Chapter 3

Symmetric Division Deg Index for Trees and Unicyclic Graphs

3.1 Introduction

In this chapter, 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. A molecular graph which has a perfect matching plays an important role in the analysis of the resonance energy and stability of the molecules [122]. So, we are interested in studying the behavior of SDD index for the class of molecular graphs that admits perfect matching.

Before proving the desired results we recall the definition of SDD index and a useful lemma. For a simple graph G, the symmetric division deg SDD index [68] is defined as

$$SDD(G) = \sum_{uv \in E(G)} \left\{ \frac{d(u)}{d(v)} + \frac{d(v)}{d(u)} \right\}, \tag{3.1}$$

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

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

$$S(i,j) = \frac{i^2 + j^2}{ij}, \tag{3.2}$$

then SDD index in Equation (3.1) can be reformulated as

$$SDD(G) = \sum_{i \leq j} e_{ij} S(i,j). \tag{3.3}$$

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 3.1.1. [75] If G has K pendants paths, then

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

The chapter is organized as follows. In Section 3.2.1 and 3.3.1 discusses the lower bounds of SDD index for the class of trees and unicyclic graph that admits perfect matching. In Section 3.2.2 and 3.3.2, we present the upper bounds of trees and unicyclic graphs with maximum degree 4 that admits perfect matching.

3.2 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 3.2.1.

Lemma 3.2.1. 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 observations 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 $(1,2)$ play 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 and having a perfect matching.

3.2.1 Lower Bounds for *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 $T \in G_i(m)$, $1 \leq i \leq 4$, 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 3.1, where $T_m^1 \in G_1(m)$, $T_m^2 \in G_2(m)$, $T_m^3 \in G_3(m)$, $T_m^4 \in G_4(m)$.

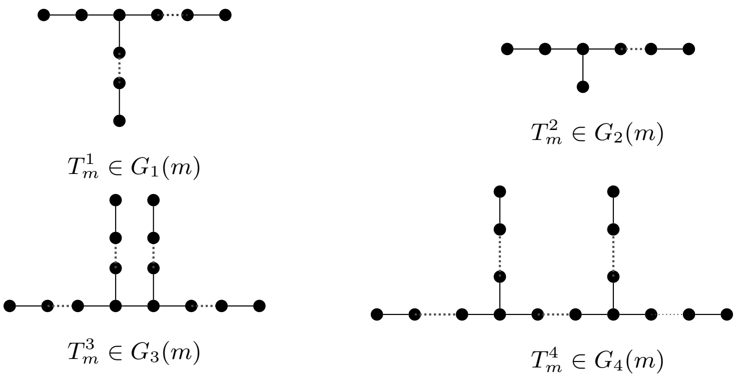


FIGURE 3.1: Representative trees from the collection $G_i(m)$, $i = 1, 2, 3, 4$.

Theorem 3.2.1. 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} is the path graph on $2m$ vertices.

2. If $T \in \mathbb{T}(m) \setminus \{P_{2m}\}, m \geq 4$, then $SDD(T) \geq 4m$. Equality holds if and only if $T \in G_1(m)$.

3. If $T \in \mathbb{T}(m) \setminus \{P_{2m}, G_1(m)\}, m \geq 4$, 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 $T \in \mathbb{T}(m) \setminus \{P_m, G_i(m)\}(i = 1, 2, 3),\ m \geq 6$, 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}. Let K denote the number of pendant paths in G. Then G has atleast 3 pendant paths, that is $K \geq 3$. 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 the following 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, $SDD(G) = S(1,3)+2S(1,2)+2S(2,3)+2(2m-6) = 4m+\frac{2}{3}$. 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 following subcases:

1. If w_1, w_2 have no pendant neighbours and w_1, w_2 are adjacent: Then, $SDD(G) = 4S(1,2) + 4S(2,3)+2(2m-9) = 4m+\frac{2}{3}$. 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 neighbours 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, $SDD(G) \geq 3S(1,2) + S(1,3) + 3S(2,3) + 2(2m-8) = 4m+\frac{4}{3} > 4m+1$.

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 3.2.1, $S(1,4) > S(1,2)$, 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 3.1.1

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

□

Corollary 3.2.1. Theorem 3.2.1 is also true for any tree that admits a perfect matching.

