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Calculation and comparison of energy and energy based on Mostar index of the double-star graph and its line graph

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Abstract

The double-star line graph is a graph built from two complete graphs of order a+1 that share a common vertex, for every positive integer $a \geq 1$. In this article, we investigate concepts of energy and energy based on the Mostar index of Ds_a and LDs_a graphs and provide a low bound for energies. We obtain general formulas for energies of Ds_a, LDs_a, $MoDs_a$, and $MoLDs_a$. This study obtains general formulas for the Mostar energy and energy of Ds_a and LDs_a. Using these formulas does not require calculating eigenvalues, and we show that the energy of these graphs only depends on a, the Number of pendeng edges. We compare energies and find relationships between them. Also, we determine the highest and lowest energy. We display the obtained results, numerically and graphically and compare energies graphically.

Subject Classification (2020): *05C90, 05C09, 05C31, 05C92.*

Keywords: *Double-star graph, Double-star line graph, Characteristic polynomial, Adjacency matrix, Eigenvalue, Spectrum, Graph energy, Mostar index.*

1. Introduction

The double-star ($Ds_{a,b}$) is a tree constructed by combining two disjoint stars $S_{1,a}$ and $S_{1,b}$, by connecting their central vertices with an additional edge, where

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a and b represent the number of edges in each star [1]. The adjacency matrix of $Ds_{a,b}$, denoted as $[(Ds_{a,b})_{ij}]$, is a matrix where $(Ds_{a,b})_{ij} = 1$ if v_i and v_j are connected, and $(Ds_{a,b})_{ij} = 0$ if they are not. The matrix size is $(a + b + 2) \times (a + b + 2)$. The characteristic polynomial $\chi(Ds_{a,b}, \lambda)$ is $det(Ds_{a,b} - \lambda I_{a+b+2})$. This can also be written as $\chi(Ds_{a,b}, \lambda) = \Pi_{i=1}^{a+b+2}(\lambda - \lambda_i(Ds_{a,b}))$, where $\lambda_1, \dots, \lambda_{a+b+2}$ are its eigenvalues. The spectrum of $Ds_{a,b}$ is as:

$$Spec(Ds_{a,b}) = \begin{pmatrix} \lambda_1, & \dots & \lambda_{a+b+2} \\ m_1, & \dots & m_{a+b+2} \end{pmatrix},$$

where $\lambda_1 \geq \cdots \geq \lambda_{a+b+2}$ [2, 3].

The number of times each eigenvalue appears is called its algebraic multiplicity, denoted by m_i, and their sum of absolute values is called the graph's energy, denoted by $E(G)$ [4, 5]. This concept is important in the discussion of graph chemical theory. In 1931, Heckel introduced graph energy as a chemical concept, and it became a mathematical interpretation years later. In 1978, graph energy was introduced as a method for evaluating chemical compounds, particularly their molecular structure and stability [2]. In 2018, Wong, Wang, and Chu [6] established bounds for the graph's energy by utilizing its matching number and derived two lower bounds for the graph's energy through this concept. In 2020, Abdullah Alazemi et al. demonstrated that the star graph yields the minimum energy among all connected chain graphs of order n, and they provided a lower bound for $LE(G)$ [7].

In general, multi-star graphs have attracted the attention of many researchers and have been studied in various fields. For example, in 2019, Rohini et al. considered a triple star graph and investigated the irregular color number for its median, total, central, and line graphs [8]. In 2019, Jianfeng Wang et al. computed the energy of double-star graphs using the Eccentricity (Ecc) matrix and explored the relationship between the energy and Ecc-energy of graphs [9]. In recent studies, Došlić et al. defined the Mostar (Mo) index as follows:

$$Mo(G) = \sum_{u \sim v} |n_u - n_v|,$$

where n_u is number of vertices of G lying closer to u [10, 11]. They determined its extremal values specified extremal trees and single-distance graphs, and computed the Mo index for the system. The Mo index has been studied in various types of graphs, including bipartite graphs and split graphs [12-15]. The line graph of G is defined as the graph whose vertex set corresponds to the edge set of G and Is denoted by $L(G)$. Two vertices within $L(G)$ are considered adjacent when the edges they represent in G are adjacent [16]. As far as known, the line graph of Ds has not been defined, and the energy concept of the double-star line graph has not yet been studied. Therefore, a new graph, called a double-star line graph, is introduced and denoted by $LDs_{a,b}$. $LDs_{a,b}$ is a graph consisting of two complete graphs K_{a+1} and K_{b+1}, such that they are connected by a common vertex. $LDs_{a,b}$ has $a + b + 1$ vertices and $\frac{a(a+1)}{2} + \frac{b(b+1)}{2}$ edges. $Ds_{a,b}$ is called regular double-star graph ($Ds_{a,a}$), when $a = b$. $Ds_{a,a}$ has $2a + 2$ vertices and $2a + 1$ edges [17].

