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Bounds of the Symmetric Division Deg Index for Trees and Unicyclic Graphs with A Perfect Matching

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ABSTRACT

The symmetric division deg (SDD) index is a well-established valuable index in the analysis of quantitative structure-property and structure-activity relationships for molecular graphs. In this paper, we study the range of SDD index for special classes of trees and unicyclic graphs. We present the first four lower bounds for SDD index of trees and unicyclic graphs, which admit a perfect matching and find the subclasses of graphs that attain these bounds. Further, we also compute the upper bounds of SDD index for the collection of molecular graphs, namely the trees and unicyclic graphs, each having maximum degree four and that admit a perfect matching.

1. INTRODUCTION

The SDD index gains its importance in the field of mathematical chemistry due to its ability to be a significant predictor of the total surface area of polychlorobiphenyls (PCB) [26]. Recently, Furtula et al. [5] concluded that SDD index has the right to be considered as a viable and applicable molecular descriptor, by a comparative analysis of SDD index with other popular descriptors such as first Zagreb index, second Zagreb index, geometric-arithmetic index, atom-bond connectivity index, and inverse sum index. For more investigation of this index, see [1, 5, 7, 8, 18, 19, 20, 21, 22, 25].

A molecular descriptor/index is a numerical function of molecular structure which plays a fundamental role in mathematical chemistry especially in the QSPR/QSAR (quantitative structure-property/activity relationship) investigation [2, 3, 9, 16, 24]. Several

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types of topological indices exist in mathematical chemistry that enables the analysis of chemicals/molecules' behaviour in a much efficient manner. In the literature, the indices are classified broadly based on the properties.

One wants to focus their study using properties, such as distances, degrees, graph spectra, etc. Among the distance-based topological indices, Wiener index [27], Hyper Wiener index [17], Hosoya index [15] are to name a few. Similarly, degree-based indices such as first Zagreb index [14], second Zagreb index [10], Randić index [23], Augmented Zagreb index [6], harmonic index [4], etc are well studied. For more detailed surveys on degree-based indices, we refer to [3, 11, 12].

In 2010, Vukičević and Gašperov [26] considered the large class of molecular descriptors, which consist of 148 discrete Adriatic descriptors for improving the various quantitative structure-property/activity relationship. They found and established that only a few of these descriptors were useful and distinct. Among these descriptors, the symmetric division deg SDD index was determined to be a useful discrete Adriatic index. The symmetric division deg, SDD, index [26] is defined as

$$SDD(G) = \sum_{uv \in E(G)} \left\{\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)}\right\}, \tag{1}$$

where $d(u)$ and $d(v)$ denotes degree of the end vertices u and v of an edge $uv \in E(G)$ in the graph G.

A molecular graph which has a perfect matching plays an important role in the analysis of the resonance energy and stability of the molecules [13]. With these motivations, we are interested in studying the behaviour of SDD index for the class of molecular graphs that admits perfect matching. To begin with, we study the range of the *SDD* index for molecular graphs, that is the upper bound and lower bound for SDD index. We also give tight bounds by presenting the first lower bound, second lower bound, third lower bound, and fourth lower bound of SDD index for trees and unicyclic graphs with maximum degree 4 that admits perfect matching. Also, we calculate the upper bounds of these trees and unicyclic graphs.

The paper is organized as follows. In Section 2, we introduce all the required definition and notations. Sections 3.1 and 4.1 discusses the lower bounds of the SDD index for the class of trees and a unicyclic graph that admits perfect matching. In Sections 3.2 and 4.2, we present the upper bounds of trees and unicyclic graphs with maximum degree 4 that admits perfect matching.

2. PRELIMINARIES

Throughout this paper, we consider only nontrivial connected simple graphs. A graph is denoted by $G = G\big(V(G), E(G)\big)$, where $V(G)$ denotes the set of vertices of the graph and the set $E(G)$ denotes the edges of the graph. Let $N(u)$ denote the set of all neighbours of a vertex $u \in V(G)$ and $d(u)$ is the degree of the vertex u, where $d(u) = |N(u)|$.

A connected acyclic graph is called a tree i.e., a tree, is a connected graph in which any two vertices have exactly one simple path connecting them. A graph is said to be unicyclic if it is connected and contains exactly one cycle. A vertex which has degree one is called a pendant vertex and a path $u_1 u_2 \ldots u_k$ is called a pendant path if $d(u_1) = 1$, $d(u_i) = 2$ for $i = 2, 3, \ldots, k-1$ and $d(u_k) \geq 3$ of graph G. Let k denote the number of pendant paths in graph G.

A matching M of a graph $G(V(G), E(G))$ is a subset of $E(G)$ such that no two edges are adjacent in G. A vertex $u \in V(G)$ is called M-saturated if it is incident to an edge of M. If all the vertex of a graph G is M-saturated, then matching M is called perfect matching. Throughout this article, when we refer to trees/unicyclic graphs we mean only those trees and unicyclic graphs which admits a perfect matching.

Suppose the degree of the vertex $u \in V(G)$ is i and the degree of the vertex $v \in V(G)$ is j, then the edge $e = uv$ is referred as ij-edge and the total number of ij-edges is denoted by e_{ij}. Let

$$S(i,j) = \frac{i^2 + j^2}{ij}. \tag{2}$$

Then SDD index in (1) can be reformulated as

$$SDD(G) = \sum_{i \leq j} e_{ij} S(i,j) \tag{3}$$

Recall that for trees and unicyclic graphs, the pair (i,j) takes values from $1 \leq i,j \leq 4$ and $(1,1)$ does not arise since we consider non-trivial and connected graphs.

Lemma 2.1. [22] If G has k pendants paths, then

$$SDD(G) \geq \frac{2}{3}k + 2|E(G)|.$$

3. Trees with Perfect Matching

In this section, we obtain the first four lower bounds and an upper bound for the SDD index of trees with a perfect matching. Also, we identify the collection of trees which attains these bounds. By definition, the SDD index depends on the degree of the vertices which can be seen immediately from the following Lemma 3.1.

Lemma 3.1. If G is a connected graph, then $min\, S(1,x) \geq max\, S(u,v)$, where $u, v, x \in \{2,3,4\}$ and equality holds only for $x = 2, u = 2$ and $v = 4$.

Proof. We prove this lemma by direct calculation. Since $S(1,2) = 5/2$,$S(1,3) = 10/3$, $S(1,4) = 17/4$, $S(2,2) = 2$, $S(2,3) = 13/6$, $S(2,4) = 5/2$, $S(3,3) = 2$,$S(3,4) = 25/12$ and $S(4,4) = 2$.

Remark. We make the following observation from the above lemma:

1. The number of edges with degree pair (i,i) contributes a very small value compared to the other degree pair edges.
2. The number of edges with degree pair $(1,2)$ plays a crucial role in determining the value of SDD index.

Based on these observations and the above lemma we proceed to determine the bounds for SDD index and the collection of trees which attains these bounds.

