The number of independent subsets and the energy of caterpillars under degree restriction

by

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Declaration

I declare that the work in the dissertation entitled "The number of independent subsets and the energy of caterpillars under degree restriction" which I hereby submit for the degree of Doctor of Philosophy in Mathematics at Rhodes University is my own work. I also declare that this research has not been submitted anywhere before and that all the sources that I have used or quoted have been indicated and acknowledged by means of complete references.

S. Xhanti	April 12, 2024
	Date signed

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Abstract

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The energy $En(G)$ of a graph G is defined as the sum of the absolute values of its eigenvalues. The Hosoya index $Z(G)$ of a graph G is the number of independent edge subsets of G, including the empty set. And, the Merrifield-Simmons index $\sigma(G)$ of a graph G is the number of independent vertex subsets of G, including the empty set. The studies of these three graph invariants are motivated by their application in chemistry, combined with pure mathematical interests. In particular, they can be used to predict boiling points of saturated hydrocarbons and estimate the total π-electron energy.

For $\ell \geq 1$, let $a_1, a_2, \ldots, a_\ell$ be non-negative integers, such that a_1 and a_ℓ are positive. The tree obtained from the path graph of vertices $v_1, v_2, \ldots, v_\ell$, by attaching a_i new leaves to v_i, for $1 \leq i \leq \ell$, is called a $(a_1, a_2, \ldots, a_\ell)$-caterpillar and denoted by $C(a_1 + 1, a_2 + 2, \ldots, a_{\ell-1} + 2, a_\ell + 1)$. In this thesis, we characterize extremal caterpillars relative to the energy, the Hosoya index and the Merrifield-Simmons index. We first study caterpillars with the same degree sequence, then compare caterpillars of the same size, same order, and different degree sequence. For any given degree sequence D, we characterize the caterpillar $\mathcal{X}(D)$ that maximizes Z and En. In $\mathcal{X}(D)$, as we move along the internal path towards the center, the degrees are in a non-decreasing order. Characterization of the caterpillar $\mathcal{S}(D)$ that has the minimum Z and En and maximum σ is also provided. In $\mathcal{S}(D)$, large and small degrees alternate.

We also compare $\mathcal{X}(D)$ with $\mathcal{X}(Y)$ and $\mathcal{S}(D)$ with $\mathcal{S}(Y)$, for a degree sequence Y majorized by a degree sequence D. Suppose $Y = (y_1, \ldots, y_n)$ and $D = (d_1, \ldots, d_n)$ are degree sequences such that Y is majorized by D and

$$\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} d_i,$$

then $Z(\mathcal{X}(D)) < Z(\mathcal{X}(Y))$, $Z(\mathcal{S}(D)) < Z(\mathcal{S}(Y))$, $En(\mathcal{X}(D)) < En(\mathcal{X}(Y))$, $En(\mathcal{S}(D)) < En(\mathcal{S}(Y))$, and $\sigma(\mathcal{S}(D)) > \sigma(\mathcal{S}(Y))$, for all positive $x \in \mathbb{R}$. From these results, one deduces that, among all caterpillars of order n and size m, the path graph P_n maximizes Z and En, and minimizes σ. The star S_n minimizes Z and En. The broom $P_{n,2}$ turns out to be the caterpillar with order n and second largest Z and En, and second smallest σ. The double star $S_{n-3,3}$ is the caterpillar with order n and second smallest Z and En.

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"But by the grace of God I am what I am, and His grace toward me was not in vain; but I labored more abundantly than they all, yet not I, but the grace of God which was with me."
1 Corinthians 15:10

Dedications

This work is dedicated to my aunt Pumla Mraji and her better half Tobekile Mraji, who took on the responsibility of raising me, from the day my late mother Nobuntu Xhanti took her last breath.

Nomenclature

Symbols	**Definitions**
$\mathbb{R}$	the set of real numbers
$\mathbb{Z}$	the set of integers
$\mathbb{N}$	the set of natural numbers
$\lceil x \rceil$	the smallest integer greater than or equal to x
$\lfloor x \rfloor$	the largest integer smaller than or equal to x
$\mathbf{I}_n$	the identity matrix of order n
$\det(A)$	the determinant of a matrix A
$V(G)$	the set of vertices of a graph G
$E(G)$	the set of edges of a graph G
$N_G(v)$	the set of vertices adjacent to v in a graph G
$N_G[v]$	the set of vertices v and all its neighbors in a graph G
$\sigma(G)$	the number of independent vertex subsets of a graph G
$m(G,k)$	the number of independent edge subsets of order k of a graph G
$Z(G)$	the number of independent edge subsets of a graph G
$\mu(G,k)$	the number of independent vertex subsets of order k of a graph G
$A(G)$	an adjacency matrix of a graph G
$\phi(G,x)$	the characteristic polynomial of a graph G
$spec(G)$	the spectrum of a graph G
$En(G)$	the energy of a graph G
P_n	the n-vertex path graph
S_n	the n-vertex star
C_n	the n-vertex cycle graph

K_n	a complete graph of order n
$\omega(G)$	the number of connected components of a graph G
$l(P_n)$	the length of the n-vertex path graph
$l(C_n)$	the length of the n-vertex cycle graph
$c(G)$	the cyclomatic number of a graph of a graph G
$A \subseteq B$	the set A is a subset of the set B
$H \subseteq G$	graph H is a subgraph of G
$A \preceq B$	B majorizes A
$K_{p,q}$	the complete bipartite graph with bipartitions of cardinality p and q
$\overline{G}$	the complement of a graph G
$\deg(v)$	the degree of a vertex v
$\delta(G)$	the minimum vertex degree in a graph G
$\Delta(G)$	the maximum vertex degree in a graph G
$\mathbb{T}(D)$	the set of trees with degree sequence D
$\mathbb{T}_{1,d}$	the set of trees with vertex degree either 1 or d
$d_G(u,v)$	the distance between vertices u and v in a graph G
$\epsilon(u)$	the eccentricity of a vertex u
$S_{p,q}$	the double star with heads of order p and q
$P_{n,k}$	the broom with head of order $k+1$ and tail of length $n-k-1$
$T_1 \approx_r T_2$	tree T_1 is root isomorphic to tree T_2
$T_1 \not\approx_r T_2$	tree T_1 is not root isomorphic to tree T_2
$r(B)$	the root of the complete branch B
$rd(B)$	the degree of the root $r(B)$ in B
$G_1 \cup G_2$	the union of the two graphs G_1 and G_2
$G_1 \cong G_2$	graph G_1 is isomorphic to graph G_2
F_n	the n-th fibonacci number
$\mathbb{C}$	the set of all caterpillars of diameter d, size m and order n
$\mathbb{C}_D$	the set of all caterpillars with degree or reduced degree sequence D
$C(d_1, \ldots, d_\ell)$	the caterpillar with ℓ non-leaf vertices $u_1, \ldots, u_\ell$, labelled from left to right, where the degree of u_i is d_i for all i
$()$	mean the zero-tuple

1 Introduction

Mathematical chemistry [133] is the field of study entailing the novel applications of mathematics to chemistry. It focuses on mathematical modelling of chemical phenomena. Chemical Graph Theory [11] is a branch of Mathematical Chemistry that uses graphs to model structure of molecules. One such model is representing atoms as vertices and chemical bonds as edges. The resulting graph is called a molecular graph. Around the middle of the 20th century, several researchers found various relations between the molecular graph and the physico-chemical properties of a molecule corresponding to it, see [64, 106, 140]. These relations drew attention of many researchers. More and more graph invariants were introduced, some have chemical interpretations and some don't: Chromatic index, Wiener index, graph energy, Hosoya index, Merrifield-Simmons index, Lovasz number, Estrada index, number of subtrees, Harary index etc. In this thesis, we will study the energy, Hosoya index and Merrifield-Simmons index of the so-called caterpillars.

Let G be a finite and undirected simple graph with vertex set $V(G)$ and edge set $E(G)$. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$. The adjacency matrix $A(G)$ of G is a square matrix of order n, whose (i, j)-entry is equal to one if the vertices v_i and v_j are adjacent and is equal to zero otherwise. The eigenvalues of $A(G)$ are called the eigenvalues of G, and are denoted as $\lambda_1, \lambda_2, \ldots, \lambda_n$. As a whole they are called the spectrum of G and denoted by $spec(G)$. The energy $En(G)$ [88] of G is defined as the sum of the absolute values of its eigenvalues. The number of independent vertex subsets $\sigma(G)$ of G, including the empty set, is called the Merrifield-Simmons index [106]. Similarly, the number of independent edge subsets $Z(G)$ of G, including the empty set, is called the Hosoya index [64]. The study of the above three mentioned graph invariants is fast growing and most of the work done is on extremal problems, see surveys [135, 153], and the book [88]. Some of the results on extremal problems will be shared in Section 1.6. This thesis is also working on extremal problems.

1.1 Outline of the thesis

This thesis is divided into 6 chapters. Chapter 1 is dedicated to the basic notions and background of the three graph invariants, graph energy, Hosoya index and the Merrifield-Simmons index. Bas-ic notation and terminology, formal definitions, and structures of some extremal graphs are provided there. We establish in Chapter 1 the connections between an auxiliary invariant $M(G, x)$ and the energy and the Hosoya index of G. Using these relations, in Chapter 3, we study $M(G, x)$ and deduce results for En and Z as corollaries. A similar invariant $\sigma(G, x)$ is also defined in Chapter 2. This invariant is introduced so that similar techniques used in Chapter 3 to characterize extremal caterpillars relative to the En and Z can also be used in Chapter 4, to characterize extremal caterpillars relative to the Merrifield-Simmons index. Chapter 2 is reserved for preliminary results that play a vital role in finding formulas and proving results in this thesis. In Chapter 3, the formula of the auxiliary invariant $M(G, x)$ of a caterpillar G is found. Then, it is used to characterize extremal caterpillars relative to the energy and Hosoya index. Simila-rly, in Chapter 4 the formula of $\sigma(G, x)$ is found and the formula is used to characterize extremal caterpillars relative to $\sigma(., x)$ and the Merrifield-Simmons index. Chapter 5 summarizes the results found in this thesis.

1.2 Basic notation and terminology

A non-oriented graph G, which we will simply call a graph, is an ordered pair of sets $G = (V(G), E(G))$, where each element of $E(G)$ is a 2-element subset of $V(G)$. The elements of the sets $V(G)$ and $E(G)$ are called vertices and edges, respectively. The cardinality of $V(G)$ is called the order of G. Similarly, the cardinality of $E(G)$ is called the size of G. In a drawing of a graph, the vertices are usually represented with dots while the edges are represented with lines joining the dots.

Every graph in this thesis is finite, simple and undirected. That is, the number of vertices and edges in a graph is finite, each pair of vertices in G is connected by at most one edge, and all the edges in G are not directed. In a graph, two vertices are said to be adjacent if there is an edge connecting them, and two edges are said to be adjacent if they share a common vertex. A vertex is said to be incident to the edge if it is one of the end points of that edge.

The identity matrix (sometimes called the unit matrix) $\mathbf{I}_n$ of order n is a square matrix of order n with all its diagonal entries equal to 1 and all other entries equal to zero. The adjacency matrix $A(G)$ of the graph G of order n is a square matrix of order n, whose (i, j)-entry is equal to 1 if the vertices v_i and v_j are adjacent and equal to zero otherwise.

A graph of order n is called an n-vertex graph. Similarly, a graph of order n and size m is called (n, m)-graph. The graph of order n and size $\binom{n}{2}$ is a complete graph and is denoted by K_n. A path in a graph is an alternating sequence $v_1, e_1, v_2, e_2 \ldots, v_k, e_k, v_{k+1}$ of distinct vertices and edges, where the edge e_i is incident to v_i and v_{i+1} for all i. The path graph is the graph consisting of only one path. The path graph of order n is denoted by P_n. It is common to find the terms path and path graph used interchangeably since they technical mean the same thing. A graph G is said to be connected if every pair of vertices is connected by some path. Otherwise, G is disconnected, and the number of connected components of G is denoted by $\omega(G)$. An articulation point or cut vertex of a connected graph G is a vertex when deleted with its incident edges from G leaves G disconnected. A cycle in a graph is an alternating sequence $v_1, e_1, v_2, e_2 \ldots, v_k, e_k, v_1$ of distinct vertices and edges, where $k \geq 3$, the edge e_i is incident to v_i and v_{i+1} for all i, and e_k is incident to v_k and v_1. The cycle graph is the graph consisting of only one cycle. It is also common to find the two terms cycle and cycle graph used interchangeable. The length $l(P_n)$ ($l(C_n)$) of a path (cycle) is the number of edges in the path (cycle).

Let G and H be simple graphs, H is said to be a subgraph of G and write $H \subseteq G$ if $V(H)$ is a subset of $V(G)$ and $E(H)$ is subset of $E(G)$. An acyclic graph is a graph without a cycle as its subgraph. An acyclic graph is also called a forest. A tree is a connected acyclic graph, and so a tree of order n has size $m = n - 1$. A graph G of order n and size m is called unicyclic, bicyclic, and tricyclic if G is connected with size $m = n$, $m = n + 1$, and $m = n + 2$, respectively. Note that the definitions of unicyclic, bicyclic and tricyclic graphs have nothing to do with the number of cycles, e.g the bicyclic graph can have three cycles. The cyclomatic number $c(G)$ of a connected graph G of order n and size m is defined as $c(G) = m - n + 1$. A graph G with $c(G) = k$ is said to be k-cyclic.

A bipartite graph $G = (V^{'}(G) \cup V^{''}(G), E(G))$ is a graph composed of two independent sets of vertices (bipartition) $V^{'}(G)$ and $V^{''}(G)$ of cardinality p and q respectively, such that for every edge $uv \in E(G)$, u and v are not in the same partition. If a bipartite graph G has partitions $V^{'}$ and $V^{''}$ of cardinality p and q respectively, and for every pair of vertices $u \in V^{'}$ and $v \in V^{''}$ there exists an edge uv in G, then G is called a complete bipartite graph and is denoted by $K_{p,q}$. Every tree is a bipartite graph and every cycle of even number of vertices is a bipartite graph. The complete bipartite graph $K_{1,n-1}$ is also called the star of order n and is denoted by S_n.

The complement $\overline{G}$ of a graph $G = (V(G), E(G))$ is the graph with the same vertex set $V(G)$, such that two vertices u and v in $\overline{G}$ are adjacent if and only if u and v are not adjacent in G. The edgeless graph of order n is the complement of the complete graph K_n and can also be denoted by $\overline{K_n}$.

The set of vertices adjacent to a vertex v in a graph G is called the neighborhood of v and is denoted by $N_G(v)$, and $N(v)$ when there is no necessity to specify the graph G. The set of vertices v and its neighbors in a graph G is denoted by $N_G[v]$ (i.e $N_G[v] = \{v\} \cup N(v)$), and by $N[v]$ when there is no necessity to specify the graph G. The cardinality of the neighborhood $N(v)$ of a vertex v in a graph G is called the degree of v and is denoted by $\deg(v)$ (i.e $\deg(v) = |N(v)|$. The minimum degree of a graph G is denoted by $\delta(G)$, while the maximum degree is denoted by $\Delta(G)$. A vertex of degree 0 is called an isolated vertex. A vertex of degree 1 is called a leaf vertex (or simply a leaf) and sometimes it is called a pendent vertex. The edge incident with a pendent vertex is called a pendent edge. The non-increasing sequence $D = (d_1, d_2, \ldots, d_n)$ of vertex degrees of a graph G is called the degree sequence of G. We sometimes write $D = \binom{d_1 \quad d_2 \quad \ldots \quad d_{n'}}{\alpha_1 \quad \alpha_2 \quad \ldots \quad \alpha_{n'}}$, where $d_1 < d_2 < \cdots < d_{n'}$ and α_i indicates the number of vertices of degree d_i in G. The reduced degree sequence of a graph G is a non-increasing sequence obtained by removing all the 1's in the degree sequence of G. The degree sequences and reduced degree sequences are equivalent for trees. The set of all trees with degree sequence D will be denoted by $\mathbb{T}(D)$. And all the set of trees with vertex degree 1 or d will be denoted by $\mathbb{T}_{1,d}$.

The distance $d_G(u, v)$ (or simply $d(u, v)$) between two vertices u and v of a graph G is the length of the shortest path joining u and v in G. If G has no path between vertices u and v, then $d_G(u, v) = +\infty$ and the trivial distance between the vertex u and itself is zero (i.e $d_G(u, u) = 0$). The diameter of a graph G is the maximum distance between any pair of vertices of G. The eccentricity of a vertex u, denoted by $\epsilon(u)$ is the maximum distance from u to any vertex v in G, i.e $\epsilon(u) = \max_{v \in V(G)} d(u, v)$. Then, the diameter of a graph G equals the maximum of the vertex eccentricities. The radius of a graph G is the minimum of the vertex eccentricities. The center of a graph is the set of vertices whose eccentricities equal the radius of the graph. The center of a tree is a single vertex called the center vertex, or the ends of an edge called the center edge, see [15]. A centered tree is a tree with only one center and a bicentered tree is a tree with two centers.

Let $P = v_0, e_0, v_1, e_1 \ldots, v_{k-1}, e_{k-1}, v_k$ be a path in a graph G. If $\deg(v_0) \geq 3$, $\deg(v_k) \geq 3$, and $\deg(v_i) = 2$, for $1 \leq i \leq k-1$, then P is said to be an internal segment of G. If $\deg(v_0) \geq 3$, $\deg(v_k) = 1$, and $\deg(v_i) = 2$, for $1 \leq i \leq k-1$, then P is said to be a pendent path of G with root v_0. A segment of a graph G is an internal segment of G, or a pendent path of G, or a cycle in G where all its vertices are of degree 2 except possibly one vertex, which is a cut vertex. The non-increasing sequence of lengths of all the segments of graph G is called the segment sequence of G.

For a given graph $G = (V(G), E(G))$, a subset $\mathbb{H}$ of $E(G)$ is called a matching of G if no two edges in $\mathbb{H}$ are adjacent in G. The edges in $\mathbb{H}$ are said to be independent. The two ends of an edge in a matching $\mathbb{H}$ of a graph G are said to be matched under $\mathbb{H}$. If every vertex in G is matched under $\mathbb{H}$, then $\mathbb{H}$ is said to be a perfect matching. $\mathbb{H}$ is a maximum matching if G has no matching $\mathbb{H}^{'}$ with $|\mathbb{H}^{'}| > |\mathbb{H}|$. Note that $\mathbb{H}$ can be empty. The number of matchings of order k of G is denoted by $m(G, k)$. Note that $m(\emptyset, k) = 0$, for all positive integers k, $m(G, 0) = 1$, and $m(G, 1) = |E(G)|$. Two vertices of a graph G are said to be independent if they are not incident to the same edge. The number of independent vertex subsets of order k of G is denoted by $\mu(G, k)$. Similarly, $\mu(\emptyset, k) = 0$, for all positive integers k, $\mu(G, 0) = 1$, and $\mu(G, 1) = |V(G)|$.

A tree obtained by joining by an edge the centers of two stars S_p and S_q is called the double star and is denoted by $S_{p,q}$. The order of a double star $S_{p,q}$ is $n = p + q$. A comet or a broom $P_{n,k}$ of order n is a tree obtained by merging the center of the star S_{k+1} with one end of the path P_{n-k}. For $n \geq 1$, let $a_1, a_2, \ldots, a_\ell$ be non-negative integers, such that a_1 and a_ℓ are positive, the tree obtained from the path graph $v_1, e_1, v_2, \ldots, e_n, v_\ell$ by attaching a_i new leaves to v_i, for $1 \leq i \leq \ell$, is called a $(a_1, a_2, \ldots, a_\ell)$-caterpillar, and is denoted by $C(a_1 + 1, a_2 + 2, \ldots, a_{\ell-1} + 2, a_\ell + 1)$. The set of all caterpillars with degree or reduced degree sequence D is denoted by $\mathbb{C}_D$. The set of all caterpillars of diameter d, size m and order n is denoted by $\mathbb{C}$. Let D be a degree sequence or a reduced degree sequence of a caterpillar

G. We say G is maximal with regard to an invariant $F(G)$, if and only if $F(G) = \max\{F(C) : C \in \mathbb{C}_D\}$. Likewise, G is said to be minimal with regard to an invariant $F(G)$, if and only if $F(G) = \min\{F(C) : C \in \mathbb{C}_D\}$. If G is either maximal or minimal with regard to an invariant $F(G)$ we say G is extremal.

For a graph G, we use $G - u$ to denote the graph obtained from G by removing the vertex u in G together with all its incident edges, while $G - uv$ denote the graph obtained from G by removing the edge $uv \in E(G)$. Similarly, for a graph G, $G + uv$ is a graph obtained from G by adding the edge $uv \notin E(G)$ in G, where $u, v \in V(G)$. Let G be a graph, $V' \subseteq V(G)$, the graph obtained from G by deleting the vertices in V' together with their incident edges is denoted by $G - V'$. Let $G_1 = (V(G_1), E(G_1))$ and $G_2 = (V(G_2), E(G_2))$ be two graphs. The union $G_1 \cup G_2$ is the graph $G = (V(G_1) \cup V(G_2), E(G_1) \cup E(G_2))$.

The subtree B of a tree T is called a complete branch of T if and only if $T - V(B)$ is connected. The vertex denoted $r(B) \in V(B)$ is called the root of B if and only if it has a neighbor in $T - V(B)$, and the neighbor of $r(B)$ in $T - V(B)$ is denoted by $rn(B)$. Note that there is only one vertex $r(B) \in V(B)$ that has a neighbor in $T - V(B)$, and that neighbor $rn(B) \in V(T - B)$ is unique. The degree of the root $r(B)$ in B is denoted by $\mathrm{rd}(B)$. Note that the degree of the vertex $r(B)$ in T is $rd(B) + 1$. If $B_1, B_2, \ldots, B_{\mathrm{rd}(B)}$ are the connected components of $B - r(B)$, we write $B = [B_1, B_2, \ldots, B_{\mathrm{rd}(B)}]$. For any two rooted trees T_1 and T_2 we write $T_1 \approx_r T_2$ if and only if there exists an isomorphism $f : V(T_1) \to V(T_2)$ which preserves the roots, that is $f(r(T_1)) = r(T_2)$, otherwise we write $T_1 \not\approx_r T_2$. A non-leaf vertex in a tree T, that has at most one neighbor of degree greater than 1 is called a pseudo-leaf. A complete branch B is called a pseudo-leaf branch if its root is a pseudo-leaf, in the original tree T containing B. A pseudo-leaf branch with d vertices is denoted by $[d]$.

Let G be a graph of order n, $A(G)$ its adjacency matrix and $\mathbf{I}_n$ the identity matrix of order n. The characteristic polynomial $\phi(G, x)$ given by $\phi(G, x) = \det(x\mathbf{I}_n - A(G))$ of the adjacency matrix $A(G)$ is the characteristic polynomial of G. Some of the well known properties of the characteristic polynomial $\phi(G, x)$ will be presented in Section 1.3. The roots of the characteristic polynomial $\phi(G, x)$ are called the eigenvalues of G and are denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$. The set of all eigenvalues of a graph G is called the spectrum of G and is denoted by $spec(G)$. For more basic notation and terminology, see standard textbook [36].

1.3 Introduction to graph energy

Let G be a graph of order n, $A(G)$ the adjacency matrix of G, and $\mathbf{I}_n$ a unit matrix of order n. The characteristic polynomial $\phi(G, x)$ of G is given by

$$\phi(G, x) = \det(x\mathbf{I}_n - A(G)) = \sum_{k=0}^{n} a_k x^{n-k}. \tag{1.1}$$

The coefficients a_k of the characteristic polynomial in Equation (1.1) can be obtained using Theorem 1.1 [21], which is best known as the Sachs Theorem.

Theorem 1.1 *(Sachs theorem) Let G be a graph with characteristic polynomial $\phi(G, x) = \sum_{k=0}^{n} a_k x^{n-k}$. Then, $a_0 = 1$ and for $k \geq 1$,*

$$a_k = \sum_{S \in L_k} (-1)^{\omega(S)} 2^{c(S)},$$

where L_k is the set of Sachs subgraphs of G with k vertices, the subgraphs in which every component is either a K_2 or a cycle, $\omega(S)$ is the number of connected components of S, and $c(S)$ is the number of cycles contained in S.

While the adjacency matrix of a graph may depend on the labelling of its vertices, the characteristic polynomial doesn't. Suppose $G_1 \cong G_2$ (G_1 is isomorphic to G_2). Then, there exists a permutation matrix Q, associated with permutations of vertex labelling of G_1, such that $A(G_2) = QA(G_1)Q^{-}$, where Q^{-} is the inverse of the invertible matrix Q. Then,

$$\begin{aligned}
\phi(G_2, x) &= \det(x\mathbf{I}_n - A(G_2)) = \det(x\mathbf{I}_n - QA(G_1)Q^{-}) \\
&= \det(xQ\mathbf{I}_nQ^{-} - QA(G_1)Q^{-}) = \det(Q(x\mathbf{I}_n - A(G_1))Q^{-}) \\
&= \det(Q)\det(x\mathbf{I}_n - A(G_1))\det(Q^{-}) = \det(Q)\det(x\mathbf{I}_n - A(G_1))\frac{1}{\det(Q)} \\
&= \det(x\mathbf{I}_n - A(G_1)) = \phi(G_1, x).
\end{aligned}$$

So, isomorphic graphs have the same characteristic polynomial. It is also possible to have non-isomorphic graphs with the same characteristic polynomial and they are said to be cospectral, see [59]. The following are some basic properties of the characteristic polynomial, which can also be found in [88].

Theorem 1.2 *If $G_1, G_2, \ldots, G_t$ are connected components of a graph G, then*

$$\phi(G,x) = \prod_{j=1}^{t} \phi(G_j, x).$$

Theorem 1.3 *Let $uv \in E(G)$ of a graph G. Then,*

$$\phi(G,x) = \phi(G-uv,x) - \phi(G-u-v,x) - 2\sum_{C\in\mathcal{L}(uv)} \phi(G-C,x),$$

where $\mathcal{L}(uv)$ is the set of cycles containing uv.

The following are direct consequence of Theorem 1.3.

Corollary 1.4 *Let G be a forest and $uv \in E(G)$. Then,*

$$\phi(G,x) = \phi(G-uv,x) - \phi(G-u-v,x).$$

Corollary 1.5 *Let P_n be a path of order n. Then, for $i = 1, 2, \ldots, n$,*

$$\phi(P_n,x) = \phi(P_i,x)\phi(P_{n-i},x) - \phi(P_{i-1},x)\phi(P_{n-i-1},x),$$

where $\phi(P_0,x) = 1$.

Theorem 1.6 *Let G be a forest and $v \in V(G)$. Then,*

$$\phi(G,x) = x\phi(G-v,x) - \sum_{u\in N(v)} \phi(G-u-v,x).$$

Theorem 1.7 *Let G be a graph. Let H be obtained from G by attaching k pendent vertices to each vertex v of G. Then,*

$$\phi(H,x) = x^{nk}\phi\left(G, x-\frac{k}{x}\right).$$

It is convenient to set $\phi(\emptyset,x) = 1$, so that the equation in Theorem 1.3 remains valid for all graphs. The following theorem was first stated explicitly in [64].

Theorem 1.8 *If G is a forest of order n, then*

$$\phi(G,x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k m(G,k) x^{n-2k},$$

where $m(G,k)$ is the number of independent edge subset of order k of G.

The roots of the characteristic polynomial $\phi(G,x)$ of a graph G are called the eigenvalues of G, and are denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$. The set of all the eigenvalues of G, listed in the set according to their multiplicities is called the spectrum of G and is denoted by $spec(G)$. The k-th spectral moment $M_k(G)$ of G is defined as $M_k(G) = \sum_{j=1}^{n} \lambda_j^k$. The Schatten k-norm of a graph G is defined as $(\sum_{j=1}^{n} |\lambda_j|^k)^{1/k}$. The spectrum and spectral moments of graphs have been studied intensively, and have their own applications, see [92, 129]. Similarly, the Schatten k-norm have been studied in matrix theory and functional analysis, see [9,98,111–113]. The k-th spectral moments and Schatten k-norm of a graph G are mentioned because the energy of a graph G seems to be related to them. One such relation is that the energy of a graph G is equivalent to the Schatten 1-norm of G, which is commonly known as the trace class norm. The sum of the absolute values of the eigenvalues of G is called the energy of G, and is denoted by $En(G)$. That is,

$$En(G) = \sum_{j=1}^{n} |\lambda_j|. \tag{1.2}$$

The energy $En(G)$ of a graph G is always greater than zero, except when G is an edgeless graph. The edgeless graph is the only graph that has all its eigenvalues zero. In 1940, Charles Coulson discovered an alternative formula for calculating the energy of a graph G, see [18]. The formula is known as the Coulson integral formula and is given by,

$$En(G) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\left[n - \frac{\mathrm{i}x\phi'(G,\mathrm{i}x)}{\phi(G,\mathrm{i}x)}\right]dx = \frac{1}{\pi}\int_{-\infty}^{+\infty}\left[n - x\frac{d}{dx}\ln\phi(G,\mathrm{i}x)\right]dx, \tag{1.3}$$

where G is a graph, $\phi(G,x)$ is the characteristic polynomial of G, $\phi'(G,x) = \frac{d}{dx}\phi(G,x)$, and $\mathrm{i} = \sqrt{-1}$.

The Coulson integral formula (1.3) shows that the energy of a graph G depends on the characteristic polynomial $\phi(G,x)$ of G, while the sachs Theorem 1.1 reveals that the $\phi(G,x)$ depends on the structure of G. This shows that the energy $En(G)$ depends on the structure of G, see [52]. Let $G_1, G_2, \ldots, G_t$ be the connected components of a graph G, and $n_1, n_2, \ldots, n_t$ their respective orders. Then, using Theorem 1.2 and the Coulson integral formula (1.3), one gets the energy of G as,

$$En(G)$$
$$= \frac{1}{\pi}\int_{-\infty}^{+\infty}\left[n - x\frac{d}{dx}\ln\phi(G,\mathrm{i}x)\right]dx$$

$$= \frac{1}{\pi}\int_{-\infty}^{+\infty}\left[n_1+n_2+\cdots+n_t - x\frac{d}{dx}\ln\phi(G_1\cup G_2\cup\cdots\cup G_t,\mathbf{i}x)\right]dx$$
$$= \frac{1}{\pi}\int_{-\infty}^{+\infty}\left[n_1+n_2+\cdots+n_t - x\frac{d}{dx}\ln\phi(G_1,\mathbf{i}x)\phi(G_2,\mathbf{i}x)\ldots\phi(G_t,\mathbf{i}x)\right]dx$$
$$= \frac{1}{\pi}\int_{-\infty}^{+\infty}\left[n_1+n_2+\cdots+n_t - x\frac{d}{dx}\left(\ln\phi(G_1,\mathbf{i}x)+\cdots+\ln\phi(G_t,\mathbf{i}x)\right)\right]dx$$
$$= \frac{1}{\pi}\int_{-\infty}^{+\infty}\left[n_1 - x\frac{d}{dx}\ln\phi(G_1,\mathbf{i}x)\right]dx+\cdots+\frac{1}{\pi}\int_{-\infty}^{+\infty}\left[n_t - x\frac{d}{dx}\ln\phi(G_t,\mathbf{i}x)\right]dx$$
$$= En(G_1)+En(G_2)+\cdots+En(G_t).$$

Therefore,

Corollary 1.9 *[4] If $G_1, G_2, \ldots, G_t$ are connected components of a graph G, then*

$$En(G) = \sum_{j=1}^{t} En(G_j).$$

There are several modifications of the Coulson integral formula (1.3), and can also be found in [19, 47, 52, 88, 100].

Corollary 1.10 *[47] If G_1 and G_2 are two graphs of the same order n, then*

$$En(G_1) - En(G_2) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\ln\frac{\phi(G_1,\mathbf{i}x)}{\phi(G_2,\mathbf{i}x)}dx. \tag{1.4}$$

Equation (1.4) is known as the Coulson-Jacobs formula, see [19] or a report in [100]. Since $En(G_1)$ and $En(G_2)$ must be real numbers, then the right handside of the Equation (1.4) must be real, that is,

$$En(G_1) - En(G_2) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\ln\left|\frac{\phi(G_1,\mathbf{i}x)}{\phi(G_2,\mathbf{i}x)}\right|dx. \tag{1.5}$$

If we choose $G_2 \cong \overline{K_n}$ and let $\phi(G,x) = \sum_{k=0}^{n} a_k x^{n-k}$, then $\phi(G_1,\mathbf{i}x) = \sum_{k=0}^{n} a_k(\mathbf{i}x)^{n-k}$, $\phi(G_2,\mathbf{i}x) = (\mathbf{i}x)^n$, $En(G_2) = En(\overline{K_n}) = 0$ and

$$En(G_1) = En(G_1) - En(G_2) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\ln\left|\frac{\phi(G_1,\mathbf{i}x)}{\phi(G_2,\mathbf{i}x)}\right|dx$$
$$= \frac{1}{\pi}\int_{-\infty}^{+\infty}\ln\left|\frac{\sum_{k=0}^{n} a_k(\mathbf{i}x)^{n-k}}{(\mathbf{i}x)^n}\right|dx = \frac{1}{\pi}\int_{-\infty}^{+\infty}\ln\left|\sum_{k=0}^{n} a_k(\mathbf{i}x)^{-k}\right|dx$$
$$= \frac{1}{\pi}\int_{-\infty}^{+\infty}\ln\left|\sum_{k\geq 0}(\mathbf{i})^{-2k}a_{2k}x^{-2k} + \sum_{k\geq 0}(\mathbf{i})^{-(2k+1)}a_{2k+1}x^{-(2k+1)}\right|dx$$
$$= \frac{1}{\pi}\int_{-\infty}^{+\infty}\ln\left|\sum_{k\geq 0}(\mathbf{i})^{-2k}a_{2k}x^{-2k} + (\mathbf{i})^{-1}\sum_{k\geq 0}(\mathbf{i})^{-2k}a_{2k+1}x^{-(2k+1)}\right|dx$$

$$= \frac{1}{\pi}\int_{-\infty}^{+\infty} \ln\left|\sum_{k\geq 0}(-1)^k a_{2k}x^{-2k} + \mathbf{i}\sum_{k\geq 0}(-1)^k a_{2k+1}x^{-(2k+1)}\right| dx$$

$$= \frac{1}{\pi}\int_{-\infty}^{+\infty} \ln\left[\sqrt{\left(\sum_{k\geq 0}(-1)^k a_{2k}x^{-2k}\right)^2 + \left(\sum_{k\geq 0}(-1)^k a_{2k+1}x^{-(2k+1)}\right)^2}\right] dx.$$

$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \ln\left[\left(\sum_{k\geq 0}(-1)^k a_{2k}x^{-2k}\right)^2 + \left(\sum_{k\geq 0}(-1)^k a_{2k+1}x^{-(2k+1)}\right)^2\right] dx.$$

Let $z = 1/x$, then

$$En(G_1) = En(G_1) - En(G_2)$$

$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{1}{z^2}\ln\left[\left(\sum_{k\geq 0}(-1)^k a_{2k}z^{2k}\right)^2 + \left(\sum_{k\geq 0}(-1)^k a_{2k+1}z^{2k+1}\right)^2\right] dz. \tag{1.6}$$

The Coulson-type formula in Equation (1.6) is commonly used in deriving explicit formulas of energies of graphs, and when comparing the energies of two graphs, see [57, 58, 151, 152, 154] and the book [88]. We have already seen in Theorem 1.8 the relationship between the number of matchings $m(G, k)$ of order k and a characteristic polynomial $\phi(G, x)$ of a forest G. This implies the following relation between the number of matchings of order k and the energy of a forest G.