Proof. If G is a tree and max degree $\triangle_G \leq 4$, then the result follows from the Theorem 3.2.1. If max degree $\triangle_G \geq 5$, then number of pendant paths K is greater than or equal to 5 in G. Therefore, by Lemma 3.1.1, we have $SDD(G) \geq \frac{2}{3}K + 2(2m-1) > 4m+1$. □

3.2.2 Upper Bounds for *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.

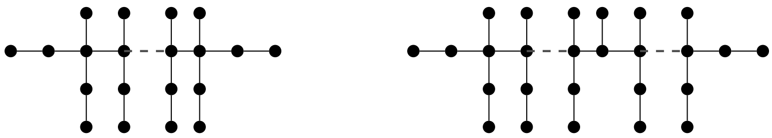
Let $G_5(m)$, (for $m \geq 4$ and m even) and $G_6(m)$ ($m \geq 7$ and m odd) be the collection of trees on $2m$ vertices with a perfect matching M, such that a tree $T \in G_5(m)$ and $T \in G_6(m)$ has the following sets of edge-degree pair cardinalities

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

and

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

respectively. See Figure 3.2, where $T_m^5 \in G_5(m)$ and $T_m^6 \in G_6(m)$ respectively.



(a) $T_m^5 \in G_5(m)$. (b) $T_m^6 \in G_6(m)$

Figure 3.2: Representative trees from the collection $G_5(m)$ and $G_6(m)$.

Theorem 3.2.2. Let $T \in \mathbb{T}(m)$, where $m \geq 4$. Then

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

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

Proof. Let

$$\phi(m) = \begin{cases} \frac{1}{8}(45m - 26) : \text{if } m \text{ is even,} \\ \frac{1}{8}(45m - 27) : \text{if } m \text{ is odd.} \end{cases} \tag{3.4}$$

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

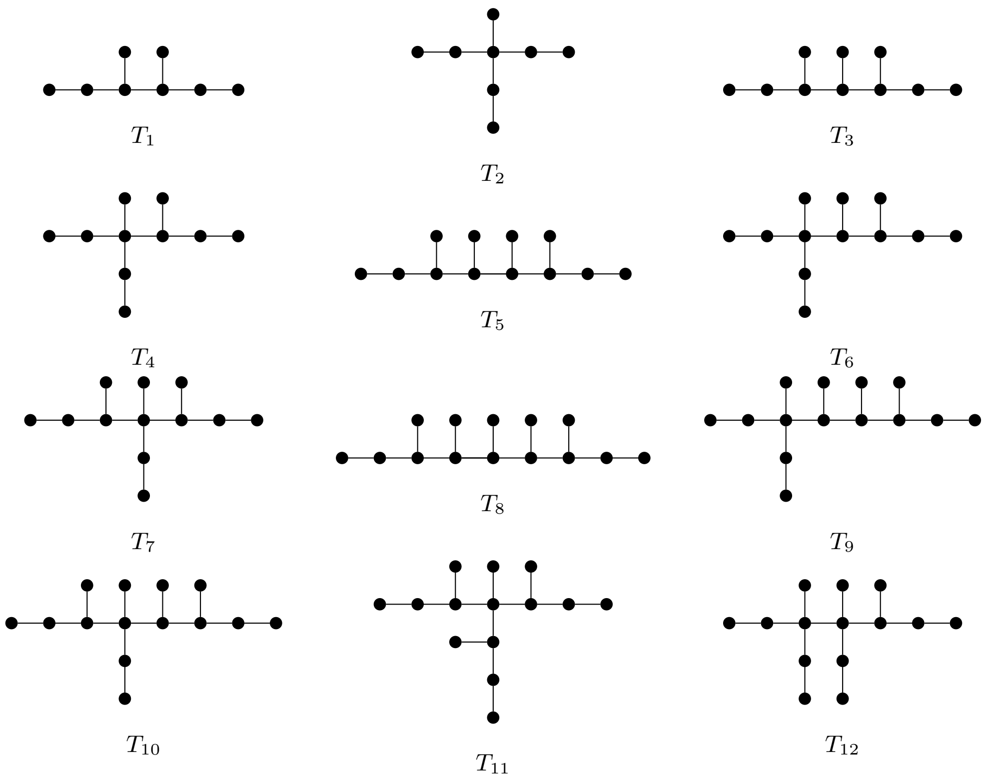


FIGURE 3.3: Collection of trees with $m-$pendant vertices on $\mathbb{T}(m)$, $m = 4, 5, 6, 7$.

