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MODIFIED SCHULTZ ENERGY OF GRAPHS

M. R. RAJESH KANNA[1] AND S. ROOPA

ABSTRACT. In this article we have defined a new matrix called modified Schultz matrix and hence modified Schultz energy. Upper and lower bounds for modified Schultz energy are presented. At the end of this article modified Schultz energies for some standard graphs like star graph, complete graph, crown graph, cocktail graph, complete bipartite graph and friendship graphs are computed.

1. INTRODUCTION

Study on energy of graphs goes back to the year 1978, when I. Gutman [7] defined this while working with energies of conjugated hydrocarbon containing carbon atoms. All graphs considered in this paper are assumed to be simple without loops and multiple edges. Let $A = (a_{ij})$ be the adjacency matrix of the graph G with its eigenvalues $\lambda_1, \lambda_2, \lambda_3, \cdots, \lambda_n$ assumed in decreasing order. Since A is real symmetric, the eigenvalues of G are real numbers whose sum equal to zero. The sum of the absolute eigenvalues values of G is called the energy $\mathcal{E}(G)$ of G, i.e., $\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|$.

Theories on the mathematical concepts of graph energy can be seen in the reviews [8], papers [5, 6, 9] and the references cited there in. For various upper and lower bounds for energy of a graph can be found in papers [12, 15] and

[1]*corresponding author*
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it was observed that graph energy has chemical applications in the molecular orbital theory of conjugated molecules [10, 11].

1.1. **Modified Schultz index.** In 1989, H.P. Schultz [17] introduced a new topological index, namely Schultz index which is defined as

$$S(G) = \sum_{\{v_i,v_j\}\subseteq V(G)} [d(v_i) + d(v_j)]d(v_i, v_j),$$

where $d(v_i, v_j)$ is the shortest distance between vertices v_i and v_j, and $d(v_i)$ is the degree of the vertex v_i in G, Similarly $d(v_j)$.

A. Dobrynin and Amide A. Kochetova in 1994 [1] also proposed the above index and called it the degree distance of a graph.

Motivated by the Schultz index, S. Klavžar and I. Gutman introduced Schultz index of the second kind in 1997 called Gutman index or modified Schlutz index [14]. It is defined by

$$S^*(G) = \sum_{\{v_i,v_j\}\subseteq V(G)} d(v_i)d(v_j)d(v_i, v_j).$$

1.2. **Modified Schultz energy.** Let G be a simple graph of order n with vertex set V and edge set $E(G)$. Let $d(v_i)$ denotes the degree of the vertex v_i. Modified Schultz matrix of a graph G is $n \times n$ matrix and is defined by $S^*(G) := (s^*_{ij})$, where

$$s^*_{ij} = d(v_i)d(v_j)d(v_i, v_j).$$

The characteristic polynomial of $S^*(G)$ is denoted by $f_n(G, \rho)= det(\rho I - S^*(G))$. The modified Schultz eigenvalues of the graph G are the eigenvalues of $S^*(G)$. Since $S^*(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$. The modified Schultz energy of G is defined as $\mathcal{E}_{S^*}(G) : = \sum_{i=1}^{n} |\rho_i|$. Here trace of $S^*(G) = 0$.

2. Main Results

2.1. Properties of Schultz eigenvalues.

Theorem 2.1. *Let G be a graph with vertex set $V = \{v_1, v_2, ..., v_n\}$, edge set E. If $\lambda_1, \lambda_2, ..., \lambda_n$ are the eigenvalues of Modified Schultz matrix $S^*(G)$ then*

(i) $\sum_{i=1}^{n} \lambda_i = 0.$

(ii) $\sum_{i=1}^{n} \lambda_i^2 = 2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2.$

Proof. (i) We know that the sum of the eigenvalues of $S^*(G)$ is the trace of $S^*(G)$

$$\therefore \sum_{i=1}^{n} \lambda_i = \sum_{i=1}^{n} s_{ii} = 0\,.$$

(ii) Similarly the sum of squares of the eigenvalues of $S^*(G)$ is trace of $[S^*(G)]^2$

$$\begin{aligned}
\therefore \sum_{i=1}^{n} \lambda_i^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n} s_{ij}s_{ji} \\
&= \sum_{i=1}^{n}(s_{ii})^2 + \sum_{i\neq j} s_{ij}s_{ji} \\
&= \sum_{i=1}^{n}(s_{ii})^2 + 2\sum_{i<j}(s_{ij})^2 \\
&= \sum_{i=1}^{n}(s_{ii})^2 + 2\sum_{i<j} d(v_i)^2 d(v_j)^2 d(v_i, v_j)^2 \\
&= 2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2 \\
&= 2M, \text{ where } M = \sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2.
\end{aligned}$$

□

2.2. **Bounds for Modified Schultz energy.** MClelland's [15] gave upper and lower bounds for ordinary energy of a graph. Similar bounds for $\mathcal{E}_{S^*}(G)$ are given in the following theorem.