Theorem 1.11 *[52] If G is a forest of order n, then*

$$En(G) = \frac{2}{\pi}\int_{0}^{+\infty} \frac{1}{x^2}\ln\left[\sum_{k\geq 0} m(G,k)x^{2k}\right] dx, \tag{1.7}$$

where $m(G, k)$ is the matching number of order k.

This relation motivates us to use the auxiliary graph invariant $M(G, x)$ of a graph G, which in turn helps us study the energy $En(G)$ and Hosoya index $Z(G)$ (to be introduced in Section 1.4) together.

Definition 1.12 Let G be a graph of order n and $m(G, k)$ the number of matchings of order k. The auxiliary invariant $M(G, x)$ is defined to be

$$M(G, x) = \sum_{k\geq 0} m(G, k)x^k.$$

Then, the Equation (1.7) can be rewritten as

$$En(G) = \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2}\ln M(G, x^2)dx. \tag{1.8}$$

Remark 1.13 It is clear from Equation (1.8), that if T and $T^{'}$ are trees and $M(T, x) \leq M(T^{'}, x)$, for all positive $x \in \mathbb{R}$, then $En(T) \leq En(T^{'})$. If furthermore, there exists a positive $x \in \mathbb{R}$, such that $M(T, x) < M(T^{'}, x)$, then $En(T) < En(T^{'})$.

The study of the energy of graphs can be traced back to the 1930s, to the German physicist Eric Hückel, who brought forward a method of finding approximate solutions of the time-independent Schrödinger equation of the conjugated hydrocarbons. His approach was later known as the "Hückel Molecular Orbital (HMO) theory". The HMO theory can be found in relevant textbooks such as [20, 30]. In his theory, he shows that the total π-electron energy of a conjugated hydrocarbon in β-units can be predicted using the eigenvalues of its molecular graph. In a chemical structure of a molecule, remove all the hydrogen atoms with their bonds, so that the carbon to carbon atom skeleton is left, then replace each carbon with a vertex and each bond (whether single, double or triple) with an edge. The newly formed structure is a molecular graph of such molecule, see the books [37,52] and the reviews [40,45,54]. The total π-electron energy being predicted by the Equation (1.9)

$$En(G) = 2\sum_{+} \lambda_j, \tag{1.9}$$

where G is the molecular graph and $\sum_{+}$ indicates summation over positive eigenvalues. Since the sum of all the eigenvalues of a molecular graph is zero, then

$$En(G) = 2\sum_{+} \lambda_j = \sum_{j=1}^{n} |\lambda_j|. \tag{1.10}$$

$En(G)$ was later known as the HMO total π-electron energy. Equation (1.10) is the same as Equation (1.2) except that at this stage it was not known that Equation (1.10) was valid for all graphs, see [18, 60, 101, 120, 121]. These results motivated Ivan Gutman to propose the energy of graphs to be that of Equation (1.2) and which was initially stated publicly in a conference held in Austria [39], in 1978. Then, later restated on several other lectures and conferences as well as the papers [42, 47] and the books [23, 52]. The study of the energy of graphs did not attract many researchers in its early days, we only saw a significant change in the number of publications between 2000 and 2001 and then between 2006 and 2007 and from then we had a significant number of publications. The survey on the growth of the study of energy of graphs, one should consult [27, 47–49], monographs [13, 21–25] and the books [6, 88, 107]. The graph energy has been found to be related to the graph entropy, see [28, 87]. The graph energy has also found its application in modelling protein properties, see [31, 141, 149, 150]. More on the applications of the energy of graphs, one should consult [1, 7, 108, 126, 127, 134, 143]. To complete this introduction on graph energy, we present in Section 1.6, some results on extremal graphs relative to the energy. We next introduce the so-called Hosoya index.

1.4 Introduction to the Hosoya index

The Hosoya index $Z(G)$ of a graph G is defined as the total number of matchings in G, that is,

$$Z(G) = \sum_{k \geq 0} m(G, k), \tag{1.11}$$

where, $m(G, k)$ is the number of matchings of order k. Recall that, $m(G, 0) = 1$, $m(G, 1) = |E(G)|$, and $m(\emptyset, k) = 0$, for all positive $k \in \mathbb{Z}$. Hence, the Hosoya index of a graph G is always greater than or equal to 1, even if G is empty.

Remark 1.14 It is clear that $Z(G) = M(G, 1)$. And if G and $G^{'}$ are two graphs, such that for all positive $x \in \mathbb{R}$, $M(G, x) \leq M(G^{'}, x)$, then $Z(G) \leq Z(G^{'})$. Note that, it is possible to have two trees T and $T^{'}$ such that, for all positive $x \in \mathbb{R}$, $M(T, x) \leq M(T^{'}, x)$, $Z(T) = Z(T^{'})$ and $En(T) < En(T^{'})$. But if $M(T, x) \leq M(T^{'}, x)$ for all positive x and $En(T) = En(T^{'})$, then $Z(T) = Z(T^{'})$.

The Hosoya index possesses the following properties, which will be realised later in Chapter 2.

Lemma 1.15 *[2] Let G and $G^{'}$ be two disjoint graphs. Then:*
(i) $Z(G \cup G^{'}) = Z(G)Z(G^{'})$.
(ii) If $v \in V(G)$, then

$$Z(G) = Z(G - v) + \sum_{w \in N(v)} Z(G - \{v, w\}).$$

(iii) If $uv \in E(G)$, then

$$Z(G) = Z(G - uv) + Z(G - \{u, v\}).$$

The Hosoya index, also known as the Z-index, was introduced by the Japanese chemist Haruo Hosoya. He discovered that this topological index (or graph invariant) can be used to characterize the topological nature of structural isomers of saturated hydrocarbons. To be more precise, in 1971 he published a paper [64] titled "Topological Index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons". In that paper, he showed that: There is a strong correlation between the Hosoya index and the characteristic polynomial of the molecular graphs of saturated hydrocarbons. By setting $x = 1$, in Theorem 1.8, we can get a sense of this correlation, when we consider the set of trees. The correlation between the Hosoya index and the boiling points of saturated hydrocarbons, the correlation between the Hosoya index and the Fibonacci numbers are also pointed out in that paper. Following this paper, several papers [35,41,66,70,74,75,99,109,110] show-ed that the Hosoya index is related with a variety of physico-chemical properties of alkanes. To illustrate, Hosoya and Gao [35] find that the boiling points of alkanes are strongly correlated to the Hosoya index. Hosoya, Gotoh, Murakami and Ikeda, also find [70] the correlation between the density of liquids and the Hosoya index, and hence the dependency of the Hosoya index to the molecular structure of alkanes. And finally, Hosoya [66] further show that a highly branched gasoline isomer must have low boiling points and smaller Hosoya index. Another series of papers pointed out the applications of the Hosoya index in the theory of conjugated π-electron systems, see [50, 55, 56, 65, 71, 72]. In particular, Gutman, Furtula, Vidovic, and Hosoya [50] in their attempt to examine the structure-dependence of the total π-electron energy, they find that all chemical trees have a positive and unique solution to the so called Coulson function ($F(G, x) = \ln Z(G)$), and that the solutions, irrespective of their size and other structural features, are nearly equal to an estimate of 1.2. More on the chemical aspects and applications of the Hosoya index one should also consult [67–69, 73]. While the Hosoya index was still enjoying the attention it was getting, about a decade later a new similar topological index was introduced by Richard E. Merrifield and Howard E. Simmons. We next introduce the Merrifield-Simmons index also known as the number σ.

1.5 Introduction to the Merrifield-Simmons index

The Merrifields-Simmons index $\sigma(G)$ of a graph G is defined as the total number of independent vertex subsets of G, including the empty set. That is,

$$\sigma(G) = \sum_{k\geq 0} \mu(G,k),$$

where $\mu(G,k)$ denotes the number of independent vertex subsets of order k of G. By definition, $\mu(G,0) = 1$, $\mu(\emptyset,k) = 0$, and $\mu(G,1) = |V(G)|$, for all positive $k \in \mathbb{Z}$. Hence, the Merrifield-Simmons index of a graph G is always greater than or equal to 1, even if G is empty. The Merrifield-Simmons index possesses the following properties, which are similar to those of the Hosoya index.

Lemma 1.16 *[106] Let G and G' be two disjoint graphs. Then:*
(i) $\sigma(G \cup G') = \sigma(G)\sigma(G')$.
(ii) If $v \in V(G)$, then

$$\sigma(G) = \sigma(G - v) + \sigma(G - N[v]).$$

(iii) If $uv \in E(G)$, then

$$\sigma(G) = \sigma(G - uv) - \sigma(G - N[u] \cup N[v]).$$

The Merrifield-Simmons index was introduced as the number σ, by the American chemists Richard E. Merrifield and Howard E. Simmons. In their attempt to give an answer to the question, "to what extent can the topological spaces be used to describe the structure of molecules?", they discovered the number σ, which was the number of open sets of the finite topology. The year was 1980 and the paper was titled "The Structures of Molecular Topological Spaces". In that paper they discovered that this number σ is equal to the number of independent vertex subsets of the associated molecular graph. They pointed out the correlation between the number σ and alkane heat formations, the correlation between the number σ and the alkane boiling points, and the correlation between the number σ and the fibonacci numbers. To which, regarding the latter, they showed that $\sigma(P_n) = F_{n+1}$. The two continued to strengthen their theory on using topological spaces to describe the structure of molecules, and published a series of articles [102–104, 106, 124] and the book [105]. Despite the hard work, their theory did not get much attention. Recognizing the similarities between the Hosoya index and the number σ, researchers did not see the number σ as a topological index on its own right, rather as the Hosoya index of the second kind, see [51]. It was until the Serbian chemist and mathematician Ivan Gutman in [43], who first mentioned the number σ as the Merrifield-Simmons index, then followed two papers [44,46], that the number σ was accepted as a topological index and the name Merrifield-Simmons index was used since then. We next highlight some of the known results on extremal graphs, relative to the energy, Hosoya index and the Merrifield-Simmons index.

1.6 Selected results on graph energy, Hosoya index, and the Merrifield-Simmons index

The energy, the Hosoya index and the Merrifield-Simmons index are among graph invariants that have applications in chemistry, in describing physico-chemical properties of molecules. In recent years, a lot of work has been done on the extremal problems, i.e. on characterizing graphs within prescribed classes that minimize or maximize the value of the index. We have seen in the previous sections that, if $G_1, G_2, \ldots, G_t$ are components of a graph G, then $En(G) = \sum_{j=1}^{t} En(G_j)$, $Z(G) = \prod_{j=1}^{t} Z(G_j)$ and $\sigma(G) = \prod_{j=1}^{t} \sigma(G_j)$. In view of these relations, most authors only study connected graphs.

We have also seen the similarities between the Hosoya index and the Merrifield-Simmons index, and the relation between the energy and the Hosoya index of trees through the auxiliary invariant $M(G,x)$. It turned out in [136], that there exists a negative correlation between the Hosoya index and the Merrifield-Simmons index, when the family of trees is considered. Even though there is no explicit formula showing the relation between the Hosoya index and the Merrifield-Simmons index, we note that in most, not all classes of graphs, the graph that maximizes the Hosoya index minimizes the Merrifield-Simmons index, and vice versa. Also the graph that maximizes/minimizes the Hosoya index maximizes/minimizes the energy, this has been proven for some non-trees, see [76].

When all graphs of order n, are considered, the edgeless graph $\overline{K_n}$ maximizes the Merrifield-Simmons index (with $\sigma(\overline{K_n}) = 2^n$, note that all the vertices in $\overline{K_n}$ are independent from each other) and minimizes the Hosoya index (with $Z(\overline{K_n}) = 1$, for only the empty set) and energy (with $En(\overline{K_n}) = 0$, since all the eigenvalues are 0). While, the complete graph K_n minimizes the Merrifield-Simmons index (with $\sigma(K_n) =$

$n+1$) and maximizes the Hosoya index (with $Z(K_n) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{2^k k!(n-2k)!}$, see [135]). Among all graphs of order n, the graph maximizing the energy is still unknown. We are aware of the recent upper bound found in [12].

When we consider only connected graphs of order n, the complete graph K_n still minimizes the Merrifield-Simmons index and maximizes the Hosoya index. While, the path graph P_n maximizes the Merrifield-Simmons index (with $\sigma(P_n) = F_{n+2}$) and minimizes the Hosoya index (with $Z(P_n) = F_{n+1}$). And the energy is minimized by a star S_n (with $En(S_n) = 2\sqrt{n-1}$). For more explanations on the above discussion, see survey [135] and book [88]. When extra conditions are imposed on connected graphs of order n, one can also consult the papers [14, 62, 115, 119, 132, 147, 155] for the Hosoya index and Merrifield-Simmons index, the book [88] for the graph energy, and the references therein.

When the family of trees of order n is considered, the star S_n maximizes the Merrifield-Simmons index (with $\sigma(S_n) = 2^{n-1}+1$) and minimizes the Hosoya index (with $Z(S_n) = n$) and the energy. While, the path graph P_n minimizes the Merrifield-Simmons index and maximizes the Hosoya index and energy, where

$$En(P_n) = \begin{cases} \frac{2}{\sin \frac{\pi}{2(n+1)}} - 2 & \text{if } n \equiv 0 (\bmod 2) \\ \frac{2\cos \frac{\pi}{2(n+1)}}{\sin \frac{\pi}{2(n+1)}} - 2 & \text{if } n \equiv 1 (\bmod 2) \end{cases}.$$

These results can also be found in [4, 38, 52, 88, 135]. It is natural that once you have characterized the graph that attains the first largest/smallest value of a certain graph invariant, one may want to characterize the graph that attains the second largest/smallest value of that invariant. Well, for the Hosoya index and the Merrifield-Simmons index one can consult the papers [38, 83, 89, 90, 137], for the trees attaining the second largest and second smallest value of the Hosoya index and the Merrifield-Simmons index. On the ordering of trees from the tree with the smallest energy, one may consult [53, 79, 84, 85, 122, 123, 125], and the ordering of trees from the tree with the largest energy, one may consult [3, 88].

The broom $P_{n,k-1}$ has been found to maximize the Merrifield-Simmons index and minimize the Hosoya index among all trees of order n and k-leaves, see [114, 146]. The characterization of a tree attaining the second largest Merrifield-Simmons index and second smallest Hosoya index can be found in [96, 138]. The characterization of a tree of order n and k-leaves that minimizes the Merrifield-Simmons index and maximizes the Hosoya index was studied in [29, 144]. For more on the number of maximal independent sets in trees with a given number of leaves, one may consult the recent paper [130]. The broom has also been found to be extremal among all trees of order n and diameter d, see [17, 83, 89, 114, 116, 145]. The broom minimizes the Hosoya index and maximizes the Merrifield-Simmons index. Among all trees of order n and diameter d, the second and third on the list of extremal trees is characterized in [91]. As we have stated earlier, that the study of these graph invariants is fast growing and we can't capture every single detail in this thesis, the interested reader is referred to the surveys [135, 153] for the Hosoya index and Merrifield-Simmons index, the book [88] for the graph energy, and for the recent results: For graph energies of general graphs, see [10,12,82,118]. For graph energies of trees, see [81]. For graph energies of unicyclic graphs, see [8, 139]. For graph energies of bicyclic graphs, see [80]. For graph energies of tricyclic graphs, see [16,86,97,128,157]. For independent subsets of general graphs, see [14, 62, 78, 115, 119, 132, 147, 155]. For independent subsets of trees, see [131, 159]. For independent subsets of unicyclic graphs, see [5, 77, 93, 95, 139, 148, 156]. For independent subsets of bicyclic graphs, see [142]. For independent subsets of tricyclic graph, see [26, 32–34, 61, 94, 117, 128, 157, 158].

Going back to the energy, Hosoya index and the Merrifield-Simmons index of trees. In [4], Eric Andriantiana investigated the energy, Hosoya index and Merrifield-Simmons index of trees under degree restrictions. In his paper, he showed that the tree $\mathcal{M}(d_1, d_2, \ldots, d_n)$ is the unique (up to isomorphism) tree that maximizes the Merrifield-Simmons index among all trees with reduced degree sequence $d_1, d_2, \ldots, d_n$, where $\mathcal{M}(d_1, d_2, \ldots, d_n)$ is constructed as follows: Let $d_1, d_2, \ldots, d_n$ be a reduced degree sequence of a tree T. If $n \leq d_n + 1$, then $\mathcal{M}(d_1, d_2, \ldots, d_n)$ is the tree obtained by merging the root of each of $[d_1], [d_2], \ldots, [d_{n-1}]$ with a leaf of $[1 + d_n]$, respectively. If $n \geq d_n + 2$, then $\mathcal{M}(d_1, d_2, \ldots, d_n)$ is constructed recursively: First label vertices as shown in Figure 1.1, such that

$$\deg(v_i) \leq \deg(v_j), \text{ if } i < j. \tag{1.12}$$

Let l be the greatest integer, such that v_l is a label in $\mathcal{M}(d_{d_n}, \ldots, d_{n-1})$. Let s be the smallest integer, such that v_s is adjacent to a leaf in $\mathcal{M}(d_{d_n}, \ldots, d_{n-1})$. Let $R_{d_n} = [[d_1], \ldots, [d_{d_n-1}]]$, where the pseudo-leaves are labelled $v_{l+1}, \ldots, v_{l+d_n-1}$, respecting Inequality (1.12). $\mathcal{M}(d_1, d_2, \ldots, d_n)$

Figure 1.1: Relabeling for the construction of $\mathcal{M}(d_1, d_2, \ldots, d_n)$.

is the tree obtained by merging the roots of R_{d_n} to a leaf adjacent to v_s. See Figure 1.2, for example. Following his work, we wondered

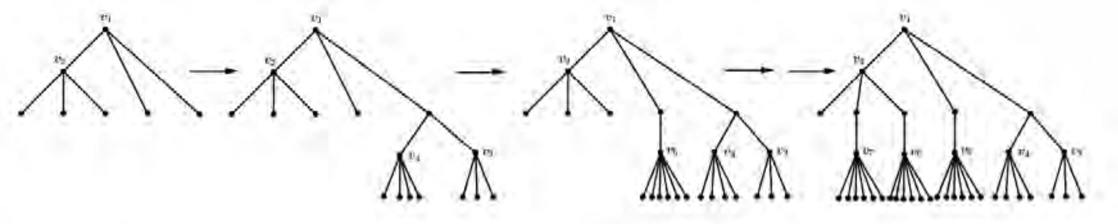

Figure 1.2: Step-by-step construction of $\mathcal{M}(7, 7, 7, 5, 4, 4, 3, 3, 2, 2, 2)$.

what would be the properties of extremal caterpillars relative to the energy, Hosoya index and the Merrifield-Simmons index, when the family of caterpillars with prescribed degree sequence is considered. In this thesis we characterize the caterpillar minimizing the Hosoya index and energy, caterpillar maximizing the Merrifield-Simmons index, and finally, we characterize the caterpillar maximizing the Hosoya index and energy. The attempt on characterization of caterpillars minimizing the Merrifield-Simmons index became a little harder, and we leave a conjecture regarding this matter. We next present preliminary results that play a vital role in the derivation of formulas and proving of results in this thesis.

2 Preliminaries

In this chapter we present basic lemmas that will be useful in Chapters 3 and 4. In Chapter 1, we defined the auxiliary invariant $M(G, x)$ of a graph G as

$$M(G, x) = \sum_{k\geq 0} m(G, k)x^k.$$

It possesses the following properties.

Lemma 2.1 ([2]) *Let G and G' be two disjoint graphs and let $x > 0$ be a real number. Then, we have*

$$M(G \cup G', x) = M(G, x)M(G', x). \tag{2.1}$$

If $v \in V(G)$, then we have

$$M(G, x) = M(G - v, x) + x \sum_{w\in N_G(v)} M(G - \{v, w\}, x). \tag{2.2}$$

For any $uv \in E(G)$ we have

$$M(G, x) = M(G - uv, x) + xM(G - \{u, v\}, x). \tag{2.3}$$

Proof. Let G and G' be two disjoint graphs and let $x > 0$ be a real number. Then, for every pair of edges e_1 and e_2 with $e_1 \in E(G)$ and $e_2 \in E(G')$, $e_1 \cap e_1 = \emptyset$. Then, in order to form an independent edge subset of cardinality k in $G \cup G'$, we take an independent edge subset of cardinality j in G and another of cardinality $k - j$ in G', for some $0 \leq j \leq k$. Hence $m(G \cup G', k) = \sum_{\substack{j+j'=k \\ j\geq 0, j'\geq 0}} m(G, j)m(G', j')$. Then,

$$M(G \cup G', x) = \sum_{k\geq 0} m(G \cup G', k)x^k = \sum_{k\geq 0} \left(\sum_{\substack{j+j'=k \\ j\geq 0, j'\geq 0}} m(G, j)m(G', j') \right) x^k$$

$$= \sum_{k\geq 0}\left(\sum_{\substack{j+j'=k\\ j\geq 0, j'\geq 0}} m(G,j)m(G',j')\right) x^{j+j'}$$
$$= \sum_{j\geq 0} m(G,j)x^j \sum_{j'\geq 0} m(G',j')x^{j'} = M(G,x)M(G',x).$$

Hence Equation (2.1).

Suppose $v \in V(G)$. Suppose we remove the vertex v from G. Then, for every pair of edges e_1 and e_2 in $G-v$, $e_1 \cap e_2 = \emptyset$ if and only if $e_1 \cap e_2 = \emptyset$ in G. Thus, any independent edge subset of $G - v$ are independent edge subsets of G. So $m(G,k) = m(G-v,k) + r$, for some positive real number r. The independent edge subsets in G that are not counted in $m(G-v,k)$ are the ones that contain v. Note that, if any subset contains v, then it can not contain the edge incident to the neighbor of v. Hence $m(G,k) = m(G-v,k) + \sum_{w\in N(v)} m(G-\{v,w\}, k-1)$. Then,

$$M(G,x) = \sum_{k\geq 0} m(G,k)x^k$$
$$= \sum_{k\geq 0}\left(m(G-v,k) + \sum_{w\in N(v)} m(G-\{v,w\},k-1)\right)x^k$$
$$= \sum_{k\geq 0} m(G-v,k)x^k + \sum_{k\geq 0}\sum_{w\in N(v)} m(G-\{v,w\},k-1)x^k$$
$$= \sum_{k\geq 0} m(G-v,k)x^k + x\sum_{w\in N(v)}\sum_{k\geq 0} m(G-\{v,w\},k-1)x^{k-1}$$
$$= M(G-v,x) + x\sum_{w\in N(v)} M(G-\{v,w\},x).$$

Hence Equation (2.2).

Suppose $uv \in E(G)$. Suppose we remove the edge uv from G. Then, for every pair of edges e_1 and e_2 in $G-uv$, $e_1 \cap e_2 = \emptyset$ if and only if $e_1 \cap e_2 = \emptyset$ in G. Thus, any independent edge subset of $G - uv$ are independent edge subsets of G. So $m(G,k) = m(G-uv,k)+r$, for some positive real number r. The independent edge subsets in G that are not counted in $m(G-uv,k)$ are the ones that contain the edge uv. Note that, if any subset contains uv, then it can not contain any other edge incident to u, and cannot contain any other edge incident to v. Hence $m(G,k) = m(G-uv,k) + m(G-\{u,v\},k-1)$. Then,

$$
\begin{aligned}
M(G,x) = \sum_{k\geq 0} m(G,k)x^k &= \sum_{k\geq 0} \left(m(G-uv,k) + m(G-\{u,v\},k-1)\right)x^k \\
&= \sum_{k\geq 0} m(G-uv,k)x^k + \sum_{k\geq 0} m(G-\{u,v\},k-1)x^k \\
&= \sum_{k\geq 0} m(G-uv,k)x^k + x\sum_{k\geq 0} m(G-\{u,v\},k-1)x^{k-1} \\
&= M(G-uv,x) + xM(G-\{u,v\},x).
\end{aligned}
$$

Hence Equation (2.3). □

Note that the Hosoya index of a graph G is given by, $Z(G) = M(G,1)$. Hence the properties of the Hosoya index in Section 1.4 follow from those of $M(G,x)$ in Lemma 2.1.

Definition 2.2 For every complete branch B of a tree, we define $m_0(B,k)$ to be the number of matchings of order k in B, not covering the root $r(B)$, $M_0(B,x) = \sum_{k\geq 0} m_0(B,k)x^k$, and $\tau(B,x) = \frac{M_0(B,x)}{M(B,x)}$. Induction on $M(B,x)$ and Lemma 2.1 give the following properties of $\tau(B,x)$.

Lemma 2.3 ([4]) *Let $B = [B_1,\ldots,B_{\mathrm{rd}(B)}]$ be a complete branch of a tree. Then, for all positive x we have*

$$\tau(B,x) = \frac{1}{1 + x\sum_{i=1}^{\mathrm{rd}(B)} \tau(B_i,x)}. \tag{2.4}$$

It is convenient to set $\tau(\emptyset,x) = 0$ for all $x > 0$, so that recurrence 2.4 still holds if some of the B_i's are empty.

Lemma 2.4 ([4]) *Let B be a complete branch of a tree and $x > 0$. Then,*

$$\frac{1}{1 + x\,\mathrm{rd}(B)} \leq \tau(B,x) \leq 1.$$

Remark 2.5 Note that the upper bound 1 is reached only if B is a leaf. It follows that the lower bound is also obtained only if B is a pseudo-leaf branch.

We define $\sigma(G,x)$ of a graph G and $\rho(B,x)$ of a complete branch B, so that the techniques used in Chapter 3 using $M(G,x)$ and $\tau(B,x)$ to characterize extremal caterpillars relative to the energy and Hosoya index, can be deployed also in Chapter 4 using $\sigma(G,x)$ and $\rho(B,x)$ to characterize extremal caterpillars relative to the Merrifield-Simmons index.

Definition 2.6 Let G be a graph. Let $\mu(G,k)$ denote the number of independent vertex subsets of order k in G. For a rooted tree T with root v, we also define $\mu_0(T,k)$ to be the number of independent vertex subsets of order k in T not containing the root v and $\mu_1(T,k)$ to be the number of independent vertex subsets of order k in T containing the root v. Let $x > 0$ be a real number, then $\sigma(T,x)$, $\sigma_0(T,x)$ and $\sigma_1(T,x)$ are defined to be:

$$\sigma(T,x) = \sum_{k\geq 0} \mu(T,k)x^k,$$

$$\sigma_0(T,x) = \sum_{k\geq 0} \mu_0(T,k)x^k$$

and

$$\sigma_1(T,x) = \sum_{k\geq 0} \mu_1(T,k)x^k,$$

respectively. We also define $\rho(T,x)$ to be $\rho(T,x) = \dfrac{\sigma_0(T,x)}{\sigma(T,x)}$. Note that $\sigma(T,x) = \sigma_0(T,x) + \sigma_1(T,x)$, and $\sigma(G,1) = \sigma(G)$.

Lemma 2.7 ([2]) *Let G be a graph.*
(i) If $uv \in E(G)$, then

$$\sigma(G,x) = \sigma(G-uv,x) - x\sigma(G-N[u]\cup N[v],x).$$

(ii) If $v \in V(G)$, then

$$\sigma(G,x) = \sigma(G-v,x) + x\sigma(G-N[v],x).$$

(iii) If $G_1, G_2, \ldots, G_t$ are the connected components of G, then

$$\sigma(G,x) = \prod_{j=1}^{t} \sigma(G_j,x).$$

Proof. (i) Let G be a graph. Suppose $uv \in E(G)$. Suppose we remove the edge uv from G. After removing uv from G, to get $G-uv$, the independent vertex subsets of order k containing both u and v are counted in $\mu(G-uv,k)$. So, to get the correct value for $\mu(G,k)$ we need to remove those subsets. Note that if both u and v are present in an idependent vertex subset, then their neighbors cannot be in that independent vertex subset. Hence

$$\mu(G,k) = \mu(G-uv,k) - \mu(G-N[u]\cup N[v],k-1).$$

Then,

$$
\begin{aligned}
\sigma(G,x) &= \sum_{k\geq 0}\sigma(G,k)x^k = \sum_{k\geq 0}\left(\mu(G-uv,k)-\mu(G-N[u]\cup N[v],k-1)\right)x^k \\
&= \sum_{k\geq 0}\mu(G-uv,k)x^k - \sum_{k\geq 0}\mu(G-N[u]\cup N[v],k-1)x^k \\
&= \sum_{k\geq 0}\mu(G-uv,k)x^k - x\sum_{k\geq 0}\mu(G-N[u]\cup N[v],k-1)x^{k-1} \\
&= \sigma(G-uv,x) - x\sigma(G-N[u]\cup N[v],x).
\end{aligned}
$$

(ii) Suppose $v \in V(G)$. Suppose we remove v from G. Then, for every pair of vertices v_1 and v_2 in $G-v$, $v_1v_2 \notin E(G-v)$ if and only if $v_1v_2 \notin E(G)$. Thus, any independent vertex subset of $G-v$ are independent vertex subsets of G. So, $\mu(G,k) = \mu(G-v,k)+r$, for some positive real number r. The independent vertex subsets with k elements in G that are not counted in $\mu(G-v,k)$ are the ones that contain v. Note that, if an independent vertex subset contains v, then it cannot contain any neighbor of v. Hence,

$$\mu(G,k) = \mu(G-v,k) + \mu(G-N[v],k-1).$$

Then,

$$
\begin{aligned}
\sigma(G,x) &= \sum_{k\geq 0}\mu(G,k)x^k = \sum_{k\geq 0}\left(\mu(G-v,k)+\mu(G-N[v],k-1)\right)x^k \\
&= \sum_{k\geq 0}\mu(G-v,k)x^k + \sum_{k\geq 0}\mu(G-N[v],k-1)x^k \\
&= \sum_{k\geq 0}\mu(G-v,k)x^k + x\sum_{k\geq 0}\mu(G-N[v],k-1)x^{k-1} \\
&= \sigma(G-v,x) + x\sigma(G-N[v],x).
\end{aligned}
$$

The proof of (iii) is the same as that of Equation (2.1) in Lemma 2.1. □

Lemma 2.8 ([63]) *Let T be a rooted tree with root v and branches $T_1,\ldots,T_k$. Then,*

(i) $\sigma_0(T,x) = \prod_{j=1}^{k}\sigma(T_j,x)$,

(ii) $\sigma_1(T,x) = x\prod_{j=1}^{k}\sigma_0(T_j,x)$,

(iii) $\rho(T,x) = \dfrac{1}{1+x\prod_{j=1}^{k}\rho(T_j,x)}$.

Proof. Let T be a rooted tree with root v and branches $T_1, \ldots, T_k$. Then,

(i) $$\sigma_0(T,x) = \sum_{k\geq 0} \mu_0(T,k)x^k = \sum_{k\geq 0} \mu(T-v,k)x^k = \sigma(T-v,x)$$
$$= \sigma(T_1,x)\sigma(T_2,x)\ldots\sigma(T_k,x) = \prod_{j=1}^{k} \sigma(T_j,x).$$

(ii) Let $v_1, \ldots, v_k$ be the roots of $T_1, \ldots, T_k$, respectively. Then, any vertex independent subset of T that contains v must not contain any of the elements in $\{v_1, \ldots, v_k\}$. Then,

$$\begin{aligned}
\sigma_1 &= \sum_{k\geq 0} \mu(T-N[v],k-1)x^k \\
&= x\sum_{k\geq 0} \mu(T-N[v],k-1)x^{k-1} = x\sigma(T-N[v],x) \\
&= x\sigma(T_1-v_1,x)\sigma(T_2-v_2,x)\ldots\sigma(T_k-v_k,x) \\
&= x\sigma_0(T_1,x)\sigma_0(T_2,x)\ldots\sigma_0(T_k,x) = x\prod_{j=1}^{k}\sigma_0(T_j,x).
\end{aligned}$$

(iii) $$\rho(T,x) = \frac{\sigma_0(T,x)}{\sigma(T,x)} = \frac{\sigma_0(T,x)}{\sigma_0(T,x)+\sigma_1(T,x)} = \frac{\sigma_0(T,x)}{\sigma_0(T,x)}\left(\frac{1}{1+\frac{\sigma_1(T,x)}{\sigma_0(T,x)}}\right)$$
$$= \frac{1}{1+\frac{\sigma_1(T,x)}{\sigma_0(T,x)}} = \frac{1}{1+\dfrac{x\prod_{j=1}^{k}\sigma_0(T_j,x)}{\prod_{j=1}^{k}\sigma(T_j,x)}} = \frac{1}{1+x\prod_{j=1}^{k}\frac{\sigma_0(T_j,x)}{\sigma(T_j,x)}}$$
$$= \frac{1}{1+x\prod_{j=1}^{k}\rho(T_j,x)}.$$

□

It is convenient to set $\rho(\emptyset,x) = 1$ for all $x > 0$, so that (iii) in Lemma 2.8 still holds if some of the T_j's are empty.

Lemma 2.9 *Let T be a rooted tree with root v and branches $T_1, \ldots, T_k$. Then,*

$$\frac{1}{1+x} \leq \rho(T,x) \leq \frac{1}{1+x\left(\frac{1}{1+x}\right)^k}.$$

Proof. Let T be a rooted tree with root v and branches $T_1, \ldots, T_k$. Then, T is not empty. Suppose T is a star rooted at its center. If T is a 1-vertex star, then

$$\rho(T,x) = \frac{\sigma_0(T,x)}{\sigma(T,x)} = \frac{1}{1+x}, \tag{2.5}$$

since there is only one vertex subset of T that does not include the root v. Otherwise, T_j is a leaf, for all $j \in \{1, \ldots, k\}$. Then, $\rho(T_j, x) = \frac{1}{1+x}$. Hence,

$$\rho(T, x) = \frac{1}{1 + x \prod_{j=1}^{k} \rho(T_j, x)} = \frac{1}{1 + x \left(\frac{1}{1+x}\right)^k}. \tag{2.6}$$

Suppose T is not a star, hence at least one branch is not a leaf. Then,

$$\rho(T, x) = \frac{\sigma_0(T, x)}{\sigma(T, x)} = \frac{\sigma_0(T, x)}{\sigma_0(T, x) + \sigma_1(T, x)} < 1,$$

since T is not empty and $\sigma_0(T, x), \sigma_1(T, x) > 0$. By similar reason, $\rho(T_j, x) < 1$ for all $j \in \{1, \ldots, k\}$. This implies that $\prod_{j=1}^{k} \rho(T_j, x) < 1$. Hence,

$$\rho(T, x) = \frac{1}{1 + x \prod_{j=1}^{k} \rho(T_j, x)} > \frac{1}{1 + x}. \tag{2.7}$$

With the same reasoning, $\rho(T_j, x) \geq \frac{1}{1+x}$, with equality only if T_j is a leaf. This implies that $\prod_{j=1}^{k} \rho(T_j, x) > \left(\frac{1}{1+x}\right)^k$ and hence

$$\rho(T, x) = \frac{1}{1 + x \prod_{j=1}^{k} \rho(T_j, x)} < \frac{1}{1 + x \left(\frac{1}{1+x}\right)^k}. \tag{2.8}$$

And therefore, from Equations (2.5) through (2.8) we get

$$\frac{1}{1 + x} \leq \rho(T, x) \leq \frac{1}{1 + x \left(\frac{1}{1+x}\right)^k},$$

both inequalities are equalities if and only if T is a star rooted at its center. $\square$

Remark 2.10 Note that the lower bound in Lemma 2.9 is reached only if T is a leaf, and the upper bound is reached only if T is a pseudo leaf or a leaf branch.