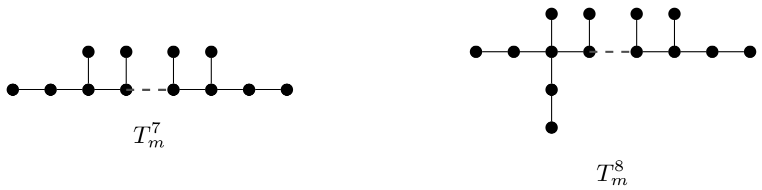


FIGURE 3.4: Collection of trees with atmost one vertex of degree 4 in $\mathbb{T}(m)$.

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 Figure 3.3). 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 Figure 3.3). 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 3.3, 3.2, 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 3.3, 3.2 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 $T \in \mathbb{T}(n)$ is adjacent to a pendant vertex. Let $T \in \mathbb{T}(m)$ and T has a perfect matching M. 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 $m \geq 4$.

If $d(w_r) = 3$. Denote $N_T(w_r) = \{v, u_r, w_{r+1}\}$, 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 3.4), 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 exist a vertex w_{r+k}, $k \geq 1$ of degree four such that $w_{r+1}, w_{r+2}, \ldots, w_{r+k-1}$ are vertices of degree three in T. Let $u_{r+1}, u_{r+2}, \ldots, u_{r+k-1}$ be 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 $\{u_{r+1}w_{r+1}, u_{r+2}w_{r+2}, \ldots, u_{r+k-1}w_{r+k-1}\} \subseteq M$. Let $H_1 = T - u_r - w_r - u_{r+1} - w_{r+1} - \cdots - u_{r+k-1} - w_{r+k-1} + vw_{r+k}$. 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 induction hypothesis, we have

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

If $m - k$ is even, then from Equation (3.4), we gets

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

If $m-k$ is odd, then from Equation (3.4), 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 $N_T(w_r)=\{v,u_r,w_{r-1},w_{r+1}\}$, where $d(u_r)=1$, $d(w_{r-1})\geq 2$, $d(w_{r+1})\geq 2$ and one of w_{r-1}, w_{r+1} has degree greater than or equal to three, since each non-pendant vertex of T has a pendant neighbour.

Let $d(w_{r-1})=2$ and $d(w_{r+1})=3$. If $T=T_m^8$ (see Figure 3.4), then $SDD(T_m^8)=\frac{1}{3}(16m-7)$ and $\phi(m)-SDD(T_m^8)=\frac{1}{24}(7m-25)\geq 0$, 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 $w_{r+1},w_{r+2},\ldots,w_{r+k-1}$ are vertices of degree three in T. Let $u_{r+1},u_{r+2},\ldots,u_{r+k-1}$ be the pendant vertices in T.

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 $\{u_{r+1}w_{r+1},u_{r+2}w_{r+2},\ldots,u_{r+k-1}w_{r+k-1}\}\subseteq M$. Let $H_2=T-u-v-u_r-w_r-u_{r+1}-w_{r+1}-\cdots-u_{r+k-1}-w_{r+k-1}+w_{r-1}w_{r+k}$. Then $M\setminus\{uv,u_rw_r,u_{r+1}w_{r+1},\ldots,u_{r+k-1}w_{r+k-1}\}$ is a perfect matching of H_2 and $H_2\in\mathbb{T}(m-k-1)$. By the induction hypothesis, we have

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

As before from Equation (3.4), we get

$$\begin{aligned} SDD(T) &\leq \phi(m)-\frac{1}{24}(7k-11), \quad \text{since } k\geq 2 \\ SDD(T) &< \phi(m). \end{aligned}$$

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 $M\setminus\{uv,u_rw_r\}$ is a perfect matching of H_4 and $H_4\in\mathbb{T}(m-2)$. By the induction hypothesis, we have

$$\begin{aligned} SDD(T) = &\ SDD(H_4)+S(1,2)+S(2,4)+S(4,1)+S(4,4) \\ \leq &\ \phi(m-2)+\frac{45}{4}=\phi(m). \end{aligned}$$

