-1)J_m & -2(r-1)(4r-1)J_{m \times m} \\ -2(r-1)(4r-1)J_{m \times m} & (\eta + 8(r-1)(2r-1))I_m - 8(r-1)(2r-1)J_m \end{vmatrix} \end{aligned}$$

Using Lemma 2.1, we get the required result. $\square$

Definition 8.12. [22] The total closed neighbourhood graph $N_{tc}(G)$ of a graph G is the graph having vertex set $V(G) \cup V'(G)$ and two vertices are adjacent if they correspond to adjacent vertices of G or one corresponds to a vertex v'_i of $V'(G)$ and the other to a vertex w_j of G and w_j is in $N_G[v_i]$.

Theorem 8.13. Let G be an r -regular graph of order n . The combined degree sum polynomial of the total closed neighbourhood graph $N_{tc}(G)$ is

$$\begin{aligned} P_{CDS(N_{tc}(G))}(\eta) &= [\eta + (2r+1)(2r+3)]^{n-1} [\eta + (r+1)(r+3)]^{n-1} \left[(\eta - (2r+1)(2r+3)(n-1))(\eta \right. \\ &\quad \left. - (r+1)(r+3)(n-1)) - n^2(2r^2 + 6r + 3)^2 \right]. \end{aligned}$$

Proof. The total closed neighbourhood graph $N_{tc}(G)$ of a r -regular graph G has two types of vertices. The n vertices with degree $2r + 1$ and n vertices are of degree $r + 1$. The combined degree sum matrix of $N_{tc}(G)$ is

$$CDS(N_{tc}(G)) = \begin{bmatrix} (2r+1)(2r+3)(J_n - I_n) & (2r^2+6r+3)J_n \\ (2r^2+6r+3)J_n & (r+1)(r+3)(J_n - I_n) \end{bmatrix}$$

Therefore,

$$\begin{aligned} P_{CDS(N_{tc}(G))}(\eta) &= |\eta I - CDS(N_{tc}(G))| \\ &= \begin{vmatrix} (\eta + (2r+1)(2r+3))I_n - (2r+1)(2r+3)J_n & -(2r^2+6r+3)J_{n \times n} \\ -(2r^2+6r+3)J_{n \times n} & (\eta + (r+1)(r+3))I_n - (r+1)(r+3)J_n \end{vmatrix} \end{aligned}$$

Using Lemma 2.1, we get the required result. $\square$

9. COMBINED DEGREE SUM POLYNOMIAL OF GRAPH OPERATIONS ON R-REGULAR GRAPHS

Definition 9.1. [16] The thorn graph of a graph G is the graph obtained from G by attaching k pendent vertices to each vertex of G .

Theorem 9.2. *The combined degree sum polynomial of the thorn graph G^{+k} of a regular graph is*

$$\begin{aligned} P_{CDS(G^{+k})}(\eta) &= (\eta + (r+k)(r+k+2))^{n-1} (\eta + 3)^{nk-1} ([\eta - (n-1)(r+k)(r+k+2)][\eta \\ &\quad - 3(nk-1)] - nk(1+2(r+k))^2). \end{aligned}$$

Proof. The thorn graph of a regular graph G of degree r has two types of vertices. The n vertices are of degree $r+k$ and the remaining nk vertices are of degree 1. Hence, the combined degree sum matrix of G^{+k} is

$$CDS(G^{+k}) = \begin{bmatrix} (r+k)(r+k+2)(J_n - I_n) & (1+2(r+k))J_{n \times nk} \\ (1+2(r+k))J_{nk \times n} & 3(J_{nk} - I_{nk}) \end{bmatrix}$$

Therefore,

$$\begin{aligned} P_{CDS(G^{+k})}(\eta) &= |\eta I - CDS(G^{+k})| \\ &= \begin{vmatrix} (\eta + (r+k)(r+k+2))I_n - (r+k)(r+k+2)J_n & -(1+2(r+k))J_{n \times nk} \\ -(1+2(r+k))J_{nk \times n} & (\eta + 3)I_{nk} - 3J_{nk} \end{vmatrix} \end{aligned}$$

Using Lemma 2.1, we get the required result. $\square$

Definition 9.3. [18] The union of the graphs G_1 and G_2 is a graph $G_1 \cup G_2$ whose vertex set is $V = V(G_1) \cup V(G_2)$ and the edge set is $E = E(G_1) \cup E(G_2)$.