Theorem 2.2. *Let G be a simple graph with n vertices and m edges and* $P = |detS^*(G)|$ *then*

$$\sqrt{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2 + n(n-1)P^{\frac{2}{n}}} \leq \mathcal{E}_{S^*}(G) \leq \sqrt{n\Big(2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2\Big)}\,.$$

Proof.

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

If $a_i = 1, b_i =\mid \lambda_i \mid$ then $\left(\sum_{i=1}^{n} \mid \lambda_i \mid\right)^2 \leq \left(\sum_{i=1}^{n} 1\right)\left(\sum_{i=1}^{n} \lambda_i^2\right)$

$$[\mathcal{E}_{S^*}(G)]^2 \leq n\Big(2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2\Big) \qquad \text{[From theorem 2.1]}$$

$$\Longrightarrow \mathcal{E}_{S^*}(G) \leq \sqrt{n\Big(2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2\Big)}\,.$$

Since arithmetic mean is greater than or equal to geometric mean we have:

$$\frac{1}{n(n-1)}\sum_{i \neq j} \mid \lambda_i \mid\mid \lambda_j \mid \geq \Big[\prod_{i \neq j} \mid \lambda_i \mid\mid \lambda_j \mid\Big]^{\dfrac{1}{n(n-1)}}$$

$$= \Big[\prod_{i=1}^{n} \mid \lambda_i \mid^{2(n-1)}\Big]^{\dfrac{1}{n(n-1)}}$$

$$= \Big[\prod_{i=1}^{n} \mid \lambda_i \mid\Big]^{\frac{2}{n}}$$

$$= \Big|\prod_{i=1}^{n} \lambda_i\Big|^{\frac{2}{n}}$$

$$= |detS^*(G)|^{\frac{2}{n}} = P^{\frac{2}{n}}$$

$$\therefore \sum_{i \neq j} \mid \lambda_i \mid\mid \lambda_j \mid \geq n(n-1)P^{\frac{2}{n}}\,.$$

Now consider,

$$[\mathcal{E}_{S^*}(G)]^2 = \Big(\sum_{i=1}^{n} \mid \lambda_i \mid\Big)^2$$

$$= \sum_{i=1}^{n} \mid \lambda_i \mid^2 + \sum_{i \neq j} \mid \lambda_i \mid\mid \lambda_j \mid,$$

$$\therefore \quad [\mathcal{E}_{S^*}(G)]^2 \geq 2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2 + n(n-1)P^{\frac{2}{n}} \qquad \text{[From theorem 2.1]}$$

$$i.e., \ \mathcal{E}_{S^*}(G) \geq \sqrt{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2 + n(n-1)P^{\frac{2}{n}}}\,.$$

□

Theorem 2.3. *If* $\lambda_1(G)$ *is the largest modified Schultz eigenvalue of* $S^*(G)$*, then* $\lambda_1(G) \geq \dfrac{S^*(G)}{n}$.

Proof. For any nonzero vector X, we have by [3], $\lambda_1(A) = \max_{X\neq 0}\left\{\dfrac{X'AX}{X'X}\right\}$

$$\therefore \lambda_1(G) \geq \frac{J'AJ}{J'J} = \frac{2\sum_{i<j} d_i d_j d_{ij}}{n} = \frac{S^*(G)}{n} \text{ where } J \text{ is a unit column matrix.}$$ □

Just like Koolen and Moulton's [13] upper bound for energy of a graph, an upper bound for $\mathcal{E}_{S^*}(G)$ is given in the following theorem.

Theorem 2.4. *If G is a (n,m) graph with* $\left(\dfrac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n}\right) \geq n$

$$\textit{then } \mathcal{E}_{S^*}(G) \leq \frac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n} + \sqrt{(n-1)\left[2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2 - \left(\frac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n}\right)^2\right]}.$$

Proof.

Cauchy-Schwartz inequality is $\left[\sum_{i=2}^{n} a_i b_i\right]^2 \leq \left(\sum_{i=2}^{n} a_i^2\right)\left(\sum_{i=2}^{n} b_j^2\right)$.