When $d(w_{r-1})=d(w_{r+1})=3$: Denote $N_T(w_{r-1})=\{w_{r-2},u_{r-1},w_r\}$ and $N_T(w_{r+1})=\{w_r,u_{r+1},w_{r+2}\}$, where u_{r-1},u_{r+1} are pendant vertices, $d(w_{r-2})\geq 2$, and $d(w_{r+2})\geq 2$. Since T has perfect matching M, then $\{u_{r-1}w_{r-1}, u_{r+1}w_{r+1}\} \subseteq M$. 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 $M \setminus \{u_{r-1}w_{r-1}, uv, u_rw_r, u_{r+1}w_{r+1}\}$ 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 $d(w_{r-2}) \geq 2$, $d(w_{r+2}) \geq 2$ and $S(3,2) > S(3,4) > S(x,x)$,where $x > 2$, we have

$$SDD(T) \leq \phi(m-4) + \frac{241}{12} + \frac{13}{3} - 2 = \phi(m) - \frac{1}{12} < \phi(m).$$

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 $M \setminus \{uv, u_rw_r\}$ is a perfect matching of H_6 and $H_6 \in \mathbb{T}(m-2)$. By the induction hypothesis, we have

$$\begin{aligned} SDD(T) &= SDD(H_6) + S(1,2) + S(2,4) + S(1,4) + S(3,4) + S(4,4) - S(3,4) \\ &\leq \phi(m-2) + \frac{45}{4} = \phi(m). \end{aligned}$$

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 $M \setminus \{uv, u_rw_r\}$ is a perfect matching of H_7 and $H_7 \in \mathbb{T}(m-2)$. By the induction hypothesis, we have

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

Hence in this case result is true.

Case 2. When $T \in \mathbb{T}(m)$ has less than m pendant vertices, that is T has at least one vertex which has no pendant neighbour.

Clearly, from Lemma 3.2.1, the contribution of a vertex in the SDD index is maximum if that vertex has a pendant neighbour. Hence $SDD(T) \leq \phi(m)$. □

3.3 Unicyclic Graphs 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.

3.3.1 Lower Bounds for *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

$$E_1(m) = \{e_{12} = 1, e_{22} = 2m - 4, e_{23} = 3\},$$

$$E_2(m) = \{e_{13} = 1, e_{22} = 2m - 3, e_{23} = 2\},$$

$$E_3(m) = \{e_{12} = 2, e_{22} = 2m - 7, e_{23} = 4, e_{33} = 1\},$$

$$E_4(m) = \{e_{12} = 2, e_{22} = 2m - 8, e_{23} = 6\},$$

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

Theorem 3.3.1. 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 $G \in \mathbb{U}(m) \setminus \{C_m\}, m \geq 3$, then $SDD(G) \geq 4m + 1$ and equality hold if and only if $G \in C_1(m)$.

3. If $G \in \mathbb{U}(m) \setminus \{C_m, C_1(m)\}, m \geq 3$, then $SDD(G) \geq 4m + \frac{5}{3}$ 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 $G \in \mathbb{U}(m) \setminus \{C_m, C_i(m)\}(i = 1, 2, 3),\ m \geq 4$, 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, say K.
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 $SDD(G) = S(1, 3) + 2S(2, 3) + 2(2m - 3) = 4m + \frac{5}{3}$. 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 subcases.

1. If w_1 and w_2 are adjacent and both w_1 and w_2 have no pendant neighbour, then $SDD(G) = 2S(1,2) + 4S(2,3) + S(3,3) + 2(2m-7) = 4m + \frac{5}{3}$. 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 both w_1 and w_2 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 or 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
$SDD(G) \geq S(1,2) + S(1,3) + 3S(2,3) + 2(2m-5) = 4m + \frac{7}{3} > 4m + 2$.

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 maximum degree of $\triangle_G = 3$, 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 the vertices w_1, w_2, w_3 are adjacent, then at least five edges connecting vertices of degree two and three exist in G. In that case
$$SDD(G) \geq 3S(1,2) + 5S(2,3) + 2(2m-8) = 2m + \frac{7}{3} > 4m + 2.$$

2. If G has a vertex of degree at least four: Then,
$$SDD(G) \geq 3S(1,2) + S(2,4) + 2(2m-5) = 4m + \frac{5}{2} > 4m + 2.$$

Subcase 4.2. If G has at least one pendant path of length one, since $S(1,4) > S(1,3)$ and $S(2,4) > S(2,3)$, then we have

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

Case 5. If $K \geq 4$, then by Lemma 3.1.1, we have $SDD(G) \geq 4m + \frac{8}{3} > 4m + 2$. □

3.3.2 Upper Bounds for *SDD* Index

In this section, we obtain upper bounds for the SDD index of unicyclic graphs (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.