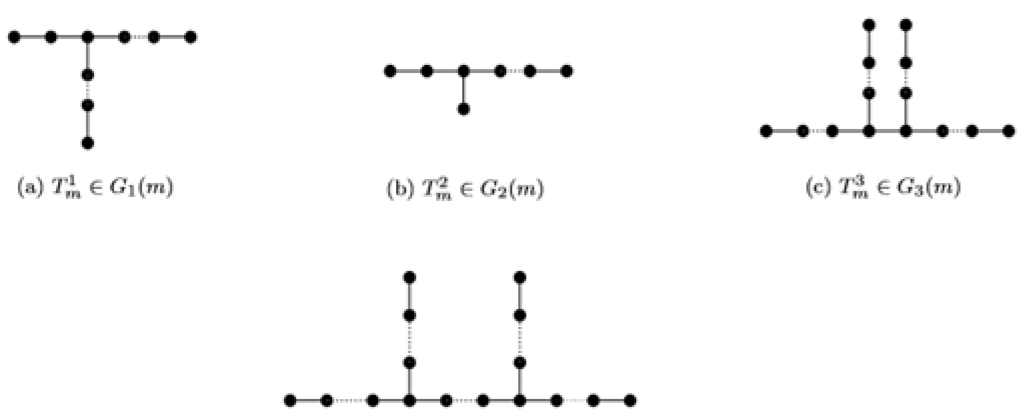
For positive integer $m \geq 2$, let $\mathbb{T}(m)$ be the set of trees on $2m$ vertices with a perfect matching.

3.1. LOWER BOUNDS OF SDD INDEX

First,we identify special classes of trees required for our proof. Let $G_i(m)$, ($i = 1, 2, 3$ and $m \geq 4$) and $G_4(m)$, for $m \geq 6$ be the collection of trees from $\mathbb{T}(m)$ such that a tree $T \in G_i(m)$ ($i = 1, 2, 3, 4$) has the following set of edge-degree pair cardinalities on $2m$ vertices:

$E_1^m = \{e_{12} = 3, e_{22} = 2m - 7, e_{23} = 3\}$,
$E_2^m = \{e_{12} = 2, e_{13} = 1 , e_{22} = 2m - 6, e_{23} = 2\}$,
$E_3^m = \{e_{12} = 4, e_{22} = 2m - 10, e_{23} = 4, e_{33} = 1\}$,
$E_4^m = \{e_{12} = 4, e_{22} = 2m - 11, e_{23} = 6\}$,

respectively. See Figure 1, where $T_m^1 \in G_1(m)$, $T_m^2 \in G_2(m)$, $T_m^3 \in G_3(m)$, $T_m^4 \in G_4(m)$.



(a) $T_m^1 \in G_1(m)$ (b) $T_m^2 \in G_2(m)$ (c) $T_m^3 \in G_3(m)$

(d) $T_m^4 \in G_4(m)$

Figure 1: Representative trees from the collection $G_i(m), i = 1,2,3,4$.

Theorem 3.1. Let $T \in \mathbb{T}(m), m \geq 2$.

1. $SDD(T) \geq 4m - 1$ and equality holds if and only if $T = P_{2m}$, where P_{2m} be a path graph on $2m$ vertices.
2. If $T \in \mathbb{T}(m) \backslash \{P_{2m}\}$, $m \geq 4$, then $SDD(T) \geq 4m$. Equality holds if and only if $T \in G_1(m)$.
3. If $T \in \mathbb{T}(m) \backslash \{P_{2m}, G_1(m)\}, m \geq 4$, then $SDD(T) \geq 4m + \frac{2}{3}$. Equality holds if and only if $T \in G_2(m), m \geq 4$, or $T \in G_3(m), m \geq 5$.
4. If $T \in \mathbb{T}(m) \backslash \{P_{2m}, G_i(m)\} (i = 1, 2, 3), m \geq 6$, then $SDD(T) \geq 4m + 1$. Equality holds if and only if $T \in G_4(m)$.

Proof. When $T = P_{2m}$, then $SDD(T) = 2S(1,2) + (2m - 3)S(2,2) = 4m - 1$. Suppose G is a graph of $2m$ vertices different from path graph P_{2m}. Then G has at least 3 pendant paths, therefore $k \geq 3$. Now we make the cases depending on k.

Case 1. If $k = 3$, then G has exactly one vertex $w \in V(G)$ of degree three. Since G has a perfect matching, any vertex of G has at most one pendant neighbour, we have two subcases.

Subcase 1.1. If w has no pendant neighbour. Then $SDD(G) = 3S(1,2) + 3S(2,3) + 2(2m - 7) = 4m$. Observe that, G satisfies the edge requirement of $G_1(m)$ and hence $G \in G_1(m)$.

Subcase 1.2. If w has a pendant neighbour. Then $SDD(G) = S(1,3) + 2S(1, 2) + 2S(2,3) + 2(2m - 6) = 4m + 2/3$. Observe that, G satisfies the edge requirement of $G_2(m)$ and hence $G \in G_2(m)$.

Case 2. If $K = 4$, then we have two subcases:

Subcase 2.1. G have two vertices $w_1, w_2 \in V(G)$ of degree three. Since G has a perfect matching, any vertex of G has at most one pendant neighbour, then we have the following subcases:

1. If w_1, w_2 have no pendant neighbour and w_1, w_2 are adjacent. Then, $SDD(G) = 4S(1, 2) + 4S(2, 3) + 2(2m - 9) = 4m + 2/3$. Observe that, G satisfies the edge requirement of $G_3(m)$ and hence $G \in G_3(m)$.
2. If w_1, w_2 have no pendant neighbour and w_1, w_2 are not adjacent. Then, $SDD(G) = 4S(1, 2) + 6S(2, 3) + 2(2m - 11) = 4m + 1$. Observe that, G satisfies the edge requirement of $G_4(m)$ and hence $G \in G_4(m)$.
3. If w_1 or w_2 have a pendant neighbour. Then
$$SDD(G) \geq 3S(1, 2) + S(1, 3) + 3S(2, 3) + 2(2m - 8)$$

$= 4m + 4/3 > 4m + 1.$

Subcase 2. 2. If G has no vertex of degree three. Then G has one vertex of degree four and other vertices are of degree one or two. Since, from Lemma 3.1, $S(1,4) > S(1,2)$, we get

$$SDD(G) \geq 4S(1, 2) + 4S(2, 4) + 2(2m - 9) = 4m + 2 > 4m + 1.$$

Case 3. If $k \geq 5$, then from Lemma 2.1

$$SDD(G) = \frac{2}{3}k + 2(2m - 1) > 4m + 1.$$

Corollary 3.2. Above result is also true for all trees that admit perfect matching.

Proof. If G is a tree and max degree $\Delta_G \leq 4$, then the result follows from the Theorem 3.1. If max degree $\Delta_G \geq 5$, then the number of pendant paths $k \geq 5$ in G, then by Lemma 2.1

$$SDD(G) = \frac{2}{3}k + 2(2m - 1) > 4m + 1.$$

3.2. UPPER BOUNDS OF SDD INDEX

In this section, we obtain the upper bounds for the SDD index of trees with a perfect matching particularly, trees with maximum degree four. Before proving the results, we define two interesting collections of trees.