3 Extremal caterpillars with regard to $M(.,x)$, energy and Hosoya index

In this chapter, we derive a formula of $M(G,x)$ of a caterpillar G, and this formula is used to characterize extremal caterpillars relative to the auxiliary invariant $M(.,x)$, Hosoya index and energy.

3.1 A formula for the auxiliary invariant $M(G,x)$ of a caterpillar G

Let G be a caterpillar and be decomposed as in Figure 3.1. Then, using Equations (2.1) and (2.3) we have:

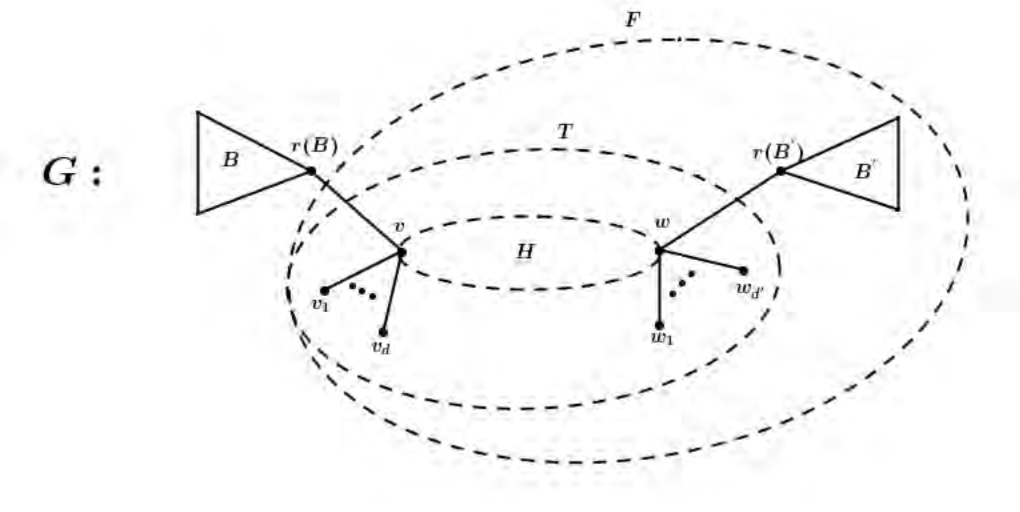

Figure 3.1: Decomposition of a caterpillar for Chapters 3 and 4.

$$
\begin{aligned}
&M(G,x)\\
&= M(G - vr(B), x) + xM(G - \{r(B), v\}, x)\\
&= M(B,x)M(F,x) + xM(G - \{r(B), v\}, x)\\
&= M(B,x)\left[M(F - wr(B^{'}), x) + xM(F - \{w, r(B^{'})\}, x)\right]\\
&\qquad\qquad\qquad\qquad\qquad\qquad + xM(G - \{r(B), v\}, x)\\
&= M(B,x)\left[M(T,x)M(B^{'},x) + xM(F - \{w, r(B^{'})\}, x)\right]\\
&\qquad\qquad\qquad\qquad\qquad\qquad + xM(G - \{r(B), v\}, x)\\
&= M(B,x)\left[M(T,x)M(B^{'},x) + xM(T - w, x)M(B^{'} - r(B^{'}), x)\right]\\
&\qquad\qquad\qquad\qquad\qquad\qquad + xM(B - r(B), x)M(F - v, x)\\
&= M(B,x)\left[M(T,x)M(B^{'},x) + xM(T - w, x)M(B^{'} - r(B^{'}), x)\right]\\
&+ xM(B - r(B), x)\left[M(F - v - wr(B^{'}), x) + xM(F - v - \{w, r(B^{'})\}, x)\right]\\
&= M(B,x)\left[M(T,x)M(B^{'},x) + xM(T - w, x)M(B^{'} - r(B^{'}), x)\right]\\
&+ xM(B - r(B), x)\left[M(T - v, x)M(B^{'}, x)\right.\\
&\qquad\qquad\qquad\qquad \left. + xM(T - \{w, v\}, x)M(B^{'} - r(B^{'}), x)\right]\\
&= M(B,x)\left[M(T,x)M(B^{'},x) + xM(T - w, x)M(B^{'} - r(B^{'}), x)\right]\\
&+ xM(B - r(B), x)\left[M(T - v, x)M(B^{'}, x)\right.\\
&\qquad\qquad\qquad\qquad \left. + xM(T - \{w, v\}, x)M(B^{'} - r(B^{'}), x)\right]\\
&= M(B,x)M(B^{'},x)M(T,x) + xM(B,x)M(B^{'} - r(B^{'}), x)M(T - w, x)\\
&\qquad\qquad\qquad + xM(B^{'},x)M(B - r(B), x)M(T - v, x)\\
&+ x^2M(B - r(B), x)M(B^{'} - r(B^{'}), x)M(T - \{v, w\}, x).
\end{aligned}
$$

Further iterative use of Equations (2.1) and (2.3) gives

$$
\begin{aligned}
&M(T,x)\\
&= M(T - v_1v, x) + xM(T - \{v_1, v\}, x)\\
&= M(T - v_1, x) + xM(T - v, x)\\
&= M(T - v_1 - v_2v, x) + xM(T - v_1 - \{v_2, v\}, x) + xM(T - v, x)\\
&= M(T - \{v_1, v_2\}, x) + xM(T - v, x) + xM(T - v, x)\\
&= M(T - \{v_1, v_2\}, x) + 2xM(T - v, x)
\end{aligned}
$$

$$
\begin{aligned}
&= M(T-\{v_1,\dots,v_d\},x) + dxM(T-v,x)\\
&= M(T-\{v_1,\dots,v_d\}-w_1w,x) + xM(T-\{v_1,\dots,v_d\}-\{w_1,w\},x)\\
&\qquad + dxM(T-v,x)\\
&= M(T-\{v_1,\dots,v_d\}-w_1,x) + xM(T-\{v_1,\dots,v_d\}-w,x)\\
&\qquad + dxM(T-v,x)\\
&= M(T-\{v_1,\dots,v_d\}-w_1-w_2w,x)\\
&\qquad + xM(T-\{v_1,\dots,v_d\}-w_1-\{w_2,w\},x)\\
&+ xM(T-\{v_1,\dots,v_d\}-w,x) + dxM(T-v,x)\\
&= M(T-\{v_1,\dots,v_d\}-\{w_1,w_2\},x) + xM(T-\{v_1,\dots,v_d\}-w,x)\\
&\qquad + xM(T-\{v_1,\dots,v_d\}-w,x) + dxM(T-v,x)\\
&= M(T-\{v_1,\dots,v_d\}-\{w_1,w_2\},x) + 2xM(T-\{v_1,\dots,v_d\}-w,x)\\
&\qquad + dxM(T-v,x)\\
&= M(T-\{v_1,\dots,v_d\}-\{w_1,\dots,w_{d'}\},x) + d'xM(T-\{v_1,\dots,v_d\}-w,x)\\
&\qquad + dxM(T-v,x)\\
&= M(H,x) + d'xM(H-w,x) + dxM(T-v,x)\\
&= M(H,x) + d'xM(H-w,x) + dx\left[M(T-v-w_1w,x)\right.\\
&\qquad \left.+xM(T-v-\{w_1,w\},x)\right]\\
&= M(H,x) + d'xM(H-w,x) + dx\left[M(T-v-w_1,x)\right.\\
&\qquad \left.+xM(T-v-w,x)\right]\\
&= M(H,x) + d'xM(H-w,x) + dx\left[M(T-v-w_1-w_2w,x)\right.\\
&\qquad \left.+ xM(T-v-w_1-\{w_2,w\},x) + xM(T-v-w,x)\right]\\
&= M(H,x) + d'xM(H-w,x)\\
&\quad + dx\left[M(T-v-\{w_1,w_2\},x) + xM(T-v-w,x) + xM(T-v-w,x)\right]\\
&= M(H,x) + d'xM(H-w,x) + dx\left[M(T-v-\{w_1,w_2\},x)\right.\\
&\qquad \left.+2xM(T-v-w,x)\right]\\
&= M(H,x) + d'xM(H-w,x) + dx\left[M(T-v-\{w_1,\dots,w_{d'}\},x)\right.\\
&\qquad \left.+d'xM(T-v-w,x)\right]\\
&= M(H,x) + d'xM(H-w,x) + dx\left[M(H-v,x) + d'xM(H-\{v,w\},x)\right],
\end{aligned}
$$

$$
\begin{aligned}
&M(T-w,x)\\
&= M(T-w-vv_1,x) + xM(T-w-\{v,v_1\},x)\\
&= M(v_1,x)M(T-w-v_1,x) + xM(T-w-\{v,v_1\},x)\\
&= M(T-w-v_1,x) + xM(T-w-\{v,v_1\},x)\\
&= M(T-w-v_1-vv_2,x) + xM(T-w-v_1-\{v,v_2\},x)\\
&\qquad + xM(T-w-\{v,v_1\},x)\\
&= M(v_2,x)M(T-w-v_1-v_2,x) + 2xM(T-w-v-\{v_1,v_2\},x)
\end{aligned}
$$

$$
\begin{aligned}
&= M(T-w-v_1-v_2,x) + 2xM(T-w-v-\{v_1,v_2\},x)\\
&= M(T-w-v_1-v_2-vv_3,x) + xM(T-w-v_1-v_2-\{v,v_3\},x)\\
&\qquad\qquad + 2xM(T-w-v-\{v_1,v_2\},x)\\
&= M(v_3,x)M(T-w-v_1-v_2-v_3,x) + 3xM(T-w-v-\{v_1,v_2,v_3\},x)\\
&= M(T-w-v_1-v_2-v_3,x) + 3xM(T-w-v-\{v_1,v_2,v_3\},x)\\
&= M(T-w-\{v_1,\ldots,v_d\},x) + dxM(T-w-v-\{v_1,\ldots,v_d\},x)\\
&= M(H-w,x) + dxM(H-w-v,x)
\end{aligned}
$$

and by similar way as above

$$M(T-v,x) = M(H-v,x) + d^{'}xM(H-w-v,x).$$

Hence,

$$
\begin{aligned}
&M(G,x)\\
&= M(B,x)M(B^{'},x)\Big[M(H,x) + d^{'}xM(H-w,x)\\
&\qquad\qquad +dx\Big[M(H-v,x) + d^{'}xM(H-\{v,w\},x)\Big]\Big]\\
&+ xM(B,x)M(B^{'}-r(B^{'}),x)\left[M(H-w,x) + dxM(H-\{v,w\},x)\right]\\
&\qquad + xM(B^{'},x)M(B-r(B),x)\Big[M(H-v,x) + d^{'}xM(H-\{v,v\},x)\Big]\\
&+ x^2M(B-r(B),x)M(B^{'}-r(B^{'}),x)M(H-\{v,w\},x)\\
&= M(B,x)M(B^{'},x)\Big[M(H,x) + d^{'}xM(H-w,x)\\
&\qquad\qquad +dx\Big[M(H-v,x) + d^{'}xM(H-\{v,w\},x)\Big]\Big]\\
&+ xM(B,x)M(B^{'},x)\tau(B^{'},x)\left[M(H-w,x) + dxM(H-\{v,w\},x)\right]\\
&\qquad + xM(B,x)M(B^{'},x)\tau(B,x)\Big[M(H-v,x) + d^{'}xM(H-\{v,w\},x)\Big]\\
&+ x^2M(B,x)M(B^{'},x)\tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x)\\
&= M(B,x)M(B^{'},x)\Big[M(H,x) + d^{'}xM(H-w,x)\\
&\qquad\qquad +dx\Big[M(H-v,x) + d^{'}xM(H-\{v,w\},x)\Big]\\
&+ x\tau(B^{'},x)\left[M(H-w,x) + dxM(H-\{v,w\},x)\right]\\
&\qquad\qquad + x\tau(B,x)\left[M(H-v,x) + d'xM(H-\{v,w\},x)\right]\\
&+ x^2\ \tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x)\Big]\\
&= M(B,x)M(B^{'},x)\Big[M(H,x) + dd^{'}x^2M(H-\{v,w\},x)\\
&+ x^2\tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x) + x\Big[d^{'}M(H-w,x) + dM(H-v,x)\Big]
\end{aligned}
$$

$$+ x\left[\tau(B^{'},x)M(H-w,x)+\tau(B,x)M(H-v,x)\right] + x^2M(H-\{v,w\},x)\left[d\tau(B^{'},x)+d^{'}\tau(B,x)\right]\Big]$$

$$= M(B,x)M(B^{'},x)\Big[M(H,x)+dd^{'}x^2M(H-\{v,w\},x) + x^2\tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x)$$

$$+ x\left[\left(d^{'}+\tau(B^{'},x)\right)M(H-w,x)+\left(d+\tau(B,x)\right)M(H-v,x)\right] + x^2M(H-\{v,w\},x)\left[d\tau(B^{'},x)+d^{'}\tau(B,x)\right]\Big]. \quad (3.1)$$

We define

$$M_v^w(G,x) = x\left[\left(d^{'}+\tau(B^{'},x)\right)M(H-w,x)+\left(d+\tau(B,x)\right)M(H-v,x)\right] + x^2M(H-\{v,w\},x)\left[d\tau(B^{'},x)+d^{'}\tau(B,x)\right],$$

so that

$$M(G,x) = M(B,x)M(B^{'},x)\Big[M(H,x)+dd^{'}x^2M(H-\{v,w\},x) + x^2\tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x)+M_v^w(G,x)\Big]. \quad (3.2)$$

3.2 Caterpillar with given degree sequence and maximum $M(.,x)$

Let G be a graph of order n and $m(G,k)$ the number of matchings of order k. Recall that the auxiliary invariant $M(G,x)$ is defined to be

$$M(G,x) = \sum_{k\geq 0} m(G,k)x^k,$$

for all positive $x \in \mathbb{R}$. The Hosoya index $Z(G)$ is given by

$$Z(G) = M(G,1)$$

and the energy $En(G)$ is given by

$$En(G) = \frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln M(G,x^2)dx.$$

In this section we characterize the caterpi-llar with given degree sequence, maximum $M(.,x)$ and hence maxim-um Hosoya index and maximum energy. We first characterize a caterpillar $\mathcal{X}(D)$ that maximizes $M(.,x)$, among all caterpillars with given degree sequence D.

This caterpillar is found to also maximize the Hosoya index and the energy. Then, we compare the two caterpi-llars $\mathcal{X}(D)$ and $\mathcal{X}(Y)$ i.e. $M(\mathcal{X}(D), x)$ with $M(\mathcal{X}(Y), x)$, $Z(\mathcal{X}(D))$ with $Z(\mathcal{X}(Y))$ and $En(\mathcal{X}(D))$ with $En(\mathcal{X}(Y))$, where the degree sequence Y is majorized by the degree sequence D. We say G is maximal with regard to an invariant $F(G)$, if and only if $F(G) = \max\{F(C) : C \in \mathbb{C}_D\}$, where D is a degree sequence of G.

The following simple technical lemma will play central role as we try to find out what exchange of branches increases $M(., x)$.

Lemma 3.1 *Let a, b, c and d be non-negative real numbers such that $a \leq b \leq c \leq d$, then $ac + bd, ad + bc \leq ab + cd$.*

Proof. Let a, b, c and d be non-negative real numbers such that $a \leq b \leq c \leq d$. Then,

$$ab+cd-(ac+bd) = ab-ac+cd-bd = -a(c-b)+d(c-b) = (c-b)(d-a) \geq 0,$$

since $c \geq b$ and $d \geq a$.

$$ab+cd-(ad+bc) = ab-ad+cd-bc = -a(d-b)+c(d-b) = (d-b)(c-a) \geq 0,$$

since $c \geq a$ and $d \geq b$. □

Lemma 3.2 *Let G be a caterpillar with degree sequence D, decomposed as in Figure 3.1 and suppose that $M(G, x) = \max\{M(C, x) : C \in \mathbb{C}_D\}$. If $\tau(B', x) > \tau(B, x)$, then either*

$$d' < d \text{ and } M(H - w, x) \leq M(H - v, x),$$

or

$$d' = d \text{ and } M(H - w, x) \geq M(H - v, x).$$

Proof. Let G be a caterpillar with degree sequence D and decomposed as in Figure 3.1. Suppose that $M(G, x) = \max\{M(C, x) : C \in \mathbb{C}_D\}$. In particular, $M(G, x)$ is maximal with respect to all possible swappings and flippings in G that preserve the degree sequence: the swapping of B and B', the swapping of d and d' (exchanging d and d') and/or the flipping of H (exchanging v and w) in G. Equation (3.2) suggests that the swapping of B and B', the swapping of d and d' and/or the flipping of H in G only affect $M_v^w(G, x)$ in $M(G, x)$. This implies that the maximality of $M_v^w(G, x)$ implies the maximality of $M(G, x)$.

Suppose $\tau(B', x) > \tau(B, x)$. The contrary to the statement results in two cases:

1.) $d^{'} \neq d$ and ($d^{'} \geq d$ or $M(H-w,x) > M(H-v,x)$) or
2.) $d^{'} \geq d$ and $M(H-w,x) < M(H-v,x)$.

To prove the two cases, we break them down into five clear different sub-cases. Let a, b, ε and η be positive real numbers.

(i) Suppose $d^{'} = a+\varepsilon > a = d$, $\tau(B^{'},x) = b+\eta > b = \tau(B,x)$ and $M(H-w,x) \leq M(H-v,x)$. Then,

$$\begin{aligned}
M_v^w(G,x) &= x\left[\left(d^{'}+\tau(B^{'},x)\right)M(H-w,x)+(d+\tau(B,x))\,M(H-v,x)\right]\\
&\qquad + x^2M(H-\{v,w\},x)\left[d\tau(B^{'},x)+d^{'}\tau(B,x)\right]\\
&= x\left[(a+\varepsilon+b+\eta)\,M(H-w,x)+(a+b)M(H-v,x)\right]\\
&\qquad + x^2M(H-\{v,w\},x)\left[a(b+\eta)+(a+\varepsilon)b\right].
\end{aligned}$$

Let $G^{'}$ be obtained from G by swapping d and $d^{'}$, then

$$\begin{aligned}
M_v^w(G^{'},x) &= x\left[\left(d+\tau(B^{'},x)\right)M(H-w,x)+\left(d^{'}+\tau(B,x)\right)M(H-v,x)\right]\\
&\qquad + x^2M(H-\{v,w\},x)\left[d^{'}\tau(B^{'},x)+d\tau(B,x)\right]\\
&= x\left[(a+b+\eta)M(H-w,x)+(a+\varepsilon+b)M(H-v,x)\right]\\
&\qquad + x^2M(H-\{v,w\},x)\left[(a+\varepsilon)(b+\eta)+ab\right]
\end{aligned}$$

and

$$\begin{aligned}
&M_v^w(G^{'},x)-M_v^w(G,x)\\
&= x\left[M(H-w,x)(a+b+\eta-(a+\varepsilon+b+\eta))\right.\\
&\qquad\qquad \left.+M(H-v,x)(a+\varepsilon+b-(a+b))\right]\\
&+ x^2M(H-\{v,w\},x)\left[(a+\varepsilon)(b+\eta)+ab-(a(b+\eta)+(a+\varepsilon)b)\right]\\
&= x\varepsilon\left[M(H-v,x)-M(H-w,x)\right]+x^2M(H-\{v,w\},x)\varepsilon\eta > 0,
\end{aligned}$$

since x,ε, $\eta > 0$, $M(H-v,x) \geq M(H-w,x)$ and $M(H-\{v,w\},x) > 0$. This implies that $M_v^w(G^{'},x) > M_v^w(G,x)$. This contradicts the maximality of $M_v^w(G,x)$.

(ii) Suppose $d^{'} = a < a+\varepsilon = d$, $\tau(B^{'},x) = b+\eta > b = \tau(B,x)$ and $M(H-w,x) > M(H-v,x)$. Then,

$$\begin{aligned}
M_v^w(G,x) &= x\left[\left(d^{'}+\tau(B^{'},x)\right)M(H-w,x)+(d+\tau(B,x))M(H-v,x)\right]\\
&\qquad + x^2M(H-\{v,w\},x)\left[d\tau(B^{'},x)+d^{'}\tau(B,x)\right]\\
&= x\left[(a+b+\eta)M(H-w,x)+(a+\varepsilon+b)M(H-v,x)\right]
\end{aligned}$$

$$+ x^2 M(H - \{v, w\}, x) \left[(a+\varepsilon)(b+\eta) + ab\right].$$

Let $G^{'}$ be obtained from G by flipping H in G, then

$$\begin{aligned} M_v^w(G^{'}, x) &= x\left[\left(d^{'} + \tau(B^{'}, x)\right) M(H - v, x) + \left(d + \tau(B, x)\right) M(H - w, x)\right] \\ &\quad + x^2 M(H - \{v, w\}, x)\left[d\tau(B^{'}, x) + d^{'}\tau(B, x)\right] \\ &= x\left[(a+b+\eta) M(H - v, x) + (a+\varepsilon+b) M(H - w, x)\right] \\ &\quad + x^2 M(H - \{v, w\}, x)\left[(a+\varepsilon)(b+\eta) + ab\right], \end{aligned}$$

and

$$\begin{aligned} & M_v^w(G^{'}, x) - M_v^w(G, x) \\ &= x\left[M(H - v, x)(a+b+\eta - (a+\varepsilon+b)) \right. \\ &\quad \left. + M(H - w, x)(a+\varepsilon+b - (a+b+\eta))\right] \\ &+ x^2 M(H - \{v, w\}, x)\left[(a+\varepsilon)(b+\eta) + ab - (a+\varepsilon)(b+\eta) - ab\right] \\ &= x(\varepsilon - \eta)\left[M(H - w, x) - M(H - v, x)\right] > 0, \text{ since } \varepsilon \geq 1 > \eta > 0, x > 0 \end{aligned}$$

and $M(H - w, x) > M(H - v, x)$.

This implies that $M_v^w(G^{'}, x) > M_v^w(G, x)$. And contradicts the maximality of $M_v^w(G, x)$.

(iii) Suppose $d^{'} = a + \varepsilon > a = d$, $\tau(B^{'}, x) = b + \eta > b = \tau(B, x)$ and $M(H - w, x) > M(H - v, x)$. Then,

$$\begin{aligned} M_v^w(G, x) &= x\left[\left(d^{'} + \tau(B^{'}, x)\right) M(H - w, x) + \left(d + \tau(B, x)\right) M(H - v, x)\right] \\ &\quad + x^2 M(H - \{v, w\}, x)\left[d\tau(B^{'}, x) + d^{'}\tau(B, x)\right] \\ &= x\left[(a+\varepsilon+b+\eta) M(H - w, x) + (a+b) M(H - v, x)\right] \\ &\quad + x^2 M(H - \{v, w\}, x)\left[a(b+\eta) + (a+\varepsilon)b\right]. \end{aligned}$$

Let $G^{'}$ be obtained from G by swapping $B^{'}$ and B, then

$$\begin{aligned} M_v^w(G^{'}, x) &= x\left[\left(d^{'} + \tau(B, x)\right) M(H - w, x) + \left(d + \tau(B^{'}, x)\right) M(H - v, x)\right] \\ &\quad + x^2 M(H - \{v, w\}, x)\left[d\tau(B, x) + d^{'}\tau(B^{'}, x)\right] \\ &= x\left[(a+\varepsilon+b) M(H - w, x) + (a+b+\eta) M(H - v, x)\right] \\ &\quad + x^2 M(H - \{v, w\}, x)\left[ab + (a+\varepsilon)(b+\eta)\right], \end{aligned}$$

and

$$M_v^w(G^{'}, x) - M_v^w(G, x)$$

$$
\begin{aligned}
&= x\left[M(H-w,x)\,(a+\varepsilon+b-(a+\varepsilon+b+\eta))\right.\\
&\qquad\qquad\qquad\qquad\left.+M(H-v,x)\,(a+b+\eta-(a+b))\right]\\
&+x^2M(H-\{v,w\},x)\left[ab+(a+\varepsilon)(b+\eta)-a(b+\eta)-(a+\varepsilon)b\right]\\
&= x\eta\left[M(H-v,x)-M(H-w,x)\right]+x^2M(H-\{v,w\},x)\varepsilon\eta\\
&= x\eta\Big[M(H-v,x)-M(H-w-vv^{'},x)-xM(H-w-\{v,v^{'}\},x)\\
&\qquad\qquad\qquad\qquad +x\varepsilon M(H-\{v,w\},x)\Big]\\
&= x\eta\Big[M(H-v,x)-M(H-\{v,w\},x)-xM(H-\{v,v^{'},w\},x)\\
&+x\varepsilon M(H-\{v,w\},x)\Big]>0,
\end{aligned}
$$

Since $x,\eta>0$, $\varepsilon\geq 1$, $M(H-v,x)>M(H-\{v,w\},x)$ and $M(H-\{v,w\},x)\geq M(H-\{v,v^{'},w\},x)$. This implies that $M_v^w(G^{'},x)>M_v^w(G,x)$. Contradicting the maximality of $M_v^w(G,x)$.

(iv) Suppose $d^{'}=a=d$, $\tau(B^{'},x)=b+\eta>b=\tau(B,x)$ and $M(H-w,x)<M(H-v,x)$. Then,

$$
\begin{aligned}
M_v^w(G,x) &= x\left[\left(d^{'}+\tau(B^{'},x)\right)M(H-w,x)+(d+\tau(B,x))\,M(H-v,x)\right]\\
&\qquad +x^2M(H-\{v,w\},x)\left[d\tau(B^{'},x)+d^{'}\tau(B,x)\right]\\
&= x\left[(a+b+\eta)\,M(H-w,x)+(a+b)M(H-v,x)\right]\\
&\qquad +x^2M(H-\{v,w\},x)\left[a(b+\eta)+ab\right].
\end{aligned}
$$

Let $G^{'}$ be obtained from G by flipping H in G, then

$$
\begin{aligned}
M_v^w(G^{'},x) &= x\left[\left(d^{'}+\tau(B^{'},x)\right)M(H-v,x)+(d+\tau(B,x))M(H-w,x)\right]\\
&\qquad +x^2M(H-\{v,w\},x)\left[d\tau(B^{'},x)+d^{'}\tau(B,x)\right]\\
&= x\left[(a+b+\eta)\,M(H-v,x)+(a+b)M(H-w,x)\right]\\
&\qquad +x^2M(H-\{v,w\},x)\left[a(b+\eta)+ab\right],
\end{aligned}
$$

and

$$
\begin{aligned}
&M_v^w(G^{'},x)-M_v^w(G,x)\\
&= x\left[M(H-v,x)(a+b+\eta-(a+b))+M(H-w,x)(a+b-(a+b+\eta))\right]\\
&= x\eta\left[M(H-v,x)-M(H-w,x)\right]>0,
\end{aligned}
$$

since $x,\eta>0$ and $M(H-v,x)>M(H-w,x)$.

This implies that $M_v^w(G^{'},x)>M_v^w(G,x)$. This contradicts the maximality of $M_v^w(G,x)$.

(v) Suppose $d' = a+\varepsilon > a = d$, $\tau(B',x) = b+\eta > b = \tau(B,x)$ and $M(H-w,x) < M(H-v,x)$. Then,

$$\begin{aligned} M_v^w(G,x) &= x\left[\left(d' + \tau(B',x)\right) M(H-w,x) + (d+\tau(B,x))\, M(H-v,x)\right] \\ &\qquad + x^2 M(H-\{v,w\},x)\left[d\tau(B',x) + d'\tau(B,x)\right] \\ &= x\left[(a+\varepsilon+b+\eta)\, M(H-w,x) + (a+b)M(H-v,x)\right] \\ &\qquad + x^2 M(H-\{v,w\},x)\left[a(b+\eta)+(a+\varepsilon)b\right]. \end{aligned}$$

Let G' be obtained from G by swapping d and d', then

$$\begin{aligned} M_v^w(G',x) &= x\left[\left(d + \tau(B',x)\right) M(H-w,x) + \left(d' + \tau(B,x)\right) M(H-v,x)\right] \\ &\qquad + x^2 M(H-\{v,w\},x)\left[d'\tau(B',x) + d\tau(B,x)\right] \\ &= x\left[(a+b+\eta)M(H-w,x) + (a+\varepsilon+b)M(H-v,x)\right] \\ &\qquad + x^2 M(H-\{v,w\},x)\left[(a+\varepsilon)(b+\eta)+ab\right], \end{aligned}$$

and

$$\begin{aligned} & M_v^w(G',x) - M_v^w(G,x) \\ &= x\left[M(H-w,x)(a+b+\eta-(a+\varepsilon+b+\eta)) \right. \\ &\qquad \left. + M(H-v,x)(a+\varepsilon+b-(a+b))\right] \\ &+ x^2 M(H-\{v,w\},x)\left[(a+\varepsilon)(b+\eta)+ab-(a(b+\eta)+(a+\varepsilon)b)\right] \\ &= x\varepsilon\left[M(H-v,x) - M(H-w,x)\right] + x^2 M(H-\{v,w\},x)\varepsilon\eta > 0, \end{aligned}$$

since x,ε,$\eta > 0$, $M(H-v,x) > M(H-w,x)$ and $M(H-\{v,w\},x) \geq 0$. This implies that $M_v^w(G',x) > M_v^w(G,x)$. This contradicts the maximality of $M_v^w(G,x)$. Since all the cases of the negation of the claim lead to contradiction, then if $\tau(B',x) > \tau(B,x)$, then either $d' < d$ and $M(H-w,x) \leq M(H-v,x)$ or $d' = d$ and $M(H-w,x) \geq M(H-v,x)$. And that completes the proof. □

Lemma 3.3 *Let G be a caterpillar. Label all the non-leaf vertices in G from left to right as $u_1, u_2, \ldots, u_\ell$. If G is maximal with respect to $M(.,x)$, then u_1 and u_ℓ have the smallest degrees among all the non-leaf vertices in G.*

Proof. Let G be a caterpillar and be decomposed as in Figure 3.1. Suppose B is a leaf adjacent to u_1 and B' a complete branch of G such that B' does not contain u_1 and u_2, and the root of B' is u_i, for $3 \leq i \leq \ell$. Then, B' is not a leaf and by Remark 2.5 we have $\tau(B,x) = 1 > \tau(B',x)$. By Lemma 3.2, we have $\deg(u_1) \leq \deg(u_{i-1})$. Hence

$$\deg(u_1) \leq \min\{\deg(u_i) : 2 \leq i \leq \ell - 1\}.$$

Same reasoning leads to

$$\deg(u_\ell) \leq \min\{\deg(u_i) : 2 \leq i \leq \ell - 1\}.$$

□

Lemma 3.4 *Let B and $B^{'}$ be complete branches of a caterpillar G, $h(B)$ and $h(B^{'})$ their respective heights. If $h(B) = h(B^{'})$, then $\tau(B, x) = \tau(B^{'}, x)$ if and only if $B \approx_r B^{'}$.*

Proof. It is clear that $B \approx_r B^{'}$ implies $\tau(B, x) = \tau(B^{'}, x)$. We only need to prove that $\tau(B, x) = \tau(B^{'}, x)$ implies $B \approx_r B^{'}$. Let $r(B)$ and $r(B^{'})$ be the roots of B and $B^{'}$, respectively. Then, B and $B^{'}$ can be decomposed as in Figure 3.2:

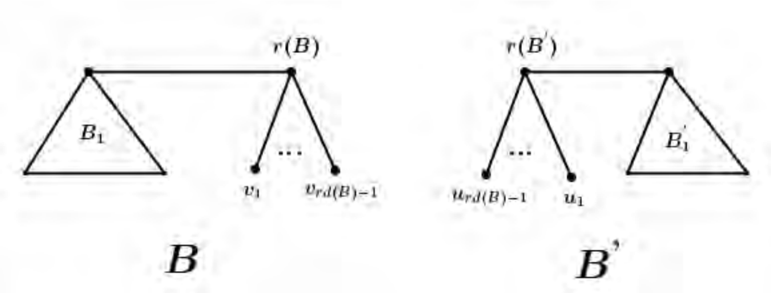

Figure 3.2: Decomposition of complete branches in Lemma 3.4.

Suppose $h(B) = h(B^{'}) = h$. If $h = 1$ and $\tau(B, x) = \tau(B^{'}, x)$, then

$$\tau(B, x) = \frac{1}{1 + x\,\mathrm{rd}(B)} = \frac{1}{1 + x\,\mathrm{rd}(B')} = \tau(B^{'}, x).$$

Then, $1 + x\,\mathrm{rd}(B) = 1 + x\,\mathrm{rd}(B^{'})$. Since $x > 0$, then $\mathrm{rd}(B) = \mathrm{rd}(B^{'})$ and $B \approx_r B^{'}$. Suppose that for $h = k \geq 1$, $\tau(B, x) = \tau(B^{'}, x) \implies B \approx_r B^{'}$. Then, for $h = k + 1:$

$$\tau(B, x) = \frac{1}{1 + x \sum_{i=1}^{\mathrm{rd}(B)} \tau(B_i, x)} = \frac{1}{1 + x\,(\mathrm{rd}(B) - 1 + \tau(B_1, x))}$$

and

$$\tau(B^{'}, x) = \frac{1}{1 + x\,\left(\mathrm{rd}(B^{'}) - 1 + \tau(B_1^{'}, x)\right)}.$$

Then, Suppose $\tau(B, x) = \tau(B^{'}, x)$. Then, $1 + x\,(\mathrm{rd}(B) - 1 + \tau(B_1, x)) = 1 + x\,\left(\mathrm{rd}(B^{'}) - 1 + \tau(B_1^{'}, x)\right)$. Since $x > 0$, then

$$\mathrm{rd}(B) + \tau(B_1, x) = \mathrm{rd}(B^{'}) + \tau(B_1^{'}, x). \tag{3.3}$$

Suppose that $\mathrm{rd}(B) \neq \mathrm{rd}(B^{'})$, without loss of generality assume $\mathrm{rd}(B) > \mathrm{rd}(B^{'})$. Then, $\mathrm{rd}(B) \geq \mathrm{rd}(B^{'}) + 1$. Since B and $B^{'}$ are non-empty and $h \geq 2$, then B_1 and $B_1^{'}$ are non-empty and $0 < \tau(B_1, x), \tau(B_1^{'}, x) \leq 1$. With $\mathrm{rd}(B) \geq \mathrm{rd}(B^{'}) + 1$ and $0 < \tau(B_1, x), \tau(B_1^{'}, x) \leq 1$, then

$$\mathrm{rd}(B) + \tau(B_1, x) > \mathrm{rd}(B^{'}) + 1 \geq \mathrm{rd}(B^{'}) + \tau(B_1^{'}, x). \tag{3.4}$$

From (3.3) and (3.4) we have $\mathrm{rd}(B) + \tau(B_1, x) = \mathrm{rd}(B^{'}) + \tau(B_1^{'}, x)$ and $\mathrm{rd}(B) + \tau(B_1, x) > \mathrm{rd}(B^{'}) + \tau(B_1^{'}, x)$ which is a contradiction, hence $\mathrm{rd}(B) = \mathrm{rd}(B^{'})$. With $\mathrm{rd}(B) = \mathrm{rd}(B^{'})$ and Equation (3.3) we have $\tau(B_1^{'}, x) = \tau(B_1, x)$. So $\mathrm{rd}(B) = \mathrm{rd}(B^{'})$ and $\tau(B_1^{'}, x) = \tau(B_1, x)$, then $B_1 \approx_r B_1^{'}$ and thus $B \approx_r B^{'}$. □

Lemma 3.5 *Let G be a caterpillar, label all the non-leaf vertices in G from left to right as u_1, u_2,...,u_ℓ. Let $s = \min\{\deg(u_i) : 1 \leq i \leq \ell\}$. Suppose $M(G, x)$ is maximum among all caterpillars of the same degree sequence as G and there are at least 2 vertices in G of degree s, then*
(i) $\deg(u_1) = \deg(u_\ell) = s$.
(ii) If $\deg(u_j) = s$ *and* $\deg(u_{j+1}) > s$, *then*

$$\deg(u_1) = \deg(u_2) = \cdots = \deg(u_j) = s.$$

Proof. Suppose G is maximal with respect to $M(., x)$ and there are at least 2 vertices of degree s. Then, by Lemma 3.3, we have $\deg(u_1) = \deg(u_\ell) = s$, which proves (i).