Let $\mathbb{C}_a(m)$ ($m \geq 6$ and m even) and $\mathbb{C}_b(m)$ ($m \geq 5$ and m is odd) be two collection 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 cardinalties on $2m$ vertices $E_a(G) = \{e_{12} = \frac{m}{2}, e_{14} = \frac{m}{2}, e_{24} = \frac{m}{2}, e_{44} = \frac{m}{2}\}$ 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 3.5, 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 3.5: Representative graphs for $\mathbb{C}_a(m), \mathbb{C}_b(m)$.

Theorem 3.3.2. Let $G \in \mathbb{U}(m)$, $m \geq 4$. Then

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

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

Proof. Let

$$\phi(m) = \begin{cases} \frac{1}{8}(45m) & : \text{if } m \text{ is even,} \\ \frac{1}{8}(45m-1) & : \text{if } m \text{ is odd.} \end{cases} \tag{3.5}$$

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 vertices.

We prove by induction on m: For $m = 4$, $\mathbb{U}(4)$ contains Q_1 and $G_d(4)$ (see Figure 3.6). By direct computation, we get $SDD(Q_1) = 22.08 < \phi(4)$ and $SDD(G_d(4)) = 21.33 < \phi(4)$. Observe that in this case, equality does not hold.

When $m = 5$, $\mathbb{U}(5)$ contains $G_b(5), G_d(5), Q_2, Q_3$ (see Figures 3.5, 3.6). Note that

$$SDD(Q_2) = 27.41 < \phi(5), \qquad SDD(Q_3) = 27.16 < \phi(4),$$
$$SDD(G_d(5)) = 26.66 < \phi(5), \qquad SDD(G_b(5)) = 28 = \phi(5).$$

Thus the result is true for $m = 5$.

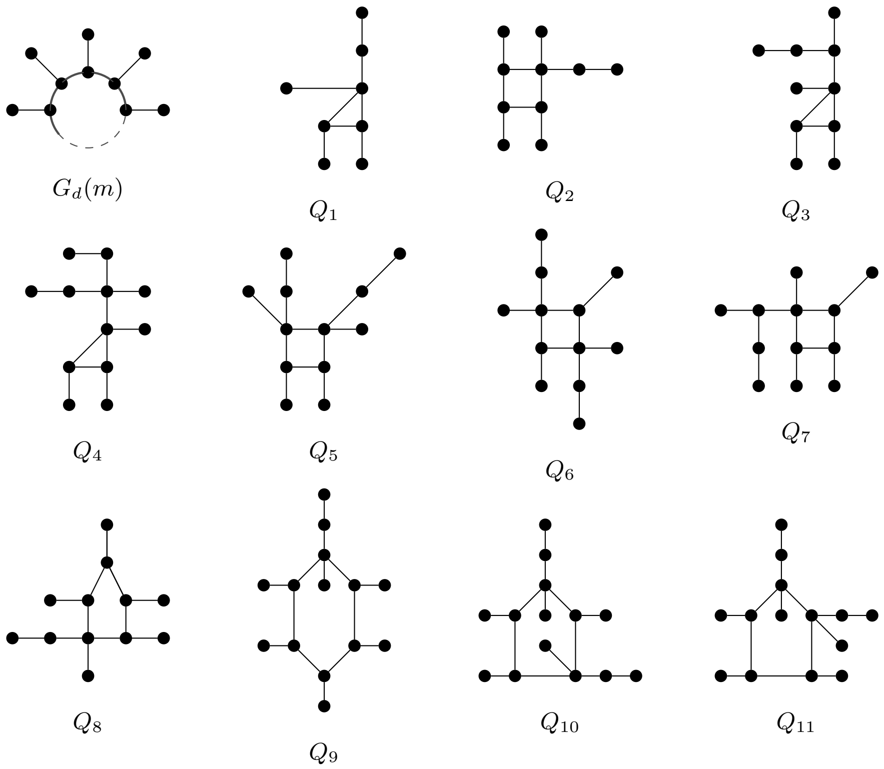


FIGURE 3.6: Collection of unicyclic graph with $m-$pendant vertices on $\mathbb{U}(m)$ for $m = 4, 5, 6, 7$.