Let $G_5(m)$, for ($m \geq 4$ and m is even) and $G_6(m)$ ($m \geq 7$ and m is odd) be the two collections of trees on $2m$ vertices with a perfect matching M, such that a tree $T \in G_5(m)$ and $T \in G_6(m)$ has the following sets of edge-degree pair cardinalities on $2m$ vertices

$$E_m^5(T) = \{e_{12} = \tfrac{m+2}{2}, e_{14} = \tfrac{m-2}{2}, e_{24} = \tfrac{m+2}{2}, e_{44} = \tfrac{m-4}{2}\},$$

and

$$E_m^6(T) = \{e_{12} = \tfrac{m+1}{2}, e_{13} = 1, e_{14} = \tfrac{m-3}{2}, e_{24} = \tfrac{m+1}{2}, e_{34} = 2, e_{44} = \tfrac{m-7}{2}\},$$

respectively. (See Figure 2, where $T_m^5 \in G_5(m)$ and $T_m^6 \in G_6(m)$, respectively).

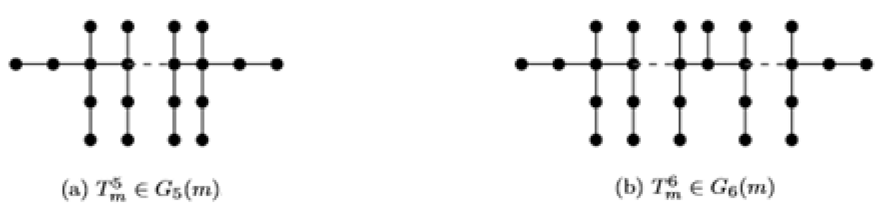


Figure 2: Representative trees from the collection $G_5(m)$ and $G_6(m)$.

Theorem 3.2. Let $\boldsymbol{T} \in \mathbb{T}(\boldsymbol{m})$, where $\boldsymbol{m} \geq \mathbf{4}$. Then

$$SDD(T) = \begin{cases} \frac{1}{8}(45m-26), & m \text{ is even}, \\ \frac{1}{8}(45m-27), & m \text{ is odd}. \end{cases}$$

Equality holds if and only if $T \in G_5(m)$ or $G_6(m)$, for $m \neq 5$.

Proof. Let

$$\phi(m) = \begin{cases} \frac{1}{8}(45m-26), & m \text{ is even}, \\ \frac{1}{8}(45m-27), & m \text{ is odd}. \end{cases} \quad (4)$$

Since under perfect matching, any non-pendant vertex has at most one pendant neighbour. Number of pendant vertices $\mathbb{T}(m) \leq m$. We prove the theorem by two cases.

Case 1. Let $T \in \mathbb{T}(m)$ has m pendant vertices. Now we prove this Case by induction on m. It is easily seen that, $\mathbb{T}(4)$ contains T_1, T_2 where $T_2 \in G_5(m)$ (see Figurers 3a, 3b) By direct calculations $SDD(T_1) = 18 < \phi(4)$ and $SDD(T_2) = 19.25 = \phi(4)$. Thus, the result is true for $m = 4$. If $m = 5$, then $\mathbb{T}(5)$ contains T_3, T_4 (see Figurers 3c, 3d, respectively). Here $SDD(T_3) = 23.33 < \phi(5)$ and $SDD(T_4) = 24.33 < \phi(5)$, in that case, equality does not hold. If $m = 6$, $\mathbb{T}(6)$ contains $T_5, T_6, T_{7,} T_6^5$ (see Figures 3e, 3f, 3g, 2a, respectively). Note that $SDD(T_5) = 28.66 \leq \phi(6)$, $SDD(T_6) = 29.66 \leq \phi(6)$ and $SDD(T_7) = 29.41 \leq \phi(6)$, $SDD(T_6^5) = 30.5 = \phi(6)$. Thus, the result is true for $m = 6$. If $m = 7$, then $\mathbb{T}(7)$ contains $T_8, T_9, T_{10,} T_{11}, T_{12,} T_7^6$ (see Figures 3h, 3i, 3j, 3k, 3l, 2b respectively). By direct calculation, we get that $SDD(T_8) = 34 \leq \phi(7)$, $SDD(T_9) = 35 \leq \phi(7)$, $SDD(T_{10}) = 34.75 \leq \phi(7)$, $SDD(T_{11}) = 34.5 \leq \phi(7)$, $SDD(T_{12}) = 35.58 \leq \phi(7)$ and $SDD(T_7^6) = 36 = \phi(7)$. The result holds for $m = 7$.

Suppose the theorem holds for $\mathbb{T}(n), n < m$ where each non-pendant vertex of $T \in \mathbb{T}(n)$ adjacent to a pendant vertex. Let $T \in \mathbb{T}(m)$ and T has a perfect matching M also each non-pendant vertex of T adjacent to a pendant vertex. Suppose u is the pendant vertex which is adjacent to a vertex v of degree two in $T \in \mathbb{T}(m)$, thus $uv \in M$. Let w_r be the neighbour vertex of v other than u, then $d(w_r) \geq 3$, since $m \geq 4$. Suppose $d(w_r) = 3$. Denote $N\{w_r\} = \{v, u_r, w_{r+1}\}$, where $d(u_r) = 1$ and $d(w_{r+1}) \geq 3$, since each non-pendant vertex of $T \in \mathbb{T}(m)$ has a pendant neighbour. If $T = T_m^7$ (see Figure 4a). Then

$$SDD(T_m^7) = \frac{1}{3}(16m-10) \text{ and } \phi(m) - SDD(T_m^7) > 0.$$

Suppose $T \neq T_m^7$, then there exists a vertex $w_{r+1}, k \geq 1$ of degree four such that $w_{r+1}, w_{r+2}, \ldots, w_{r+k-1}$ are vertices of degree three in T. Let $u_{r+1}, u_{r+2}, \ldots, u_{r+k-1}$ are pendant vertices in T. Since each non-pendant vertex of T has a pendant neighbour. Suppose $u_{r+1}, u_{r+2}, \ldots, u_{r+k-1}$ are adjacent to $w_{r+1}, w_{r+2}, \ldots, w_{r+k-1}$, respectively, then

$$\{u_{r+1}w_{r+1}, u_{r+2}w_{r+2}, \ldots, u_{r+k-1}w_{r+k-1}\} \in M.$$

Let $H_1 = T - u_r - w_r - u_{r+1} - w_{r+1} - \ldots - u_{r+k-1} - w_{r+k-1} + vw_{r+k}$. Then $M \setminus \{u_r w_r, u_{r+1} w_{r+1}, \ldots, u_{r+k-1} w_{r+k-1}\}$ is a perfect matching of H_1 and $H_1 \in \mathbb{T}(m-k)$. By the induction hypothesis, we have

$$SDD(T) = SDD(H_1) + kS(1,3) + (k-1)S(3,3) + S(3,2) + S(3,4) - S(2,4)$$
$$\leq \phi(m-k) + \frac{1}{12}(64k-3).$$

If $m-k$ is even, then from Equation 4, we get

$$SDD(T) \leq \frac{1}{8}(45m - 45k - 26) + \frac{1}{12}(64k-3) = \phi(m) - \frac{1}{24}(7k+6) < \phi(m).$$

If $m-k$ is odd, then from Equation 4, we have

$$SDD(T) \leq \frac{1}{8}(45m - 45k - 27) + \frac{1}{12}(64k-3) = \phi(m) - \frac{1}{24}(7k+6) < \phi(m).$$

If $d(w_r) \neq 3$, then $d(w_r) = 4$. Denote $N\{w_r\} = \{v, u_r, w_{r-1}, w_{r+1}\}$, where $d(u_r) = 1$, $d(w_{r-1}), d(w_{r+1}) \geq 2$ and one of them w_{r-1}, w_{r+1} have degree greater than or equal to three, since each non-pendant vertex of T has a pendant neighbour.