Theorem 9.4. *Let G be an r_1 -regular graph of order n_1 and H be an r_2 -regular graph of order n_2 . Then, the combined degree sum polynomial of the graph $G \cup H$ is*

$$\begin{aligned} P_{CDS(G \cup H)}(\eta) &= P_{CDS(G)}(\eta)P_{CDS(H)}(\eta) - (\eta + r_1(r_1+2))^{n_1-1} (\eta + r_2(r_2 \\ &\quad + 2))^{n_2-1} (r_1 + r_2 + r_1r_2)^2 n_1 n_2. \end{aligned}$$

Proof. The combined degree sum matrix of $G \cup H$ is

$$CDS(G \cup H) = \begin{bmatrix} r_1(r_1 + 2)(J_{n_1} - I_{n_1}) & (r_1 + r_2 + r_1 r_2)J_{n_1 \times n_2} \\ (r_1 + r_2 + r_1 r_2)J_{n_2 \times n_1} & r_2(r_2 + 2)(J_{n_2} - I_{n_2}) \end{bmatrix}$$

Therefore,

$$\begin{aligned} P_{CDS(G \cup H)}(\eta) &= |\eta I - CDS(G \cup H)| \\ &= \begin{vmatrix} (\eta + r_1(r_1 + 2))I_{n_1} - r_1(r_1 + 2)J_{n_1} & -(r_1 + r_2 + r_1 r_2)J_{n_1 \times n_2} \\ -(r_1 + r_2 + r_1 r_2)J_{n_2 \times n_1} & (\eta + r_2(r_2 + 2))I_{n_2} - r_2(r_2 + 2)J_{n_2} \end{vmatrix} \end{aligned}$$

Using Lemma 2.1, we get

$$P_{CDS(G \cup H)}(\eta) = (\eta + r_1(r_1 + 2))^{n_1 - 1} (\eta + r_2(r_2 + 2))^{n_2 - 1} \left([\eta - (n_1 - 1)r_1(r_1 + 2)][\eta - (n_2 - 1)r_2(r_2 + 2)] - n_1 n_2 (r_1 + r_2 + r_1 r_2)^2 \right) \quad (9.1)$$

But G is an r_1 -regular graph of order n_1 and H is an r_2 -regular graph of order n_2 . Then by Theorem 4.1, we have

$$P_{CDS(G)}(\eta) = (\eta + r_1(r_1 + 2))^{n_1 - 1} (\eta - r_1(r_1 + 2)(n_1 - 1)). \quad (9.2)$$

and

$$P_{CDS(H)}(\eta) = (\eta + r_2(r_2 + 2))^{n_2 - 1} (\eta - r_2(r_2 + 2)(n_2 - 1)). \quad (9.3)$$

By substituting Eq. 9.2 and Eq. 9.3 in Eq. 9.1, we get the desired result. $\square$

Definition 9.5. The corona [18] $G \circ H$ of graphs G and H is a graph obtained from G and H by taking one copy of G and $|V(G)|$ copies of H and then joining i^{th} vertex of G to every vertex in the i^{th} copy of H .

Theorem 9.6. Let G be an r_1 -regular graph of order n_1 and H be an r_2 -regular graph of order n_2 . The combined degree sum polynomial of the graph $G \circ H$ is

$$\begin{aligned} P_{CDS(G \circ H)}(\eta) &= [\eta + R_1(R_1 + 2)]^{n_1} [\eta + R_2(R_2 + 2)]^{n_1 n_2 - 1} \left[(\eta - R_1(R_1 + 2)(n_1 - 1)) (\eta \right. \\ &\quad \left. - R_2(R_2 + 2)(n_1 n_2 - 1)) - n_1^2 n_2 (R_1 + R_2 + R_1 R_2)^2 \right], \end{aligned}$$

where $R_1 = r_1 + n_2$ and $R_2 = r_2 + 1$.

Proof. If G is an r_1 -regular graph of order n_1 and H is an r_2 -regular graph of order n_2 , then $G \circ H$ has two types of vertices, the n_1 vertices are of degree $R_1 = r_1 + n_2$ and the remaining $n_1 n_2$ vertices are of degree $R_2 = r_2 + 1$. Hence The combined degree sum matrix of $G \circ H$ is

$$CDS(G \circ H) = \begin{bmatrix} R_1(R_1 + 2)(J_{n_1} - I_{n_1}) & (R_1 + R_2 + R_1 R_2)J_{n_1 \times n_1 n_2} \\ (R_1 + R_2 + R_1 R_2)J_{n_1 n_2 \times n_1} & R_2(R_2 + 2)(J_{n_1 n_2} - I_{n_1 n_2}) \end{bmatrix}$$

Therefore,

$$\begin{aligned} P_{CDS(G \circ H)}(\eta) &= |\eta I - CDS(G \circ H)| \\ &= \begin{vmatrix} (\eta + R_1(R_1 + 2))I_{n_1} - R_1(R_1 + 2)J_{n_1} & -(R_1 + R_2 + R_1 R_2)J_{n_1 \times n_1 n_2} \\ -(R_1 + R_2 + R_1 R_2)J_{n_1 n_2 \times n_1} & (\eta + R_2(R_2 + 2))I_{n_1 n_2} - R_2(R_2 + 2)J_{n_1 n_2} \end{vmatrix} \end{aligned}$$

Using Lemma 2.1, we get the required result. $\square$

Definition 9.7. [18] The join $G + H$ of two graphs G_1 and G_2 is the graph obtained from G_1 and G_2 by joining every vertex of G_1 to all vertices of G_2 .