Suppose $\deg(u_j) = s$ and $\deg(u_{j+1}) > s$. $j = 1$ is trivial. If $j = 2$ we are done because $\deg(u_1) = \deg(u_2) = s$. Otherwise decompose G as in Figure 3.3, such that $\deg(u_i) = \deg(u_j) = s$ with $i + 1 < j$ and each of B_1 and $B_1^{'}$ non-empty. Then,

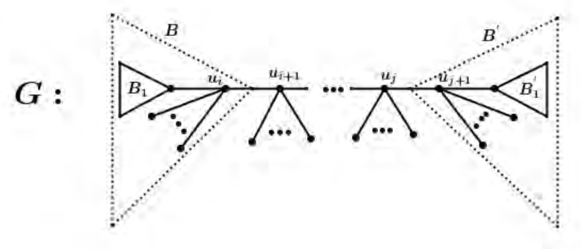

Figure 3.3: Decomposition of caterpillar G in Lemma 3.5.

$$\tau(B, x) = \frac{1}{1 + x\,(s - 2 + \tau(B_1, x))}$$

and

$$\tau(B^{'},x) = \frac{1}{1 + x\left(\deg(u_{j+1}) - 2 + \tau(B_1^{'},x)\right)}.$$

Since both $B_1^{'}$ and B_1 are non-empty and $\deg(u_j) = s < \deg(u_{j+1})$, then $0 < \tau(B_1,x), \tau(B_1^{'},x) \leq 1$ and

$$s - 2 + \tau(B_1,x) \leq \deg(u_{j+1}) - 2 < \deg(u_{j+1}) - 2 + \tau(B_1^{'},x).$$

Hence $\tau(B,x) > \tau(B^{'},x)$. Since $\tau(B,x) > \tau(B^{'},x)$, then by Lemma 3.2, we must have $\deg(u_{i+1}) \leq \deg(u_j) = s$. But s is the smallest degree among all non-leaf vertices in G, hence $\deg(u_{i+1}) = s$ and that proves (ii). □

Lemma 3.6 *Let G be a caterpillar, label all the non-leaf vertices in G from left to right as u_1, u_2,. . . ,u_ℓ. Suppose G is maximal with respect to $M(.,x)$ and suppose j is the largest positive integer with*

$$\deg(u_1) = \deg(u_2) = \cdots = \deg(u_j) = s.$$

If $j \geq 2$ and G have at least 1 vertex of degree greater than s, then $\deg(u_{\ell-1}) > s$ and $\deg(u_\ell) = s$.

Proof. Suppose G is maximal with respect to $M(.,x)$, $j \geq 2$ is the largest integer with

$$\deg(u_1) = \deg(u_2) = \cdots = \deg(u_j) = s$$

and there exists vertex u_i in G with degree greater than s. Since $j \geq 2$, then by Lemma 3.5, we must have $\deg(u_\ell) = s$. If $j = \ell - 2$ we are done. Suppose that $2 \leq j \leq \ell - 3$. Then, decompose G as in Figure 3.4. Then,

$$\tau(B,x) = \frac{1}{1 + x\left(s - 2 + \tau(B_1,x)\right)}$$

and

$$\tau(B^{'},x) = \frac{1}{1 + x(s-1)}.$$

Since $j \geq 2$, then B_1 is non-empty and not a leaf. Since B_1 is non-empty and not a leaf, then by Remark 2.5 we must have

$$0 < \tau(B_1,x) < 1.$$

Since $0 < \tau(B_1,x) < 1$, then $s - 1 > s - 2 + \tau(B_1,x)$ and hence $\tau(B^{'},x) < \tau(B,x)$. Since $\tau(B,x) > \tau(B^{'},x)$, then by Lemma 3.2, we must have $\deg(u_{j+1}) \leq \deg(u_{\ell-1})$. Since $\deg(u_j) < \deg(u_{j+1}) \leq \deg(u_{\ell-1})$, then $s = \deg(u_j) < \deg(u_{\ell-1})$. □

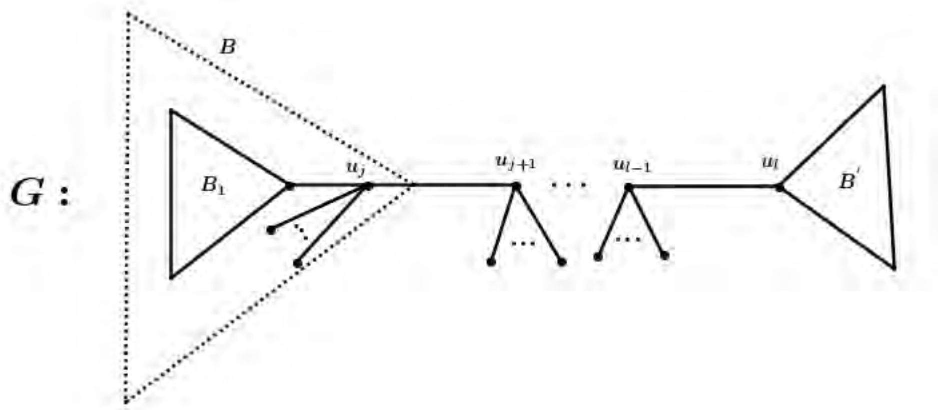

Figure 3.4: Decomposition of a caterpillar G in Lemma 3.6.

Lemma 3.7 *Let G be a caterpillar, label all the non-leaf vertices in G from left to right as u_1, u_2,..., u_ℓ. Suppose G is maximal with respect to $M(.,x)$ among all caterpillars with the same degree sequence as G. And suppose j is the largest positive integer with*

$$\deg(u_1) = \deg(u_2) = \cdots = \deg(u_j) = s.$$

If $j \geq 2$ and G have at least 1 vertex of degree greater than s, then

$$\deg(u_{j+1}) = \min\{\deg(u_i) : \deg(u_i) \neq s \text{ and } 1 \leq i \leq \ell\}$$

and

$$\deg(u_{\ell-1}) = \min\{\deg(u_i) : \deg(u_i) \neq s \text{ and } j+2 \leq i \leq \ell\}.$$

Proof. Suppose G is maximal with regard to $M(.,x)$, $j \geq 2$ is the largest integer with

$$\deg(u_1) = \deg(u_2) = \cdots = \deg(u_j) = s$$

and there exists vertex v in G with degree greater than s. Then, decompose G as in Figure 3.5. Then,

$$\tau(B,x) = \frac{1}{1 + x\left(\deg(u_k) - 2 + \tau(B_1,x)\right)}$$

and

$$\tau(B',x) = \frac{1}{1 + x(s-1)}.$$

If $j+1 \leq k \leq \ell-1$, then by Lemmas 3.5 and 3.6 and by the assumption $\deg(u_k) > s$. Since $j \geq 2$, then B_1 is non-empty and not a leaf hence

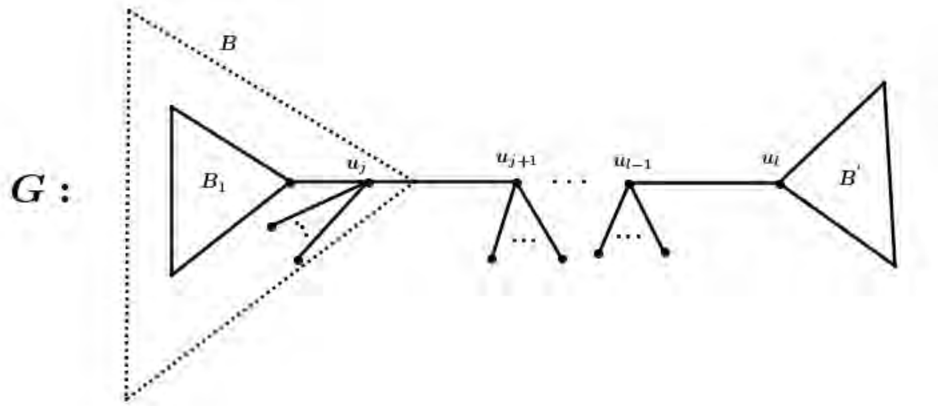

Figure 3.5: Decomposition of a caterpillar G in Lemma 3.7.

by Remark 2.5 we must have $0 < \tau(B_1, x) < 1$. Since $0 < \tau(B_1, x) < 1$ and $\deg(u_k) > s$, then

$$s - 1 \leq \deg(u_k) - 2 < \deg(u_k) - 2 + \tau(B_1, x).$$

Since $s - 1 < \deg(u_k) - 2 + \tau(B_1, x)$, then $\tau(B^{'}, x) > \tau(B, x)$. $\tau(B^{'}, x) > \tau(B, x)$, then by Lemma 3.2, we have $\deg(u_{\ell-1}) \leq \deg(u_{k+1})$, for all $j + 1 \leq k \leq \ell - 3$. Hence,

$$\deg(u_{\ell-1}) \leq \min\{\deg(u_i) : j + 2 \leq i \leq \ell - 1\}. \tag{3.5}$$

If $k = j$, then $\deg(u_k) = s$ and

$$\deg(u_k) - 2 + \tau(B_1, x) = s - 2 + \tau(B_1, x).$$

Since $0 < \tau(B_1, x) < 1$, then

$$\deg(u_k) - 2 + \tau(B_1, x) = s - 2 + \tau(B_1, x) < s - 1,$$

hence $\tau(B, x) > \tau(B^{'}, x)$. Since $\tau(B, x) > \tau(B^{'}, x)$, then by Lemma 3.2, we get

$$\deg(u_{k+1}) \leq \deg(u_{\ell-1}). \tag{3.6}$$

Equations (3.5) and (3.6) imply

$$\deg(u_{k+1}) \leq \deg(u_{\ell-1}) \leq \min\{\deg(u_i) : j + 2 \leq i \leq \ell - 1\}.$$

And hence,

$$\deg(u_{j+1}) = \min\{\deg(u_i) : \deg(u_i) \neq s \text{ and } 1 \leq i \leq \ell\}$$

and

$$\deg(u_{\ell-1}) = \min\{\deg(u_i) : \deg(u_i) \neq s \text{ and } j + 2 \leq i \leq \ell\}.$$

□

Lemma 3.8 *Let B and $B^{'}$ be two complete branches of a caterpillar G. Label all the non-leaf vertices in B starting from its root as u_1, u_2,…,u_ℓ and let their degrees be d_1, d_2,…,d_ℓ, respectively. Label all the non-leaf vertices in $B^{'}$ starting from its root as v_1, v_2,…,$v_{m'}$ and let their degrees be $d_1^{'}$, $d_2^{'}$,…,$d_{m'}^{'}$, respectively. Let B_i be a complete branch of G such that B_i is in B and the root of B_i is u_i. Let $B_j^{'}$ be a complete branch of G such that $B_j^{'}$ is in $B^{'}$ and the root of $B_j^{'}$ is v_j. If $1 \le m < \min\{\ell, m^{'}\}$, $d_1 = d_1^{'}$, $d_2 = d_2^{'}$,…,$d_m = d_m^{'}$ and $\tau(B_{m+1}^{'}, x) > \tau(B_{m+1}, x)$, then the following holds:*
(i) if m is odd, then $\tau(B^{'}, x) < \tau(B, x)$,
(ii) if m is even, then $\tau(B^{'}, x) > \tau(B, x)$.

Proof. Suppose $1 \le m < \min\{\ell, m^{'}\}$, $d_1 = d_1^{'}$, $d_2 = d_2^{'}$,…,$d_m = d_m^{'}$ and $\tau(B_{m+1}^{'}, x) > \tau(B_{m+1}, x)$. By assumption $m \ge 1$, $B = B_1$ and $B^{'} = B_1^{'}$.

Base case: Suppose $m = 1$ (odd). By assumption

$$\begin{aligned}\tau(B^{'}, x) = \tau(B_1^{'}, x) &= \frac{1}{1 + x\left(d_1 - 2 + \tau(B_2^{'}, x)\right)} < \frac{1}{1 + x\left(d_1 - 2 + \tau(B_2, x)\right)} \\ &= \tau(B_1, x) = \tau(B, x).\end{aligned}$$

Suppose that the lemma holds for $m = k$, for some $k \ge 1$. Consider $m = k + 1$.
(a) Suppose $k + 1$ is odd so that k is even. Suppose $d_1 = d_1^{'}, \ldots, d_{k+1} = d_{k+1}^{'}$ and $\tau(B_{k+2}^{'}, x) > \tau(B_{k+2}, x)$. Since

$$\tau(B_{k+1}, x) = \frac{1}{1 + x\left(d_{k+1} - 2 + \tau(B_{k+2}, x)\right)}$$

and

$$\tau(B_{k+1}^{'}, x) = \frac{1}{1 + x\left(d_{k+1} - 2 + \tau(B_{k+2}^{'}, x)\right)},$$

then $\tau(B_{k+1}, x) > \tau(B_{k+1}^{'}, x)$. So, $d_1 = d_1^{'}, \ldots, d_k = d_k^{'}$, $\tau(B_{k+1}, x) > \tau(B_{k+1}^{'}, x)$ and k is even. By the induction assumption $\tau(B, x) > \tau(B^{'}, x)$. And hence, if $k + 1$ is odd, then $\tau(B^{'}, x) < \tau(B, x)$.

(b) Suppose that $k + 1$ is even so that k is odd. Suppose $d_1 = d_1^{'}, \ldots, d_{k+1} = d_{k+1}^{'}$ and $\tau(B_{k+2}^{'}, x) > \tau(B_{k+2}, x)$. Since

$$\tau(B_{k+1}, x) = \frac{1}{1 + x\left(d_{k+1} - 2 + \tau(B_{k+2}, x)\right)}$$

and

$$\tau(B_{k+1}^{'}, x) = \frac{1}{1 + x\left(d_{k+1} - 2 + \tau(B_{k+2}^{'}, x)\right)},$$

then $\tau(B_{k+1},x) > \tau(B'_{k+1},x)$. So, $d_1 = d'_1,\dots,d_k = d'_k$, $\tau(B_{k+1},x) > \tau(B'_{k+1},x)$ and k is odd. By the induction assumption $\tau(B,x) < \tau(B',x)$. And hence, if $k+1$ is even, then $\tau(B',x) > \tau(B,x)$. □

Lemma 3.9 *Let G be a caterpillar, label all the non-leaf vertices in G from left to right as u_1, u_2,...,u_ℓ and let their degrees be d_1, d_2,...,d_ℓ, respectively. If G is maximal with respect to $M(.,x)$, all the d_i's are different and $d_1 < d_\ell$, then*

$$d_1 < d_\ell < d_2 < d_{\ell-1} < d_3 < d_{\ell-2} < \cdots < d_j < d_{\ell-j+1},$$

for some positive integer j.

Proof. Suppose G is maximal with respect to $M(.,x)$, all the d_i's are different and $d_1 < d_\ell$. Then, by Lemma 3.3, u_1 and u_ℓ must have the smallest degrees among all non-leaf vertices in G hence

$$d_1 < d_\ell < \min\{d_2, d_3, \dots, d_{\ell-1}\}. \tag{3.7}$$

Let G be decomposed as in Figure 3.6. If the root of B is u_1 and the

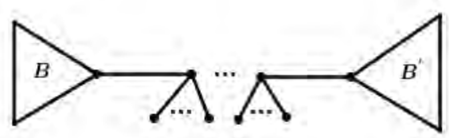

Figure 3.6: Decomposition of a caterpillar G in Lemma 3.9.

root of B' is u_ℓ, then

$$\tau(B,x) = \frac{1}{1 + x\,(d_1 - 1)}$$

and

$$\tau(B',x) = \frac{1}{1 + x\,(d_\ell - 1)}.$$

Since $d_1 < d_\ell$ and $x > 0$, then $\tau(B,x) > \tau(B',x)$. Then, by Lemma 3.2, we have $d_2 \le d_{\ell-1}$. d_2 and $d_{\ell-1}$ are different hence

$$d_2 < d_{\ell-1}. \tag{3.8}$$

If the root of B is u_i such that $2 \le i \le \ell - 3$ and the root of B' is u_ℓ, then

$$\tau(B,x) = \frac{1}{1 + x\,(d_i - 2 + \tau(B_{i-1},x))}$$

and

$$\tau(B^{'},x)=\frac{1}{1+x\,(d_\ell-1)}.$$

Since $i\geq 2$, then B_{i-1} is non-empty and not a leaf. Then, by Lemma 2.3 and Remark 2.5, we have $0<\tau(B_{i-1},x)<1$. Since $d_\ell<d_i$ and $x>0$, then $d_\ell-1\leq d_i-2<d_i-2+\tau(B_{i-1},x)$ and hence $\tau(B^{'},x)>\tau(B,x)$. Then, by Lemma 3.2, we must have $d_{\ell-1}\leq d_{i+1}$. But $d_{\ell-1}$ and d_{i+1} are different hence

$$d_{\ell-1}<d_{i+1} \text{ for all } 2\leq i\leq \ell-3. \tag{3.9}$$

Then, from (3.7), (3.8) and (3.9)

$$d_1<d_\ell<d_2<d_{\ell-1}<\min\{d_3,d_4,\ldots,d_{\ell-2}\}.$$

Now suppose that

$$d_1<d_\ell<d_2<d_{\ell-1}<\cdots<d_k<d_{\ell-k+1}<\min\{d_{k+1},d_{k+2},\ldots,d_{\ell-k}\},$$

for $k\geq 1$. If the root of B is u_k and the root of $B^{'}$ is $u_{\ell-k+1}$, then

$$\tau(B,x)=\frac{1}{1+x\,(d_k-2+\tau(B_{k-1},x))}$$

and

$$\tau(B^{'},x)=\frac{1}{1+x\left(d_{\ell-k+1}-2+\tau(B^{'}_{\ell-k+2},x)\right)}.$$

Since $k\geq 1$, then B_{k-1} and $B^{'}_{\ell-k+2}$ are non-empty. Then, by Lemma 2.3 and Remark 2.5, we have $0<\tau(B_{k-1},x),\tau(B^{'}_{\ell-k+2},x)\leq 1$. Since $d_k<d_{\ell-k+1}$ and $0<\tau(B_{k-1},x),\tau(B^{'}_{\ell-k+2},x)\leq 1$, then

$$d_k-2+\tau(B_{k-1},x)\leq d_{\ell-k+1}-2<d_{\ell-k+1}-2+\tau(B^{'}_{\ell-k+2},x).$$

Then, $\tau(B,x)>\tau(B^{'},x)$. By Lemma 3.2, we get $d_{k+1}\leq d_{\ell-k}$. But d_{k+1} and $d_{\ell-k}$ are different, then

$$d_{k+1}<d_{\ell-k}. \tag{3.10}$$

Suppose the root of B is u_i with $k+1\leq i\leq \ell-k-2$ and the root of $B^{'}$ is $u_{\ell-k+1}$, then

$$\tau(B,x)=\frac{1}{1+x\,(d_i-2+\tau(B_{i-1},x))}$$

and

$$\tau(B^{'},x)=\frac{1}{1+x\left(d_{\ell-k+1}-2+\tau(B^{'}_{\ell-k+2},x)\right)}.$$

Since $i \geq k+1 \geq 2$, then B_{i-1} and $B'_{\ell-k+2}$ are non-empty. Then, by Lemma 2.3 and Remark 2.5, we have $0 < \tau(B_{i-1},x), \tau(B'_{\ell-k+2},x) \leq 1$. Since $d_{\ell-k+1} < d_i$ and $0 < \tau(B_{i-1},x), \tau(B'_{\ell-k+2},x) \leq 1$, then

$$d_{\ell-k+1} - 2 + \tau(B'_{\ell-k+2},x) \leq d_i - 2 < d_i - 2 + \tau(B_{i-1},x).$$

Then, $\tau(B',x) > \tau(B,x)$. Then, by Lemma 3.2, we have $d_{\ell-k} \leq d_{i+1}$ for all $k+1 \leq i \leq \ell-k-2$. Since $d_{\ell-k}$ and d_{i+1} are different, then

$$d_{\ell-k} < d_{i+1}. \tag{3.11}$$

Then, from (3.10) and (3.11) and the hypothesis we have

$$d_1 < d_\ell < d_2 < d_{\ell-1} < \cdots < d_k < d_{\ell-k+1} < d_{k+1} < d_{\ell-k} < \min\{d_{k+2}, d_{k+3}, \ldots, d_{\ell-k-1}\}.$$

□

The following form of writing a reduced degree sequence makes it easy to define the extremal caterpillar $\mathcal{X}(D)$. While the standard way $(d_1, d_2, \ldots, d_n)$ is convenient to define the extremal caterpillar $\mathcal{S}(D)$.

Definition 3.10 Let G be a connected, simple graph. The reduced degree sequence of G will be written in the following form:

$$D = \begin{pmatrix} s_1 & s_2 & \ldots & s_t \\ r_1 & r_2 & \ldots & r_t \end{pmatrix},$$

where $1 < s_1 < s_2 < \cdots < s_t$ and r_i is the number of repetitions of s_i in the degree sequence of G.

The following definition will be needed for describing the structure of extremal caterpillar.

Definition 3.11 Let $D = \begin{pmatrix} s_1 & s_2 & \ldots & s_t \\ r_1 & r_2 & \ldots & r_t \end{pmatrix}$ be a reduced degree sequence of a tree, for some positive integer t. Let k be a positive integer such that $k \leq t$ and let i and j be nonnegative integers such that $i + j \leq r_k$. Then, $B_L^{k,i}(D)$ and $B_R^{k,j}(D)$ are two disjoint complete branches such that:

(i) If $k = 1$, then $B_L^{1,0}(D) = B_R^{1,0}(D) = [1]$, otherwise

$$B_L^{1,i\geq 1}(D) = [\underbrace{[1],\ldots,[1]}_{s_1-2 \text{ times}}, \underbrace{[[1],\ldots,[1]}_{s_1-2 \text{ times}}, [\ldots, \underbrace{[[1],\ldots,[1]}_{s_1-2 \text{ times}}, \underbrace{[s_1]\ ]\ldots]]]}_{i-1 \text{ times}}$$

and

$$B_R^{1,j\geq 1}(D) = [\underbrace{[1],\ldots,[1]}_{s_1-2 \text{ times}}, [\underbrace{[1],\ldots,[1]}_{s_1-2 \text{ times}}, [\ldots, [\underbrace{[1],\ldots,[1]}_{s_1-2 \text{ times}}, [s_1] \underbrace{]\ldots]]]}_{j-1 \text{ times}} .$$

See Figure 3.7 for an example.

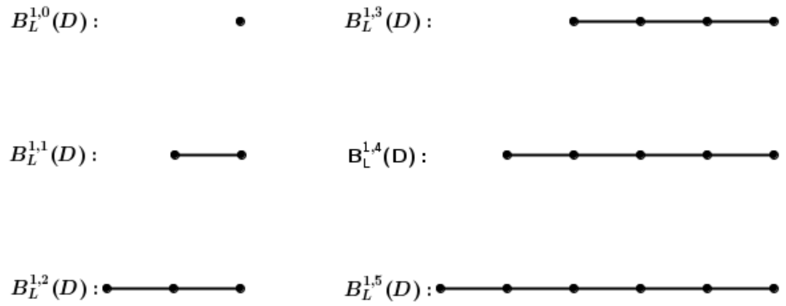

Figure 3.7: Graph representations of $B_L^{1,0}(D)$, $B_L^{1,1}(D)$, $B_L^{1,2}(D)$, $B_L^{1,3}(D)$, $B_L^{1,4}(D)$ and $B_L^{1,5}(D)$, for a reduced degree sequence $D = \binom{2\ \ 3\ \ 4\ \ 5\ \ 7}{5\ \ 4\ \ 4\ \ 4\ \ 3}$.

(ii) If $k \geq 2$ and k is even, then

$$B_L^{k,i}(D) = [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, [\ldots, [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, B_L^{k-1,1}(D) \underbrace{]\ldots]]]}_{i \text{ times}}$$

and

$$B_R^{k,j}(D) = [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, [\ldots, [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, B_R^{k-1,r_{k-1}-1}(D) \underbrace{]\ldots]]]}_{j \text{ times}} .$$

See Figure 3.8 for an example.
(iii) If $k \geq 2$ and k is odd, then

$$B_L^{k,i}(D) = [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, [\ldots, [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, B_L^{k-1,r_{k-1}-1}(D) \underbrace{]\ldots]]]}_{i \text{ times}}$$

and

$$B_R^{k,j}(D) = [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, [\ldots, [\underbrace{[1],\ldots,[1]}_{s_k-2 \text{ times}}, B_R^{k-1,1}(D) \underbrace{]\ldots]]]}_{j \text{ times}} .$$

See Figure 3.9 for an example.

Remark 3.12 Note that $B_L^{k,0}(D) = B_L^{k-1,r_{k-1}-1}(D)$ and $B_R^{k,0}(D) = B_R^{k-1,1}(D)$, if $k \geq 2$ and k is odd. $B_L^{k,0}(D) = B_L^{k-1,1}(D)$ and $B_R^{k,0}(D) = B_R^{k-1,r_{k-1}-1}(D)$, if $k \geq 2$ and k is even.

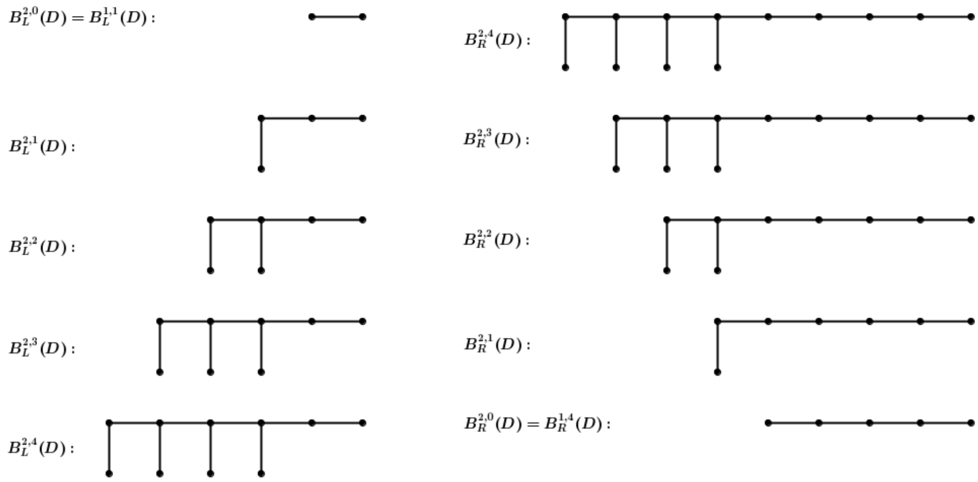

Figure 3.8: Graph representations of $B_L^{2,0}(D)$, $B_L^{2,1}(D)$, $B_L^{2,2}(D)$, $B_L^{2,3}(D)$, $B_L^{2,4}(D)$, $B_R^{2,4}(D)$, $B_R^{2,3}(D)$, $B_R^{2,2}(D)$, $B_R^{2,1}(D)$ and $B_R^{2,0}(D)$, for a reduced degree sequence $D = \binom{2 \quad 3 \quad 4 \quad 5 \quad 7}{5 \quad 4 \quad 4 \quad 4 \quad 3}$.

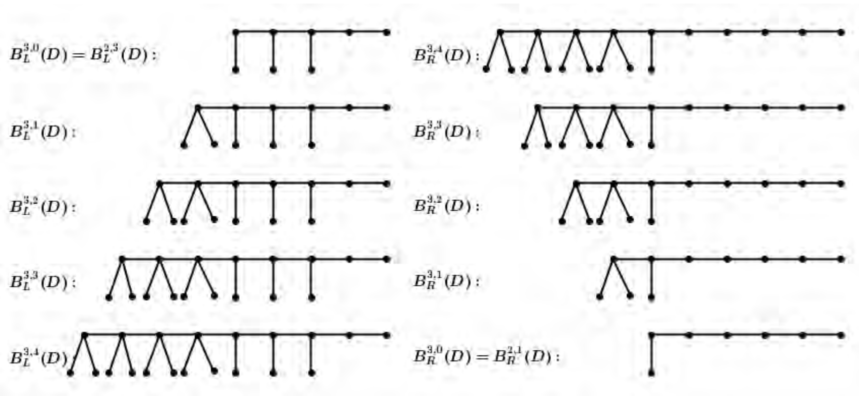

Figure 3.9: Graph representations of $B_L^{3,0}(D)$, $B_L^{3,1}(D)$, $B_L^{3,2}(D)$, $B_L^{3,3}(D)$, $B_L^{3,4}(D)$, $B_R^{3,4}(D)$, $B_R^{3,3}(D)$, $B_R^{3,2}(D)$, $B_R^{3,1}(D)$ and $B_R^{3,0}(D)$, for a reduced degree sequence $D = \binom{2 \quad 3 \quad 4 \quad 5 \quad 7}{5 \quad 4 \quad 4 \quad 4 \quad 3}$.

Definition 3.13 Let $D = \binom{s_1 \quad s_2 \quad \cdots \quad s_t}{r_1 \quad r_2 \quad \cdots \quad r_t}$ be a reduced degree sequence of a caterpillar, for some positive integer t. Then, we define $\mathcal{X}(D)$ to be the caterpillar, with reduced degree sequence D, obtained by joining by an edge the roots of $B_L^{t,i}(D)$ and $B_R^{t,j}(D)$ where: if t is odd, then $i = 1$ and $j = r_t - 1$ and if t is even, then $i = r_t - 1$ and $j = 1$, see Figure 3.10 for an example.

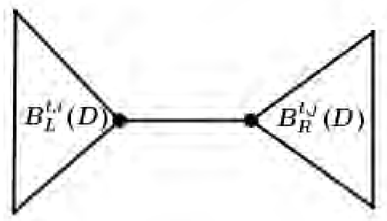

Figure 3.10: Graph representation of $\mathcal{X}(D)$, where $D = \binom{s_1 \quad s_2 \quad \cdots \quad s_t}{r_1 \quad r_2 \quad \cdots \quad r_t}$

The roots of $B_L^{t,i}(D)$ and $B_R^{t,j}(D)$ is selected as follows: Suppose $t = 1$. Then $i = 1$ and the root of $B_L^{t,i}(D)$ is the pseudo-leaf or a leaf of degree $s_1 - 1$ in $B_L^{t,i}(D)$. If $j = 0$, then the root of $B_R^{t,j}(D)$ is an isolated vertex $B_R^{t,j}(D)$. If $j \geq 1$, then the root of $B_R^{t,j}(D)$ is the pseudo-leaf or a leaf of degree $s_1 - 1$ in $B_R^{t,j}(D)$.

Suppose $t \geq 2$ and t is even. If $i = 0$, then the root of $B_L^{t,i}(D)$ is the root of $B_L^{t-1,1}(D)$. If $i \geq 1$, then the root of $B_L^{t,i}(D)$ is the pseudo-leaf of degree $s_t - 1$, adjacent to the root of $B_L^{t,i-1}(D)$. Conversely, if t is even, then $j = 1$ and the root of $B_R^{t,j}(D)$ is the pseudo-leaf of degree $s_t - 1$, adjacent to the root of $B_R^{t-1,r_{t-1}-1}(D)$.

Suppose $t \geq 2$ and t is odd. Then, $i = 1$ and the root of $B_L^{t,i}(D)$ is the pseudo-leaf of degree $s_t - 1$, adjacent to the root of $B_L^{t-1,r_{t-1}-1}(D)$. Conversely, if $j = 0$, then the root of $B_R^{t,j}(D)$ is the root of $B_R^{t-1,1}(D)$. If $j \geq 1$, then the root of $B_R^{t,j}(D)$ is the pseudo-leaf of degree $s_t - 1$, adjacent to the root of $B_R^{t,j-1}(D)$. That is,

$$\mathcal{X}(D) = C(s_1, \underbrace{s_2, \ldots, s_2}_{r_2-1}, s_3, \ldots, \underbrace{s_t, \ldots, s_t}_{r_t}, \ldots, \underbrace{s_3, \ldots, s_3}_{r_3-1}, s_2, \underbrace{s_1, \ldots, s_1}_{r_1-1}),$$

if $r_i > 1$ for all i. See Figure 3.11 for an example.

Lemma 3.14 *Let $D = \binom{s_1 \quad s_2 \quad \cdots \quad s_t}{r_1 \quad r_2 \quad \cdots \quad r_t}$ be a reduced degree sequence of a tree, for some positive integer t. Let k be a positive integer such that $k \leq t$. Let i and j be nonnegative integers such that $i + j = r_k$.*

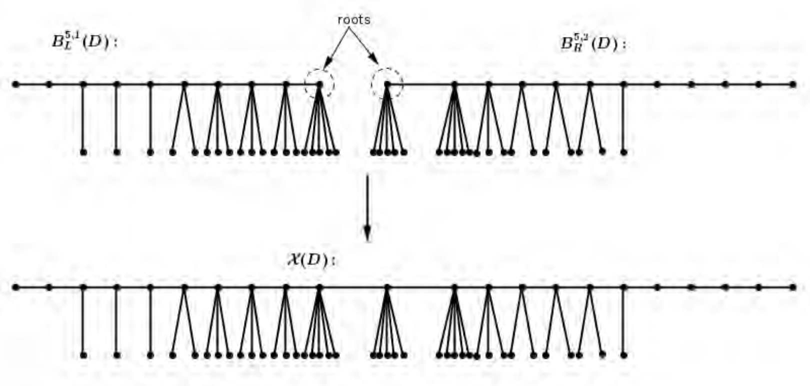

Figure 3.11: Graph representations of $\mathcal{X}(D)$, with $D = \binom{2\ 3\ 4\ 5\ 7}{5\ 4\ 4\ 4\ 3}$.

If k is odd, then $\tau(B_L^{k,1}(D),x) \leq \tau(B_R^{k,j}(D),x)$, with equality if and only if $B_L^{k,1}(D) \approx_r B_R^{k,j}(D)$, for all $0 \leq j \leq r_k - 1$. If k is even, then $\tau(B_L^{k,i}(D),x) \geq \tau(B_R^{k,1}(D),x)$, with equality if and only if $B_L^{k,i}(D) \approx_r B_R^{k,1}(D)$, for all $0 \leq i \leq r_k - 1$ and $x > 0$.