Put $a_i = 1, b_i = \mid \lambda_i \mid$ then $\left(\sum_{i=2}^{n} \mid \lambda_i \mid\right)^2 = \sum_{i=2}^{n} 1 \sum_{i=2}^{n} \mid \lambda_i \mid^2$

$$\Rightarrow [\mathcal{E}_{S^*}(G) - \lambda_1]^2 \leq (n-1)\left(2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2 - \lambda_1^2\right)$$

$$\Rightarrow \mathcal{E}_{S^*}(G) \leq \lambda_1 + \sqrt{(n-1)\left(2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2 - \lambda_1^2\right)}$$

$$\text{Let } f(x) = x + \sqrt{(n-1)\left(2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2 - x^2\right)}.$$

For decreasing function

$$f'(x) \le 0 \Rightarrow 1 - \frac{x(n-1)}{\sqrt{(n-1)\left(2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2 - x^2\right)}} \le 0$$

$$\Rightarrow x \ge \sqrt{\frac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n}}.$$

Since $\left(\dfrac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n}\right) \ge n$, we have $\sqrt{\dfrac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n}} \le \dfrac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n} \le \lambda_1$

$$\therefore f(\lambda_1) \le f\left(\frac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n}\right)$$

$$i.e., \mathcal{E}_{S^*}(G) \le f(\lambda_1) \le f\left(\frac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n}\right)$$

$$i.e., \mathcal{E}_{S^*}(G) \le f\left(\frac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n}\right)$$

$$i.e., \mathcal{E}_{S^*}(G) \le \frac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n} + \sqrt{(n-1)\left[2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2 - \left(\frac{2\sum_{i<j} {d_i}^2 {d_j}^2 d_{ij}^2}{n}\right)^2\right]}.$$

□

Milovanović [16] bounds for Modified Schultz energy of a graph are given in the following theorem.

Theorem 2.5. *Let G be a graph with n vertices and m edges. Let $|\lambda_1| \ge |\lambda_2| \ge \ldots \ge |\lambda_n|$ be a non-increasing order of Schultz eigenvalues of $S^*(G)$ then*

$\mathcal{E}_{S^*}(G) \geq \sqrt{n\Big(2\sum\limits_{i<j} {d_i}^2{d_j}^2d_{ij}^2\Big) - \alpha(n)(|\lambda_1| - |\lambda_n|)^2}$ *where* $\alpha(n) = n[\frac{n}{2}](1 - \frac{1}{n}[\frac{n}{2}])$ *and* $[x]$ *denotes the integral part of a real number.*

Proof. For real numbers $a, a_1, a_2, \ldots, a_n, A$ and $b, b_1, b_2, \ldots, b_n, B$ with $a \leq a_i \leq A$ and $b \leq b_i \leq B \; \forall \; i = 1, 2, \ldots n$ the following inequality is valid.
$\Big|n\sum\limits_{i=1}^{n} a_ib_i - \sum\limits_{i=1}^{n} a_i \sum\limits_{i=1}^{n} b_i\Big| \leq \alpha(n)(A-a)(B-b)$ where $\alpha(n) = n[\frac{n}{2}](1 - \frac{1}{n}[\frac{n}{2}])$ and equality holds if and only if $a_1 = a_2 = \ldots = a_n$ and $b_1 = b_2 = \ldots = b_n$.
If $a_i = |\lambda_i|$, $b_i = |\lambda_i|$, $a = b = |\lambda_n|$ and $A = B = |\lambda_1|$, then

$$\Big|n\sum_{i=1}^{n}|\lambda_i|^2 - \Big(\sum_{i=1}^{n}|\lambda_i|\Big)^2\Big| \leq \alpha(n)(|\lambda_1| - |\lambda_n|)^2 .$$

But $\sum\limits_{i=1}^{n}|\lambda_i|^2 = 2\sum\limits_{i<j} {d_i}^2{d_j}^2d_{ij}^2$ and $\mathcal{E}_{S^*}(G) \leq \sqrt{n\Big(2\sum\limits_{i<j} {d_i}^2{d_j}^2d_{ij}^2\Big)}$ then the above inequality becomes

$$n\Big(2\sum_{i<j} {d_i}^2{d_j}^2d_{ij}^2\Big) - (\mathcal{E}_{S^*}(G))^2 \leq \alpha(n)(|\lambda_1| - |\lambda_n|)^2$$

$$\text{i,e., } \mathcal{E}_{S^*}(G) \geq \sqrt{n\Big(2\sum_{i<j} {d_i}^2{d_j}^2d_{ij}^2\Big) - \alpha(n)(|\lambda_1| - |\lambda_n|)^2} .$$

□

Theorem 2.6. *Let* G *be a graph with* n *vertices and* m *edges. Let* $|\lambda_1| \geq |\lambda_2| \geq \ldots \geq |\lambda_n| > 0$ *be a non-increasing order of eigenvalues of* $S^*(G)$ *then*

$$\mathcal{E}_{S^*}(G) \geq \frac{2\sum\limits_{i<j} {d_i}^2{d_j}^2d_{ij}^2 + n|\lambda_1||\lambda_n|}{(|\lambda_1| + |\lambda_n|)} .$$