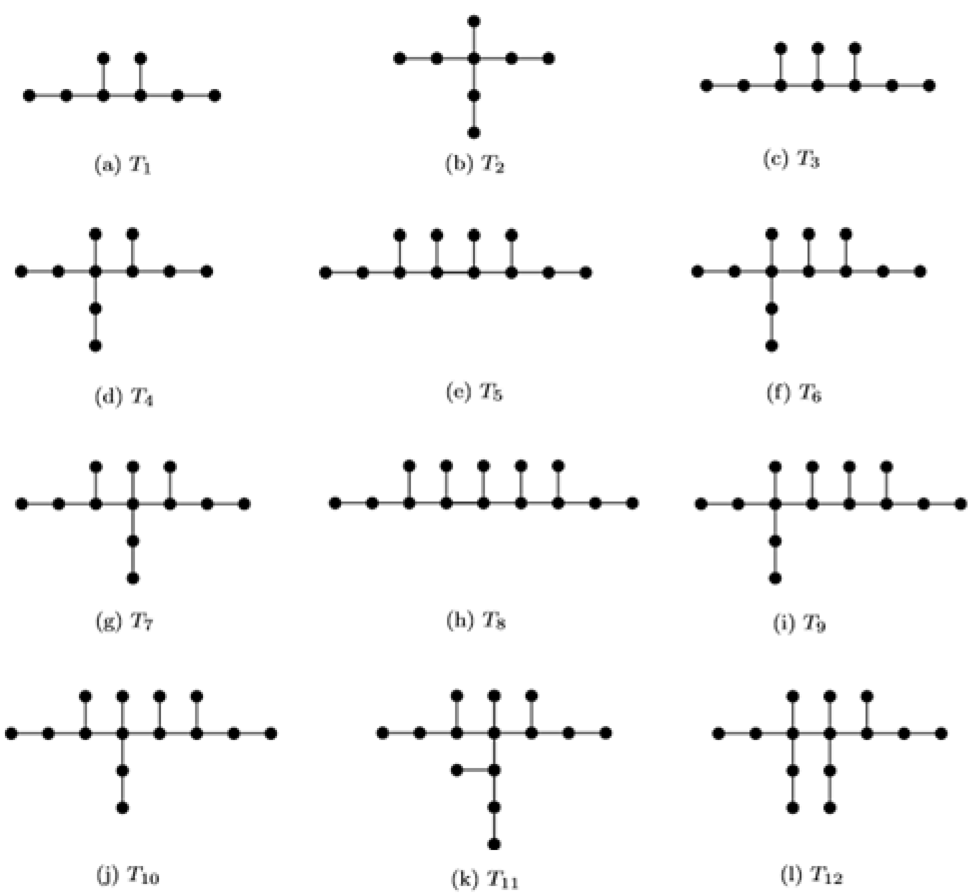


Figure 3: Collection of trees with $m-$pendant vertices on $\mathbb{T}(m)$ $m = 4,5,6,7$.

(a) T_m^7 (b) T_m^8

Figure 4. Collection of trees with atmost one vertex of degree 4 in $\mathbb{T}(m)$**.**

Let $d(w_{r-1}) = 2$ and $d(w_{r+1}) = 3$. If $T = T_m^8$ (see Figure 4b), then $SDD(T_m^8) = 1/3(16m - 7)$ and $\phi(m) - SDD(T_m^8) = 1/24(7m - 25) \geq 0$, since $m \geq 7$. If $T \neq T_m^8$, then there exists a vertex $w_{r+k}, k \geq 2$ of degree four such that, $w_{r+1}, w_{r+2}, \dots, w_{r+k-1}$ are vertices of degree three in T. Let $u_{r+1}, u_{r+2}, \dots, u_{r+k-1}$ are pendant vertices in T. Since each non-pendant vertex of T has a pendant neighbour. Suppose $u_{r+1}, u_{r+2}, \dots, u_{r+k-1}$ are adjacent to $w_{r+1}, w_{r+2}, \dots, w_{r+k-1}$ respectively, then $\{u_{r+1}w_{r+1}, u_{r+2}w_{r+2}, \dots, u_{r+k-1}w_{r+k-1}\} \in M$. Let $H_2 = T - u - v - u_r - w_r - u_{r+1} - w_{r+1} - \dots - u_{r+k-1} - w_{r+k-1} + w_{r-1}w_{r+k}$. Then

$$M \backslash \{uv, u_r w_r, u_{r+1}w_{r+1}, \dots, u_{r+k-1}w_{r+k-1}\}$$

is a perfect matching of H_2 and $H_2 \in \mathbb{T}(m - k - 1)$. By the induction hypothesis, we have

$$\begin{aligned} SDD(T) &= SDD(H_2) + S(1,2) + S(2,4) + S(1,4) + S(3,4) + (k-1)S(1,3) \\ &\quad + (k-2)S(3,3) + S(4,3) + S(4,2) - S(2,4) \\ &\leq \phi(m - k - 1) + \frac{1}{12}(64k + 73). \end{aligned}$$

As before from Equation 4, we get $SDD(T) \leq \phi(m) - 1/24(7k - 11)$, since $k \geq 2$, $SDD(T) < \phi(m)$. Let $d(w_{r-1}) = 2, d(w_{r+1}) = 4$ and $H_4 = T - u - v - u_r - w_r + w_{r-1}w_{r+1}$, then $M \backslash \{uv, u_r w_r\}$ is a perfect matching of H_4 and $H_4 \in \mathbb{T}(m-2)$. By the induction hypothesis, we have $SDD(T) = SDD(H_4) + S(1,2) + S(2,4) + S(4,1) + S(4,4) \leq \phi(m-2) + \frac{45}{4} = \phi(m)$.