Note that when $B_L^{k,1}(D) \approx_r B_R^{k,j}(D)$ or $B_L^{k,i}(D) \approx_r B_R^{k,1}(D)$, then

$$r_1 = r_2 = \cdots = r_k = 2.$$

Proof. (i) If $k = 1$, then $B_L^{1,1}(D) = [s_1]$ and

$$\tau(B_L^{1,1}(D),x) = \frac{1}{1 + x(s_1 - 1)}.$$

$$B_R^{1,j}(D) = \begin{cases} [1], & \text{if } j = 0. \\ [\underbrace{[1],\ldots,[1]}_{s_1-2 \text{ times}}, [\underbrace{[1],\ldots,[1]}_{s_1-2 \text{ times}}, [\ldots, [\underbrace{[1],\ldots,[1]}_{s_1-2 \text{ times}}, [s_1] \underbrace{]\ldots]]]}_{j-1 \text{ times}}, & \text{if } 1 \leq j \leq r_1 - 1. \end{cases}$$

Then,

$$\tau(B_R^{1,0}(D),x) = 1 > \frac{1}{1 + x(s_1 - 1)} = \tau(B_L^{1,1}(D),x)$$

and for $r_k > 1$, we have

$$\tau(B_R^{1,1}(D),x) = \frac{1}{1 + x(s_1 - 1)} = \tau(B_L^{1,1}(D),x).$$

In this case $B_R^{1,1}(D) \approx_r B_L^{1,1}(D)$.

$$\tau(B_R^{1,j\geq 2}(D),x) = \frac{1}{1 + x(s_1 - 2 + \tau(B_R^{1,j-1}(D),x))}.$$

Since $j \geq 2$, then $B_R^{1,j-1}(D)$ is neither a leaf nor empty, hence by Lemma 2.4 and Remark 2.5, we must have $0 < \tau(B_R^{1,j-1}(D), x) < 1$. Then, $s_1 - 2 + \tau(B_R^{1,j-1}(D), x) < s_1 - 1$. Hence

$$\tau(B_R^{1,j\geq 2}(D), x) > \tau(B_L^{1,1}(D), x).$$

Therefore, if $k = 1$ the lemma holds.

(ii) If $k = 2$, then

$$B_L^{2,i}(D) = [\underbrace{[1], \ldots, [1]}_{s_2-2 \text{ times}}, [\underbrace{[1], \ldots, [1]}_{s_2-2 \text{ times}}, [\ldots, [\underbrace{[1], \ldots, [1]}_{s_2-2 \text{ times}}, B_L^{1,1}(D) \underbrace{] \ldots]]}_{i \text{ times}},$$

for $0 \leq i \leq r_2 - 1$, $B_R^{2,1}(D) = [\underbrace{[1], \ldots, [1]}_{s_2-2 \text{ times}}, B_R^{1,r_1-1}(D)]$ and

$$\tau(B_R^{2,1}(D), x) = \frac{1}{1 + x\left(s_2 - 2 + \tau(B_R^{1,r_1-1}(D), x)\right)}.$$

(a) If $i = 0$, then

$$\tau(B_L^{2,0}(D), x) = \tau(B_L^{1,1}(D), x) = \frac{1}{1 + x(s_1 - 1)}.$$

Since $B_R^{1,r_1-1}(D)$ is not empty and $s_1 < s_2$, then by Lemma 2.4 and Remark 2.5, we have $0 < \tau(B_R^{1,r_1-1}(D), x) \leq 1$. Then, $s_1 - 1 \leq s_2 - 2 < s_2 - 2 + \tau(B_R^{1,r_1-1}(D), x)$. Hence $\tau(B_L^{2,0}(D), x) > \tau(B_R^{2,1}(D), x)$.

(b) If $i = 1$, then

$$\tau(B_L^{2,1}(D), x) = \frac{1}{1 + x(s_2 - 2 + \tau(B_L^{1,1}(D), x))}$$

From (i), $\tau(B_L^{1,1}(D), x) \leq \tau(B_R^{1,r_1-1}(D), x)$, hence

$$\tau(B_L^{2,1}(D), x) \geq \tau(B_R^{2,1}(D), x).$$

If $\tau(B_L^{2,1}(D), x) = \tau(B_R^{2,1}(D), x)$, then by Lemma 3.4, we get $B_L^{2,1}(D) \approx_r B_R^{2,1}(D)$.

(c) If $i \geq 2$, then

$$\tau(B_L^{2,i}(D), x) = \frac{1}{1 + x(s_2 - 2 + \tau(B_L^{2,i-1}(D), x))},$$

$$\tau(B_L^{2,i-1}(D), x) = \frac{1}{1 + x(s_2 - 2 + \tau(B_L^{2,i-2}(D), x))}$$

and

$$\tau(B_R^{1,r_1-1}(D),x) = \begin{cases} \frac{1}{1+x(s_1-2+\tau(B_R^{1,r_1-2}(D),x))}, & \text{if } r_1 \geq 2 \\ \\ 1, & \text{otherwise.} \end{cases}$$

Since $i \geq 2$, $B_L^{2,i-2}(D)$ is neither empty nor a leaf. If $r_1 \geq 2$, then $B_R^{1,r_1-2}(D)$ is not empty. Then, by Lemma 2.4 and Remark 2.5, we have $0 < \tau(B_L^{2,i-2}(D),x) < 1$ and $0 < \tau(B_R^{2,r_1-2}(D),x) \leq 1$. Then,

$$\begin{aligned} \tau(B_L^{2,i-1}(D),x) &= \frac{1}{1+x(s_2-2+\tau(B_L^{2,i-2}(D),x))} < \frac{1}{1+x(s_2-2)} \\ &\leq \frac{1}{1+x(s_1+1-2)} \leq \frac{1}{1+x(s_1-2+\tau(B_R^{1,r_1-2}(D),x))} \\ &\leq \begin{cases} \frac{1}{1+x(s_1-2+\tau(B_R^{1,r_1-2}(D),x))}, & \text{if } r_1 \geq 2 \\ \\ 1, & \text{otherwise} \end{cases} \\ &= \tau(B_R^{1,r_1-1}(D),x). \end{aligned}$$

Hence $\tau(B_L^{2,i-1}(D),x) < \tau(B_R^{1,r_1-1}(D),x)$ and thus

$$\tau(B_L^{2,i}(D),x) > \tau(B_R^{2,1}(D),x).$$

Therefore, if $k = 2$ the lemma holds.

(iii) Suppose the lemma is true for $k = m \geq 2$. That is, if m is odd, then $\tau(B_L^{m,1}(D),x) \leq \tau(B_R^{m,j}(D),x)$, where $0 \leq j \leq r_m - 1$ and $x > 0$. If m is even, then $\tau(B_L^{m,i}(D),x) \geq \tau(B_R^{m,1}(D),x)$, where $0 \leq i \leq r_m - 1$ and $x > 0$. With equality if and only if $B_L^{m,i}(D) \approx_r B_R^{m,j}(D)$.

(a) If $m+1$ is odd, then

$$\tau(B_L^{m+1,1}(D),x) = \frac{1}{1+x(s_{m+1}-2+\tau(B_L^{m,i}(D),x))},$$

for some i with $0 \leq i \leq r_m - 1$ and

$\tau(B_R^{m+1,j'}(D),x)$

$$= \begin{cases} \dfrac{1}{1+x(s_m-2+\tau(B_R^{m-1,j''}(D),x))}, & \text{for some } j'' \text{ with } 0 \le j'' \le r_{m-1}-1, \text{ if } j'=0, \\ \dfrac{1}{1+x(s_{m+1}-2+\tau(B_R^{m,1}(D),x))}, & \text{if } j'=1, \\ \dfrac{1}{1+x(s_{m+1}-2+\tau(B_R^{m+1,j'-1}(D),x))}, & \text{if } j' \ge 2. \end{cases}$$

Since $m \ge 2$, then neither $B_L^{m,i}(D)$ nor $B_R^{m-1,j''}(D)$ is empty, where $0 \le i \le r_m - 1$ and $0 \le j'' \le r_{m-1}-1$. Then, by Lemma 2.4 and Remark 2.5, we have $0 < \tau(B_L^{m,i}(D),x), \tau(B_R^{m-1,j''}(D),x) \le 1$. Then,

$$\begin{aligned} \tau(B_L^{m+1,1}(D),x) &= \frac{1}{1+x(s_{m+1}-2+\tau(B_L^{m,i}(D),x))} < \frac{1}{1+x(s_{m+1}-2)} \\ &\le \frac{1}{1+x(s_m+1-2)} \le \frac{1}{1+x(s_m-2+\tau(B_R^{m-1,j''}(D),x))} \\ &= \tau(B_R^{m+1,0}(D),x). \end{aligned}$$

Thus, $\tau(B_L^{m+1,1}(D),x) < \tau(B_R^{m+1,0}(D),x)$. This completes the case of $j'=0$.

Now we consider the case of $j'=1$. Since $m+1$ is odd, then m is even. From the inductive hypothesis $\tau(B_L^{m,i}(D),x) \ge \tau(B_R^{m,1}(D),x)$, with equality if and only if $B_L^{m,i}(D) \approx_r B_R^{m,1}(D)$. Hence,

$$\begin{aligned} &\tau(B_L^{m+1,1}(D),x) \\ &= \frac{1}{1+x(s_{m+1}-2+\tau(B_L^{m,i}(D),x))} \le \frac{1}{1+x(s_{m+1}-2+\tau(B_R^{m,1}(D),x))} \\ &= \tau(B_R^{m+1,1}(D),x), \end{aligned}$$

with equality if and only if $B_L^{m,i}(D) \approx_r B_R^{m,1}(D)$.

We are left with the case of $j' \ge 2$.

$$\tau(B_L^{m,i}(D),x) = \frac{1}{1+x(\mathrm{rd}(B_L^{m,i}(D))-1+\tau(C,x))},$$

where C is the largest branch of the root of $B_L^{m,i}(D)$, and $0 \le i \le r_m - 1$. Since $m \ge 2$, then C is not empty, then by Lemma 2.4 and Remark 2.5, we have $0 < \tau(C,x) \le 1$. If $i=0$, then $\mathrm{rd}(B_L^{m,0}(D)) = s_{m-1}-1$, otherwise $i \ge 1$ and $\mathrm{rd}(B_L^{m,i}(D)) = s_m - 1$. Now

$$\tau(B_R^{m+1,j'-1}(D),x) = \frac{1}{1+x(s_{m+1}-2+\tau(B_R^{m+1,j'-2}(D),x))}.$$

Since $m \geq 2$ and $j' \geq 2$, then $B_R^{m+1,j'-2}(D)$ is neither empty nor a leaf. Then, by Lemma 2.4 and Remark 2.5, we have $0 < \tau(B_R^{m+1,j'-2}(D), x) < 1$. Then,

$$\begin{aligned}
&\tau(B_R^{m+1,j'-1}(D), x) \\
&= \frac{1}{1 + x(s_{m+1} - 2 + \tau(B_R^{m+1,j'-2}(D), x))} < \frac{1}{1 + x(s_{m+1} - 2)} \\
&\leq \frac{1}{1 + x(s_m + 1 - 2)} = \frac{1}{1 + x(s_m - 1 - 1 + 1)} \\
&\leq \frac{1}{1 + x(\mathrm{rd}(B_L^{m,i}(D)) - 1 + 1)} \leq \frac{1}{1 + x(\mathrm{rd}(B_L^{m,i}(D)) - 1 + \tau(C, x))} \\
&= \tau(B_L^{m,i}(D), x).
\end{aligned}$$

Hence $\tau(B_L^{m,i}(D), x) > \tau(B_R^{m+1,j'-1}(D), x)$, if $j' \geq 2$. Therefore, if $m + 1$ is odd the lemma holds.

(b) If $m + 1$ is even, then $\tau(B_R^{m+1,1}(D), x) = \frac{1}{1+x(s_{m+1}-2+\tau(B_R^{m,j}(D),x))}$, where $0 \leq j \leq r_m - 1$ and

$$\tau(B_L^{m+1,i'}(D), x) = \begin{cases} \frac{1}{1+x(s_m-2+\tau(B_L^{m-1,i''}(D),x))}, & \text{for some } i'' \text{ with } 0 \leq i'' \leq r_{m-1} - 1, \text{ if } i' = 0, \\ \frac{1}{1+x(s_{m+1}-2+\tau(B_L^{m,1}(D),x))}, & \text{if } i' = 1, \\ \frac{1}{1+x(s_{m+1}-2+\tau(B_L^{m+1,i'-1}(D),x))}, & \text{if } i' \geq 2. \end{cases}$$

Reasoning as in (iii) (a) we conclude the proof. □

Proposition 3.15 Let G be a caterpillar with reduced degree sequence $D = \binom{s_1 \ s_2 \ \dots \ s_t}{r_1 \ r_2 \ \dots \ r_t}$, for some positive integer t. If G is maximal with respect to $M(.,x)$, then G has disjoint complete branches $B_L^{1,1}(D)$ and $B_R^{1,r_1-1}(D)$. That is G can be decomposed as in Figure 3.12:

Proof. Label all the non-leaf vertices in G from left to right as v_1, $v_2, \dots, v_\ell$. Suppose G is maximal with respect to $M(.,x)$. Then, by Lemma 3.3, v_1 and v_ℓ must have the smallest degrees among all non-leaf vertices in G. We choose $\deg(v_1) \leq \deg(v_\ell)$. If $r_1 = 1$, then $\deg(v_1) = s_1$ and $\deg(v_\ell) = s_2$. Then, G can be decomposed as in Figure 3.12 with v_1 being the root of $B_L^{1,1}(D)$ and $B_R^{1,0}(D)$ as a leaf. If $r_1 = 2$, then by Lemma 3.5 (i), we must have $\deg(v_1) = \deg(v_\ell) = s_1$. Then, G

Figure 3.12: Decomposition of a caterpillar in Proposition 3.15.

can be decomposed as in Figure 3.12 with $B_L^{1,1}(D) \approx_r B_R^{1,1}(D) = [s_1]$.

Suppose $r_1 \geq 3$. If $t = 1$, we are done, because $\deg(v_1) = \deg(v_2) = \cdots = \deg(v_\ell) = s_1$. Hence G can be decomposed as in Figure 3.12. Suppose $t \geq 2$. By reversing the labelling if needed in the non-leaf vertices in G, we can assume there is a positive integer j such that $2 \leq j < \ell - 1$ and $\deg(v_j) > \deg(v_{j+1}) = s_1$. By Lemma 3.5 (ii), we must have

$$\deg(v_{j+1}) = \deg(v_{j+2}) = \cdots = \deg(v_\ell) = s_1.$$

By Lemma 3.6, we get that $\deg(v_2) > s_1$. By Lemma 3.7, we get that

$$\deg(v_j) = \min\{\deg(v_i) : 2 \leq i \leq j\}$$

and

$$\deg(v_2) = \min\{\deg(v_i) : 2 \leq i \leq j-1\}.$$

Then, G can be decomposed as in Figure 3.12. Therefore in all the cases G can be decomposed as in Figure 3.12. □

Definition 3.16 Let G be a caterpillar and label all its non-leaf vertices from left to right as u_1, u_2,…,u_ℓ. We define $B_L^{u_i}$ to be a complete branch of G that contains u_i but not u_{i+1} and $B_R^{u_i} = G - B_L^{u_{i-1}}$ for $i \in \{1, \ldots, \ell - 1\}$.

Lemma 3.17 *Let G be a caterpillar with reduced degree sequence $D = \binom{s_1 \ s_2 \ \cdots \ s_t}{r_1 \ r_2 \ \cdots \ r_t}$, for some positive integer t. Suppose that C and C' are disjoint complete branches of G, with roots y_1 and y_2, respectively. Let $u_1, \ldots, u_j$ be the internal vertices of the path from y_1 to y_2 in this order. See Figure 3.13. Suppose G is maximal with respect to $M(.,x)$.*

(i) If $\deg(y_1) < \deg(u_1) = \deg(u_2) = s = \deg(u_{j-1}) = \deg(u_j)$ and $\deg(u_i) \geq s$, for any $1 \leq i \leq j$, then $\deg(u_i) = s$, for all $i \in \{1, \ldots, j\}$.

(ii) If $\deg(u_1) = s = \deg(u_{j-1}) < \deg(u_j)$ and $\deg(u_i) \geq s$, for any $1 \leq i \leq j$, then $\deg(u_1) = \deg(u_2) = \cdots = \deg(u_{j-1})$.

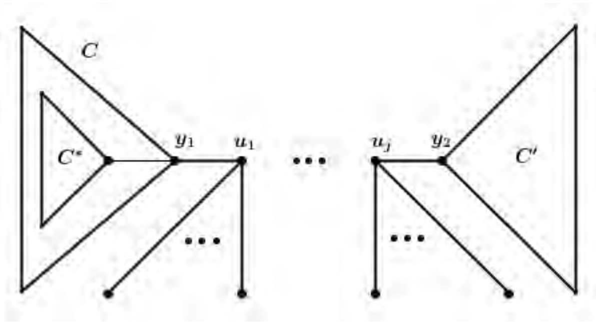

Figure 3.13: Decomposition of caterpillar G in Lemma 3.17.

Proof. Since C and C' are non-empty and non-leaves, then by Lemma 2.4 and Remark 2.5, we have $0 < \tau(C,x), \tau(C',x) < 1$.

$$\begin{aligned}
\tau(C,x) &= \frac{1}{1+x(\deg(y_1)-2+\tau(C^*,x))} \\
&\geq \frac{1}{1+x(\deg(y_1)-2+1)}, \text{ with equality if } C^* \text{ is a leaf.} \\
&\geq \frac{1}{1+x(\deg(u_j)-2)}, \text{ with equality if } \deg(u_j)=\deg(y_1)+1. \\
&> \frac{1}{1+x(\deg(u_j)-2+\tau(C',x))}, \text{ since } C' \text{ is not empty.} \\
&= \tau(B_R^{u_j},x).
\end{aligned}$$

Therefore, $\tau(C,x) > \tau(B_R^{u_j},x)$. Then,

$$\begin{aligned}
\tau(B_L^{u_1},x) &= \frac{1}{1+x(\deg(u_1)-2+\tau(C,x))} = \frac{1}{1+x(s-2+\tau(C,x))} \\
&< \frac{1}{1+x(s-2+\tau(B_R^{u_j},x))} = \frac{1}{1+x(\deg(u_{j-1})-2+\tau(B_R^{u_j},x))} \\
&= \tau(B_R^{u_{j-1}},x).
\end{aligned}$$

Therefore, $\tau(B_L^{u_1},x) < \tau(B_R^{u_{j-1}},x)$. Then, by Lemma 3.2, we have $\deg(u_2)$
$\geq \deg(u_{j-2}) \geq s$. Since $\deg(u_2)=s$, we have $\deg(u_{j-2})=s$. Since $\deg(u_{j-2})=\deg(u_{j-1})=s$, then with the same reasoning as above with $\deg(y_1)<\deg(u_1)=\deg(u_2)=s$, we get $\deg(u_{j-3})=s$. By iterating the process, we get $\deg(u_1)=\deg(u_2)=\cdots=\deg(u_j)=s$. This completes the proof of (i).

Now, we prove (ii).

$$\tau(B_L^{u_1},x) = \frac{1}{1+x(\deg(u_1)-2+\tau(C,x))}$$

$$
\begin{aligned}
&> \frac{1}{1+x(\deg(u_1)-2+1)}, \text{ since } C \text{ is not a leaf.}\\
&\geq \frac{1}{1+x(\deg(u_j)-2)}, \text{ with equality if } \deg(u_j)=\deg(u_1)+1.\\
&> \frac{1}{1+x(\deg(u_j)-2+\tau(C',x))}, \text{ since } C' \text{ is not empty.}\\
&= \tau(B_R^{u_j},x).
\end{aligned}
$$

Therefore, $\tau(B_L^{u_1},x) > \tau(B_R^{u_j},x)$. Then, by Lemma 3.2, we have $\deg(u_2) \leq \deg(u_{j-1})$. Since $\deg(u_i) \geq s$ for any $1 \leq i \leq j$ and $\deg(u_{j-1}) = s$, then $s \leq \deg(u_2) \leq \deg(u_{j-1}) = s$. Hence $\deg(u_2) = s$. Since $s = \deg(u_2) = \deg(u_{j-1}) < \deg(u_j)$, then with the same reasoning we get $\deg(u_3) = s$. Then, by iterating the process we get $\deg(u_1) = \deg(u_2) = \cdots = \deg(u_{j-1}) = s$. □

Theorem 3.18 *Let $\mathbb{C}_D$ be the set of all caterpillars with reduced degree sequence $D = \binom{s_1 \ s_2 \ \cdots \ s_t}{r_1 \ r_2 \ \cdots \ r_t}$, for some positive integer t. Let $x > 0$. If $G \in \mathbb{C}_D$ such that for all $H \in \mathbb{C}_D$ $M(H,x) \leq M(G,x)$, then $G \cong \mathcal{X}(D)$.*

Proof. Suppose $G \in \mathbb{C}_D$ such that for all $H \in \mathbb{C}_D$ $M(H,x) \leq M(G,x)$. Label all the non-leaf vertices in G from left to right as u_1, u_2,…,u_ℓ and their degrees as d_1, d_2,…,d_ℓ, respectively.

1.) If $t = 1$, there is only one caterpillar of reduced degree sequence D, as all the internal degrees are the same, and its $\mathcal{X}(D)$.

2.) If $t = 2$, then by Proposition 3.15 G can be decomposed as in Figure 3.14. Which we can view as in Figure 3.15. Hence $G \cong \mathcal{X}(D)$.

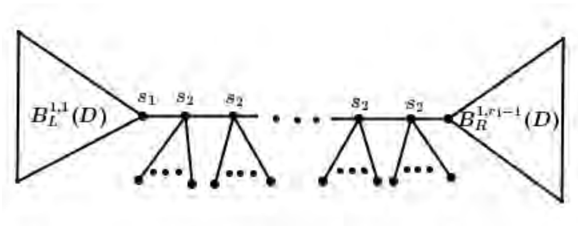

Figure 3.14: Decomposition of a caterpillar G in the proof of Theorem 3.18.

3.) Now assume that $t \geq 3$. Then, by Proposition 3.15 G can be decomposed as in Figure 3.16, for some positive integer j with $\deg(u_2)$, $\deg(u_j) > s_1$. Then, $\tau(B_L^{1,1}(D),x) = \frac{1}{1+x(s_1-1)}$.

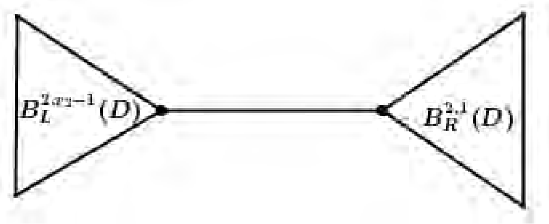

Figure 3.15: Alternative view of Figure 3.14.

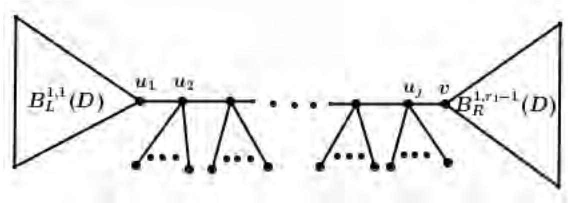

Figure 3.16: Decomposition of the caterpillar G in the proof of Theorem 3.18.

(i) If $r_1 = 1$, then by Lemma 2.4 and Remark 2.5, we have

$$\tau(B_R^{1,r_1-1}(D),x) = \tau(B_R^{1,0}(D),x) = 1 > \frac{1}{1+x\,(s_1-1)} = \tau(B_L^{1,1}(D),x),$$

since $B_R^{1,0}(D)$ is a leaf.

(ii) If $r_1 = 2$, then $B_R^{1,r_1-1}(D) = B_R^{1,1}(D) \approx_r B_L^{1,1}(D)$ and by Lemma 3.4, we get that

$$\tau(B_R^{1,r_1-1}(D),x) = \tau(B_R^{1,1}(D),x) = \tau(B_L^{1,1}(D),x) = \frac{1}{1+x\,(s_1-1)}.$$

(iii) If $r_1 \geq 3$, then

$$\tau(B_R^{1,r_1-1}(D),x) = \frac{1}{1+x\left(s_1-2+\tau(B_R^{1,r_1-2}(D),x)\right)}.$$

Since $r_1 \geq 3$, then $B_R^{1,r_1-2}(D)$ is not empty and not a leaf. Then, by Lemma 2.4 and Remark 2.5, we have $0 < \tau(B_R^{1,r_1-2}(D),x) < 1$. Then, $s_1-2+\tau(B_R^{1,r_1-2}(D),x) < s_1-1$ and hence $\tau(B_R^{1,r_1-1}(D),x) > \tau(B_L^{1,1}(D),x)$. Therefore $\tau(B_R^{1,r_1-1}(D),x) \geq \tau(B_L^{1,1}(D),x)$ in all the cases, with equality if and only if $B_R^{1,r_1-1}(D) \approx_r B_L^{1,1}(D)$.

Let i be a positive integer such that $2 \leq i < j$. Then, $s_1 = d_1 < d_l$ for all $2 \leq l \leq j$. Since $2 \leq i < j$, then $B_R^{u_{i+2}}$ is non-empty. Then, by Lemma 2.4 and Remark 2.5, we have $0 < \tau(B_R^{u_{i+2}},x) \leq 1$. Then,

$$\tau(B_L^{1,1}(D),x)$$

$$= \frac{1}{1+x\,(s_1-1)} = \frac{1}{1+x\,(d_1-1)} > \frac{1}{1+x\,(d_{i+1}-2+\tau(B_R^{u_{i+2}},x))}$$
$$= \tau(B_R^{u_{i+1}},x).$$

Since $\tau(B_L^{1,1}(D),x) > \tau(B_R^{u_{i+1}},x)$, then by Lemma 3.2, we get that

$$d_2 \leq d_i. \qquad (3.12)$$

By Lemma 3.14, we have, $\tau(B_L^{1,1}(D),x) \leq \tau(B_R^{1,r_1-1}(D),x)$. If $\tau(B_L^{1,1}(D),x) < \tau(B_R^{1,r_1-1}(D),x)$, then by Lemma 3.2, we get that $d_2 \geq d_j$.
If $\tau(B_L^{1,1}(D),x) = \tau(B_R^{1,r_1-1}(D),x)$, we choose $d_2 \geq d_j$. So we can assume

$$d_2 \geq d_j. \qquad (3.13)$$

Then, from (3.12) and (3.13), if $\tau(B_L^{1,1}(D),x) \leq \tau(B_R^{1,r_1-1}(D),x)$, then

$$s_2 = d_j \leq d_2 \leq d_i. \qquad (3.14)$$

Now, if $r_2 = 1$, then $d_j = s_2$ and $d_2 = s_3$. If $r_2 \geq 2$, then $d_j = d_2 = s_2$.

Suppose $r_2 \geq 3$. Suppose $d_2 = d_3 = s_2 = d_{j-1} = d_j$. Since $s_1 = d_1 < d_2 = d_3 = s_2 = d_{j-1} = d_j$, then by Lemma 3.17 (i), we must have $d_2 = d_3 = \cdots = d_j = s_2$. Which is a contradiction since $t \geq 3$. Hence

$$d_2 = d_3 \implies d_{j-1} \neq d_j \text{ and } d_{j-1} = d_j \implies d_2 \neq d_3. \qquad (3.15)$$

Since $\tau(B_L^{1,1}(D),x) \leq \tau(B_R^{1,r_1-1}(D),x)$, then

$$\begin{aligned}
&\tau(B_L^{u_2},x)\\
&= \frac{1}{1+x\left(d_2-2+\tau(B_L^{1,1}(D),x)\right)}\\
&= \frac{1}{1+x\left(s_2-2+\tau(B_L^{1,1}(D),x)\right)}, \quad \text{since } d_2 = s_2\\
&\geq \frac{1}{1+x\left(s_2-2+\tau(B_R^{1,r_1-1}(D),x)\right)}, \text{ since } \tau(B_L^{1,1}(D),x) \leq \tau(B_R^{1,r_1-1}(D),x).\\
&= \frac{1}{1+x\left(d_j-2+\tau(B_R^{1,r_1-1}(D),x)\right)}, \text{ since } d_j = s_2\\
&= \tau(B_R^{u_j},x).
\end{aligned}$$

Therefore, $\tau(B_L^{u_2},x) \geq \tau(B_R^{u_j},x)$, with equality if and only $\tau(B_L^{1,1}(D),x) = \tau(B_R^{1,r_1-1}(D),x)$ i.e $B_L^{1,1}(D) \approx_r B_R^{1,r_1-1}(D)$.

If $\tau(B_L^{u_2},x) = \tau(B_R^{u_j},x)$, then we choose $d_3 \leq d_{j-1}$, otherwise $\tau(B_L^{u_2},x) > \tau(B_R^{u_j},x)$ and by Lemma 3.2, we get that $d_3 \leq d_{j-1}$. Hence

$$s_2 = d_3 \leq d_{j-1}. \qquad (3.16)$$

Let h and h' be two positive integers such that $4 \leq h \leq j-2$, $2 \leq h' < h-1$ and $s_2 = d_{h'} = d_h < d_{h+1}$. Since $d_i \geq s_2$, for all $2 \leq i \leq h$, then by Lemma 3.17 (ii), we must have $d_{h'} = d_{h'+1} = \cdots = d_h = s_2$. Hence

$$d_2 = d_3 = \cdots = d_h = s_2, \text{ for all } 4 \leq h \leq j-2. \tag{3.17}$$

From (3.15), (3.16) and (3.17) we have, $d_{j-1} > d_3 = s_2$. Therefore G can be decomposed as in Figure 3.17, for some positive integer n'. Now, suppose G can be decomposed as in Figure 3.18, for some

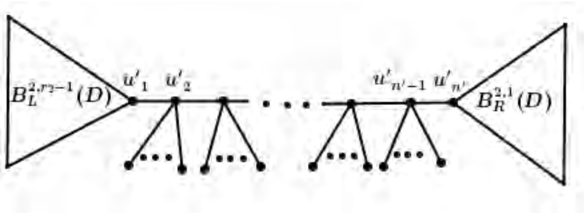

Figure 3.17: Decomposition of the caterpillar G in the proof of Theorem 3.18.

positive integers $k \leq t \geq 2$ and n'', such that if k is odd, then $i' = 1$ and $j' = r_k - 1$ and if k is even, then $i' = r_k - 1$ and $j' = 1$. If $k = t$,

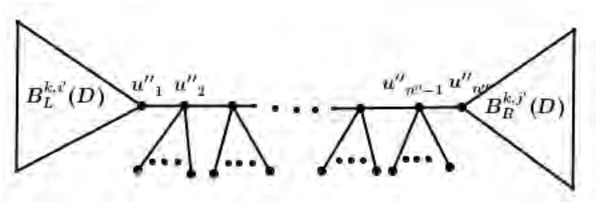

Figure 3.18: Decomposition of the caterpillar G in the proof of Theorem 3.18.

then $n''-1 = 0$ and we are done, because $G \cong \mathcal{X}(D)$. If $k = t-1$, then $\deg(u''_2) = \deg(u''_3) = \cdots = \deg(u''_{n''-1}) = s_{k+1}$ and G can be decomposed as in Figure 3.19, such that if k is odd, then $i'' = r_{k+1} - 1$ and $j'' = 1$ and if k is even, then $i'' = 1$ and $j'' = r_{k+1} - 1$. This is just $\mathcal{X}(D)$, hence $G \cong \mathcal{X}(D)$.

Suppose $2 \leq k < t-1$. Then $B_L^{u''_{i'''}}$ and $B_R^{u''_{i'''}}$ are non-empty and non-leaves, for all $2 \leq i''' \leq n''-1$. Then, $B_L^{u''_{i'''-1}}$ and $B_R^{u''_{i'''+1}}$ are non-empty and by Lemma 2.4 and Remark 2.5, we have

$$0 < \tau(B_L^{u''_{i'''-1}}, x), \tau(B_R^{u''_{i'''+1}}, x) \leq 1.$$

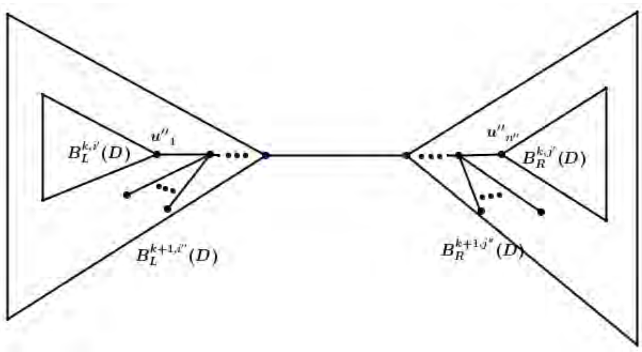

Figure 3.19: Decomposition of the caterpillar G in the proof of Theorem 3.18.

Then,

$$\begin{aligned}
&\tau(B_L^{k,i'}(D),x)\\
&= \frac{1}{1+x\left(\deg(u''_1)-2+\tau(B_L^{k,i'-1}(D),x)\right)}\\
&\geq \frac{1}{1+x\left(\deg(u''_{i'''})-2\right)}, && \text{since } s_k=\deg(u''_1)<\deg(u''_{i'''})\\
&> \frac{1}{1+x\left(\deg(u''_{i'''})-2+\tau(B_R^{u''_{i'''+1}},x)\right)}, && \text{since } 0<\tau(B_R^{u''_{i'''+1}},x)\\
&= \tau(B_R^{u''_{i'''}},x).
\end{aligned}$$

Therefore, $\tau(B_L^{k,i'}(D),x) > \tau(B_R^{u''_{i'''}},x)$. Similarly,

$$\begin{aligned}
&\tau(B_R^{k,j'}(D),x)\\
&= \frac{1}{1+x\left(\deg(u''_{n''})-2+\tau(B_R^{k,j'-1}(D),x)\right)}\\
&\geq \frac{1}{1+x\left(\deg(u''_{i'''})-2\right)}, && \text{since } \deg(u''_{n''})<\deg(u''_{i'''})\\
&> \frac{1}{1+x\left(\deg(u''_{i'''})-2+\tau(B_L^{u''_{i'''-1}},x)\right)}, && \text{since } 0<\tau(B_L^{u''_{i'''-1}},x)\\
&= \tau(B_L^{u''_{i'''}},x).
\end{aligned}$$

Therefore, $\tau(B_R^{k,j'}(D),x) > \tau(B_L^{u''_{i'''}},x)$. Then, by Lemma 3.2, we get that

$$\deg(u''_2) \leq \deg(u''_{i'''-1}) \text{ and } \deg(u''_{n''-1}) \leq \deg(u''_{i'''+1}). \tag{3.18}$$

(a) If k is odd, then by Lemma 3.14, we have

$$\tau(B_L^{k,1}(D),x) \leq \tau(B_R^{k,r_k-1}(D),x),$$

with equality if and only if $B_L^{k,1}(D) \approx_r B_R^{k,r_k-1}(D)$. If $\tau(B_L^{k,1}(D),x) = \tau(B_R^{k,r_k-1}(D),x)$, we choose $\deg(u''_2) \geq \deg(u''_{n''-1})$. Otherwise $\tau(B_L^{k,1}(D),x) < \tau(B_R^{k,r_k-1}(D),x)$ and by Lemma 3.2, we get that $\deg(u''_2) \geq \deg(u''_{n''-1})$. Therefore

$$\deg(u''_2) \geq \deg(u''_{n''-1}). \tag{3.19}$$

Then, from (3.18) and (3.19) we have,

$$\deg(u''_{n''-1}) \leq \deg(u''_2) \leq \deg(u''_{i'''}), \text{ for } 2 \leq i''' \leq n''-2. \tag{3.20}$$

Then, from (3.20) if $r_{k+1} = 1$, then $\deg(u''_{n''-1}) = s_{k+1}$ and $\deg(u''_2) = s_{k+2}$. If $r_{k+1} = 2$, then $\deg(u''_{n''-1}) = \deg(u''_2) = s_{k+1}$.