When $m = 6$, $\mathbb{U}(6)$ contains Q_i $(i = 4, 5, 6, 7, 8)$, $G_a(6)$ and $G_d(6)$ (see Figures 3.5, 3.6). Note that by direct computation, we have

$SDD(Q_4) = 33.33 < \phi(6)$, $SDD(Q_5) = 33.33 < \phi(6)$, $SDD(Q_6) = 33.5 < \phi(6)$,

$SDD(Q_7) = 32.5 < \phi(6)$, $SDD(Q_8) = 32.75 < \phi(6)$, $SDD(G_d(6)) = 32 < \phi(6)$,

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

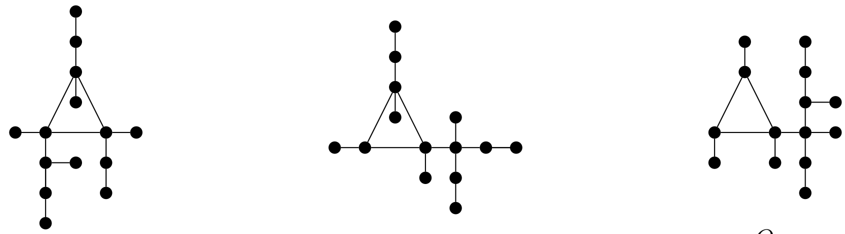
When $m = 7$, $\mathbb{U}(6)$ contains Q_i $(i = 9, 10, 11, 12, 13, 14)$, $G_d(7)$ and $G_b(7)$ (see Figures 3.5, 3.6, 3.7), then by direct calculation, we have

$SDD(Q_9) = 38.083 < \phi(7)$, $\quad SDD(Q_{10}) = 38.83 < \phi(7)$, $\quad SDD(Q_{11}) = 38.66 < \phi(7)$,

$SDD(Q_{12}) = 36.33 < \phi(7)$, $\quad SDD(Q_{13}) = 39.25 \leq \phi(7)$, $\quad SDD(Q_{14}) = 38.41 \leq \phi(7)$,

$SDD(G_d(7)) = 37.33 < \phi(7)$, $\quad$ and $SDD(G_b(7)) = 39.25 = \phi(7)$.

Thus equality holds for $m = 6$ and $m = 7$.



Q_{12} $\quad Q_{13}$ $\quad Q_{14}$

FIGURE 3.7: Collection of unicyclic graph with $m-$pendant vertices on $\mathbb{U}(m)$ for $m = 7$.

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

Subcase 1. 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 of v other than u in G. Then $d(w_r) \geq 3$.

If $d(w_r) = 3$, denote $N_G(w_r) = \{v, u_r, w_{r+1}\}$, 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 exist 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 $\{uv, u_rw_r, u_{r+1}w_{r+1}, \ldots, u_{r+k-1}w_{r+k-1}\} \subseteq M$. Let $C_1 = G - u_r - w_r - u_{r+1} - w_{r+1} - \ldots -$

$u_{r+k-1} - w_{r+k-1} + vw_{r+k}$. 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 C_1 and $C_1 \in \mathbb{U}(m-k)$. By induction hypothesis, we have

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

If $m-k$ is even, then from Equation (3.5), we have

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

If $m-k$ is odd, then from Equation (3.5), we have

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

When $d(w_r) \neq 3$, then $d(w_r) = 4$. Denote $N_G(w_r) = \{w_{r-1}, u_r, v, w_{r+1}\}$, where $d(u_r) = 1$, $d(w_{r-1}) \geq 2$, $d(w_{r+1}) \geq 2$ 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.

When $d(w_{r-1}) = 2$ and $d(w_{r+1}) = 3$. Denote $N_G(w_{r-1}) = \{u_{r-1}, w_r\}$ and $N_G(w_{r+1}) = \{w_r, u_{r+1}, w_{r+2}\}$, where $d(w_{r+2}) \geq 3$. Suppose G has no vertex of degree four except $\{w_r\}$, then G cannot be unicyclic in this subcase. Hence there exists a vertex w_{r+k}, $k \geq 2$ of degree four in G such that $w_{r+1}, w_{r+2}, \ldots, w_{r+k-1}$ are all vertices of degree three. Since G has a perfect matching M, then $\{uv, u_r w_r, u_{r+1}w_{r+1}, \ldots, u_{r+k-1}w_{r+k-1}\} \subseteq M$. Let $C_2 = G - u_r - w_r - u_{r+1} - w_{r+1} - \cdots - u_{r+k-1}w_{r+k-1} + w_{r-1}w_{r+k}$. Then $M \setminus \{uv, u_r w_r, u_{r+1}w_{r+1}, \ldots, u_{r+k-1}w_{r+k-1}\}$ is a perfect matching of C_2 and $C_2 \in \mathbb{U}(m-k-1)$. By induction hypothesis, we have