Let $d(w_{r-1}) = d(w_{r+1}) = 3$. Denotes $N\{w_{r-1}\} = \{w_{r-2}, u_{r-1}, w_r\}$ and $N\{w_{r+1}\} = \{w_r, u_{r+1}, w_{r+2}\}$, where u_{r-1}, u_{r+1} are pendant vertex and $d(w_{r-2}), d(w_{r+2}) \geq 2$. Since T has perfect matching M, then $\{u_{r-1}w_{r-1}, u_{r+1}w_{r+1}\} \in M$. Suppose that $H_5 = T - u - v - w_r - u_r - u_{r-1} - w_{r-1} - u_{r+1} - w_{r+1} + w_{r-2}w_{r+2}$. Then $M \backslash \{u_{r-1}w_{r-1}, uv, u_r w_r, u_{r+1}w_{r+1}\}$ is a perfect matching of H_5 *and* $H_5 \in \mathbb{T}(m-4)$. By the induction hypothesis, we have $SDD(T) = SDD(H_5) + S(1,2) + S(2,4) + S(1,4) + 2S(3,4) + 2S(1,3) + S(3, d(w_{r-2})) + S(3, d(w_{r+2})) - S(d(w_{r-2}), d(w_{r+2}))$. Since $d(w_{r-2}), d(w_{r+2}) \geq 2$ and $S(3,2) > S(3,4) > S(x,x)$, where $x > 2$. Then we have $SDD(T) \leq \phi(m-4) + 241/12 + 13/3 - 2 = \phi(m) - 1/12 < \phi(m)$. Let $d(w_{r-1}) = 3$, $d(w_{r+1}) = 4$ and $H_6 = T - u - v - u_r - w_r + w_{r-1}w_{r+1}$. Then $M \backslash \{uv, u_r w_r\}$ is a perfect matching of H_6 and $H_6 \in \mathbb{T}(m-2)$. By the induction hypothesis, we have

$$SDD(T) = SDD(H_6) + S(1,2) + S(2,4) + S(1,4) + S(3,4) + S(4,4) - S(3,4)$$

$\leq \phi(m-2) + \frac{45}{4} = \phi(m)$.

Let $d(w_{r-1}) = d(w_{r+1}) = 4$ and $H_7 = T - u - v - u_r - w_r + w_{r-1}w_{r+1}$. Then $M\backslash\{uv, u_r w_r\}$ is a perfect matching of H_7 and $H_7 \in \mathbb{T}(m-2)$. By the induction hypothesis, we have

$$SDD(T) = SDD(H_7) + S(1,2) + S(2,4) + S(1,4) + S(4,4)$$
$$\leq \phi(m-2) + \frac{45}{4} = \phi(m).$$

Hence in this case result is true.

Case 2. When $T \in \mathbb{T}(m)$ has less than m pendant vertex, that is T has at least a vertex which has no pendant neighbour. Clearly, from Lemma 3.1, note that the contribution of a vertex in the SDD index is maximum if that vertex has a pendant neighbour. Hence $SDD(T) \leq \phi(m)$.

4. UNICYCLIC GRAPH WITH PERFECT MATCHING

For positive integer $m \geq 2$, let $\mathbb{U}(m)$ be the set of unicyclic graphs of $2m$ vertices with a perfect matching.

4.1. LOWER BOUNDS OF SDD INDEX

In this section, we obtain the first four lower bounds for the SDD index of unicyclic graphs with a perfect matching. Also, we identify the collection of unicyclic graphs which attains these bounds. Before proving the main result, we define some collection of unicyclic graphs. Let C_1, C_2, for $m \geq 3$, C_3, for $m \geq 4, C_4$, for $m \geq 4$, and C_5, for $m \geq 5$ be the collections of unicyclic graphs, such that for $G \in C_i(m)(i = 1,2,3,4,5)$ has an edge set

$$E_1(m) = \{e_{12} = 1, e_{22} = 2m-4, e_{23} = 3\},$$
$$E_2(m) = \{e_{13} = 1, e_{22} = 2m-3, e_{23} = 2\},$$
$$E_3(m) = \{e_{12} = 1, e_{22} = 2m-7, e_{23} = 4, e_{33} = 1\},$$
$$E_4(m) = \{e_{12} = 2, e_{22} = 2m-8, e_{23} = 6\}$$

and $E_5(m) = \{e_{12} = 3, e_{22} = 2m-9, e_{23} = 3, e_{33} = 3\}$, respectively.

Theorem 4.1. Let $G \in \mathbb{U}(m), m \geq 2$.

1. $SDD(G) \geq 4m$ and equality holds if and only if $G = C_{2m}$, where C_{2m} be a cyclic graph of $2m$ vertices.
2. If $G \in \mathbb{U}(m)\backslash\{C_m\},\ m \geq 3$, then $SDD(G) \geq 4m + 1$ and equality hold if and only if $G \in C_1(m)$.
3. If $G \in \mathbb{U}(m)\backslash\{C_m, C_1(m)\},\ m \geq 3$, then $SDD(G) \geq 4m + 5/3$ and equality holds if and only if $G \in C_2(m), m \geq 3$ or $G \in C_3(m), m \geq 4$.

4. If $G \in \mathbb{U}(m)\backslash\{C_m, C_i(m)\}$ $(i = 1,2,3)$, $m \geq 4$, then $SDD(G) \geq 4m + 2$ and equality holds if and only if $G \in C_4(m \geq 4)$, or $G \in C_5(m \geq 5)$.

Proof. For $m \geq 2$, let $G \in \mathbb{U}(m)$ be a $2m$ vertex unicyclic graph. We prove the theorem by making cases on the number of pendant paths.

Case 1. If $k = 0$, then G has no pendant path, therefore $G = C_{2m}$ and $SDD(G) = 4m$.

Case 2. If $k = 1$, then G has exactly one vertex $w \in V(G)$ of maximum degree three. If w has no pendant neighbour, then $SDD(G) = S(1,2) + 3S(2,3) + 2(2m-4) = 4m + 1$. Observe that, G satisfies the edge requirement of $C_1(m)$ and hence $G \in C_1(m)$. If w has a pendant neighbour, then $SDD(G) = S(1,3) + 2S(2,3) + 2(2m-3) = 4m + 5/3$. Observe that, G satisfies the edge requirement of $C_2(m)$and hence $G \in C_2(m)$.

Case 3. If $k = 2$, then we have two subcases: Either G has no vertex of degree four or G has a vertex of degree four.

Subcase 3.1. If G has no vertex of degree four, then G contains two vertices $w_1, w_2 \in V(G)$ of degree three. Now we have the following subcase.

1. If w_1 and w_2 are adjacent and have no pendant neighbour, then
$$SDD(G) = 2S(1,2) + 4S(2,3) + S(3,3) + 2(2m-7) = 4m + 5/3,$$
Observe that G satisfies the edge requirement of $C_3(m)$ and hence $G \in C_3(m)$.
2. If w_1 and w_2 are not adjacent and have no pendant neighbour, then $SDD(G) = 2S(1,2) + 6S(2,3) + 2(2m-8) = 4m + 2$. Observe that, G satisfies the edge requirement of $C_4(m)$ and hence $G \in C_4(m)$.
3. If w_1 and w_2 has a pendant neighbour: Then, there are at least three edges in G connecting the vertices of degree two and three, we have $SDD(G) \geq S(1,2) + S(1,3) + 3S(2,3) + 2(2m-5) = 4m + 7/3 > 4m + 2$.

Subcase 3.2. If G has one vertex of degree four: Then, $SDD(G) \geq 2S(1,2) + 4S(2,4) + 2(2m-6) = 4m + 3 > 4m + 2$, since $S(1,4) > S(1,2)$.