Proof. Let $a_i \neq 0$, b_i, r and R be real numbers satisfying $ra_i \leq b_i \leq Ra_i$, then the following inequality holds. [Theorem 2, [16]]

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i \leq (r+R)\sum_{i=1}^{n} a_ib_i .$$

Put $b_i = |\lambda_i|$, a_i =1, $r = |\lambda_n|$ and $R = |\lambda_1|$ then

$$\sum_{i=1}^{n}|\lambda_i|^2 + |\lambda_1||\lambda_n|\sum_{i=1}^{n}1 \leq (|\lambda_1| + |\lambda_n|)\sum_{i=1}^{n}|\lambda_i|$$

$$i.e.,\ 2\sum_{i<j} {d_i}^2{d_j}^2d_{ij}^2 + |\lambda_1||\lambda_n|n \leq (|\lambda_1| + |\lambda_n|)\mathcal{E}_{S^*}(G)$$

$$\therefore \mathcal{E}_{S^*}(G) \geq \frac{2\sum_{i<j} {d_i}^2{d_j}^2d_{ij}^2 + n|\lambda_1||\lambda_n|}{(|\lambda_1| + |\lambda_n|)}.$$

□

The question of when does the graph energy becomes a rational number was answered by Bapat and S. Pati in their paper [4]. Similar result for Modified Schultz energy is obtained in the following theorem.

Theorem 2.7. *If the minimum Modified Schultz energy $\mathcal{E}_{S^*}(G)$ is a rational number,then $\mathcal{E}_{S^*}(G) \equiv 0$(mod 2).*

Proof. The proof is similar to theorem 3.7 of [2]. □

2.3. Modified Schultz energy of some standard graphs.

Theorem 2.8. *For $n \geq 2$, the Modified Schultz energy of complete graph K_n is $2(n-1)^3$.*

Proof. Let K_n be a complete graph with vertex set $V = \{v_1, v_2, v_3, ..., v_n\}$. Then the modified Schultz matrix of complete graph is,

$$MS^*(K_n) = \begin{pmatrix} 0 & (n-1)^2 & (n-1)^2 & \dots & (n-1)^2 & (n-1)^2 & (n-1)^2 \\ (n-1)^2 & 0 & (n-1)^2 & \dots & (n-1)^2 & (n-1)^2 & (n-1)^2 \\ (n-1)^2 & (n-1)^2 & 0 & \dots & (n-1)^2 & (n-1)^2 & (n-1)^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ (n-1)^2 & (n-1)^2 & (n-1)^2 & \dots & 0 & (n-1)^2 & (n-1)^2 \\ (n-1)^2 & (n-1)^2 & (n-1)^2 & \dots & (n-1)^2 & 0 & (n-1)^2 \\ (n-1)^2 & (n-1)^2 & (n-1)^2 & \dots & (n-1)^2 & (n-1)^2 & 0 \end{pmatrix}_{n\times n}$$

Characteristic polynomial is $(-1)^n[\lambda - (n-1)^3][\lambda + (n-1)^2]^{n-1}$.
Characteristic equation is $(-1)^n[\lambda - (n-1)^3][\lambda + 2(n-1)^2]^{n-1} = 0$.

$$\text{Spec}(MS^*(K_n)) = \begin{pmatrix} (n-1)^3 & -(n-1)^2 \\ \\ 1 & n-1 \end{pmatrix}.$$

The Modified Schultz energy is,

$\mathcal{ME}_{S^*}(K_n) = |(n-1)^3|(1) + |-(n-1)^2|(n-1)$

$\mathcal{ME}_{S^*}(K_n) = (n-1)^3 + (n-1)^2(n-1)$

$\mathcal{ME}_{S^*}(K_n) = 2(n-1)^3$. □

Theorem 2.9. *The Modified Schultz energy of star graph $K_{1,n-1}$ is*

$$\begin{cases} 4 & \text{if } n = 2 \\ 2(n-1) + \sqrt{n^3 + n^2 - 2n + 1} & \text{if } n > 2 \end{cases}$$

Proof. Let $K_{1,n-1}$ be a star graph with vertex set $V = \{v_0, v_1, v_2, ..., v_{n-1}\}$.