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

From Equation (3.5), we have

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

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

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

From Equation (3.5), we have

$$SDD(G) \leq \phi(m).$$

When $d(w_{r-1}) = 3 = d(w_{r+1})$: Denote $N_G(w_{r-1}) = \{w_{r-2}, u_{r-1}, w_r\}$ and $N_G(w_{r+1}) = \{w_r, u_{r+1}, w_{r+2}\}$, where u_{r-1}, u_{r+1} are pendant vertices and $d(w_{r-2}) \geq 2$ and $d(w_{r+2}) \geq 2$. Since G has a perfect matching M, then $\{u_{r-1}w_{r-1}, u_{r+1}w_{r+1}\} \subseteq M$. Let $C_4 = G - u - v - w_r - u_r - u_{r-1} - w_{r-1} - u_{r+1} - w_{r+1} + w_{r-2}w_{r+2}$. Then $M \setminus \{u_{r-1}w_{r-1}, uv, u_rw_r, u_{r+1}w_{r+1}\}$ is a perfect matching of C_4 and $C_4 \in \mathbb{U}(m-4)$. By induction hypothesis, we have

$$\begin{aligned} SDD(G) =& SDD(C_4) + S(1,2) + S(2,4) + S(1,4) + 2S(3,4) + 2S(1,3) \\ &+ S(3, d(w_{r-2})) + S(3, d(w_{r+2})) - S(d(w_{r-2}), d(w_{r+2})). \end{aligned}$$

Since $d(w_{r-2}) \geq 2$, $d(w_{r+2}) \geq 2$ and $S(3,2) > S(3,4) > S(x,x)$, for $x > 2$, we have

$$SDD(G) \leq \phi(m-4) + \frac{241}{12} + \frac{13}{3} - 2.$$

From Equation (3.5), we have

$$SDD(G) \leq \phi(m) - \frac{1}{12} < \phi(m).$$

When $d(w_{r-1}) = 3$ and $d(w_{r+1}) = 4$: Let $C_5 = T - u - v - u_r - w_r + w_{r-1}w_{r+1}$, then $M \setminus \{uv, u_rw_r\}$ is a perfect matching of C_5 and $C_5 \in \mathbb{U}(m-2)$. By induction hypothesis, we have

$$\begin{aligned} SDD(G) &= SDD(C_5) + S(1,2) + S(2,4) + S(1,4) + S(3,4) + S(4,4) - S(3,4) \\ &\leq \phi(m-2) + \frac{45}{4}. \end{aligned}$$

From Equation (3.5), we have

$$SDD(G) \leq \phi(m).$$

When $d(w_{r-1}) = d(w_{r+1}) = 4$: Let $C_6 = G - u - v - u_r - w_r + w_{r-1}w_{r+1}$. Then $M \setminus \{uv, u_r w_r\}$ is a perfect matching of C_6 and $C_6 \in \mathbb{U}(m-2)$. By induction hypothesis, we have

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

Hence in this subcase, the result is true.

Subcase 2. No neighbour of pendant vertices has degree two in G.

Since G is unicyclic graph which has a perfect matching and where each vertex of G has a pendant neighbour, we have $G \cong C_d(m)$, where $C_d(m)$ is shown in (Figure 3.6) and $SDD(C_d(m)) = \frac{16}{3}m$. If m is even, then

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

If m is odd, then

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

Hence in this case the result is true.

Case 2. When $G \in \mathbb{U}(m)$ has less than m pendant vertices, that is G has a vertex which has no pendant neighbour. Clearly, from Lemma 3.2.1, we can easily say that the SDD value of any vertex is maximum if it has a pendant neighbour. Hence $SDD(G) \leq \phi(m)$. □

3.4 Summary

In this chapter, 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.

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