2. Main Results

In this article, $Ds_{a,b}$ and $LDs_{a,b}$ are investigated when $a = b$. $Ds_{a,a}$ and $LDs_{a,a}$ denoted as Ds_a and LDs_a, respectively, for $a \geq 1$. Assume that Ds_a is a double-star graph with at least a pendeng edge of any ended vertex of the central edge. Let Ds_a be a double-star graph. LDs_a be their line graph. $E.Ds_a$ and $E.LDs_a$ are Ds_a energy and LDs_a energy, respectively. $E.MoDs_a$, $E.MoLDs_a$ are the Mo index-based Ds_a energy and the Mo index-based LDs_a energy, respectively. The number of pendeng edges of the central edge is denoted by a. Some symbols used throughout the paper are explained.

Definition 2.1: Consider the adjacency matrix Ds_a. The entry at position (i, j) is as follows:

$$(Ds_a)_{ij} = \begin{cases} 1, & v_i v_j \in E(Ds_a), \\ 0, & o.w. \end{cases}$$

where, $1 \leq i, j \leq 2a + 2, a \geq 1$.

Definition 2.2: Consider the adjacency matrix LDs_a. The entry at position (i, j) is as follows:

$$(LDs_a)_{ij} = \begin{cases} 1, & v_i v_j \in E(LDs_a), \\ 0, & o.w. \end{cases}$$

where, $1 \leq i, j \leq 2a + 1, a \geq 1$.

Definition 2.3: For the matrix $MoDs_a$, the element at position (i, j) is defined as follows:

$$(MoDs_a)_{ij} = \begin{cases} |n_{v_i} - n_{v_j}|, & \text{if } v_i v_j \in E(Ds_a), \\ 0, & o.w. \end{cases}$$

Definition 2.4: In the case of the matrix $MoLDs_a$, the (i, j)-th element is represented by:

$$(MoLDs_a)_{ij} = \begin{cases} |n_{v_i} - n_{v_j}|, & \text{if } v_i v_j \in E(LDs_a), \\ 0, & o.w. \end{cases}$$

where, $1 \leq i, j \leq 2a + 1, a \geq 1$.

Theorem 2.1: *If Ds_a is a double-star graph, then*

$$Spec(Ds_a) = \begin{pmatrix} 0 & \frac{\sqrt{4a+1}-1}{2} & -\frac{\sqrt{4a+1}-1}{2} & \frac{\sqrt{4a+1}+1}{2} & -\frac{\sqrt{4a+1}+1}{2} \\ 2a-2 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

Proof: We prove this Theorem by using Definitions 2.1:

$$Ds_a = \begin{pmatrix} 0 & \cdots & 0 & 1 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & 0 & 0 & \cdots & 0 \\ 1 & \cdots & 1 & 0 & 1 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 & 0 & 1 & \cdots & 1 \\ 0 & \cdots & 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & 1 & 0 & \cdots & 0 \end{pmatrix},$$

The characteristic polynomial of Ds_a is obtained from $\chi(Ds_a;\lambda) = det(Ds_a - \lambda I_{2a+2})$. To calculate $det(Ds_a - \lambda I_{2a+2})$, we $Ds_a - \lambda I_{2a+2}$ convert first to a block diagonal matrix. Then we get its determinant from the product of the determinants of the blocks on the Main diagonal. So, the characteristic polynomial is as follows:

$$\chi(D_a;\lambda) = (-\lambda)^{2a-2}(\lambda^4 - (2a+1)\lambda^2 + a^2),$$

The roots of $\chi(Ds_a;\lambda) = 0$ are the eigenvalues of Ds_a. So, we obtain its eigenvalues. Hence,

$$Spec(Ds_a) = \begin{pmatrix} 0 & \frac{\sqrt{4a+1}-1}{2} & -\frac{\sqrt{4a+1}-1}{2} & \frac{\sqrt{4a+1}+1}{2} & -\frac{\sqrt{4a+1}+1}{2} \\ 2a-2 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