Case: 1 If $n > 2$, then the Modified Schultz matrix of star graph is,

$$S^*(K_{1,n-1}) = \begin{pmatrix} 0 & n & n & n & \dots & n \\ n & 0 & 2 & 2 & \dots & 2 \\ n & 2 & 0 & 2 & \dots & 2 \\ n & 2 & 2 & 0 & \dots & 2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ n & 2 & 2 & 2 & \dots & 0 \end{pmatrix}_{n \times n}$$

Characteristic polynomial is $(-1)^{n-1}(\lambda+2)^{n-1}[\lambda^2 - 2(n-1)\lambda - n^3]$.
Characteristic equation is $(-1)^{n-1}(\lambda+2)^{n-1}[\lambda^2 - 2(n-1)\lambda - n^3] = 0$.
Spec$(K_{1,n-1}) =$

$$\begin{pmatrix} -2 & (n-1) + \sqrt{n^3 + n^2 - 2n + 1} & (n-1) - \sqrt{n^3 + n^2 - 2n + 1} \\ \\ n-1 & 1 & 1 \end{pmatrix}$$

The Modified Schultz energy is,

$$\mathcal{E}_{S^*}(K_{1,n-1}) = |-2|(n-1) + \left|(n-1) + \sqrt{n^3 + n^2 - 2n + 1}\right|(1) +$$

$$+ \left|(n-1) - \sqrt{n^3 + n^2 - 2n + 1}\right|(1)$$

$$\mathcal{E}_{S^*}(K_{1,n-1}) = 2(n-1) + (n-1) + \sqrt{n^3+n^2-2n+1}$$
$$+\sqrt{n^3+n^2-2n+1} - (n-1)$$
$$\mathcal{E}_{S^*}(K_{1,n-1}) = 2[(n-1) + \sqrt{n^3+n^2-2n+1}].$$

Case: 2 if $n = 2$

Then Modified Schultz matrix of is,

$$S^*(K_{1,n-1}) = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}_{2\times 2}$$

Characteristic polynomial is $(\lambda-4)^2$.
Characteristic equation is $(\lambda-4)^2 = 0$.

$$\text{Spec}(K_{1,n-1}) = \begin{pmatrix} 2 \\ 2 \end{pmatrix}.$$

The Modified Schultz energy is, $\mathcal{E}_{S^*}(K_{1,n-1}) = |2|(2) = 4$.

□

Definition 2.1. *Cocktail party graph is denoted by $K_{n\times 2}$, is a graph having the vertex set $V = \bigcup_{i=1}^{n}\{u_i, v_i\}$ and the edge set $E = \{u_iu_j, v_iv_j : i \neq j\} \bigcup \{u_iv_j, v_iu_j : 1 \leq i < j \leq n\}$.*

Theorem 2.10. *The Modified Schultz energy of cocktail party graph is $16n(n-1)^2$.*

Proof. For $n > 2$, consider cocktail party graph $K_{n\times 2}$ with vertex set $V = \bigcup_{i=1}^{n}\{u_i, v_i\}$. Then the Modified Schultz matrix of cocktail party is $MS^*(K_{n\times 2}) =$

$$\left(\begin{array}{c|ccccc|ccccc}
 & u_1 & u_2 & \dots & u_{n-1} & u_n & v_1 & v_2 & \dots & v_{n-1} & v_n \\
\hline
u_1 & 0 & 4(n-1)^2 & \dots & 4(n-1)^2 & 4(n-1)^2 & 4(n-1)^2 & 4(n-1)^2 & \dots & 4(n-1)^2 & 4(n-1)^2 \\
u_2 & 4(n-1)^2 & 0 & \dots & 4(n-1)^2 & 4(n-1)^2 & 8(n-1)^2 & 4(n-1)^2 & \dots & 4(n-1)^2 & 4(n-1)^2 \\
u_3 & 4(n-1)^2 & 4(n-1)^2 & \dots & 4(n-1)^2 & 4(n-1)^2 & 4(n-1)^2 & 8(n-1)^2 & \dots & 4(n-1)^2 & 4(n-1)^2 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
u_{n-1} & 4(n-1)^2 & 4(n-1)^2 & \dots & 0 & 4(n-1)^2 & 4(n-1)^2 & 4(n-1)^2 & \dots & 8(n-1)^2 & 4(n-1)^2 \\
u_n & 4(n-1)^2 & 4(n-1)^2 & \dots & 4(n-1)^2 & 0 & 4(n-1)^2 & 4(n-1)^2 & \dots & 4(n-1)^2 & 8(n-1)^2 \\
\hline
v_1 & 8(n-1)^2 & 4(n-1)^2 & \dots & 4(n-1)^2 & 4(n-1)^2 & 0 & 4(n-1)^2 & \dots & 4(n-1)^2 & 4(n-1)^2 \\
v_2 & 4(n-1)^2 & 8(n-1)^2 & \dots & 4(n-1)^2 & 4(n-1)^2 & 4(n-1)^2 & 0 & \dots & 4(n-1)^2 & 4(n-1)^2 \\
v_3 & 4(n-1)^2 & 4(n-1)^2 & \dots & 4(n-1)^2 & 4(n-1)^2 & 4(n-1)^2 & 4(n-1)^2 & \dots & 4(n-1)^2 & 4(n-1)^2 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
v_{n-1} & 4(n-1)^2 & 4(n-1)^2 & \dots & 8(n-1)^2 & 4(n-1)^2 & 4(n-1)^2 & 4(n-1)^2 & \dots & 0 & 4(n-1)^2 \\
v_n & 4(n-1)^2 & 4(n-1)^2 & \dots & 4(n-1)^2 & 8(n-1)^2 & 4(n-1)^2 & 4(n-1)^2 & \dots & 4(n-1)^2 & 0
\end{array}\right)$$