Theorem 9.8. *Let G be an r_1 -regular graph of order n_1 and H be an r_2 -regular graph of order n_2 . Then, combined degree sum polynomial of the graph $G + H$ is*

$$P_{CDS(G+H)}(\eta) = [\eta + R_1(R_1 + 2)]^{n_1-1} [\eta + R_2(R_2 + 2)]^{n_1 n_2 - 1} \left[(\eta - R_1(R_1 + 2)(n_1 - 1)) (\eta - R_2(R_2 + 2)(n_1 n_2 - 1)) - n_1^2 n_2 (R_1 + R_2 + R_1 R_2)^2 \right],$$

where $R_1 = r_1 + n_2$ and $R_2 = r_2 + n_1$.

Proof. If G is an r_1 -regular graph of order n_1 and H is an r_2 -regular graph of order n_2 , then $G \circ H$ has two types of vertices, the n_1 vertices are of degree $R_1 = r_1 + n_2$ and the remaining $n_1 n_2$ vertices are of degree $R_2 = r_2 + n_1$. Hence The combined degree sum matrix of $G + H$ is

$$CDS(G + H) = \begin{bmatrix} R_1(R_1 + 2)(J_{n_1} - I_{n_1}) & (R_1 + R_2 + R_1 R_2)J_{n_1 \times n_1 n_2} \\ (R_1 + R_2 + R_1 R_2)J_{n_1 n_2 \times n_1} & R_2(R_2 + 2)(J_{n_1 n_2} - I_{n_1 n_2}) \end{bmatrix}$$

Therefore,

$$\begin{aligned} P_{CDS(G+H)}(\eta) &= |\eta I - CDS(G + H)| \\ &= \begin{vmatrix} (\eta + R_1(R_1 + 2))I_{n_1} - R_1(R_1 + 2)J_{n_1} & -(R_1 + R_2 + R_1 R_2)J_{n_1 \times n_1 n_2} \\ -(R_1 + R_2 + R_1 R_2)J_{n_1 n_2 \times n_1} & (\eta + R_2(R_2 + 2))I_{n_1 n_2} - R_2(R_2 + 2)J_{n_1 n_2} \end{vmatrix} \end{aligned}$$

Using Lemma 2.1, we get the required result. $\square$

Definition 9.9. [18] The product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G \times H$ if and only if $[a = b \text{ and } xy \in E(H)]$ or $[x = y \text{ and } ab \in E(G)]$.

Theorem 9.10. *Let G be an r_1 -regular graph of order n_1 and H be an r_2 -regular graph of order n_2 . Then*

$$P_{CDS(G \times H)}(\eta) = [\eta + (r_1 + r_2)(r_1 + r_2 + 2)]^{n_1 n_2 - 1} [\eta + (r_1 + r_2)(r_1 + r_2 + 2)(n_1 n_2 - 1)].$$

Proof. If G and H are r_1 and r_2 regular graphs, respectively, then $G \times H$ is a $(r_1 + r_2)$ -regular graph with $n_1 n_2$ vertices. Hence, the result follows from Theorem 2.1. $\square$

Definition 9.11. [18] The composition $G[H]$ of graphs G and H with disjoint vertex sets $V(G)$ and $V(H)$ and edge sets $E(G)$ and $E(H)$ is the graph with vertex set $V(G[H]) = V(G) \cup V(H)$ and $(a, x)(b, y)$ is an edge of $G[H]$ if and only if $[a \text{ is adjacent to } b]$ or $[a = b \text{ and } x \text{ is adjacent to } y]$.

Theorem 9.12. *Let G be an r_1 -regular graph of order n_1 and H be an r_2 -regular graph of order n_2 . Then*

$$P_{CDS(G[H])}(\eta) = [\eta + (n_2 r_1 + r_2)(n_2 r_1 + r_2 + 2)]^{n_1 n_2 - 1} [\eta + (n_2 r_1 + r_2)(n_2 r_1 + r_2 + 2)(n_1 n_2 - 1)].$$

Proof. If G and H are r_1 and r_2 regular graphs, respectively, then $G[H]$ is a $n_2 r_1 + r_2$ -regular graph with $n_1 n_2$ vertices. Hence, the result follows from Theorem 2.1. $\square$

10. CONCLUSION

In this paper, we have introduced a new graph matrix called combined degree sum matrix and its energy. $E_{CDS}(G)$ values of some molecules containing hetero atoms are correlated with their total π -electron energy, we got a good correlation with the correlation coefficient $r=0.9823$. Further, we obtained CDS polynomials and CDS energy of some graphs. Bounds for the largest CDS eigenvalues and CDS energy of a graph are investigated. We gave the correct expression for the degree sum polynomial of semi-total line graph of r -regular graph of G . The characteristic polynomial of the combined degree sum matrix of graph valued functions and graph operations on regular graphs are obtained.

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