Theorem 2.2: *If Ds_a is a double-star graph, then $E.D_a = 2\sqrt{4a+1}$.*

Proof: We prove this Theorem by using Theorm 2.1, we get its energy as following:

$$\begin{aligned} E.D_a &= \Sigma_{i=1}^{2a+2}|\lambda_i| = |\lambda_1| + |\lambda_2| + \cdots + |\lambda_{2a+2}| \\ &= |\tfrac{\sqrt{4a+1}-1}{2}| + |-\tfrac{\sqrt{4a+1}-1}{2}| + |\tfrac{\sqrt{4a+1}+1}{2}| + |-\tfrac{\sqrt{4a+1}+1}{2}| \\ &+(2a-2)(0) = 2\sqrt{4a+1}. \end{aligned}$$

Hence proved, $E.D_a = 2\sqrt{4a+1}$.

Corollary 2.1: $E.Ds_a \geq 2\sqrt{5}$, *for* $a \geq 1$.

Theorem 2.3: *If LDs_a is the line graph of Ds_a, then*

$$Spec(LDs_a) = \begin{pmatrix} -1 & a-1 & \frac{\sqrt{a^2+6a+1}-(a-1)}{2} & -\frac{\sqrt{a^2+6a+1}-(a-1)}{2} \\ 2a-2 & 1 & 1 & 1 \end{pmatrix}.$$

Proof: The proof follows a similar approach to that of Theorem 2.1. We have from Definition 2.2,

$$LDs_a = \begin{pmatrix} 0 & 1 & \cdots & 1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & \ddots & \ddots & \vdots & 1 & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & 1 & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \dots & 1 & 0 & 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & \cdots & 1 & 0 & 1 & 1 & \cdots & 1 \\ 0 & 0 & \cdots & 0 & 1 & 0 & 1 & \cdots & 1 \\ 0 & 0 & \cdots & 0 & \vdots & 1 & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots & 1 & \vdots & \ddots & \ddots & 1 \\ 0 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1 & 0 \end{pmatrix},$$

By using its characteristic polynomial, we obtain its eigenvalues.

$$\begin{aligned} \chi(LDs_a;\lambda) = (\lambda+1)^{2a-2}(\lambda - a + 1)&\left(\lambda - \left(\tfrac{\sqrt{a^2+6a+1}+(a-1)}{2}\right)\right) \\ &\left(\lambda - \left(\tfrac{-\sqrt{a^2+6a+1}+(a-1)}{2}\right)\right). \end{aligned}$$

Hence,

$$Spec(LDs_a) = \begin{pmatrix} -1 & a-1 & \frac{\sqrt{a^2+6a+1}-(a-1)}{2} & -\frac{\sqrt{a^2+6a+1}-(a-1)}{2} \\ 2a-2 & 1 & 1 & 1 \end{pmatrix}.$$

Theorem 2.4: *If LDs_a is the line graph of Ds_a, then $E.LD_a = 3a-3+\sqrt{a^2+6a+1}$.*

Proof: We prove this Theorem by using Theorem 2.3:

$$\begin{aligned} E.LDs_a &= \Sigma_{i=1}^{2a+1}|\lambda_i| \\ &= |\tfrac{\sqrt{a^2+6a+1}+(a-1)}{2}| + |\tfrac{-\sqrt{a^2+6a+1}+(a-1)}{2}| \\ &+|a-1| + (2a-2)| - 1| = 3a-3+\sqrt{a^2+6a+1}. \end{aligned}$$

Hence, $E.LDs_a = 3a-3+\sqrt{a^2+6a+1}$.

Corollary 2.2: $E.LD_a \geq 2\sqrt{2}$, *for* $a \geq 1$.

Theorem 2.5: $MoDs_a$ *is assumed. Then,*

$$Spec(MoDs_a) = \begin{pmatrix} 0 & 2a\sqrt{a} & -2a\sqrt{a} \\ 2a-2 & 2 & 2 \end{pmatrix}.$$

Proof: The argument is analogous to the proofs of Theorems 2.1 and 2.3. We have from Definition 2.3:

$$MoDs_a = \begin{pmatrix} 0 & \cdots & 0 & 2a & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 2a & 0 & 0 & \cdots & 0 \\ 2a & \cdots & 2a & 0 & 0 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 0 & 0 & 2a & \cdots & 2a \\ 0 & \cdots & 0 & 0 & 2a & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & 2a & 0 & \cdots & 0 \end{pmatrix},$$

By using its characteristic polynomial, we obtain its eigenvalues.

$$\chi(MoD_a;\lambda) = (-\lambda)^{2a-2}(-\lambda^2+4a^3)^2,$$

Hence,

$$Spec(MoDs_a) = \begin{pmatrix} 0 & 2a\sqrt{a} & -2a\sqrt{a} \\ 2a-2 & 2 & 2 \end{pmatrix}.$$

Theorem 2.6: $MoDs_a$ *is assumed. Then,* $E.MoDs_a = 8a\sqrt{a}$.