Characteristic polynomial is, $[\lambda - 8n(n-1)^2]\lambda^{n-1}[\lambda + 8(n-1)^2]^n$.
Characteristic equation is, $[\lambda - 8n(n-1)^2][\lambda^{n-1}][\lambda + 8(n-1)^2]^n = 0$.

$$\text{Spec}(MS^*(K_{n\times 2})) = \begin{pmatrix} 8n(n-1)^2 & 0 & -8(n-1)^2 \\ \\ 1 & n-1 & n \end{pmatrix}$$

The Modified Schultz energy is,

$$\mathcal{ME}_{S^*}(K_{n\times 2}) = |8n(n-1)^2|(1) + |0|(n-1) + |-8(n-1)^2|(n)$$
$$\mathcal{E}_{S^*}(K_{n\times 2}) = 8n(n-1)^2 + 8n(n-1)^2$$
$$\mathcal{E}_{S^*}(K_{n\times 2}) = 16n(n-1)^2.$$ □

Definition 2.2. *Crown graph S_n^0 for an integer $n \geq 2$ is the graph with vertex set $\{u_1, u_2, ..., u_n, v_1, v_2, ..., v_n\}$ and edge set $\{u_i v_j : 1 \leq i, j \leq n, i \neq j\}$.*

Theorem 2.11. *For $n \geq 2$, the Modified Schultz energy of the crown graph is*

$$\begin{cases} 4 & \textit{if } n = 2 \\ 8(n-1)^3 & \textit{if } n \geq 3 \end{cases}$$

Proof. **Case: 1** if $n \geq 3$,
The Modified Schultz matrix of crown graph is $MS^*(S_n^0) =$

$$\left(\begin{array}{c|ccccc|ccccc} & v_1 & v_2 & v_3 & \dots & v_n & u_1 & u_2 & u_3 & \dots & u_n \\ \hline v_1 & 0 & 2(n-1)^2 & 2(n-1)^2 & \dots & 2(n-1)^2 & 3(n-1)^2 & (n-1)^2 & (n-1)^2 & \dots & (n-1)^2 \\ v_2 & 2(n-1)^2 & 0 & 2(n-1)^2 & \dots & 2(n-1)^2 & (n-1)^2 & 3(n-1)^2 & (n-1)^2 & \dots & (n-1)^2 \\ v_3 & 2(n-1)^2 & 2(n-1)^2 & 0 & \dots & 2(n-1)^2 & (n-1)^2 & (n-1)^2 & 3(n-1)^2 & \dots & (n-1)^2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ v_n & 2(n-1)^2 & 2(n-1)^2 & 2(n-1)^2 & \dots & 0 & (n-1)^2 & (n-1)^2 & (n-1)^2 & \dots & 3(n-1)^2 \\ \hline u_1 & 3(n-1)^2 & (n-1)^2 & (n-1)^2 & \dots & (n-1)^2 & 0 & 2(n-1)^2 & 2(n-1)^2 & \dots & 2(n-1)^2 \\ u_2 & (n-1)^2 & 3(n-1)^2 & (n-1)^2 & \dots & (n-1)^2 & 2(n-1)^2 & 0 & 2(n-1)^2 & \dots & 2(n-1)^2 \\ u_3 & (n-1)^2 & (n-1)^2 & 3(n-1)^2 & \dots & (n-1)^2 & 2(n-1)^2 & 2(n-1)^2 & 0 & \dots & 2(n-1)^2 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ u_n & (n-1)^2 & (n-1)^2 & (n-1)^2 & \dots & 3(n-1)^2 & 2(n-1)^2 & 2(n-1)^2 & 2(n-1)^2 & \dots & 0 \end{array}\right)$$

Characteristic polynomial is $[\lambda - 3n(n-1)^2][\lambda - (n-4)(n-1)^2]\lambda^{n-1}[\lambda + 4(n-1)^2]^{n-1}$.
Characteristic equation is $[\lambda - 3n(n-1)^2][\lambda - (n-4)(n-1)^2]\lambda^{n-1}[\lambda + 4(n-1)^2]^{n-1} = 0$.

$$\text{Spec}(S_n^0) = \begin{pmatrix} 3n(n-1)^2 & (n-4)(n-1)^2 & 0 & -4(n-1)^2 \\ 1 & 1 & n-1 & n-1 \end{pmatrix}$$