Case 4. If $k = 3$, then we have two subcases: Either G has at least one pendant path of length one or has no pendant path of length one.

Subcase 4.1. If G has no pendant path of length one, then we have following subcases.

1. If the maximum degree of $\Delta_G = 3$, then there exist three vertices $w_1, w_2, w_3 \in V(G)$ of degree three. If w_1, w_2, w_3 are pairwise adjacent, then $G \in C_5(m)$ and

$$SDD(G) = 3S(1,2) + 3S(2,3) + 3S(3,3) + 2(2m-9) = 4m+2.$$

Observe that, G satisfies the edge requirement of $C_5(m)$ and hence $G \in C_5(m)$. If at most two pairs of vertices w_1, w_2, w_3 are adjacent, then at least five edges which are connecting vertices of degree two and three. In that case

$$SDD(G) \geq 3S(1,2) + 5S(2,3) + 2(2m-8) = 4m + \frac{7}{3} > 4m+2.$$

2. If G has a vertex of degree at least four, then,

$$SDD(G) \geq 3S(1,2) + S(2,4) + 2(2m-5) = 4m + 5/2 > 4m+2.$$

3. If G has at least one pendant path of length one, then,

$$SDD(G) \geq 2S(1,2) + S(1,3) + 2(2m-3) = 4m + 7/3 > 4m+2,$$

since $S(1,4) > S(1,3)$ and $S(2,4) > S(2,3)$.

Case 5. If $k \geq 4$, then by Lemma 2.1, we have $SDD(G) \geq 4m + 8/3 > 4m+2$.

4.2. UPPER BOUNDS OF SDD INDEX

In this section, we obtain upper bounds for the SDD index of unicyclic graph (which has maximum degree four) with a perfect matching. Before proving the results, we define two collections of unicyclic graphs which are required for our proof.

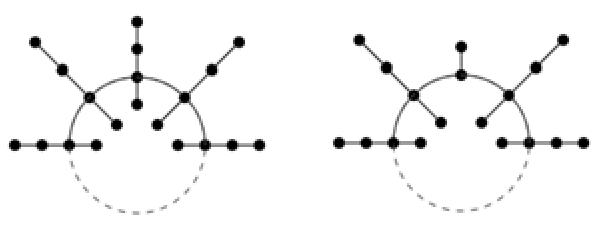
$\mathbb{C}_a(m)$ $(m \geq 6 \; and \; m \; even)$, $\mathbb{C}_b(m)$ $(m \geq 5 \; and \; m \; odd)$ are two collections of unicyclic graphs, such that for each $G \in \mathbb{C}_a(m), \mathbb{C}_b(m)$ has the following sets of edge-degree pair cardinalities on $2m$ vertices

$$E_a(G) = \left\{e_{12} = \frac{m}{2}, e_{14} = \frac{m}{2}, e_{24} = \frac{m}{2}, e_{44} = \frac{m}{2}\right\}$$

and

$$E_b(G) = \{e_{12} = \frac{m-1}{2}, e_{13} = 1, e_{14} = \frac{m-1}{2}, e_{24} = \frac{m-1}{2}, \; e_{34} = 2, \; e_{44} = \frac{m-3}{2}\}$$

respectively. See Figure 5, where $G_a(m) \in \mathbb{C}_a(m)$ and $G_b(m) \in \mathbb{C}_b(m)$.



(a) $G_a(m) \in \mathbb{C}_a(m)$ (b) $G_b(m) \in \mathbb{C}_b(m)$

Figure 5: Representative graphs for $\mathbb{C}_a(m), \mathbb{C}_b(m)$.

Theorem 4.2. Let $G \in \mathbb{U}(m), m \geq 4$. Then

$$SDD(\mathrm{G}) \leq \begin{cases} \frac{1}{8}(45m), & m \text{ is even}, \\ \frac{1}{8}(45m-1), & m \text{ is odd}. \end{cases}$$

Equality holds if and only if $G \in \mathbb{C}_a(m)$ or $\mathbb{C}_b(m), (m \geq 5)$.

Proof. Let

$$\phi(m) \leq \begin{cases} \frac{1}{8}(45m), & m \text{ is even}, \\ \frac{1}{8}(45m-1), & m \text{ is odd}. \end{cases} \quad (5)$$

Since under perfect matching, any non-pendant vertex has at-most one pendant neighbour, the number of pendant vertices in $G \leq m$. We now make cases based on number of pendants.

Case 1. Let $G \in \mathbb{U}(m)$has m pendant vertex.We prove by induction: For $m = 4, \mathbb{U}(4)$ contains Q_1 and $G_d(4)$ (see Figures 6a, 6b). By direct computation, we get $SDD(Q_1) = 22.08 < \phi(4)$ and $SDD\big(G_d(4)\big) = 21.33 < \phi(4)$. In this case, equality does not hold. If $m = 5, \mathbb{U}(5)$ contains $G_b(5), G_d(5), Q_2, Q_3$ (see Figures 5b, 6a, 6c, 6d). Note that

$$SDD(Q_2) = 27.41 < \phi(5),\ SDD(Q_3) = 27.16 < \phi(5),$$
$$SDD\big(G_d(5)\big) = 26.66 < \phi(5), SDD\big(G_b(5)\big) = 28 = \phi(5).$$

Thus, the result is true for $m = 5$. If $m = 6, \mathbb{U}(6)$ contains Q_i $(i = 4,5,6,7,8)$, $G_a(6)$ (see Figures 5b, 6e, 6f, 6g, 6h, 6i) and $G_d(6)$ (see Figure 6a). Note that

$$SDD(Q_4) = 33.33 < \phi(6), SDD(Q_5) = 33.33 < \phi(6), SDD(Q_6) = 33.5 < \phi(6),$$
$$SDD(Q_7) = 32.5 < \phi(6), SDD(Q_8) = 32.75 < \phi(6), SDD\big(G_d(6)\big) = 32 < \phi(6),$$

and $SDD(G_a(6)) = 33.75 = \phi(6)$.

If $m = 7, \mathbb{U}(7)$ contains Q_i $(i = 9,10,11,12,13,14)$, $G_d(7)$ (see Figures 6a, 6j, 6k, 6l, 7a, 7b, 7c) and $G_b(7)$ (see Figure 5b), then by a direct calculation, we have

$$SDD(Q_9) = 38.083 < \phi(7), SDD(Q_{10}) = 38.83 < \phi(7), SDD(Q_{11}) = 38.66 < \phi(7),$$
$$SDD(Q_{12}) = 36.33 < \phi(7), SDD(Q_{13}) = 39.25 \leq \phi(7), SDD(Q_{14}) = 38.41 \leq \phi(7),$$

$SDD(G_d(7)) = 37.33 < \phi(7)$ and $SDD(G_b(7)) = 39.25 = \phi(7)$. Thus the equality holds for $m = 6$ and $m = 7$.

Suppose result holds for $\mathbb{U}(n), (n < m)$, where each non-pendant vertex of $G \in \mathbb{U}(n)$ has a pendant neighbour. Let M be the perfect matching of $G \in \mathbb{U}(m)$ and suppose each non-pendant vertex of G has a pendant neighbour.