Suppose $r_{k+1} \geq 3$. Suppose

$$\deg(u''_2) = \deg(u''_3) = s_{k+1} = \deg(u''_{n''-2}) = \deg(u''_{n''-1}).$$

Since $\deg(u''_1), \deg(u''_{n''}) \leq s_k < s_{k+1}$ and $\deg(u''_{i'''}) > s_k$, for all $2 \leq i''' \leq n''-1$, then by Lemma 3.17 (i), we must have

$$\deg(u''_2) = \deg(u''_3) = \cdots = \deg(u''_{n''-2}) = \deg(u''_{n''-1}) = s_{k+1}.$$

Since $k < t-1$, then there exists a vertex $u''_{i'''}$ such that $\deg(u''_{i'''}) = s_t > s_{t-1} \geq s_{k+1}$, for some $2 \leq i''' \leq n''-1$. This is a contradiction. Hence, we have the following labeled statements. The statements are labeled as we will refer to them later in the proof.

If $\deg(u''_2) = \deg(u''_3)$, then $\deg(u''_{n''-2}) \neq \deg(u''_{n''-1})$ and if $\deg(u''_{n''-1}) = \deg(u''_{n''-2})$, then $\deg(u''_2) \neq \deg(u''_3)$. (3.21)

Since $\tau(B_L^{k,1}(D),x) \leq \tau(B_R^{k,r_k-1}(D),x)$, with equality if and only if $B_L^{k,1}(D) \approx_r B_R^{k,r_k-1}(D)$, then

$$\begin{aligned}
&\tau(B_L^{u''_2},x)\\
&= \frac{1}{1+x\left(\deg(u''_2)-2+\tau(B_L^{k,1}(D),x)\right)} = \frac{1}{1+x\left(s_{k+1}-2+\tau(B_L^{k,1}(D),x)\right)}\\
&\geq \frac{1}{1+x\left(s_{k+1}-2+\tau(B_R^{k,r_k-1}(D),x)\right)}\\
&= \frac{1}{1+x\left(\deg(u''_{n''-1})-2+\tau(B_R^{k,r_k-1}(D),x)\right)} = \tau(B_R^{u''_{n''-1}},x).
\end{aligned}$$

Therefore, $\tau(B_L^{u_2''}, x) \geq \tau(B_R^{u_{n''-1}''}, x)$, with equality if and only if $B_L^{k,1}(D) \approx_r B_R^{k,r_k-1}(D)$. If $\tau(B_L^{u_2''}, x) = \tau(B_R^{u_{n''-1}''}, x)$, we choose $\deg(u_3'') \leq \deg(u_{n''-2}'')$, otherwise $\tau(B_L^{u_2''}, x) > \tau(B_R^{u_{n''-1}''}, x)$ and by Lemma 3.2, we get that $\deg(u_3'') \leq \deg(u_{n''-2}'')$. Therefore

$$\deg(u_3'') \leq \deg(u_{n''-2}''). \tag{3.22}$$

Let m and m' be two positive integers such that $4 \leq m \leq n'' - 2$, $2 \leq m' < m - 1$ and $s_{k+1} = \deg(u_{m'}'') = \deg(u_m'') < \deg(u_{m+1}'')$. Since $s_{k+1} \leq \deg(u_{i'''}'')$, for any $2 \leq i''' \leq n'' - 1$, then by Lemma 3.17 (ii), we must have

$$\deg(u_{m'}'') = \deg(u_{m'+1}'') = \cdots = \deg(u_m'') = s_{k+1}. \tag{3.23}$$

Since $r_{k+1} \geq 3$, then from (3.20) we have $\deg(u_{n''-1}'') = \deg(u_2'') = s_{k+1}$. From (3.23) we have either $\deg(u_3'') = s_{k+1}$ or $\deg(u_{n''-2}'') = s_{k+1}$. From (3.21) and (3.22) we have $s_{k+1} = \deg(u_3'') < \deg(u_{n''-2}'')$. By (3.23) we have

$$\deg(u_2'') = \deg(u_3'') = \cdots = \deg(u_m'') = s_{k+1}.$$

Therefore, $\deg(u_q'') \geq s_{k+2}$, for all $m + 1 \leq q \leq n'' - 2$. And G can be decomposed as in Figure 3.20.

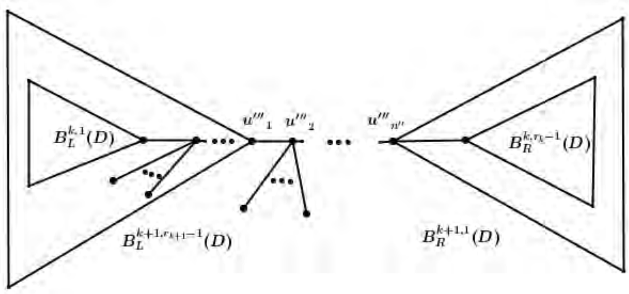

Figure 3.20: Decomposition of the caterpillar G in the proof of Theorem 3.18.

(b) If k is even, then by Lemma 3.14, we have

$$\tau(B_L^{k,r_k-1}(D), x) \geq \tau(B_R^{k,1}(D), x),$$

with equality if and only if $B_L^{k,r_k-1}(D) \approx_r B_R^{k,1}(D)$. By replacing $B_L^{k,1}(D)$ with $B_R^{k,1}(D)$, $B_R^{k,r_k-1}(D)$ with $B_L^{k,r_k-1}(D)$ and keeping the other notation in (a), we arrive to G decomposed as in Figure 3.21. Hence we conclude that $G \cong \mathcal{X}(D)$. □

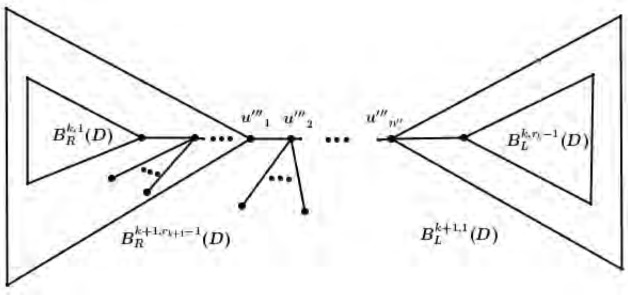

Figure 3.21: Decomposition of the caterpillar G in the proof of Theorem 3.18.

Remark 3.19 In Chapter 1, we saw that if T and $T^{'}$ are trees, such that $M(T,x) \leq M(T^{'},x)$ for all positive $x \in \mathbb{R}$, then

$$Z(T) = M(T,1) \leq M(T^{'},1) = Z(T^{'}),$$

and

$$En(T) = \frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln M(T,x^2)dx \leq \frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln M(T^{'},x^2)dx = En(T^{'}).$$

Then, from Theorem 3.18 we deduce the following theorem.

Theorem 3.20 *Let $\mathbb{C}_D$ be the set of all caterpillars with reduced degree sequence $D = \binom{s_1 \;\; s_2 \;\; \cdots \;\; s_t}{r_1 \;\; r_2 \;\; \cdots \;\; r_t}$, for some positive integer t.*
(i) If $G \in \mathbb{C}_D$ such that for all $H \in \mathbb{C}_D$ $Z(H) \leq Z(G)$, then $G \cong \mathcal{X}(D)$.

(ii) If $G \in \mathbb{C}_D$ such that for all $H \in \mathbb{C}_D$ $En(H) \leq En(G)$, then $G \cong \mathcal{X}(D)$.

Lemma 3.21 *Let $D = (d_1,\ldots,d_i,\ldots,d_j,\ldots,d_n)$ be a reduced degree sequence, for some positive integers i and j. Let $d = d_i - 2$ and $d^{'} = d_j - 2$. Decompose $\mathcal{X}(D)$ as in Figure 3.1, such that either*
(i) $\deg(v) = d_i$, $\deg(w) = d_j$ and $d_i \geq d_j + 3$, or
(ii) $\deg(v) = d_i = d_j + 2 = \deg(w) + 2$ and H is either a 2-vertex path with end vertices v and w or H is a $d_j + 2$-star. Note that v and w are leaves of H.

Let v_1 be a leaf adjacent to v, such that $v_1 \neq B$. Let G be obtained from $\mathcal{X}(D)$ by removing the edge vv_1 and then adding the edge wv_1. Then, the reduced degree sequence of G is
$D^{'} = (d_1,\ldots,d_{i-1},d_i-1,d_{i+1},\ldots,d_{j-1},d_j+1,d_{j+1},\ldots,d_n)$ *and*

$$M(\mathcal{X}(D),x) < M(G,x) \leq M(\mathcal{X}(D^{'}),x).$$

Proof. Since G and $\mathcal{X}(D^{'})$ have the same reduced degree sequence $D^{'}$, then by Theorem 3.18, $M(G,x) \leq M(\mathcal{X}(D^{'}),x)$.

(i) Suppose $\deg(v) = d_i$, $\deg(w) = d_j$ and $d_i \geq d_j + 3$. Then, from Equation (3.1) we have

$$\begin{aligned}
&M(\mathcal{X}(D), x)\\
&= M(B,x)M(B^{'},x)\Big[M(H,x) + dd^{'}x^2M(H-\{v,w\},x)\\
&\qquad + x^2\tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x)\\
&+ x\Big[\left(d^{'} + \tau(B^{'},x)\right)M(H-w,x) + \left(d+\tau(B,x)\right)M(H-v,x)\Big]\\
&\qquad + x^2M(H-\{v,w\},x)\Big[d\tau(B^{'},x) + d^{'}\tau(B,x)\Big]\Big],
\end{aligned}$$

$$\begin{aligned}
&M(G,x)\\
&= M(B,x)M(B^{'},x)\Big[M(H,x) + (d-1)\left(d^{'}+1\right)x^2M(H-\{v,w\},x)\\
&\qquad + x^2\tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x)\\
&+ x\Big[\left(d^{'} + \tau(B^{'},x)+1\right)M(H-w,x) + \left(d+\tau(B,x)-1\right)M(H-v,x)\Big]\\
&\qquad + x^2M(H-\{v,w\},x)\Big[(d-1)\tau(B^{'},x) + \left(d^{'}+1\right)\tau(B,x)\Big]\Big]
\end{aligned}$$

and

$$\begin{aligned}
&M(\mathcal{X}(D), x) - M(G,x)\\
&= M(B,x)M(B^{'},x)\Big[x^2M(H-\{v,w\},x)\left(dd^{'} - (d-1)\left(d^{'}+1\right)\right)\\
&\qquad + x\Big[M(H-w,x)\left(d^{'}+\tau(B^{'},x) - \left(d^{'}+\tau(B^{'},x)+1\right)\right)\\
&+ M(H-v,x)\left(d+\tau(B,x)-(d+\tau(B,x)-1)\right)]\\
&\quad + x^2M(H-\{v,w\},x)\Big[\tau(B^{'},x)(d-(d-1)) + \tau(B,x)\left(d^{'} - \left(d^{'}+1\right)\right)\Big]\Big]\\
&= M(B,x)M(B^{'},x)\Big[x^2M(H-\{v,w\},x)\left(-d+d^{'}+1\right)\\
&\qquad + x\left[-M(H-w,x) + M(H-v,x)\right]\\
&+ x^2M(H-\{v,w\},x)\Big[\tau(B^{'},x) - \tau(B,x)\Big]\Big]\\
&= M(B,x)M(B^{'},x)\Big[x^2M(H-\{v,w\},x)\left(d^{'}+\tau(B^{'},x)+1-(d+\tau(B,x))\right)\\
&\qquad + x\left[M(H-v,x) - M(H-w,x)\right]\Big]. \qquad (3.24)
\end{aligned}$$

Let $v^{'}$ be a neighbor of v in H and let $w^{'}$ be a neighbor of w in H. Then,

$$M(\mathcal{X}(D), x) - M(G,x)$$

$$= M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(d^{'}+\tau(B^{'},x)+1-(d+\tau(B,x))\right)\right.$$
$$+x\left[M(H-v-ww^{'},x)+xM(H-\{v,w,w^{'}\},x)-M(H-w-vv^{'},x)\right.$$
$$\left.\left.-\ xM(H-\{v,v^{'},w\},x)\right]\right]$$
$$= M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(d^{'}+\tau(B^{'},x)+1-(d+\tau(B,x))\right)\right.$$
$$+x\left[M(H-\{v,w\},x)+xM(H-\{v,w,w^{'}\},x)-M(H-\{v,w\},x)\right.$$
$$\left.\left.-\ xM(H-\{v,v^{'},w\},x)\right]\right]$$
$$= M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(d^{'}+\tau(B^{'},x)+1-(d+\tau(B,x))\right)\right.$$
$$\left.+x^2\left[M(H-\{v,w,w^{'}\},x)-M(H-\{v,v^{'},w\},x)\right]\right]$$
$$= M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(d^{'}+\tau(B^{'},x)+1\right.\right.$$
$$\left.-(d^{'}+3+a+\tau(B,x))\right)$$
$$\left.+x^2\left[M(H-\{v,w,w^{'}\},x)-M(H-\{v,v^{'},w\},x)\right]\right]$$
$$= M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(\tau(B^{'},x)-(2+a+\tau(B,x))\right)\right.$$
$$\left.+x^2\left[M(H-\{v,w,w^{'}\},x)-M(H-\{v,v^{'},w\},x)\right]\right],$$

where a is a nonnegative integer. Since $-a \leq 0$, B and $B^{'}$ non-empty and $\tau(B^{'},x)-\tau(B,x)<1$, then $\tau(B^{'},x)-\tau(B,x)-a-2<-1$. So

$$\begin{aligned}
M(\mathcal{X}(D),x)-M(G,x) &< M(B,x)M(B^{'},x)\left[-x^2M(H-\{v,w\},x)\right.\\
&\quad \left.+x^2\left[M(H-\{v,w,w^{'}\},x)-M(H-\{v,v^{'},w\},x)\right]\right]\\
&= M(B,x)M(B^{'},x)\left[-x^2\left(M(H-\{v,w,w^{'}\},x)+a^{'}\right)\right.\\
&\quad \left.+x^2\left[M(H-\{v,w,w^{'}\},x)-M(H-\{v,v^{'},w\},x)\right]\right]\\
&< 0, \text{ where } a^{'} \text{ is a nonnegative real number.}
\end{aligned}$$

The last inequality followed from the fact that $M(B,x), M(B^{'},x), M(H-\{v,w,w^{'}\},x), M(H-\{v,v^{'},w\},x)>0$ and $x>0$. Hence

$$M(\mathcal{X}(D),x) < M(G,x) \leq M(\mathcal{X}(D^{'}),x).$$

(ii) Suppose $\deg(v)=d_i=d_j+2=\deg(w)+2$ and H is either a 2-vertex path with end vertices v and w or H is a d_j+2-star and v and w are leaves of H. Then, $H-v \cong H-w$ and hence $M(H-v,x) = M(H-w,x)$. Then, from Equation (3.24) we have

$$\begin{aligned}
&M(\mathcal{X}(D),x) - M(G,x)\\
&= M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(d^{'}+\tau(B^{'},x)+1-(d+\tau(B,x))\right)\right.\\
&\qquad\qquad\qquad\qquad\qquad\qquad\left. + x\left[M(H-v,x)-M(H-w,x)\right]\right]\\
&= M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(d^{'}+\tau(B^{'},x)+1-(d+\tau(B,x))\right)\right]\\
&= M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(d^{'}+\tau(B^{'},x)+1\right.\right.\\
&\qquad\qquad\qquad\qquad\qquad\qquad\left.\left.-(d^{'}+2+\tau(B,x))\right)\right]\\
&= M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(\tau(B^{'},x)-\tau(B,x)-1\right)\right]
\end{aligned}$$

< 0, since B and $B^{'}$ are non-empty, $\tau(B^{'},x)-\tau(B,x) < 1$ and $M(B,x)$, $M(B^{'},x), M(H-\{v,w\},x) > 0$.

Hence

$$M(\mathcal{X}(D),x) < M(G,x) \leq M(\mathcal{X}(D^{'}),x).$$

□

Lemma 3.22 *Let G be a caterpillar and be decomposed as in Figure 3.22, such that $\deg(w) = 1$, $\deg(v) = d+2 \geq 3$ and $v^{'}$ a leaf adjacent to v. Let $G^{'}$ be obtained from G by removing the edge $vv^{'}$ and then adding the edge $wv^{'}$. If $d \geq 2$ or H is a path, then*

$$M(G,x) < M(G^{'},x).$$

Proof.

$$\begin{aligned}
&M(G,x)\\
&= M(G-vv^{'},x) + xM(G-\{v,v^{'}\},x) = M(G-v^{'},x) + xM(G-\{v,v^{'}\},x)\\
&= M(G-v^{'}-vr(B),x) + xM(G-v^{'}-\{v,r(B)\},x) + xM(G-\{v,v^{'}\},x)\\
&= M(B,x)M(T,x) + xM(B-r(B),x)M(H-v,x) + xM(B,x)M(H-v,x)\\
&= M(B,x)M(T,x) + xM(B-r(B),x)M(H-v,x)\\
&\qquad\qquad + xM(B,x)\left[M(H-v-ww^{'},x) + xM(H-v-\{w,w^{'}\},x)\right],
\end{aligned}$$

where $w^{'}$ is a neighbor of w in H. Therefore,

$$M(G,x) = M(B,x)M(T,x) + xM(B-r(B),x)M(H-v,x)$$

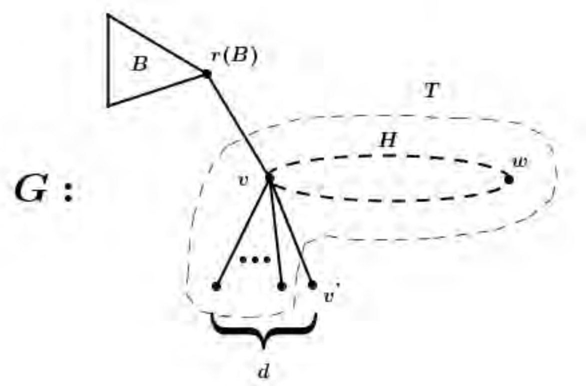

Figure 3.22: The caterpillar G in Lemma 3.22, $T = G - B - v'$.

$$+ xM(B,x)\left[M(H-\{v,w\},x) + xM(H-\{v,w,w'\},x)\right].$$

$$\begin{aligned}
&M(G',x)\\
&= M(G'-wv',x) + xM(G'-\{w,v'\},x)\\
&= M(G'-v',x) + xM(G'-\{w,v'\},x)\\
&= M(G'-v'-vr(B),x) + xM(G'-v'-\{v,r(B)\},x)\\
&\qquad\qquad + xM(G'-\{w,v'\},x)\\
&= M(B,x)M(T,x) + xM(B-r(B),x)M(H-v,x) + xM(G'-\{w,v'\},x)\\
&= M(B,x)M(T,x) + xM(B-r(B),x)M(H-v,x)\\
&\qquad + x\left[M(G'-\{w,v'\}-vr(B),x) + xM(G'-\{w,v'\}-\{v,r(B)\},x)\right]\\
&= M(B,x)M(T,x) + xM(B-r(B),x)M(H-v,x)\\
&\qquad + x\left[M(B,x)M(T-w,x) + xM(B-r(B),x)M(H-\{v,w\},x)\right]\\
&= M(B,x)M(T,x) + xM(B-r(B),x)M(H-v,x)\\
&\qquad + xM(B,x)M(T-w,x) + x^2M(B-r(B),x)M(H-\{v,w\},x)\\
&= M(B,x)M(T,x) + xM(B-r(B),x)M(H-v,x)\\
&\qquad + xM(B,x)\left[M(H-w,x) + (d-1)xM(H-\{v,w\},x)\right]\\
&+ x^2M(B-r(B),x)M(H-\{v,w\},x)
\end{aligned}$$

and

$$\begin{aligned}
&M(G,x) - M(G',x)\\
&= xM(B,x)\left[M(H-\{v,w\},x) + xM(H-\{v,w,w'\},x)\right]\\
&\qquad - xM(B,x)\left[M(H-w,x) + (d-1)xM(H-\{v,w\},x)\right]\\
&- x^2M(B-r(B),x)M(H-\{v,w\},x)
\end{aligned}$$

$$= xM(B,x)\left[M(H-\{v,w\},x) + xM(H-\{v,w,w^{'}\},x)\right]$$
$$- xM(B,x)\Big[M(H-w-vv^{''},x)$$
$$+xM(H-w-\{v,v^{''}\},x) + x(d-1)M(H-\{v,w\},x)\Big]$$

$- x^2M(B-r(B),x)M(H-\{v,w\},x)$, where $v^{''}$ is a neighbor of v in H.

$$= xM(B,x)\left[M(H-\{v,w\},x) + xM(H-\{v,w,w^{'}\},x)\right]$$
$$- xM(B,x)\big[M(H-\{v,w\},x)$$
$$+xM(H-\{v,v^{''},w\},x) + x(d-1)M(H-\{v,w\},x)\Big]$$
$$- x^2M(B-r(B),x)M(H-\{v,w\},x)$$
$$= x^2M(B,x)M(H-\{v,w,w^{'}\},x)$$
$$- x^2M(B,x)\left[M(H-\{v,v^{''},w\},x) + (d-1)M(H-\{v,w\},x)\right]$$
$$- x^2M(B-r(B),x)M(H-\{v,w\},x).$$

If $d \geq 2$, then $d-1 \geq 1$. Since $M(H-\{v,w\},x) \geq M(H-\{v,w,w^{'}\},x)$, $M(B,x), M(H-\{v,w\},x), M(H-\{v,w,w^{'}\},x), M(H-\{v,v^{''},w\},x), M(B-r(B),x) > 0$, $x > 0$, then

$$M(G,x) - M(G^{'},x)$$
$$= x^2M(B,x)M(H-\{v,w,w^{'}\},x)$$
$$- x^2M(B,x)\left[M(H-\{v,v^{''},w\},x) + (d-1)M(H-\{v,w\},x)\right]$$
$$- x^2M(B-r(B),x)M(H-\{v,w\},x)$$
$$\leq x^2M(B,x)M(H-\{v,w,w^{'}\},x)$$
$$- x^2M(B,x)\left[M(H-\{v,v^{''},w\},x) + M(H-\{v,w\},x)\right]$$
$$- x^2M(B-r(B),x)M(H-\{v,w\},x) < 0.$$

If H is a path, then $H-\{v,w,w^{'}\} \cong H-\{v,v^{''},w\}$ and $M(H-\{v,w,w^{'}\},x) = M(H-\{v,v^{''},w\},x)$. Then,

$$M(G,x) - M(G^{'},x)$$
$$= x^2M(B,x)M(H-\{v,w,w^{'}\},x)$$
$$- x^2M(B,x)\left[M(H-\{v,v^{''},w\},x) + (d-1)M(H-\{v,w\},x)\right]$$
$$- x^2M(B-r(B),x)M(H-\{v,w\},x)$$
$$= -x^2M(B,x)(d-1)M(H-\{v,w\},x)$$
$$- x^2M(B-r(B),x)M(H-\{v,w\},x) < 0.$$

Hence
$$M(G,x) < M(G^{'},x).$$

□

The transformation in Lemma 3.22 may form a tree that is not a caterpillar. If the neighbor of w is a pseudo leaf, then the new graph $G^{'}$ is a caterpillar.

Definition 3.23 Let $(b_1, \ldots, b_n)$ and $(d_1, \ldots, d_n)$ be two degree sequences of trees. We say that $(d_1, \ldots, d_n)$ majorizes $(b_1, \ldots, b_n)$ and write $(b_1, \ldots, b_n) \preceq (d_1, \ldots, d_n)$, if and only if for all $k \in \{1, \ldots, n\}$ we have

$$\sum_{i=1}^{k} b_i \leq \sum_{i=1}^{k} d_i.$$

If furthermore there exists i_0, such that $d_{i_0} \neq b_{i_0}$, then we write $(b_1, \ldots, b_n) \prec (d_1, \ldots, d_n)$.

Theorem 3.24 *Let $(y_1, \ldots, y_n)$ and $(d_1, \ldots, d_n)$ be two degree sequences of caterpillars. If $(y_1, \ldots, y_n) \prec (d_1, \ldots, d_n)$ and $\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} d_i$, then there exists a caterpillar G with degree sequence $(y_1, \ldots, y_n)$ such that*

$M(\mathcal{X}(d_1, \ldots, d_n), x) < M(G, x) \leq M(\mathcal{X}(y_1, \ldots, y_n), x)$, *for all positive* $x \in \mathbb{R}$

and hence

$$Z(\mathcal{X}(d_1, \ldots, d_n)) < Z(G) \leq Z(\mathcal{X}(y_1, \ldots, y_n))$$

and

$$En(\mathcal{X}(d_1, \ldots, d_n)) < En(G) \leq En(\mathcal{X}(y_1, \ldots, y_n)),$$

with equality if and only if $G \cong \mathcal{X}(y_1, \ldots, y_n)$.

Proof. Suppose $Y = (y_1, \ldots, y_n)$ and $D = (d_1, \ldots, d_n)$ are two degree sequences of caterpillars, $Y \prec D$ and $\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} d_i$. Then, there exists i_0, such that $d_{i_0} \neq y_{i_0}$. In fact, the set $\mathbb{I} = \{i : d_i \neq y_i\}$ must have at least two elements, otherwise $\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} d_i$ would be impossible. Let $l = \min\{i : d_i \neq y_i\}$ and $m = \max\{i : d_i \neq y_i\}$. We must have $y_m > d_m \geq 1$ and we must also have $d_l > y_l$. We define D_1 to be a degree sequence consisting of the numbers $d_1, \ldots, d_{l-1}, d_l - 1, d_{l+1}, \ldots, d_{m-1}, d_m + 1, d_{m+1}, \ldots, d_n$. Since $d_l > y_l \geq y_m > d_m \geq 1$, then $d_l \geq y_l + 1 \geq y_m + 1 > d_m + 1$. Then $d_l \geq y_l + 1 \geq y_m + 1 \geq d_m + 2$. Hence $d_l \geq d_m + 2$ and $d_l - 1 \geq d_m + 1 \geq 2$. Therefore D_1 is indeed a valid degree sequence. It is clear that $D_1 \prec D$. If $d_l > d_m + 2$ and $d_m = 1$, decompose $\mathcal{X}(D)$ as in Figure 3.22 such that $\deg(w) = d_m = 1$ and

$\deg(v) = d_l > 3$. Since $d_l \geq 4 = 2 + 2$, then by Lemma 3.22, we can obtain a caterpillar G from $\mathcal{X}(D)$, by removing the edge $vv^{'}$ and then adding the edge $wv^{'}$ and get $M(\mathcal{X}(D), x) < M(G, x)$. Since the degree sequence of G is D_1, then by Theorem 3.18, we must also have

$$M(\mathcal{X}(D), x) < M(G, x) \leq M(\mathcal{X}(D_1), x).$$

If $d_l > d_m + 2$ and $d_m \geq 2$, decompose $\mathcal{X}(D)$ as in Figure 3.1, such that $\deg(v) = d_l \geq d_m + 3 = \deg(w) + 3$. Let v_1 be a leaf adjacent to v, such that $v_1 \neq B$. Let G be obtained from $\mathcal{X}(D)$, by removing the edge vv_1 and then adding the edge wv_1. Then, the degree sequence of G is D_1 and by Lemma 3.21 (i), we must have

$$M(\mathcal{X}(D), x) < M(G, x) \leq M(\mathcal{X}(D_1), x).$$

If $d_l = d_m + 2$ and $d_m \geq 2$, decompose $\mathcal{X}(D)$ as in Figure 3.1, such that $\deg(v) = d_l$ and $\deg(w) = d_m$. Let v_1 be a leaf adjacent to v, such that $v_1 \neq B$. Let G be obtained from $\mathcal{X}(D)$, by removing the edge vv_1 and then adding the edge wv_1. Then, the degree sequence of G is D_1. Then, from Equation (3.1) we must have

$$\begin{aligned}
&M(\mathcal{X}(D), x)\\
&= M(B, x)M(B^{'}, x)\big[M(H, x) + d(d-2)x^2 M(H - \{v, w\}, x)\\
&\qquad\qquad + x^2\tau(B, x)\tau(B^{'}, x)M(H - \{v, w\}, x)\\
&+ x\left[\left(d + \tau(B^{'}, x) - 2\right) M(H - w, x) + (d + \tau(B, x))\, M(H - v, x)\right]\\
&\qquad\qquad + x^2 M(H - \{v, w\}, x)\left[d\tau(B^{'}, x) + (d-2)\tau(B, x)\right]\Big]
\end{aligned}$$

and

$$\begin{aligned}
&M(G, x)\\
&= M(B, x)M(B^{'}, x)\big[M(H, x) + (d-1)(d-1)x^2 M(H - \{v, w\}, x)\\
&\qquad\qquad + x^2\tau(B, x)\tau(B^{'}, x)M(H - \{v, w\}, x)\\
&+ x\left[\left(d + \tau(B^{'}, x) - 1\right) M(H - w, x) + (d + \tau(B, x) - 1)\, M(H - v, x)\right]\\
&\qquad\qquad + x^2 M(H - \{v, w\}, x)\left[(d-1)\tau(B^{'}, x) + (d-1)\tau(B, x)\right]\Big].
\end{aligned}$$

Let $G^{'}$ be obtained from G by swapping B and $B^{'}$. Let $v^{'}$ be a neighbor of v in H and let $w^{'}$ be a neighbor of w in H. Then,

$$\begin{aligned}
&M(G^{'}, x)\\
&= M(B, x)M(B^{'}, x)\big[M(H, x) + (d-1)(d-1)x^2 M(H - \{v, w\}, x)\\
&\qquad\qquad + x^2\tau(B, x)\tau(B^{'}, x)M(H - \{v, w\}, x)
\end{aligned}$$

$$+ x\left[(d+\tau(B,x)-1)\,M(H-w,x)+\left(d+\tau(B^{'},x)-1\right)M(H-v,x)\right]$$
$$+ x^2M(H-\{v,w\},x)\left[(d-1)\tau(B,x)+(d-1)\tau(B^{'},x)\right]\Big]$$

and

$$\begin{aligned}
&M(\mathcal{X}(D),x)-M(G^{'},x)\\
&=M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(d(d-2)-(d-1)^2\right)\right.\\
&\qquad+x\left[\left(\tau(B^{'},x)-\tau(B,x)-1\right)M(H-w,x)\right.\\
&+\left.\left(\tau(B,x)-\tau(B^{'},x)+1\right)M(H-v,x)\right]\\
&\quad\left.+x^2M(H-\{v,w\},x)\left[\tau(B^{'},x)(d-(d-1))+\tau(B,x)(d-2-(d-1))\right]\right]\\
&=M(B,x)M(B^{'},x)\left[-x^2M(H-\{v,w\},x)\right.\\
&\qquad+x\left(\tau(B^{'},x)-\tau(B,x)-1\right)(M(H-w,x)-M(H-v,x))\\
&\left.+x^2M(H-\{v,w\},x)\left(\tau(B^{'},x)-\tau(B,x)\right)\right]\\
&=M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left(\tau(B^{'},x)-\tau(B,x)-1\right)\right.\\
&\qquad\left.+x\left(\tau(B^{'},x)-\tau(B,x)-1\right)(M(H-w,x)-M(H-v,x))\right]\\
&=M(B,x)M(B^{'},x)\left(\tau(B^{'},x)-\tau(B,x)-1\right)\left[x^2M(H-\{v,w\},x)\right.\\
&\qquad\left.+x\,(M(H-w,x)-M(H-v,x))\right]\\
&=xM(B,x)M(B^{'},x)\left(\tau(B^{'},x)-\tau(B,x)-1\right)\left[xM(H-\{v,w\},x)\right.\\
&\qquad\left.+M(H-w,x)-M(H-v,x)\right]\\
&=xM(B,x)M(B^{'},x)\left(\tau(B^{'},x)-\tau(B,x)-1\right)\left[xM(H-\{v,w\},x)\right.\\
&\qquad+M(H-\{v,w\},x)+xM(H-\{v,v^{'},w\},x)-M(H-\{v,w\},x)\\
&\left.-xM(H-\{v,w,w^{'}\},x)\right]\\
&=xM(B,x)M(B^{'},x)\left(\tau(B^{'},x)-\tau(B,x)-1\right)\left[xM(H-\{v,w\},x)\right.\\
&\qquad\left.+xM(H-\{v,v^{'},w\},x)-xM(H-\{v,w,w^{'}\},x)\right]<0,
\end{aligned}$$

since $x>0$, $M(.,x)>0$, $0<\tau(B,x),\tau(B^{'},x)\le 1$, $\tau(B^{'},x)-\tau(B,x)-1<0$ and $M(H-\{v,w\},x)\ge M(H-\{v,w,w^{'}\},x)$. Therefore, if $d_l=d_m+2$, then $M(\mathcal{X}(D),x)<M(G^{'},x)$. Since the degree sequence of $G^{'}$ is D_1, then by Theorem 3.18, we must also have

$$M(\mathcal{X}(D),x)<M(G^{'},x)\le M(\mathcal{X}(\mathcal{D}_1),x).$$

If $d_l = d_m + 2$ and $d_m = 1$, decompose $\mathcal{X}(D)$ as in Figure 3.22 such that $\deg(w) = d_m = 1$, $\deg(v) = d_l = 3$, H is a path with end vertices v and w and v' a leaf adjacent to v. Let G be obtained from $\mathcal{X}(D)$, by removing the edge vv' and then adding the edge wv'. Since H is a path then $M(H-w,x) = M(H-v,x)$. Then by Lemma 3.22, we must have $M(\mathcal{X}(D),x) < M(G,x)$. Since the degree sequence of G is D_1, then by Theorem 3.18, we must also have

$$M(\mathcal{X}(D),x) < M(G,x) \le M(\mathcal{X}(D_1),x).$$

If $D_1 = Y$, then we are done. Otherwise, we iterate the process. We set $D = D_0$, and if k is a positive integer and $D_k \neq Y$, then we construct D_{k+1} in exactly the same way as D_1 was constructed from D. After a finite number $J = \frac{1}{2}\sum_{i\in\mathbb{I}} |d_i - y_i|$ of iterations, we will get the chain

$$D = D_0 \succ D_1 \succ D_2 \succ \cdots \succ D_{J-1} \succ D_J = Y.$$

For any $k \in \{1,\ldots,J-1\}$, we can apply Lemmas 3.21 and 3.22 with Theorem 3.18 to $\mathcal{X}(D_k)$ as we did above, to deduce that there exists a caterpillar G_{k+1} with degree sequence D_{k+1} such that

$$M(\mathcal{X}(D_k),x) < M(G_{k+1},x) \le M(\mathcal{X}(D_{k+1}),x)$$

and hence

$$M(\mathcal{X}(D),x) < M(\mathcal{X}(D_1),x) < \cdots < M(\mathcal{X}(D_J),x) = M(\mathcal{X}(Y),x).$$

□

From Theorem 3.24, we can conclude that among all caterpillars of size m, the path graph is maximal with respect to $M(.,x)$ and hence maximal with respect to Z and En. This is well-known see [38] and [88]. The path graph was found to be extremal, when the family of trees is considered. Since the family of caterpillars is within the class of trees, the path graph must also be extremal among all caterpillars. The following corollaries can also be deduced from Theorem 3.24.