The Modified Schultz energy,

$$\mathcal{ME}_{S^*}(S_n^0) = |3n(n-1)^2|(1) + |(n-4)(n-1)^2|(1) + |0|(n-1) + |-4(n-1)^2|(n-1)$$
$$\mathcal{ME}_{S^*}(S_n^0) = 3n(n-1)^2 + (n-4)(n-1)^2 + 4(n-1)^2(n-1)$$
$$\mathcal{ME}_{S^*}(S_n^0) = 8(n-1)^3.$$

Case: 2 if $n = 2$

Then the Modified Schultz matrix is crown graph is,

$$MS^*(S_n^0) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}_{4\times 4}$$

Characteristic polynomial is $(\lambda - 1)^2(\lambda + 1)^2$.
Characteristic equation is $(\lambda - 1)^2(\lambda + 1)^2 = 0$.

$$\text{Spec}(S_n^0) = \begin{pmatrix} 1 & -1 \\ 2 & 2 \end{pmatrix}$$

The Modified Schultz energy,

$$\mathcal{ME}_{S^*}(S_n^0) = |1|(2) + |-1|(2)$$
$$\mathcal{ME}_{S^*}(S_n^0) = 4.$$
□

Definition 2.3. *Friendship graph is the graph obtained by taking n copies of the cycle graph C_3 with a vertex in common. It is denoted by F_3^n. Friendship graph F_3^n contains $2n+1$ vertices and $3n$ edges.*

Theorem 2.12. *The Modified Schultz energy of friendship graph $\mathcal{ME}_{S^*}(F_3^n)$ is equal to* $2[(3n-1)+2\sqrt{8n^3+16n^2-24n+9}]$.

Proof. For a friendship graph F_3^n with vertex set $V = \{v_o, v_1, v_2, ..., v_n, v_{n+1}, v_{n+2}, ..., v_{2n}\}$ Then the Schultz matrix of friendship graph is $MS^*(F_3^n) =$

$$\left(\begin{array}{c|cccccccccc} & v_0 & v_1 & v_2 & v_3 & v_4 & v_5 & v_6 & v_7 & \dots & v_{2n} \\ \hline v_0 & 0 & 2^2n & 2^2n & 2^2n & 2^2n & 2^2n & 2^2n & 2^2n & \dots & 2^2n \\ v_1 & 2^2n & 0 & 2^2 & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & \dots & (3^2-1) \\ v_2 & 2^2n & 2^2 & 0 & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & \dots & (3^2-1) \\ v_3 & 2^2n & (3^2-1) & (3^2-1) & 0 & 2^2 & (3^2-1) & (3^2-1) & (3^2-1) & \dots & (3^2-1) \\ v_4 & 2^2n & (3^2-1) & (3^2-1) & 2^2 & 0 & (3^2-1) & (3^2-1) & (3^2-1) & \dots & (3^2-1) \\ v_5 & 2^2n & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & 0 & 2^2 & (3^2-1) & \dots & (3^2-1) \\ v_6 & 2^2n & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & 2^2 & 0 & (3^2-1) & \dots & (3^2-1) \\ v_7 & 2^2n & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & 0 & \dots & (3^2-1) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ v_{2n} & 2^2n & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & (3^2-1) & \dots & 0 \end{array}\right)_{(2n+1)\times(2n+1)}$$

Characteristic polynomial is

$(-1)(\lambda+4)^n(\lambda+2)^{n-1}[\lambda^2-(16n-12)\lambda-32n^3]$.

Characteristic equation is

$(-1)(\lambda+4)^n(\lambda+2)^{n-1}[\lambda^2-(16n-12)\lambda-32n^3] = 0$.

Spec$(F_3^n) =$

$$\begin{pmatrix} -4 & -2 & (8n-6)+2\sqrt{8n^3+16n^2-24n+9} & (8n-6)-2\sqrt{8n^3+16n^2-24n+9} \\ n & n-1 & 1 & 1 \end{pmatrix}$$

Modified Schultz energy is,

$$\mathcal{ME}_{S^*}(F_3^n) = \left|-4\right|(n) + \left|-2\right|(n-1) + \left|(8n-6)+2\sqrt{8n^3+16n^2-24n+9}\right|(1)$$

$$\left|(8n-6)-2\sqrt{8n^3+16n^2-24n+9}\right|(1)$$

$$=4n+2n-2+(8n-6)+2\sqrt{8n^3+16n^2-24n+9}+2\sqrt{8n^3+16n^2-24n+9}-(8n-6)$$

$$\mathcal{ME}_{S^*}(F_3^n) = 2[(3n-1)+2\sqrt{8n^3+16n^2-24n+9}].$$ □

Theorem 2.13. *The Modified Schultz energy of the complete bipartite graph is* $4[m^2n+mn^2-m^2-n^2]$.