Let $u, u_1, u_2, \ldots, u_r, \ldots, u_{m-1}$ are pendant vertices, which is adjacent to the vertices $v, w_1, w_2, \ldots, w_r, \ldots, w_{m-1}$ respectively, where $d(v), d(w_i) \geq 2$ $(i = 1$ to $m - 1)$. Then $\{uv, u_i w_i\} \in M, (i = 1$ to $m - 1)$. Now we consider the following two subcases.

Subcase 1. If G has a pendant vertex u adjacent to a vertex v of degree two. In this subcase, $uv \in M$. Let w_r be the neighbour vertex of v other than u in G, then

$d(w_r) \geq 3$. If $d(w_r) = 3$. Denote $N\{w_r\} = \{v, u_r, w_{r+1}\}$, where $d(w_{r+1}) \geq 3$. If G has no vertex of degree four, then G is not unicyclic since each non-pendant vertex of G must have a pendant neighbour, and we get a contradiction. Hence, there exists a vertex $w_{r+k}, k \geq 1$ of degree four in G, such that $w_{r+1}, w_{r+2}, \ldots, w_{r+k-1}$ are vertices of degree three in G. Since G has a perfect matching M, then $\{uv, u_r w_r, u_{r+1} w_{r+1}, \ldots, u_{r+k-1} w_{r+k-1}\} \in M$. Let

$$C_1 = G - u_r - w_r - u_{r+1} - w_{r+1} - \cdots - u_{r+k-1} - w_{r+k-1} + v w_{r+k}.$$

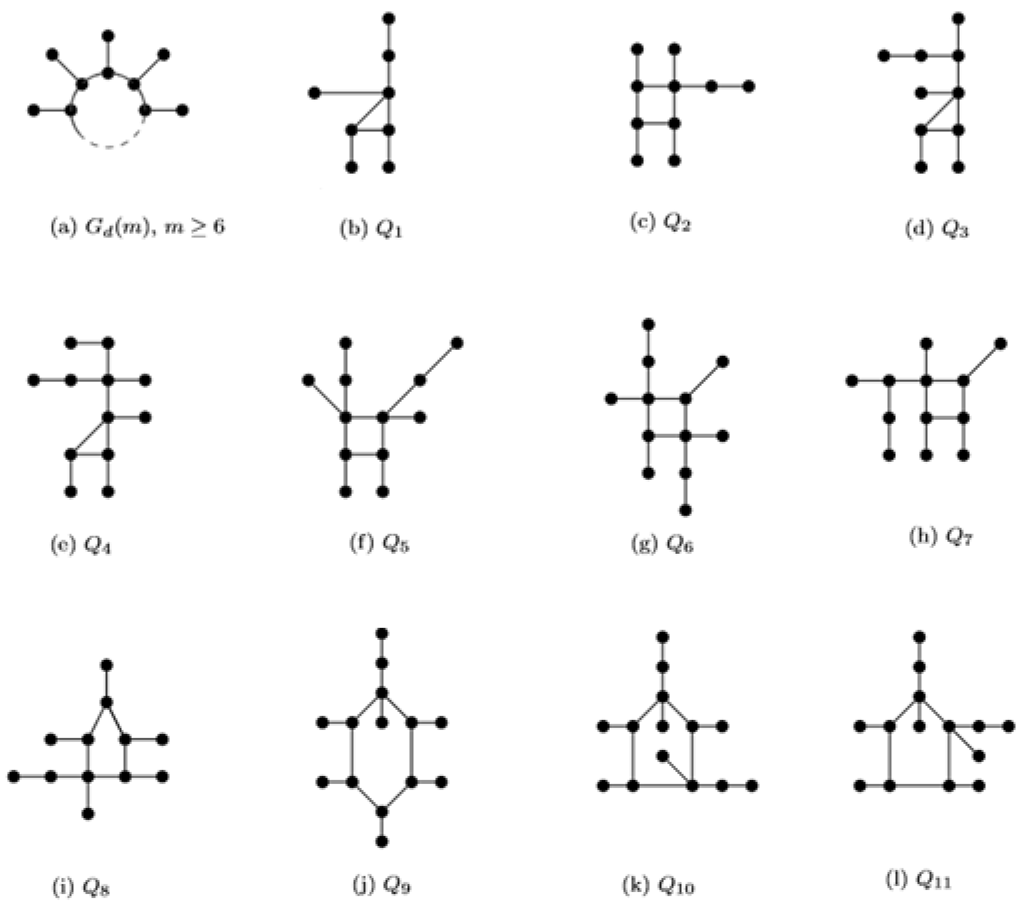


Figure 6: Collection of unicyclic graph with $m-$pendant vertices on $\mathbb{U}(m)$ for $m = 4,5,6,7$.

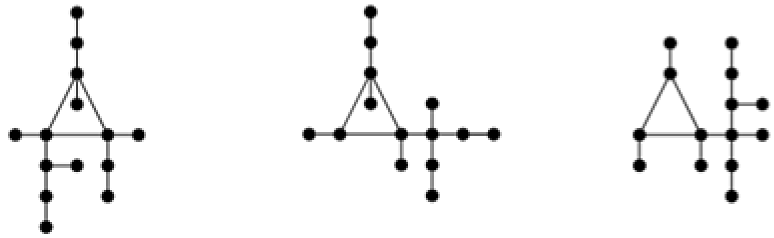


Figure 7: Collection of unicyclic graph with $m-$pendant vertices on $\mathbb{U}(m)$ for $m = 7$.

Then $M = \{u_r w_r,\ u_{r+1}w_{r+1}, \dots, u_{r+k-1}w_{r+k-1}\}$ is a perfect matching of C_1 and $C_1 \in \mathbb{U}(m-k)$. By the induction hypothesis, we have

$$SDD(G) = SDD(C_1) + kS(1,3) + (k-1)S(3,3) + S(2,3) + S(3,4) - S(2,4)$$
$$\leq \phi(m-k) + \frac{1}{12}(64k-3).$$

If $m-k$ is even, then from Equation 5, we have

$$SDD(G) \leq \frac{1}{8}(45m - 45\text{k}) + \frac{1}{12}(64k-3) = \phi(m) - \frac{1}{24}(7k+6) < \phi(m).$$

If $m-k$ is odd, then from Equation 5, we have

$$SDD(G) \leq \frac{1}{8}(45m - 45k - 1) + \frac{1}{12}(64k-3) = \phi(m) - \frac{1}{24}(7k+6) < \phi(m).$$