Remark 3.25 Let d, m and l be positive integers. Let d and m be diameter and size of a caterpillar G, respectively. Let

$$D = (\underbrace{l+1,\ldots,l+1}_{r \text{ times}}, \underbrace{l,\ldots,l}_{d-r-1 \text{ times}}, \underbrace{1,\ldots,1}_{m-d+2 \text{ times}})$$

be a degree sequence of a caterpillar G. Then, the total number of internal vertices in the backbone of G is $d-1$. The number of leaves is $m-d+2$. Let d_i be a degree of a vertex in G, for $1 \le i \le m+1$. The degree sum of the vertices of G is given by

$$\sum_{i=1}^{m+1} d_i = (l+1)r + (d-r-1)l + m - d + 2.$$

The degree sum of the vertices of G is also given by

$$\sum_{i=1}^{m+1} d_i = 2(d-1) + 2(m-d+2) - 2.$$

This implies that

$$\begin{aligned} &(l+1)r + (d-r-1)l = 2(d-1) + m - d \\ \implies &(l+1)r + (d-1)l - lr = 2(d-1) + m - d \\ \implies &(l+1)r - lr = 2(d-1) + m - d - (d-1)l \\ \implies &(l+1-l)r = 2(d-1) - (d-1)l + m - d \\ \implies &r = (d-1)(2-l) + m - d = m - d - (d-1)(l-2). \end{aligned}$$

Therefore,

$$r = m - d - (d-1)(l-2). \tag{3.25}$$

Equivalently,

$$l - 2 = \frac{m-d}{d-1} - \frac{r}{d-1}.$$

Note that if $r = d-1$, then

$$D = (\underbrace{l+1, \ldots, l+1}_{d-1 \text{ times}}, \underbrace{1, \ldots, 1}_{m-d+2 \text{ times}}).$$

This is equivalent to $d-r-1=0$. If $r < d-1$, then $\frac{r}{d-1} < 1$. Hence,

$$l = 2 + \left\lfloor \frac{m-d}{d-1} \right\rfloor$$

and from Equation (3.25)

$$r = m - d - (d-1)\left(2 + \left\lfloor \frac{m-d}{d-1} \right\rfloor - 2\right) = m - d - (d-1)\left\lfloor \frac{m-d}{d-1} \right\rfloor < d-1.$$

Corollary 3.26 *Let d, m and n be positive integers. Let $\mathbb{C}$ be the set of all caterpillars of diameter d, size m and order n. Then, among all caterpillars in $\mathbb{C}$, the caterpillar $\mathcal{X}(D)$ maximizes $M(.,x)$ and hence Z and En, where*

$$D = (\underbrace{l+1, \ldots, l+1}_{r \text{ times}}, \underbrace{l, \ldots, l}_{d-r-1 \text{ times}}, \underbrace{1, \ldots, 1}_{m-d+2 \text{ times}})$$

is a degree sequence, $l = 2 + \left\lfloor \frac{m-d}{d-1} \right\rfloor$ and $r = (m-d) - (d-1)\left\lfloor \frac{m-d}{d-1} \right\rfloor < d-1$.

Remark 3.27 Let m and δ be positive integers. Let m and δ be the size and minimum internal vertex degree of a caterpillar G, respectively. Suppose

$$D = (\underbrace{\delta+1,\ldots,\delta+1}_{r \text{ times}}, \underbrace{\delta,\ldots,\delta}_{d-r-1 \text{ times}}, \underbrace{1,\ldots,1}_{m-d+2 \text{ times}})$$

is a degree sequence of G, such that $r < \delta$. Then, using the handshake lemma we have

$$\begin{aligned}
&2m-(m-d+2)=(d-1)\delta+r \implies m+d-2=(d-1)\delta+r\\
&\implies m-2-r=(d-1)\delta-d \implies m-2-r=d\delta-\delta-d\\
&\implies m+\delta-2-r=d\delta-d\\
&\implies m+\delta-2-r=d(\delta-1) \qquad (3.26)\\
&\implies m+\delta-3-(r-1)=d(\delta-1) \implies \frac{m+\delta-3}{\delta-1}-\frac{r-1}{\delta-1}=d.
\end{aligned}$$

Since $r < \delta$ and d is an integer, then $0 \leq \frac{r-1}{\delta-1} < 1$ and $d = \lfloor\frac{m+\delta-3}{\delta-1}\rfloor$. Then, from Equation (3.26), we have

$$r = m-d(\delta-1)+\delta-2 = m-\left\lfloor\frac{m+\delta-3}{\delta-1}\right\rfloor(\delta-1)+\delta-2 < d-1.$$

Note that $r < d-1$ as suggested in Remark 3.25.

Corollary 3.28 *Among all caterpillars of size m and minimum internal degree δ, $\mathcal{X}(D)$ maximizes $M(.,x)$ and hence Z and En, where*

$$D = (\underbrace{\delta+1,\ldots,\delta+1}_{r \text{ times}}, \underbrace{\delta,\ldots,\delta}_{d-r-1 \text{ times}}, \underbrace{1,\ldots,1}_{m-d+2 \text{ times}})$$

is a degree sequence, $d = \lfloor\frac{m+\delta-3}{\delta-1}\rfloor$ and

$$r = m-\left\lfloor\frac{m+\delta-3}{\delta-1}\right\rfloor(\delta-1)+\delta-2 < d-1.$$

Corollary 3.29 *Among all caterpillars of size m and number of leaves k, $\mathcal{X}(D)$ maximizes $M(.,x)$ and hence Z and En, where*

$$D = (\underbrace{3,\ldots,3}_{k-2 \text{ times}}, \underbrace{2,\ldots,2}_{m-2k+3 \text{ times}}, \underbrace{1,\ldots,1}_{k \text{ times}})$$

is a degree sequence.

Since there are are m edges and k leaves in Corollary 3.29, once all the leaves are removed, there are $m-k$ edges remaining and $m-k+1$ vertices making up the backbone. To get a degree sequence that is majorised by all degree sequences of caterpillars with m edges and k leaves, the degrees of the vertices in the backbone have to be as small as possible. Then, out of those $k-2$ have degree 3. Leaving out $m-k+1-(k-2)=m-2k+3$ vertices of degree 2.

3.3 Caterpillars with given degree sequence and minimum $M(.,x)$

In this section we first characterize a caterpillar $\mathcal{S}(D)$ that minimizes $M(.,x)$ and hence Hosoya index and energy, among all caterpillars with given degree sequence D. This caterpillar is found to also maximize $\sigma(.,x)$. Then, we compare the two caterpillars $\mathcal{S}(D)$ and $\mathcal{S}(Y)$ i.e. $M(\mathcal{S}(D),x)$ with $M(\mathcal{S}(Y),x)$, $Z(\mathcal{S}(D))$ with $Z(\mathcal{S}(Y))$ and- $En(\mathcal{S}(D))$ with $En(\mathcal{S}(Y))$, where the degree sequence Y is majorized by the degree sequence D. We say G is minimal with regard to an invariant $F(G)$, if and only if $F(G)=\min\{F(C) : C \in \mathbb{C}_D\}$, where D is a degree sequence of G.

The following simple technical lemma will play central role as we try to find out what exchange of branches reduces $M(.,x)$.

Lemma 3.30 *Let a,b,c and d be nonnegative real numbers. If $a \le b$ and $c \le d$, then $ac+bd \ge ad+bc$. If $a \le b \le c \le d$, then $ab+cd \ge ac+bd \ge ad+bc$.*

Proof. Let a,b,c and d be nonnegative real numbers. Suppose $a \le b$ and $c \le d$. Then, $ac+bd-(ad+bc)=(b-a)(d-c) \ge 0$. Hence

$$ac+bd \ge ad+bc. \tag{3.27}$$

Suppose $a \le b \le c \le d$. Then, $ab+cd-(ac+bd)=(d-a)(c-b) \ge 0$, since $d \ge a$ and $c \ge b$. Hence

$$ab+cd \ge ac+bd. \tag{3.28}$$

Therefore, from (3.27) and (3.28) we have $ab+cd \ge ac+bd \ge ad+bc$. □

Lemma 3.31 *Let G be a caterpillar and be decomposed as in Figure 3.1, with both B and B' non-empty. Suppose G is minimal with respect to $M(.,x)$.*

(i) If $\tau(B^{'},x) > \tau(B,x)$, then $d^{'} \geq d$ and $M(H-w,x) \leq M(H-v,x)$.
(ii) If $d^{'} > d$ and $\tau(B^{'},x) \neq \tau(B,x)$, then $\tau(B^{'},x) > \tau(B,x)$ and $M(H-w,x) \leq M(H-v,x)$.
(iii) If $d^{'} > d$ and $\tau(B^{'},x) = \tau(B,x)$, then $M(H-w,x) \leq M(H-v,x)$.

Proof. Let G be a caterpillar and be decomposed as in Figure 3.1. Suppose G is minimal with respect to $M(.,x)$. In particular, $M(G,x)$ is minimal with respect to all possible swappings of branches and flippings of H in G that preserves the degree sequence while keeping the graph to be caterpillar. That is, the swapping of B and $B^{'}$, the swapping of d and $d^{'}$, and/or the flipping of H in G.

(i) Suppose $\tau(B^{'},x) > \tau(B,x)$. Equation (3.2) suggests that the swapping of B and $B^{'}$, the swapping of d and $d^{'}$ and/or the flipping of H in G only affect $M_v^w(G,x)$ in $M(G,x)$. This implies that the minimality of $M_v^w(G,x)$ implies the minimality of $M(G,x)$. Since

$$\begin{aligned} &M_v^w(G,x) \\ &= x\left[d^{'}M(H-w,x) + dM(H-v,x)\right] \\ &\qquad\qquad + x\left[\tau(B^{'},x)M(H-w,x) + \tau(B,x)M(H-v,x)\right] \\ &+ x^2 M(H-\{v,w\},x)\left[d\tau(B^{'},x) + d^{'}\tau(B,x)\right]. \end{aligned}$$

Then, $M_v^w(G,x)$ is minimal if each of the expressions: $d^{'}M(H-w,x) + dM(H-v,x)$, $\tau(B^{'},x)M(H-w,x) + \tau(B,x)M(H-v,x)$ and $d\tau(B^{'},x) + d^{'}\tau(B,x)$ is smallest. Since $\tau(B^{'},x) > \tau(B,x)$, then by Lemma 3.30, $d\tau(B^{'},x) + d^{'}\tau(B,x)$ is smallest only if $d \leq d^{'}$. Again, since $\tau(B^{'},x) > \tau(B,x)$, then by Lemma 3.30, $\tau(B^{'},x)M(H-w,x) + \tau(B,x)M(H-v,x)$ is smallest only if $M(H-w,x) \leq M(H-v,x)$. $\tau(B^{'},x) > \tau(B,x)$, $d^{'} \geq d$, $M(H-w,x) \leq M(H-v,x)$ and Lemma 3.30 correspond to $d^{'}M(H-w,x)+dM(H-v,x)$ being smallest. Hence, if $\tau(B^{'},x) > \tau(B,x)$, then $d^{'} \geq d$ and $M(H-w,x) \leq M(H-v,x)$.

(ii) Suppose $d^{'} > d$, $\tau(B^{'},x) \neq \tau(B,x)$ and either $\tau(B^{'},x) < \tau(B,x)$ or $M(H-w,x) > M(H-v,x)$.

Suppose $\tau(B^{'},x) < \tau(B,x)$. Then, from (i) we must have $d^{'} \leq d$. But $d^{'} > d$. This is a contradiction. Hence $\tau(B^{'},x) \geq \tau(B,x)$. Since $\tau(B^{'},x) \neq \tau(B,x)$, then we conclude that $\tau(B^{'},x) > \tau(B,x)$. Furthermore, suppo-se $M(H-w,x) > M(H-v,x)$. Since $\tau(B^{'},x) > \tau(B,x)$, then from (i) we must have $M(H-w,x) \leq M(H-v,x)$. This is a contradiction. Hence we must have $M(H-w,x) \leq M(H-v,x)$. And therefore, if $d^{'} > d$ and $\tau(B^{'},x) \neq \tau(B,x)$, then $\tau(B^{'},x) > \tau(B,x)$ and $M(H-w,x) \leq M(H-v,x)$.

(iii) We proceed as in (i). Since $\tau(B',x) = \tau(B,x)$, then $M_v^w(G,x)$ is minimal only if the expression $d'M(H-w,x)+dM(H-v,x)$ is smallest. Since $d' > d$, then by Lemma 3.30, $d'M(H-w,x)+dM(H-v,x)$ is smallest only if $M(H-w,x) \leq M(H-v,x)$. Hence, we conclude that, if $d' > d$ and $\tau(B',x) = \tau(B,x)$, then $M(H-w,x) \leq M(H-v,x)$. □

Lemma 3.32 *Let G be a caterpillar. Label all the non-leaf vertices in G from left to right as $u_1, u_2, \ldots, u_\ell$. If G is minimal with respect to $M(.,x)$, then u_1 and u_ℓ have the largest degrees in G.*

Proof. If $\ell = 1$, then G is a star and has only one non-leaf vertex, which is of largest degree. If $\ell = 2$, then G has two non-leaf vertices and they have the largest degrees in G. If $\ell \geq 3$, decompose G as in Figure 3.1 with B a leaf adjacent to u_1 and B' a complete branch of G such that B' does not contain u_1 and u_2 and the root of B' is u_i, for $3 \leq i \leq \ell$. Then, B' is not empty and not a leaf. By Lemma 2.4 and Remark 2.5, we have $\tau(B,x) = 1 > \tau(B',x)$. By Lemma 3.31, we get that $\deg(u_1) \geq \deg(u_{i-1})$. Hence $\deg(u_1) \geq \max\{\deg(u_i) : 2 \leq i \leq \ell-1\}$. Same reasoning leads to $\deg(u_\ell) \geq \max\{\deg(u_i) : 2 \leq i \leq \ell-1\}$. □

Definition 3.33 Let $D = (d_1, d_2, \ldots, d_n)$ be a reduced degree sequence of a caterpillar. Let $k = \lceil \frac{n}{2} \rceil$. Then, $C_L^k(D)$ and $C_R^k(D)$ are defined as two disjoint complete branches such that:

(i) If $n = 1$, then $C_L^k(d_1) = C_L^1(d_1) = C(d_1)$ and $C_R^k(D) = C_R^1(d_1) = ()$.
(ii) If $n = 2$, then $C_L^k(d_1,d_2) = C_L^1(d_1,d_2) = C(d_1-1)$ and $C_R^k(d_1,d_2) = C_R^1(d_1,d_2) = C(d_2-1)$.
(iii) If $n = 3$, then $C_L^k(d_1,d_2,d_3) = C_L^2(d_1,d_2,d_3) = C(d_1,d_3-1)$ and $C_R^k(d_1,d_2,d_3) = C_R^2(d_1,d_2,d_3) = C(d_2-1)$.
(iv) If $n = 4$, then $C_L^k(d_1,d_2,d_3,d_4) = C_L^2(d_1,d_2,d_3,d_4) = C(d_1,d_4-1)$ and $C_R^k(d_1,d_2,d_3,d_4) = C_R^2(d_1,d_2,d_3,d_4) = C(d_2,d_3-1)$.
(v) If $n \geq 5$, then

$$C_L^k(d_1,d_2,\ldots,d_n) = C_L^{\lceil \frac{n}{2} \rceil}(d_1,d_2,\ldots,d_n)$$

$$= \begin{cases} C(d_1, d_n, d_3, d_{n-2}, \ldots, d_{2i+1}, d_{n-2i}, \ldots, d_{\lceil \frac{n}{2} \rceil +2}, d_{\lceil \frac{n}{2} \rceil} - 1), \\ \text{if both } n \text{ and } \lceil \frac{n}{2} \rceil \text{ are odd,} \\ \\ C(d_1, d_n, d_3, d_{n-2}, \ldots, d_{2i+1}, d_{n-2i}, \ldots, d_{\lceil \frac{n}{2} \rceil -1}, d_{\lceil \frac{n}{2} \rceil +1} - 1), \\ \text{if } n \text{ is odd and } \lceil \frac{n}{2} \rceil \text{ is even,} \\ \\ C(d_1, d_n, d_3, d_{n-2}, \ldots, d_{2i+1}, d_{n-2i}, \ldots, d_{\lceil \frac{n}{2} \rceil}, d_{\lceil \frac{n}{2} \rceil +1} - 1), \\ \text{if } n \text{ is even and } n/2 \text{ is odd,} \\ \\ C(d_1, d_n, d_3, d_{n-2}, \ldots, d_{2i+1}, d_{n-2i}, \ldots, d_{\lceil \frac{n}{2} \rceil -1}, d_{\lceil \frac{n}{2} \rceil +2} - 1), \\ \text{if both } n \text{ and } n/2 \text{ are even,} \end{cases}$$

and

$$C_R^k(d_1, d_2, \ldots, d_n) = C_R^{\lceil \frac{n}{2} \rceil}(d_1, d_2, \ldots, d_n)$$

$$= \begin{cases} C(d_2, d_{n-1}, d_4, d_{n-3}, \ldots, d_{2i+2}, d_{n-2i-1}, \ldots, d_{\lceil \frac{n}{2} \rceil -1}, d_{\lceil \frac{n}{2} \rceil +1} - 1), \\ \text{if both } n \text{ and } \lceil \frac{n}{2} \rceil \text{ are odd,} \\ \\ C(d_2, d_{n-1}, d_4, d_{n-3}, \ldots, d_{2i+2}, d_{n-2i-1}, \ldots, d_{\lceil \frac{n}{2} \rceil +2}, d_{\lceil \frac{n}{2} \rceil} - 1), \\ \text{if } n \text{ is odd and } \lceil \frac{n}{2} \rceil \text{ is even,} \\ \\ C(d_2, d_{n-1}, d_4, d_{n-3}, \ldots, d_{2i+2}, d_{n-2i-1}, \ldots, d_{\lceil \frac{n}{2} \rceil -1}, d_{\lceil \frac{n}{2} \rceil +2} - 1), \\ \text{if } n \text{ is even and } n/2 \text{ is odd,} \\ \\ C(d_2, d_{n-1}, d_4, d_{n-3}, \ldots, d_{2i+2}, d_{n-2i-1}, \ldots, d_{\lceil \frac{n}{2} \rceil}, d_{\lceil \frac{n}{2} \rceil +1} - 1), \\ \text{if both } n \text{ and } n/2 \text{ are even,} \end{cases}$$

for a nonnegative integer i.

Definition 3.34 Let $D = (d_1, d_2, \ldots, d_n)$ be a reduced degree sequence of a caterpillar G. Then, we define $\mathcal{S}(D)$ to be the caterpillar of reduced degree sequence D, obtained by joining by an edge the root of $C_L^k(D)$ and the root of $C_R^k(D)$, where $k = \lceil \frac{n}{2} \rceil$. The roots of $C_L^k(D)$ and $C_R^k(D)$ are identified as follows. If $n = 1$, then the root of $C_L^k(D)$ is the pseudo-leaf or a leaf of degree d_1, and the root of $C_R^k(D)$ is empty. If $n = 2$, then the root of $C_L^k(D)$ is the pseudo-leaf or a leaf of degree $d_1 - 1$, and the root of $C_R^k(D)$ is the pseudo-leaf or a leaf of degree $d_2 - 1$. If $n = 3$, then the root of $C_L^k(D)$ is the pseudo-leaf or a leaf of degree $d_3 - 1$, and the root of $C_R^k(D)$ is the pseudo-leaf or a leaf of degree $d_2 - 1$. If $n = 4$, then the root of $C_L^k(D)$ is the pseudo-leaf or a leaf of degree $d_4 - 1$, and the root of $C_R^k(D)$ is the pseudo-leaf or a leaf of degree $d_3 - 1$.

Suppose $n \geq 5$. If both n and $\lceil \frac{n}{2} \rceil$ are odd, then the root of $C_L^k(D)$ is the pseudo-leaf, or a leaf attached to a pseudo-leaf, of degree $d_{\lceil \frac{n}{2} \rceil} - 1$, that also has a neighbor of degree $d_{\lceil \frac{n}{2} \rceil + 2}$. The root of $C_R^k(D)$ is the pseudo-leaf, or a leaf attached to a pseudo-leaf, of degree $d_{\lceil \frac{n}{2} \rceil + 1} - 1$, that also has a neighbor of degree $d_{\lceil \frac{n}{2} \rceil - 1}$. If n is odd and $\lceil \frac{n}{2} \rceil$ is even, then the root of $C_L^k(D)$ is the pseudo-leaf, or a leaf attached to a pseudo leaf, of degree $d_{\lceil \frac{n}{2} \rceil + 1} - 1$, that also has a neighbor of degree $d_{\lceil \frac{n}{2} \rceil - 1}$. The root of $C_R^k(D)$ is the pseudo-leaf, or a leaf attached to a pseudo-leaf, of degree $d_{\lceil \frac{n}{2} \rceil} - 1$, that also has a neighbor of degree $d_{\lceil \frac{n}{2} \rceil + 2}$. If n is even and $n/2$ is odd, then the root of $C_L^k(D)$ is the pseudo-leaf, or a leaf attached to a pseudo-leaf, of degree $d_{\lceil \frac{n}{2} \rceil + 1} - 1$, that also has a neighbor of degree $d_{\lceil \frac{n}{2} \rceil}$. The root of $C_R^k(D)$ is the pseudo-leaf, or a leaf attached to a pseudo-leaf, of degree $d_{\lceil \frac{n}{2} \rceil + 2} - 1$, that also has a neighbor of degree $d_{\lceil \frac{n}{2} \rceil - 1}$. If both n and $n/2$ are even, then the root of $C_L^k(D)$ is the pseudo-leaf, or a leaf attached to a pseudo-leaf, of degree $d_{\lceil \frac{n}{2} \rceil + 2} - 1$, that also has a neighbor of degree $d_{\lceil \frac{n}{2} \rceil - 1}$. The root of $C_R^k(D)$ is the pseudo-leaf, or a leaf attached to a pseudo-leaf, of degree $d_{\lceil \frac{n}{2} \rceil + 1} - 1$, that also has a neighbor of degree $d_{\lceil \frac{n}{2} \rceil}$. That is: If $n = 1$, then $\mathcal{S}(D) = C(d_1)$, if $n = 2$, then $\mathcal{S}(D) = C(d_1, d_2)$, if $n = 3$, then $\mathcal{S}(D) = C(d_1, d_3, d_2)$, if $n = 4$, then $\mathcal{S}(D) = C(d_1, d_4, d_3, d_2)$, and if $n \geq 5$, then

$$\mathcal{S}(D) = \begin{cases} C(d_1, d_n, d_3, d_{n-2}, \ldots, d_{\lceil \frac{n}{2} \rceil + 2}, d_{\lceil \frac{n}{2} \rceil}, d_{\lceil \frac{n}{2} \rceil + 1}, d_{\lceil \frac{n}{2} \rceil - 1}, \ldots, d_{n-3}, d_4, d_{n-1}, d_2), \\ \text{if both } n \text{ and } \lceil \frac{n}{2} \rceil \text{ are odd,} \\ C(d_1, d_n, d_3, d_{n-2}, \ldots, d_{\lceil \frac{n}{2} \rceil - 1}, d_{\lceil \frac{n}{2} \rceil + 1}, d_{\lceil \frac{n}{2} \rceil}, d_{\lceil \frac{n}{2} \rceil + 2}, \ldots, d_{n-3}, d_4, d_{n-1}, d_2), \\ \text{if } n \text{ is odd and } \lceil \frac{n}{2} \rceil \text{ is even,} \\ C(d_1, d_n, d_3, d_{n-2}, \ldots, d_{\lceil \frac{n}{2} \rceil}, d_{\lceil \frac{n}{2} \rceil + 1}, d_{\lceil \frac{n}{2} \rceil + 2}, d_{\lceil \frac{n}{2} \rceil - 1}, \ldots, d_{n-3}, d_4, d_{n-1}, d_2), \\ \text{if } n \text{ is even and } n/2 \text{ is odd,} \\ C(d_1, d_n, d_3, d_{n-2}, \ldots, d_{\lceil \frac{n}{2} \rceil - 1}, d_{\lceil \frac{n}{2} \rceil + 2}, d_{\lceil \frac{n}{2} \rceil + 1}, d_{\lceil \frac{n}{2} \rceil}, \ldots, d_{n-3}, d_4, d_{n-1}, d_2), \\ \text{if both } n \text{ and } n/2 \text{ are even.} \end{cases}$$

See Figure 3.23, for a reduced degree sequence $D = (5, 5, 5, 4, 4, 4, 4, 3, 3, 3)$.

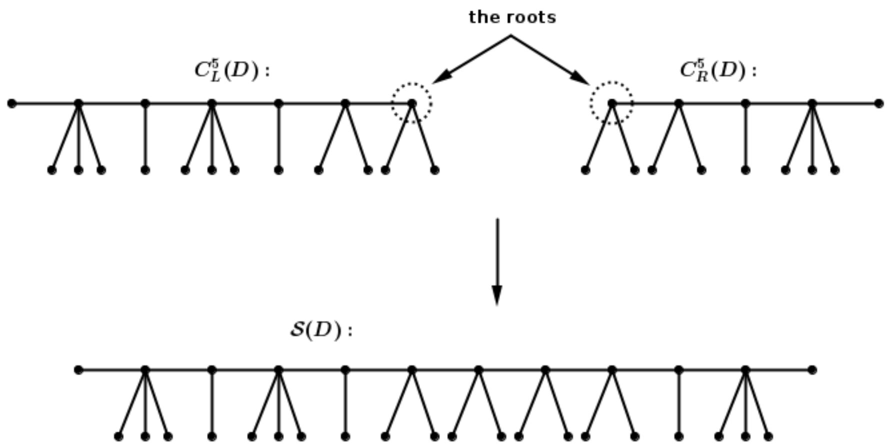

Figure 3.23: The graph representation of $C_L^5(D)$, $C_R^5(D)$ and $\mathcal{S}(D)$, for a reduced degree sequence $D = (5, 5, 5, 4, 4, 4, 4, 3, 3, 3)$.

Theorem 3.35 *Let $\mathbb{C}_D$ be the set of all caterpillars with reduced degree sequence D. Then, $M(\mathcal{S}(D), x) \le M(H, x)$ for all $H \in \mathbb{C}_D$.*

Proof. Let H be a caterpillar with reduced degree sequence $D = (d_1, d_2, \ldots, d_n)$. Suppose H is minimal with respect to $M(., x)$. Label all the non-leaf vertices in H from left to right as $u_1, u_2, \ldots, u_n$.

(i) If $n = 1$, then H is a star and $H = C(d_1) = C_L^1(d_1)$. Hence $H = \mathcal{S}(D)$, with $C_R^1(d_1) = ()$.

(ii) If $n = 2$, then $H = C(d_1, d_2)$. $C(d_1, d_2)$ can be viewed as a caterpillar obtained by joining the roots of $C(d_1 - 1) = C_L^1(d_1, d_2)$ and $C(d_2 - 1) = C_R^1(d_1, d_2)$. Hence $H = C(d_1, d_2) = \mathcal{S}(D)$.

(iii) If $n = 3$, then by Lemma 3.32, u_1 and u_3 attains the largest degrees in H. Assume $\deg(u_1) \ge \deg(u_3)$. Then, H is the caterpillar of Figure 3.24 (a), which can be viewed as in Figure 3.24 (b), with $C_L^2(d_1, d_2, d_3) = C(d_1, d_3 - 1)$ and $C_R^2(d_1, d_2, d_3) = C(d_2 - 1)$. This is just $\mathcal{S}(D)$, and hence $H \cong \mathcal{S}(D)$.

(iv) If $n = 4$, then by Lemma 3.32, u_1 and u_4 must have the largest degrees in H. Assume $\deg(u_1) \ge \deg(u_4)$. Then,

$$\tau(B_L^{u_1}, x) = \frac{1}{1 + x\,(\deg(u_1) - 1)} \le \frac{1}{1 + x\,(\deg(u_4) - 1)} = \tau(B_R^{u_4}, x),$$

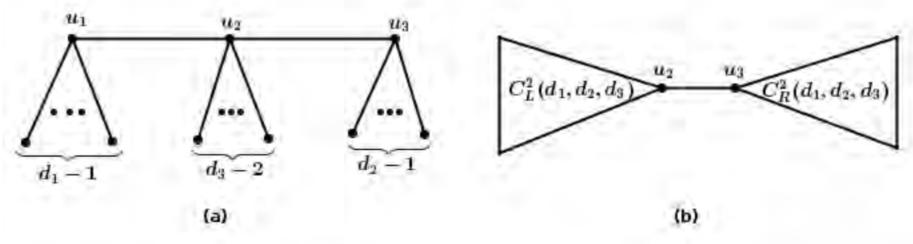

Figure 3.24: The caterpillar H in the proof of Theorem 3.35 for $n = 3$.

with equality if and only if $\deg(u_1) = \deg(u_4)$. If $\tau(B_L^{u_1}, x) = \tau(B_R^{u_4}, x)$, then we choose $\deg(u_2) \leq \deg(u_3)$. Otherwise $\tau(B_L^{u_1}, x) < \tau(B_R^{u_4}, x)$ and by Lemma 3.31, we get that $\deg(u_2) \leq \deg(u_3)$. Hence $\deg(u_2) \leq \deg(u_3)$. Then, H is the caterpillar of Figure 3.25 (a), which can be viewed as in Figure 3.25 (b). This is just $\mathcal{S}(D)$ and hence $H \cong \mathcal{S}(D)$.

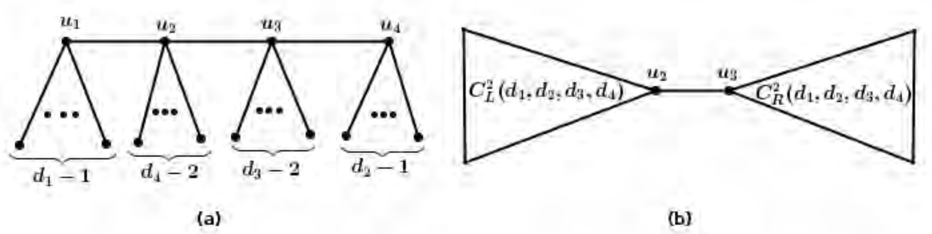

Figure 3.25: The caterpillar H in the proof of Theorem 3.35 for $n = 4$.

(v) Suppose $n \geq 5$. Note that it is enough to show that for all integers $1 \leq j < n$, if j is odd, then

$$\tau(B_L^{u_{j-1}}, x) \geq \tau(B_R^{u_{n-j+2}}, x) > \tau(B_L^{u_{i-2}}, x), \text{ for all } j+2 \leq i \leq n-j-1$$

and

$$\deg(u_j) \geq \deg(u_{n-j+1}) \geq \max\{\deg(u_{j+1}), \ldots, \deg(u_{n-j})\}.$$

And if j is even, then

$$\tau(B_L^{u_{j-1}}, x) \leq \tau(B_R^{u_{n-j+2}}, x) < \tau(B_L^{u_{i-2}}, x), \text{ for all } j+2 \leq i \leq n-j-1$$

and

$$\deg(u_j) \leq \deg(u_{n-j+1}) \leq \min\{\deg(u_{j+1}), \ldots, \deg(u_{n-j})\}.$$

As the former characterizes the caterpillar $\mathcal{S}(D)$.