Proof. For the complete bipartite graph $K_{m,n}$ $(m \leq n)$ with vertex set $V = \{u_1,u_2,...,u_m,v_1,v_2,...,v_n\}$
The a Modified Schultz matrix of complete bipartite graph is $S^*(K_{m,n}) =$

	v_1	v_2	v_3	$\ldots$	v_m	u_1	u_2	u_3	$\ldots$	u_n
v_1	0	$2n^2$	$2n^2$	$\ldots$	$2n^2$	mn	mn	mn	$\ldots$	mn
v_2	$2n^2$	0	$2n^2$	$\ldots$	$2n^2$	mn	mn	mn	$\ldots$	mn
v_3	$2n^2$	$2n^2$	0	$\ldots$	$2n^2$	mn	mn	mn	$\ldots$	mn
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
v_m	$2n^2$	$2n^2$	$2n^2$	$\ldots$	0	mn	mn	mn	$\ldots$	mn
u_1	mn	mn	mn	$\ldots$	mn	0	$2m^2$	$2m^2$	$\ldots$	$2m^2$
u_2	mn	mn	mn	$\ldots$	mn	$2m^2$	0	$2m^2$	$\ldots$	$2m^2$
u_3	mn	mn	mn	$\ldots$	mn	$2m^2$	$2m^2$	0	$\ldots$	$2m^2$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
u_n	mn	mn	mn	$\ldots$	mn	$2m^2$	$2m^2$	$2m^2$	$\ldots$	0

Characteristic polynomial is

$$(-1)^{m+n}(\lambda+2m^2)^{n-1}(\lambda+2n^2)^{m-1}(\lambda^2-2((m-1)n^2+m^2n-m^2)\lambda+ n^2(m^2(3m-4)n-4m^2(m-1))).$$

Characteristic equation is

$$(-1)^{m+n}(\lambda+2m^2)^{n-1}(\lambda+2n^2)^{m-1}(\lambda^2-2((m-1)n^2+m^2n-m^2)\lambda+ n^2(m^2(3m-4)n-4m^2(m-1)))=0$$

$$Spec(K_{m,n}) = \begin{pmatrix} -2m^2 & -2n^2 & X+\sqrt{Y} & X-\sqrt{Y} \\ n-1 & m-1 & 1 & 1 \end{pmatrix},$$

where $X=(m-1)n^2+m^2n-m^2$ and $Y=(m^2-2m+1)n^4+(2m^2-m^3)n^3+(m^4+2m^3-2m^2)n^2-2m^4n+m^4$.

Modified Schultz energy is:

$$\begin{aligned}
\mathcal{E}_{S^*}(K_{m,n}) &= |-2m^2|(n-1)+|-2n^2|(m-1)+|[(m-1)n^2+m^2n-m^2]+\\
&\sqrt{(m^2-2m+1)n^4+(2m^2-m^3)n^3+(m^4+2m^3-2m^2)n^2-2m^4n+m^4}|(1)\\
&+|[(m-1)n^2+m^2n-m^2]-\\
&\sqrt{(m^2-2m+1)n^4+(2m^2-m^3)n^3+(m^4+2m^3-2m^2)n^2-2m^4n+m^4}|(1).\\
\mathcal{E}_{S^*}(K_{m,n}) &= 2m^2(n-1)\ +\ 2n^2(m-1)\ +\ (m-1)n^2+m^2n-m^2+\\
&\sqrt{(m^2-2m+1)n^4+(2m^2-m^3)n^3+(m^4+2m^3-2m^2)n^2-2m^4n+m^4}+\\
&(m-1)n^2+m^2n-m^2-\\
&\sqrt{(m^2-2m+1)n^4+(2m^2-m^3)n^3+(m^4+2m^3-2m^2)n^2-2m^4n+m^4}\\
\mathcal{E}_{S^*}(K_{m,n}) &= 4(m^2n+mn^2-m^2-n^2).
\end{aligned}$$

□

3. CONCLUSION

In this article we defined Modified Schultz energy of a graph. Upper and lower bounds for Modified Schultz energy are established. A generalized expression for Schultz energies for star graph, complete graph, crown graph, complete bipartite graph, cocktail party graph and friendship graphs are also computed.

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DEPARTMENT OF MATHEMATICS
SRI.D DEVARAJA URS GOVERNEMENT FIRST GRADE COLLEGE
HUNSUR - 571 105, INDIA
Email address: mr.rajeshkanna@gmail.com

SCHOOL OF SCIENCES
CAREER POINT UNIVERSITY
KOTA, INDIA
Email address: rooopa.s.kumar@gmail.com