If $d(w_r) \neq 3$, then $d(w_r) = 4$. Denote $N\{w_r\} = \{w_{r-1}, u_r, v, w_{r+1}\}$, where $d(u_r) = 1$, $d(w_{r-1}), d(w_{r+1}) \geq 2$ and one of w_{r-1}, w_{r+1} have degree greater than or equal to three, since each non-pendant vertex of $G \in \mathbb{U}(n)$ has a pendant neighbour. If $d(w_{r-1}) = 2$ and $d(w_{r+1}) = 3$. Denote $N\{w_{r-1}\} = \{u_{r-1}, w_r\}$, and $N\{w_{r+1}\} = \{w_r, u_{r+1}, w_{r+2}\}$, where $d(w_{r+2}) \geq 3$. Suppose G has no vertex of degree four except $\{w_r\}$. Then G has no unicyclic in that subcase, hence there exist a vertex $w_{r+k}, k \geq 2$ of degree four in G such that $w_{r+1}, w_{r+2}, \dots, w_{r+k-1}$ are vertices of degree three. Since G has a perfect matching M, then $\{uv, u_r w_r, u_{r+1}w_{r+1}, \dots, u_{r+k-1}w_{r+k-1}\} \in M$. Let

$$C_2 = G - u_r - w_r - u_{r+1} - w_{r+1} - \cdots - u_{r+k-1} - \mathrm{w}_{r+k-1} + \mathrm{w}_{r-1}w_{r+k}.$$

Then $M \backslash \{\text{uv}, u_r w_r, u_{r+1}w_{r+1}, \dots, u_{r+k-1}w_{r+k-1}\}$ is a perfect matching of C_2 and $C_2 \in \mathbb{U}(m-k-1)$. By the induction hypothesis, we have

$$SDD(G) = SDD(C_2) + S(1{,}2) + S(2{,}4) + S(1{,}4) + S(3{,}4)$$
$$+(k-1)S(1{,}3) + (k-2)S(3{,}3) + S(2{,}4) + S(3{,}4) - S(2{,}4)$$
$$\leq \phi(m-k-1) + \frac{1}{12}(64k+73).$$

From Equation 5, we have

$$SDD(G) \leq \phi(m) - \frac{1}{24}(7k-11),\quad k \geq 2$$
$$< \phi(m).$$

If $d(w_{r-1}) = 2$ and $d(w_{r+1}) = 4$: Suppose $C_3 = G - \mathrm{u} - \mathrm{v} - u_r - w_r + \mathrm{w}_{r-1}w_{r+1}$, then $M\backslash\{\mathrm{uv}, u_r w_r\}$ is a perfect matching of C_3 and $C_3 \in \mathbb{U}(m-2)$. By the induction hypothesis, we have

$$SDD(G) = SDD(C_3) + S(1,2) + S(2,4) + S(4,1) + S(4,4)$$
$$\leq \phi(m-2) + \tfrac{45}{4}.$$

From Equation 5, we have $SDD(G) \leq \phi(m)$. If both neighbour of w_r have degree three. Denote $N\{w_{r-1}\} = \{w_{r-2}, u_{r-1}, w_r\}$ and $N\{w_{r+1}\} = \{w_r, u_{r+1}, w_{r+2}\}$, where $\mathrm{u}_{r-1}, \mathrm{u}_{r+1}$ are pendant vertices and $d(w_{r-2}), d(w_{r+2}) \geq 2$. Since G has a perfect matching M, then $\{u_{r-1}w_{r-1}, u_{r+1}w_{r+1}\} \in M$. Let

$$C_4 = G - \mathrm{u} - \mathrm{v} - w_r - \mathrm{u}_r - u_{r-1} - w_{r-1} - u_{r+1} - \mathrm{w}_{r+1} + \mathrm{w}_{r-2}w_{r+2}.$$

Then $M\backslash\{u_{r-1}w_{r-1}, \mathrm{uv}, u_r w_r, u_{r+1}w_{r+1}\}$ is a perfect matching of C_4 and $C_4 \in \mathbb{U}(m-4)$. By the induction hypothesis, we have

$$SDD(G) = SDD(\mathrm{C}_4) + S(1,2) + S(2,4) + S(1,4) + 2S(3,4) + 2S(1,3)$$
$$+S(3, d(w_{r-2})) + S(3, d(w_{r+2})) - S(d(w_{r-2}), d(w_{r+2})).$$

Since $d(w_{r-2}), d(w_{r+2}) \geq 2$, $\mathrm{S}(3,2) > S(3,4) > S(x,x)$, where $\mathrm{x} > 2$. Then, we have $SDD(G) \leq \phi(m-4) + 241/12 + 13/3 - 2.$ From Equation 5, we have $SDD(G) \leq \phi(m) - 1/12 \leq \phi(m)$. If $d(w_{r-1}) = 3$ and $d(w_{r+1}) = 4$: Let $C_5 = G - \mathrm{u} - \mathrm{v} - u_r - w_r + \mathrm{w}_{r-1}w_{r+1}$, then $M\backslash\{\mathrm{uv}, u_r w_r\}$ is a perfect matching of C_5 and $C_5 \in \mathbb{U}(m-2)$. By the induction hypothesis, we have

$$SDD(G) = SDD(C_5) + S(1,2) + S(2,4) + S(1,4) + S(3,4) + \mathrm{S}(4,4) - \mathrm{S}(3,4)$$
$$\leq \phi(m-2) + \tfrac{45}{4}.$$

From Equation 5, we have $SDD(G) \leq \phi(m)$. If $d(w_{r-1}) = d(w_{r+1}) = 4$. Let $C_6 = G - \mathrm{u} - \mathrm{v} - u_r - w_r + \mathrm{w}_{r-1}w_{r+1}$, then $M\backslash\{\mathrm{uv}, u_r w_r\}$ is a perfect matching of C_6 and $C_6 \in \mathbb{U}(m-2)$. By the induction hypothesis, we have

$$SDD(G) = SDD(C_6) + S(1,2) + S(2,4) + S(1,4) + \mathrm{S}(4,4)$$
$$\leq \phi(m-2) + \tfrac{45}{4}$$
$$= \phi(m).$$

Hence in that subcase result is true.

Subcase 2. If no neighbour of pendant vertex has degree two in G. Since G is a unicyclic graph and it has a perfect matching also each vertex of G has a pendant neighbour, we have $G \cong C_d(m)$ where $C_d(m)$ is shown in (Figure 6a) and $SDD(C_d(m)) = 16m/3$. If m is even, then

$$\phi(m) - SDD(C_d(m)) = 7m/24m \geq 0, m \geq 6.$$

If m is odd, then

$$\phi(m) - SDD(C_d(m)) = \frac{7m-3}{24} \geq 0, m \geq 7.$$

Hence in this case result is true.

Case 2. When $G \in \mathbb{U}(m)$ has less than m pendant vertex, that is G has a vertex which has no pendant neighbour. Clearly, Lemma 3.1, we can easily say that the SDD value of any vertex is maximum if it has a pendant neighbour. Hence $SDD(G) \leq \phi(m)$.

5. CONCLUSION

In this paper, we have found the first four lower bounds for SDD index of trees and unicyclic graphs which admit a perfect matching and the subclasses of graphs that attain these bounds. Further, we have also computed the upper bounds of SDD index for the collection of molecular graphs, namely the trees and unicyclic graphs with maximum degree four that admits a perfect matching.

In view of our results, we would like to pose the following open problem: Determine the upper bounds for SDD index of trees and unicyclic graphs that admits perfect matching having the maximum degree Δ_G.

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