Proof: We prove this Theorem by using Theorm 2.5, we get its energy as following:

$E.MoD_a = \Sigma_{i=1}^{2a+2}|\lambda_i| = 2|\sqrt{4a^3}| + 2| - \sqrt{4a^3}| + (2a+2)(0) = 4\sqrt{4a^3} = 8a\sqrt{a}$, hence, $E.MoD_a = 8a\sqrt{a}$.

Corollary 2.3: $E.MoD_a \geq 8$, *for* $a \geq 1$.

Theorem 2.7: $MoLDs_a$ *is assumed. Then,*

$$Spec(MoLDs_a) = \begin{pmatrix} 0 & a\sqrt{2a} & -a\sqrt{2a} \\ 2a-1 & 1 & 1 \end{pmatrix}.$$

Proof: A similar proof to theorems 2.1, 2.3, and 2.5 is proceeded. We have from Definition 2.3,

$$MoLDs_a = \begin{pmatrix} 0 & \cdots & 0 & a & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & a & 0 & \cdots & 0 \\ a & \cdots & a & 0 & a & \cdots & a \\ 0 & \cdots & 0 & a & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & a & 0 & \cdots & 0 \end{pmatrix},$$

By using its characteristic polynomial, we obtain its eigenvalues.

$$\chi(MoLDs_a; \lambda) = (-\lambda)^{2a-1}(\lambda^2 - 2a^3),$$

Hence proved,

$$Spec(MoLDs_a) = \begin{pmatrix} 0 & a\sqrt{2a} & -a\sqrt{2a} \\ 2a-1 & 1 & 1 \end{pmatrix}.$$

Theorem 2.8: $MoLDs_a$ *is assumed. Then,* $E.MoLDs_a = 2a\sqrt{2a}$.

Proof: We prove this Theorem by using Theorm 2.7, we get its energy as following:

$$E.MoLDs_a = \Sigma_{i=1}^{2a+1}|\lambda_i| = (2a-1)(0) + |\sqrt{2a^3}| + |-\sqrt{2a^3}| = 2\sqrt{2a^3}.$$

Therefore, $E.MoLDs_a$ are obtained as following:

$$E.MoLDs_a = 2a\sqrt{2a^3}.$$

Corollary 2.4: $E.LMoDs_a \geq 2\sqrt{2}$, *when* $a \geq 1$.

Proposition 2.1: Show that, $E.MoDs_a = (2\sqrt{2})E.MoLDs_a$.

Proof: See Theromes 2.6 and 2.8. we get from their comparison:

$$\frac{E.MoDs_a}{E.MoLDs_a} = 2\sqrt{2},$$

$$E.MoDs_a = (2\sqrt{2})E.MoLDs_a.$$

Proposition 2.2: Show that, $E.MoLDs_{2a} = E.MoDs_a$.

Proof: By using Theorems 2.6 and 2.8, we have $MoDs_a$ and $MoLDs_a$ as following:

$$E.MoDs_a = 8a\sqrt{a},$$
$$E.MoLDs_a = 2\sqrt{2}a\sqrt{a}.$$

From $E.MoLDs_a = 2\sqrt{2}a\sqrt{a}$, we have:

$$E.MoLDs_{2a} = 2\sqrt{2}(2a)\sqrt{2a} = 4(\sqrt{2})^2 a\sqrt{a} = 8a\sqrt{a},$$

Hence,

$$E.MoLDs_{2a} = E.MoDs_a.$$

Proposition 2.3: Show that, $E.MoLDs_{2a2^n} = (2\sqrt{2})^{n+1}E.MoLDs_a$.

Proof: By using Proposition 2.2, we get following:

$$\begin{aligned} E.MoLDs_{2a2^n} = E.MoLDs_{(2(a2^n)} &= (2\sqrt{2})E.MoLDs_{a2^n} \\ &= (2\sqrt{2})^2 E.MoLDs_{a2^{n-1}} \\ &\vdots \\ &= (2\sqrt{2})^{n+1}E.MoLDs_{a2^{n-n}} \\ &= (2\sqrt{2})^{n+1}E.MoLDs_a. \end{aligned}$$

Proposition 2.4: Show that, $E.MoLDs_{2a} = (2\sqrt{2})E.MoLDs_a$.

Proof: It is obtained from the proposition 2.3, For $n = 0$.

3. Numerical and Graphical Representation

Table 1 shows that as the value of a increases, all discussed energies also increase. The graphic representation of these energies shows that the plot of $MoDs_a$ is higher than other energies. The plot of Ds_a is lower than other energies except when $a = 1$. In $a = 1$, $E.LDs_a$ have the same value $E.MoLDs_a$ and it is lower than others, see Figures 1, 2, 3, and 4. For each $a \geq 1$, the $E.MoDs_a$ plot was higher than their plot of the line graph. For any $a > 1$, the plot of $E.Ds_a$ was lower than their line graph, except $a = 1$.

Table 1

Numerical comparison of $E.Ds_a$, $E.LDs_a$, $E.MoDs_a$ and $E.MoLDs_a$.

a	1	2	3	4	5	6	7	8	9	10
$E.Ds_a$	4.47	6	7.21	8.25	9.16	10	10.77	11.49	12.16	12.80
$E.LDs_a$	2.83	7.12	11.30	15.40	19.48	23.54	27.59	31.63	35.66	39.69
$E.MoDs_a$	8	22.63	41.57	64	89.44	117.57	148.16	181.02	216	252.98
$E.MoLDs_a$	2.83	8	14.70	22.63	31.62	41.57	52.38	64	76.37	89.44

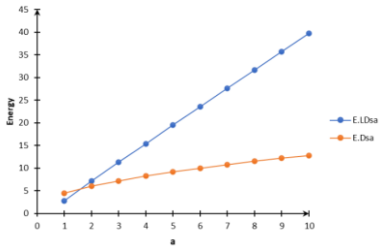

Figure 1
Comparison of $E.LDs_a$ and $E.Ds_a$

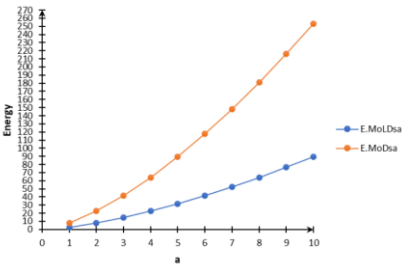

Figure 2
Comparison of $E.MoLDs_a$ and $E.MoDs_a$

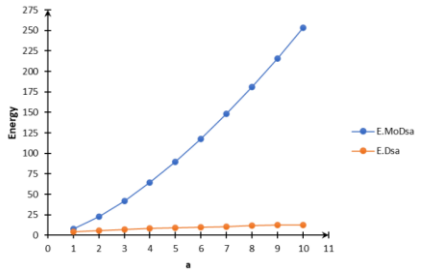

Figure 3
Comparison of $E.MoDs_a$ and $E.Ds_a$

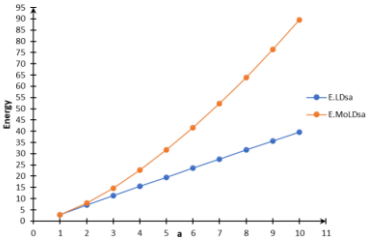

Figure 4
Comparison of $E.MoLDs_a$ and $E.LDs_a$

4. Conclusion

In this article, we obtained the eigenvalues of the adjacency matrices, and the Mo index matrices of the double-star graph and their line graph. We calculated the spectrum of these graphs. We found general formulas for their energies based on the number of pendeng edges. To calculate the energies with these formulas, there is no need to calculate the eigenvalues, only the number of pendeng edges is needed. We found relationships between the energies and we abtained lower bounds for them. As the value of a increased, all energies were ascending. For each $a \geq 1$, the $E.MoDs_a$ plot was higher than their plot of the line graph. For any $a > 1$, the plot of $E.Ds_a$ was lower than their line graph, except $a = 1$. The obtained results were displayed graphically and numerically. The energy of the Mo line graph of the double-stars for the even number of pendeng edges and Mo energy of double-star was obtained from a similar formula. These results can be used for the next studies because there is no need to write the adjacency matrix, the characteristic polynomial, and find the eigenvalues, also calculations are less than before methods.

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