Base case: By Lemma 3.32, u_1 and u_n must have the largest degrees in H. Assume $\deg(u_1) \geq \deg(u_n)$. Therefore

$$\deg(u_1) \geq \deg(u_n) \geq \max\{\deg(u_2), \ldots, \deg(u_{n-1})\}. \quad (3.29)$$

Then,

$$\tau(B_L^{u_1},x) = \frac{1}{1+x\,(\deg(u_1)-1)} \le \frac{1}{1+x\,(\deg(u_n)-1)} = \tau(B_R^{u_n},x), \quad (3.30)$$

with equality if and only if $\deg(u_1) = \deg(u_n)$. If $\tau(B_L^{u_1},x) = \tau(B_R^{u_n},x)$, we then choose $\deg(u_2) \le \deg(u_{n-1})$. Otherwise, $\tau(B_L^{u_1},x) < \tau(B_R^{u_n},x)$ and by Lemma 3.31, we get that $\deg(u_2) \le \deg(u_{n-1})$. Hence

$$\deg(u_2) \le \deg(u_{n-1}). \quad (3.31)$$

From (3.29) $\deg(u_n) \ge \max\{\deg(u_i) : 2 \le i \le n-1\}$. Since $n \ge 5$, then for $2 \le i \le n-1$ $B_L^{u_{i-1}}$ is neither empty nor a leaf. Then, by Lemma 2.4 and Remark 2.5, we have $0 < \tau(B_L^{u_{i-1}},x) < 1$. Then, for $2 \le i \le n-1$

$$\begin{aligned}
\tau(B_R^{u_n},x) &= \frac{1}{1+x\,(\deg(u_n)-1)} \\
&\le \frac{1}{1+x\,(\deg(u_i)-1)}, && \text{since } \deg(u_n) \ge \deg(u_i) \\
&< \frac{1}{1+x\,(\deg(u_i)-2+\tau(B_L^{u_{i-1}},x))}, && \text{since } 0 < \tau(B_L^{u_{i-1}},x) < 1 \\
&= \tau(B_L^{u_i},x).
\end{aligned}$$

Hence

$$\tau(B_R^{u_n},x) < \tau(B_L^{u_i},x), \text{ for all } 2 \le i \le n-1. \quad (3.32)$$

By Lemma 3.31,

$$\deg(u_{n-1}) \le \deg(u_{i+1}), \text{ for all } 2 \le i \le n-3. \quad (3.33)$$

From (3.31) and (3.33) we get that $\deg(u_2) \le \deg(u_{n-1}) \le \deg(u_{i+1})$, for all $2 \le i \le n-3$. Therefore,

$$\deg(u_2) \le \deg(u_{n-1}) \le \min\{\deg(u_3),\ldots,\deg(u_{n-2})\}. \quad (3.34)$$

From (3.30) we have $\tau(B_L^{u_1},x) \le \tau(B_R^{u_n},x)$, with equality if and only if $\deg(u_1) = \deg(u_n)$. From (3.34) we get that $\deg(u_2) \le \deg(u_{n-1})$. Since $\deg(u_2) \le \deg(u_{n-1})$ and $\tau(B_L^{u_1},x) \le \tau(B_R^{u_n},x)$, then

$$\begin{aligned}
\tau(B_L^{u_2},x) &= \frac{1}{1+x\,(\deg(u_2)-2+\tau(B_L^{u_1},x))} \\
&\ge \frac{1}{1+x\,(\deg(u_{n-1})-2+\tau(B_R^{u_n},x))} = \tau(B_R^{u_{n-1}},x).
\end{aligned}$$

Therefore,

$$\tau(B_L^{u_2},x) \ge \tau(B_R^{u_{n-1}},x). \quad (3.35)$$

By Lemma 3.4, we get $\tau(B_L^{u_2},x)=\tau(B_R^{u_{n-1}},x)$ if and only if $B_L^{u_2}\approx_r B_R^{u_{n-1}}$, that is, if $\deg(u_2)=\deg(u_{n-1})$ and $\deg(u_1)=\deg(u_n)$. If $\tau(B_L^{u_2},x)=\tau(B_R^{u_{n-1}},x)$, then choose $\deg(u_3)\geq\deg(u_{n-2})$. Otherwise $\tau(B_L^{u_2},x)>\tau(B_R^{u_{n-1}},x)$ and by Lemma 3.31, we get $\deg(u_3)\geq\deg(u_{n-2})$. Hence

$$\deg(u_3)\geq\deg(u_{n-2}). \tag{3.36}$$

For any $3\leq i\leq n-2$, $B_L^{u_{i-2}}$ is neither empty nor a leaf. Then, by Lemma 2.4 and Remark 2.5, we have $0<\tau(B_L^{u_{i-2}},x)<1$. And for any $3\leq i\leq n-2$, we get

$$\begin{aligned}&\tau(B_R^{u_n},x)\\ &=\frac{1}{1+x\left(\deg(u_n)-1\right)}\\ &\leq\frac{1}{1+x\left(\deg(u_{i-1})-1\right)},\text{ since }\deg(u_n)\geq\deg(u_{i-1})\text{ in (3.29)}\\ &<\frac{1}{1+x\left(\deg(u_{i-1})-2+\tau(B_L^{u_{i-2}},x)\right)},\text{ since }0<\tau(B_L^{u_{i-2}},x)<1\\ &=\tau(B_L^{u_{i-1}},x).\end{aligned}$$

Therefore,

$$\tau(B_R^{u_n},x)<\tau(B_L^{u_{i-1}},x),\text{ for any }3\leq i\leq n-2. \tag{3.37}$$

From (3.34) and (3.37) we get

$$\begin{aligned}&\tau(B_R^{u_{n-1}},x)\\ &=\frac{1}{1+x\left(\deg(u_{n-1})-2+\tau(B_R^{u_n},x)\right)}>\frac{1}{1+x\left(\deg(u_i)-2+\tau(B_L^{u_{i-1}},x)\right)}\\ &=\tau(B_L^{u_i},x).\end{aligned}$$

Therefore,

$$\tau(B_R^{u_{n-1}},x)>\tau(B_L^{u_i},x),\text{ for any }3\leq i\leq n-2. \tag{3.38}$$

By Lemma 3.31, we get that $\deg(u_{n-2})\geq\deg(u_{i+1})$ for any $3\leq i\leq n-4$. Hence

$$\deg(u_{n-2})\geq\max\left\{\deg(u_4),\ldots,\deg(u_{n-3})\right\}. \tag{3.39}$$

From (3.36) and (3.39) we get that

$$\deg(u_3)\geq\deg(u_{n-2})\geq\max\left\{\deg(u_4),\ldots,\deg(u_{n-3})\right\}. \tag{3.40}$$

Therefore, from (3.29) we have

$$\deg(u_1)\geq\deg(u_n)\geq\max\left\{\deg(u_2),\ldots,\deg(u_{n-1})\right\},$$

from (3.30) and (3.32) we have

$$\tau(B_L^{u_1},x) \leq \tau(B_R^{u_n},x) < \tau(B_L^{u_{i-2}},x), \text{ for any } 4 \leq i \leq n-3$$

and from (3.34) we have

$$\deg(u_2) \leq \deg(u_{n-1}) \leq \min\{\deg(u_3),\dots,\deg(u_{n-2})\}.$$

From (3.35) and (3.38) we have

$$\tau(B_L^{u_2},x) \geq \tau(B_R^{u_{n-1}},x) > \tau(B_L^{u_{i-2}},x), \text{ for any } 5 \leq i \leq n-4$$

and from (3.40) we have

$$\deg(u_3) \geq \deg(u_{n-2}) \geq \max\{\deg(u_4),\dots,\deg(u_{n-3})\}.$$

Suppose that for all integers $1 \leq j < n$:
(a) If j is odd, then

$$\tau(B_L^{u_{j-1}},x) \geq \tau(B_R^{u_{n-j+2}},x) > \tau(B_L^{u_{i-2}},x), \text{ for any } j+2 \leq i \leq n-j-1, \tag{3.41}$$

and

$$\deg(u_j) \geq \deg(u_{n-j+1}) \geq \max\{\deg(u_{j+1}),\dots,\deg(u_{n-j})\}. \tag{3.42}$$

(b) If j is even, then

$$\tau(B_L^{u_{j-1}},x) \leq \tau(B_R^{u_{n-j+2}},x) < \tau(B_L^{u_{i-2}},x), \text{ for any } j+2 \leq i \leq n-j-1 \tag{3.43}$$

and

$$\deg(u_j) \leq \deg(u_{n-j+1}) \leq \min\{\deg(u_{j+1}),\dots,\deg(u_{n-j})\}. \tag{3.44}$$

(i) Suppose j is odd. Then, from (3.41) and (3.42) we have $\tau(B_L^{u_{j-1}},x) \geq \tau(B_R^{u_{n-j+2}},x)$ and $\deg(u_j) \geq \deg(u_{n-j+1})$. Hence,

$$\begin{aligned}\tau(B_L^{u_j},x) &= \frac{1}{1+x\left(\deg(u_j)-2+\tau(B_L^{u_{j-1}},x)\right)}\\ &\leq \frac{1}{1+x\left(\deg(u_{n-j+1})-2+\tau(B_R^{u_{n-j+2}},x)\right)} = \tau(B_R^{u_{n-j+1}},x).\end{aligned}$$

Therefore,

$$\tau(B_L^{u_j},x) \leq \tau(B_R^{u_{n-j+1}},x). \tag{3.45}$$

By Lemma 3.4, $\tau(B_L^{u_j},x) = \tau(B_R^{u_{n-j+1}},x)$ if and only if $B_L^{u_j} \approx_r B_R^{u_{n-j+1}}$, in such a case $\deg(u_j) = \deg(u_{n-j+1})$ and $\tau(B_L^{u_{j-1}},x) = \tau(B_R^{u_{n-j+2}},x)$. Otherwise, $\tau(B_L^{u_j},x) < \tau(B_R^{u_{n-j+1}},x)$. If $\tau(B_L^{u_j},x) = \tau(B_R^{u_{n-j+1}},x)$, then we choose $\deg(u_{j+1}) \leq \deg(u_{n-j})$. Otherwise $\tau(B_L^{u_j},x)$

$< \tau(B_R^{u_{n-j+1}}, x)$ and by Lemma 3.31, we must have $\deg(u_{j+1}) \leq \deg(u_{n-j})$. Hence,

$$\deg(u_{j+1}) \leq \deg(u_{n-j}). \tag{3.46}$$

From (3.41), we have $\tau(B_R^{u_{n-j+2}}, x) > \tau(B_L^{u_{i-2}}, x)$, for any $j+2 \leq i \leq n-j-1$. Then, by Lemma 3.31, we must have $\deg(u_{n-j+1}) \geq \deg(u_{i-1})$ and hence,

$$\begin{aligned}\tau(B_R^{u_{n-j+1}}, x) &= \frac{1}{1 + x\left(\deg(u_{n-j+1}) - 2 + \tau(B_R^{u_{n-j+2}}, x)\right)} \\ &< \frac{1}{1 + x\left(\deg(u_{i-1}) - 2 + \tau(B_L^{u_{i-2}}, x)\right)} = \tau(B_L^{u_{i-1}}, x).\end{aligned}$$

Therefore,

$$\tau(B_R^{u_{n-j+1}}, x) < \tau(B_L^{u_{i-1}}, x), \text{ for any } j+2 \leq i \leq n-j-1. \tag{3.47}$$

Hence, from (3.45) and (3.47) we get

$$\tau(B_L^{u_j}, x) \leq \tau(B_R^{u_{n-j+1}}, x) < \tau(B_L^{u_{i-1}}, x), \text{ for any } j+2 \leq i \leq n-j-1. \tag{3.48}$$

From (3.48) we have $\tau(B_R^{u_{n-j+1}}, x) < \tau(B_L^{u_{i-1}}, x)$. By Lemma 3.31, we must have $\deg(u_{n-j}) \leq \deg(u_i)$. Hence

$$\deg(u_{n-j}) \leq \min\left\{\deg(u_{j+2}), \ldots, \deg(u_{n-j-1})\right\}. \tag{3.49}$$

Therefore, from (3.46) and (3.49) we must have

$$\deg(u_{j+1}) \leq \deg(u_{n-j}) \leq \min\left\{\deg(u_{j+2}), \ldots, \deg(u_{n-j-1})\right\}. \tag{3.50}$$

Hence, from (3.48) and (3.50) if j is odd, then

$$\tau(B_L^{u_j}, x) \leq \tau(B_R^{u_{n-j+1}}, x) < \tau(B_L^{u_{i-1}}, x), \text{ for any } j+2 \leq i \leq n-j-1$$

and

$$\deg(u_{j+1}) \leq \deg(u_{n-j}) \leq \min\left\{\deg(u_{j+2}), \ldots, \deg(u_{n-j-1})\right\}.$$

(ii) Suppose j is even. From (3.43) and (3.44) we have $\tau(B_L^{u_{j-1}}, x) \leq \tau(B_R^{u_{n-j+2}}, x)$ and $\deg(u_j) \leq \deg(u_{n-j+1})$. Then,

$$\begin{aligned}\tau(B_L^{u_j}, x) &= \frac{1}{1 + x\left(\deg(u_j) - 2 + \tau(B_L^{u_{j-1}}, x)\right)} \\ &\geq \frac{1}{1 + x\left(\deg(u_{n-j+1}) - 2 + \tau(B_R^{u_{n-j+2}}, x)\right)} = \tau(B_R^{u_{n-j+1}}, x).\end{aligned}$$

Therefore,

$$\tau(B_L^{u_j}, x) \geq \tau(B_R^{u_{n-j+1}}, x). \tag{3.51}$$

By Lemma 3.4, $\tau(B_L^{u_j},x)=\tau(B_R^{u_{n-j+1}},x)$ if and only if $B_L^{u_j}\approx_r B_R^{u_{n-j+1}}$, in such a case $\deg(u_j)=\deg(u_{n-j+1})$ and $\tau(B_L^{u_{j-1}},x)=\tau(B_R^{u_{n-j+2}},x)$. Otherwise $\tau(B_L^{u_j},x)>\tau(B_R^{u_{n-j+1}},x)$. If $\tau(B_L^{u_j},x)=\tau(B_R^{u_{n-j+1}},x)$, then we choose $\deg(u_{j+1})\geq\deg(u_{n-j})$. Otherwise, $\tau(B_L^{u_j},x)>\tau(B_R^{u_{n-j+1}},x)$ and by Lemma 3.31, we must have $\deg(u_{j+1})\geq\deg(u_{n-j})$. Hence,

$$\deg(u_{j+1})\geq\deg(u_{n-j}). \tag{3.52}$$

From (3.43) we have $\tau(B_R^{u_{n-j+2}},x)<\tau(B_L^{u_{i-2}},x)$, for any $j+2\leq i\leq n-j-1$. By Lemma 3.31, we must have $\deg(u_{n-j+1})\leq\deg(u_{i-1})$ and hence

$$\begin{aligned}\tau(B_R^{u_{n-j+1}},x)&=\frac{1}{1+x\left(\deg(u_{n-j+1})-2+\tau(B_R^{u_{n-j+2}},x)\right)}\\&>\frac{1}{1+x\left(\deg(u_{i-1})-2+\tau(B_L^{u_{i-2}},x)\right)}=\tau(B_L^{u_{i-1}},x).\end{aligned}$$

Therefore,

$$\tau(B_R^{u_{n-j+1}},x)>\tau(B_L^{u_{i-1}},x),\text{ for any } j+2\leq i\leq n-j-1. \tag{3.53}$$

Hence, from (3.51) and (3.53) we must have

$$\tau(B_L^{u_j},x)\geq\tau(B_R^{u_{n-j+1}},x)>\tau(B_L^{u_{i-1}},x),\text{ for any } j+2\leq i\leq n-j-1. \tag{3.54}$$

From (3.54) we have $\tau(B_R^{u_{n-j+1}},x)>\tau(B_L^{u_{i-1}},x)$, for any $j+2\leq i\leq n-j-1$. By Lemma 3.31, we must have $\deg(u_{n-j})\geq\deg(u_i)$. Hence

$$\deg(u_{n-j})\geq\max\left\{\deg(u_{j+2}),\ldots,\deg(u_{n-j-1})\right\}. \tag{3.55}$$

From (3.52) and (3.55) we have

$$\deg(u_{j+1})\geq\deg(u_{n-j})\geq\max\left\{\deg(u_{j+2}),\ldots,\deg(u_{n-j-1})\right\}. \tag{3.56}$$

Hence, from (3.54) and (3.56) if j is even, then

$$\tau(B_L^{u_j},x)\geq\tau(B_R^{u_{n-j+1}},x)>\tau(B_L^{u_{i-1}},x),\text{ for all } j+2\leq i\leq n-j-1$$

and

$$\deg(u_{j+1})\geq\deg(u_{n-j})\geq\max\left\{\deg(u_{j+2}),\ldots,\deg(u_{n-j-1})\right\}.$$

□

Remark 3.36 In Chapter 1, we saw that if T and T' are trees, such that $M(T,x)\leq M(T',x)$ for all positive $x\in\mathbb{R}$, then

$$Z(T)=M(T,1)\leq M(T',1)=Z(T'),$$

and

$$En(T)=\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln M(T,x^2)dx\leq\frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\ln M(T',x^2)dx=En(T').$$

Then, from Theorem 3.35 we deduce the following theorem.

Theorem 3.37 *Let $\mathbb{C}_D$ be the set of all caterpillars with reduced degree sequence D. Then, $Z(\mathcal{S}(D)) \leq Z(H)$ and $En(\mathcal{S}(D)) \leq En(H)$ for all $H \in \mathbb{C}_D$.*

Lemma 3.38 *Let i, j and n be positive integers such that $1 \leq i < j \leq n$. Let $D = (d_1, \dots, d_i, \dots, d_j, \dots, d_n)$ be reduced degree sequence of a caterpillar C, such that $d_i \geq d_j > 2$. Decompose $\mathcal{S}(D)$ as in Figure 3.26, with B, $B^{'}$ and H non-empty. Let v and w be vertices of $\mathcal{S}(D)$ such that $\deg(v) = d_i$ and $\deg(w) = d_j$. Let w' be a leaf adjacent to w. Let G be obtained from $\mathcal{S}(D)$ by removing the edge ww' and then adding the edge vw'. If either (i) $d_i > d_j$ or (ii) $d_i = d_j$ and $M(H-w,x) \geq M(H-v,x)$, then*

$$M(\mathcal{S}(D), x) > M(G, x) \geq M(\mathcal{S}(D^{'}), x),$$

where $D^{'} = (d_1, \dots, d_{i-1}, d_i + 1, d_{i+1}, \dots, d_{j-1}, d_j - 1, d_{j+1}, \dots, d_n)$.

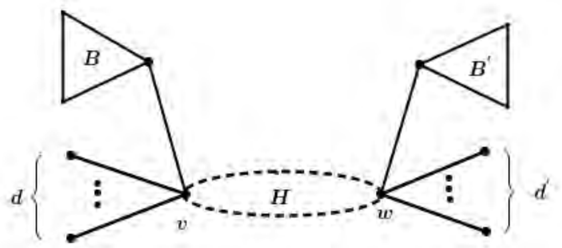

Figure 3.26: Decomposition of the caterpillar $\mathcal{S}(D)$ in Lemma 3.38.

Proof. Let $d = d_i - 2$ and $d^{'} = d_j - 2$. Suppose $\deg(v) = d_i > d_j = \deg(w)$. Then, $d > d^{'}$. Since $\mathcal{S}(D)$ is minimal with respect to $M(.,x)$ and $d > d^{'}$, then by Lemma 3.31 (ii) and (iii), we must have $\tau(B,x) \geq \tau(B^{'},x)$ and $M(H-v,x) \leq M(H-w,x)$. From Equation (3.2), we have

$$M(\mathcal{S}(D),x) = M(B,x)M(B^{'},x)\Big[M(H,x) + dd^{'}x^2M(H-\{v,w\},x) + x^2\tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x) + M_v^w(\mathcal{S}(D),x)\Big]$$

where,

$$M_v^w(\mathcal{S}(D),x) = x\left[\left(d^{'} + \tau(B^{'},x)\right)M(H-w,x) + (d+\tau(B,x))\,M(H-v,x)\right] + x^2M(H-\{v,w\},x)\left[d\tau(B^{'},x) + d^{'}\tau(B,x)\right]$$

and

$$M(G,x) = M(B,x)M(B^{'},x)\Big[M(H,x) + (d+1)(d^{'}-1)x^2M(H-\{v,w\},x)$$

$$+ x^2\tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x) + M_v^w(G,x)\Big]$$

where,

$$\begin{aligned}
&M_v^w(G,x)\\
&= x\left[\left(d^{'}+\tau(B^{'},x)-1\right)M(H-w,x)+(d+\tau(B,x)+1)M(H-v,x)\right]\\
&\qquad + x^2M(H-\{v,w\},x)\left[(d+1)\tau(B^{'},x)+\left(d^{'}-1\right)\tau(B,x)\right].
\end{aligned}$$

Then,

$$\begin{aligned}
&M(\mathcal{S}(D),x)-M(G,x)\\
&= M(B,x)M(B^{'},x)\left[\left(dd^{'}-(d+1)\left(d^{'}-1\right)\right)x^2M(H-\{v,w\},x)\right.\\
&\qquad \left.+M_v^w(\mathcal{S}(D),x)-M_v^w(G,x)\right]\\
&= M(B,x)M(B^{'},x)\left[\left(dd^{'}-dd^{'}+d-d^{'}+1\right)x^2M(H-\{v,w\},x)\right.\\
&\qquad \left.+M_v^w(\mathcal{S}(D),x)-M_v^w(G,x)\right]\\
&= M(B,x)M(B^{'},x)\left[\left(d-d^{'}+1\right)x^2M(H-\{v,w\},x)\right.\\
&\qquad \left.+M_v^w(\mathcal{S}(D),x)-M_v^w(G,x)\right].
\end{aligned}$$

But,

$$\begin{aligned}
&M_v^w(\mathcal{S}(D),x)-M_v^w(G,x)\\
&= x\left[\left(d^{'}+\tau(B^{'},x)-\left(d^{'}+\tau(B^{'},x)-1\right)\right)M(H-w,x)\right.\\
&\qquad \left.+((d+\tau(B,x))-(d+\tau(B,x)+1))M(H-v,x)\right]\\
&+ x^2M(H-\{v,w\},x)\left[d\tau(B^{'},x)+d^{'}\tau(B,x)\right.\\
&\qquad \left.-(d+1)\tau(B^{'},x)-(d^{'}-1)\tau(B,x)\right]\\
&= x\left[M(H-w,x)-M(H-v,x)\right]+x^2M(H-\{v,w\},x)\left[\tau(B,x)-\tau(B^{'},x)\right].
\end{aligned}$$

Therefore,

$$\begin{aligned}
&M(\mathcal{S}(D),x)-M(G,x)\\
&= M(B,x)M(B^{'},x)\left[\left(d-d^{'}+1\right)x^2M(H-\{v,w\},x)\right.\\
&\qquad +x\left[M(H-w,x)-M(H-v,x)\right]\\
&\left.+ x^2M(H-\{v,w\},x)\left[\tau(B,x)-\tau(B^{'},x)\right]\right]\\
&= M(B,x)M(B^{'},x)\left[x^2M(H-\{v,w\},x)\left[(d+\tau(B,x)+1)\right.\right.\\
&\qquad \left.-\left(d^{'}+\tau(B^{'},x)\right)\right]
\end{aligned}$$

$+ x\,(M(H-w,x) - M(H-v,x))]$
> 0, since $x > 0, 0 < \tau(B,x), \tau(B^{'},x) \leq 1, d > d^{'}$ and $M(H-w,x) \geq M(H-v,x)$.

Suppose $d_i = d_j$ and $M(H-w,x) \geq M(H-v,x)$. Then, $d = d^{'}$ and

$$\begin{aligned}
&M(\mathcal{S}(D),x) - M(G,x)\\
&= M(B,x)M(B^{'},x)\left[x^2 M(H-\{v,w\},x)\left[(d+\tau(B,x)+1)\right.\right.\\
&\qquad\qquad \left.\left. - \left(d^{'} + \tau(B^{'},x)\right)\right] + x\,(M(H-w,x) - M(H-v,x))\right]\\
&= M(B,x)M(B^{'},x)\left[x^2 M(H-\{v,w\},x)\left(\tau(B,x)+1-\tau(B^{'},x)\right)\right.\\
&\qquad\qquad \left. + x\,(M(H-w,x) - M(H-v,x))\right]
\end{aligned}$$

> 0, since $x > 0, 0 < \tau(B,x), \tau(B^{'},x) \leq 1$ and $M(H-w,x) \geq M(H-v,x)$. Hence $M(\mathcal{S}(D),x) > M(G,x)$. Since $\mathcal{S}(D^{'})$ and G have the same reduced degree sequence $D^{'}$ and are both caterpillars, then by Theorem 3.35, we must have $M(G,x) \geq M(\mathcal{S}(D^{'}),x)$. Hence, we conclude

$$M(\mathcal{S}(D),x) > M(G,x) \geq M(\mathcal{S}(D^{'}),x).$$

□

Lemma 3.39 *Let G be a caterpillar and be decomposed as in Figure 3.1, with B, $B^{'}$ and H non-empty. Let $G^{'}$ be obtained from G by removing the edge $wr(B^{'})$ and then adding the edge $vr(B^{'})$. Suppose G is minimal with respect to $M(.,x)$. If either*

1.) $\tau(B,x) > \tau(B^{'},x)$,
2.) $d > d^{'}$, or
3.) $\tau(B,x) = \tau(B^{'},x)$, $d = d^{'}$ and $M(H-v,x) \leq M(H-w,x)$,
then

$$M(G,x) > M(G^{'},x).$$

Proof. Suppose G is a caterpillar and decomposed as in Figure 3.1. Suppose G is minimal with respect to $M(.,x)$. Suppose $\tau(B,x) > \tau(B^{'},x)$, then by Lemma 3.31 (i), we must have $d \geq d^{'}$ and $M(H-v,x) \leq M(H-w,x)$. Suppose $d > d^{'}$, then by Lemma 3.31 (ii) and (iii), we must have $M(H-v,x) \leq M(H-w,x)$. Therefore, if 1.), 2.) or 3.) holds, then $d \geq d^{'}$ and $M(H-v,x) \leq M(H-w,x)$. $G^{'}$ can be decomposed as in Figure 3.27. Then,

$$M(G^{'},x) = M(G^{'} - vr(B),x) + xM(G^{'} - \{v, r(B)\},x)$$

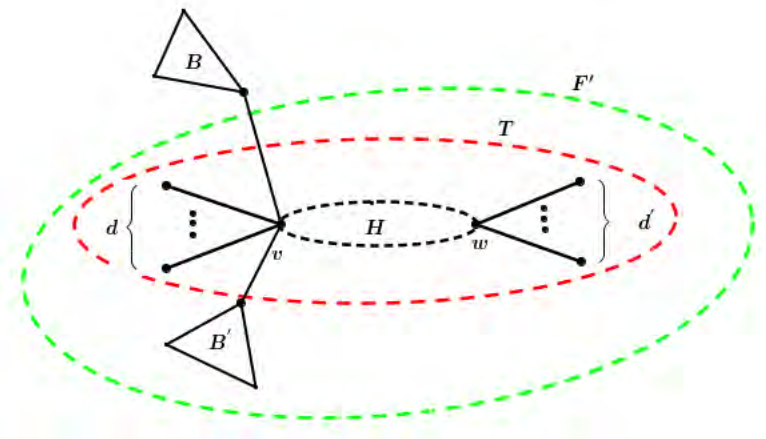

Figure 3.27: Decomposition of the tree $G^{'}$ in the proof of Lemma 3.39.

$$
\begin{aligned}
&= M(B,x)M(F',x) + xM(G^{'} - \{v, r(B)\}, x)\\
&= M(B,x)M(F',x) + xM(B - r(B), x)M(B^{'}, x)M(T - v, x)\\
&= M(B,x)\left[M(F' - vr(B^{'}), x) + xM(F' - \{v, r(B^{'})\}, x)\right]\\
&\qquad + xM(B - r(B), x)M(B^{'}, x)M(T - v, x)\\
&= M(B,x)\left[M(B^{'}, x)M(T,x) + xM(B^{'} - r(B^{'}), x)M(T - v, x)\right]\\
&\qquad + xM(B - r(B), x)M(B^{'}, x)M(T - v, x)\\
&= M(B,x)M(B^{'},x)M(T,x)\\
&\qquad + xM(B,x)M(B^{'} - r(B^{'}), x)M(T - v, x)\\
&+ xM(B - r(B), x)M(B^{'}, x)M(T - v, x)
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&M(G^{'}, x)\\
&= M(B,x)M(B^{'},x)M(T,x) + xM(B,x)M(B^{'} - r(B^{'}), x)M(T - v, x)\\
&\qquad + xM(B - r(B), x)M(B^{'}, x)M(T - v, x)
\end{aligned}
$$

and

$$
\begin{aligned}
&M(G, x)\\
&= M(B,x)M(B^{'},x)M(T,x) + xM(B,x)M(B^{'} - r(B^{'}), x)M(T - w, x)\\
&\qquad + xM(B^{'}, x)M(B - r(B), x)M(T - v, x)\\
&+ x^2 M(B - r(B), x)M(B^{'} - r(B^{'}), x)M(T - \{v, w\}, x).
\end{aligned}
$$

Then,

$M(G,x) - M(G^{'}, x)$

$$
\begin{aligned}
&= xM(B,x)M(B^{'}-r(B^{'}),x)\left[M(T-w,x)-M(T-v,x)\right]\\
&\qquad + x^2M(B-r(B),x)M(B^{'}-r(B^{'}),x)M(T-\{v,w\},x)\\
&= xM(B,x)M(B^{'}-r(B^{'}),x)\Big[M(H-w,x)+dxM(H-\{v,w\},x)\\
&\qquad - M(H-v,x)-d^{'}xM(H-\{v,w\},x)\Big]\\
&+ x^2M(B-r(B),x)M(B^{'}-r(B^{'}),x)M(H-\{v,w\},x)\\
&= xM(B,x)M(B^{'}-r(B^{'}),x)\Big[M(H-w,x)-M(H-v,x)\\
&\qquad +xM(H-\{v,w\},x)(d-d^{'})\Big]\\
&+ x^2M(B-r(B),x)M(B^{'}-r(B^{'}),x)M(H-\{v,w\},x)>0,
\end{aligned}
$$

since $x>0, M(B-r(B),x), M(B^{'}-r(B^{'}),x), M(H-\{v,w\},x)>0, M(H-w,x)\geq M(H-v,x)$ and $d\geq d^{'}$. □

Lemma 3.40 *Let G be a caterpillar and be decomposed as in Figure 3.1, with B, $B^{'}$ and H non-empty. Let $w^{'}$ be a leaf adjacent to w. Let $G^{'}$ be obtained from G by removing the edge ww' and then adding the edge $vw^{'}$. If $\tau(B,x)\geq\tau(B^{'},x)$, $d\geq d^{'}$ and $M(H-v,x)\leq M(H-w,x)$, then $M(G,x)>M(G^{'},x)$.*

Proof. Suppose B, $B^{'}$ and H are non-empty. Suppose $\tau(B,x)\geq\tau(B^{'},x)$, $d\geq d^{'}$ and $M(H-v,x)\leq M(H-w,x)$.

$$
\begin{aligned}
M(G,x) = M(B,x)M(B^{'},x)\Big[&M(H,x)+dd^{'}x^2M(H-\{v,w\},x)\\
&+ x^2\tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x)+M_v^w(G,x)\Big]
\end{aligned}
$$

and

$$
\begin{aligned}
&M(G^{'},x)\\
&= M(B,x)M(B^{'},x)\Big[M(H,x)+(d+1)\left(d^{'}-1\right)x^2M(H-\{v,w\},x)\\
&\qquad + x^2\tau(B,x)\tau(B^{'},x)M(H-\{v,w\},x)+M_v^w(G^{'},x)\Big].
\end{aligned}
$$

Then,

$$
\begin{aligned}
&M(G,x)-M(G^{'},x)\\
&= M(B,x)M(B^{'},x)\Big[x^2M(H-\{v,w\},x)\left(dd^{'}-(d+1)\left(d^{'}-1\right)\right)\\
&\qquad + M_v^w(G,x)-M_v^w(G^{'},x)\Big]\\
&= M(B,x)M(B^{'},x)\Big[x^2M(H-\{v,w\},x)\left(dd^{'}-\left(dd^{'}-d+d^{'}-1\right)\right)\\
&\qquad + M_v^w(G,x)-M_v^w(G^{'},x)\Big]
\end{aligned}
$$

$$= M(B,x)M(B',x)\left[x^2M(H-\{v,w\},x)\left(d-d'+1\right) + M_v^w(G,x) - M_v^w(G',x)\right].$$

But

$$M_v^w(G,x) - M_v^w(G',x)$$
$$= x\left[\left(d'+\tau(B',x)\right)M(H-w,x) + (d+\tau(B,x))M(H-v,x)\right] + x^2M(H-\{v,w\},x)\left[d\tau(B',x)+d'\tau(B,x)\right]$$
$$- x\left[\left(d'+\tau(B',x)-1\right)M(H-w,x) + (d+\tau(B,x)+1)M(H-v,x)\right] - x^2M(H-\{v,w\},x)\left[(d+1)\tau(B',x)+\left(d'-1\right)\tau(B,x)\right]$$
$$= x\left[M(H-w,x)-M(H-v,x)\right] + x^2M(H-\{v,w\},x)\left[\tau(B,x)-\tau(B',x)\right].$$

This implies that,

$$M(G,x) - M(G',x)$$
$$= M(B,x)M(B',x)\left[x^2M(H-\{v,w\},x)\left(d-d'+1\right)\right.$$
$$\left. + x\left[M(H-w,x)-M(H-v,x)\right] + x^2M(H-\{v,w\},x)\left[\tau(B,x)-\tau(B',x)\right]\right.$$
$$= M(B,x)M(B',x)\left[x^2M(H-\{v,w\},x)\left(d+\tau(B,x)+1-\left(d'+\tau(B',x)\right)\right) + x\left[M(H-w,x)-M(H-v,x)\right]\right]$$

> 0, since $d \geq d', \tau(B,x) \geq \tau(B',x)$ and $M(H-w,x) \geq M(H-v,x)$.

□

Theorem 3.41 *Let $(y_1,\ldots,y_n)$ and $(d_1,\ldots,d_n)$ be two degree sequences of caterpillars. If $(y_1,\ldots,y_n) \prec (d_1,\ldots,d_n)$ and $\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} d_i$, then for all $x > 0$ we have*

$$M(\mathcal{S}(y_1,\ldots,y_n),x) > M(\mathcal{S}(d_1,\ldots,d_n),x)$$

and hence,

$$Z(\mathcal{S}(y_1,\ldots,y_n)) > Z(\mathcal{S}(d_1,\ldots,d_n))$$

and

$$En(\mathcal{S}(y_1,\ldots,y_n)) > En(\mathcal{S}(d_1,\ldots,d_n)).$$

Proof. Suppose $Y = (y_1,\ldots,y_n)$ and $D = (d_1,\ldots,d_n)$ are two degree sequences of caterpillars, $Y \prec D$ and $\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} d_i$. Then, there exists i_0, such that $d_{i_0} \neq y_{i_0}$. In fact, the set $\mathbb{I} = \{i : d_i \neq y_i\}$ must have at least two elements, otherwise $\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} d_i$ would be impossible. Let $l = \min\{i : d_i \neq y_i\}$ and $m = \max\{i : d_i \neq y_i\}$. We must have $y_m > d_m \geq 1$ and we must also have $d_l > y_l$. We define

$$Y_1 = (y_1, \ldots, y_{l-1}, y_l + 1, y_{l+1}, \ldots, y_{m-1}, y_m - 1, y_{m+1}, \ldots, y_n).$$

Note that Y_1 is still a valid degree sequence. If $l > 1$, then $y_{l-1} = d_{l-1} \geq d_l \geq y_l + 1 > d_m + 1 \geq 2$ and if $l = 1$, then $d_l \geq y_l + 1 > d_m + 1 \geq 2$. If $m < n$, then $y_m - 1 \geq d_m \geq d_{m+1} = y_{m+1} \geq 1$ and if $m = n$, then $y_m - 1 \geq d_m \geq 1$. It is clear that $Y \prec Y_1$. If $y_m > 2$, then by applying Lemma 3.38 to $\mathcal{S}(Y)$, we know that there exists a caterpillar G with degree sequence Y_1 such that

$$M(\mathcal{S}(Y), x) > M(G, x) \geq M(\mathcal{S}(Y_1), x).$$

Otherwise $y_m = 2$. In such case, decompose $\mathcal{S}(Y)$ as in Figure 3.28, with B non-empty, $\deg(v) = y_l$ and $\deg(w) = y_m = 2$. In view of the

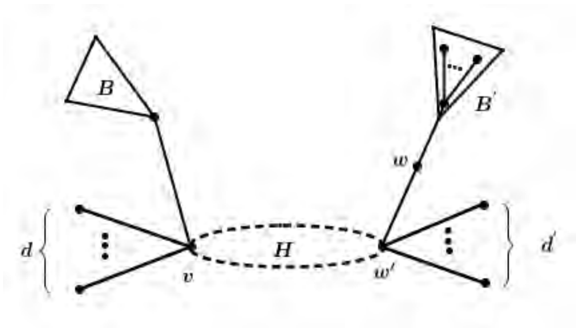

Figure 3.28: Decomposition of the caterpillar $\mathcal{S}(Y)$ in the proof of Theorem 3.41.

structure of $\mathcal{S}(Y)$, we can choose w so that $\deg(r(B')) \geq \deg(u')$, for all non-leaf vertices u' in $\mathcal{S}(Y)$. Since

$$\tau(B', x) = \frac{1}{1 + x\,(\deg(r(B')) - 1)},$$

$$\tau(B_L^{u'}, x) = \frac{1}{1 + x\,(\deg(u') - 2 + \tau(B^*, x))}, \text{ for some branch } B^* \text{ in } B_L^{u'}$$

and $\deg(r(B')) \geq \deg(u')$, for all non-leaf vertices u' in $\mathcal{S}(Y)$, then $\tau(B', x) \leq \tau(B_L^{u'}, x)$, with equality if and only if $\deg(u') = \deg(r(B'))$, u' is a pseudo leaf and u' is not $r(B')$. Let G be a caterpillar obtained from $\mathcal{S}(Y)$, by removing the edge $wr(B')$ and then adding the edge $w'r(B')$. Since $\deg(w') \geq 2 = \deg(w)$, $\tau(B_L^{u'}, x) \geq \tau(B', x)$ and $M(H' - w', x) =$

$M(H' - w, x)$ (H' is the two vertex path with end vertices w and $w^{'}$), then by Lemma 3.39, we must have $M(\mathcal{S}(Y), x) > M(G, x)$.

Note that $\tau(B, x) \geq \tau(B^{'}, x)$. Let w'' be a leaf adjacent to $w^{'}$ in G. Let $G^{'}$ be a caterpillar obtained from G as follows: if $\deg(v) \geq \deg(w^{'})$ and $M(H - v, x) \leq M(H - w^{'}, x)$, then remove the edge $w^{'}w''$ and then add the edge vw''. Otherwise, $\deg(v) \leq \deg(w^{'})$ or $M(H-v, x) \geq M(H-w^{'}, x)$. If $\deg(v) \leq \deg(w^{'})$ and $M(H-v, x) \geq M(H-w^{'}, x)$, then swap B and $B^{'}$, remove the edge $w^{'}w''$ and then add the edge vw''. If $\deg(v) > \deg(w^{'})$ and $M(H-v, x) \geq M(H-w^{'}, x)$, then flip H, remove the edge $w^{'}w''$ and then add the edge vw'' (note that when flipping H, we assume v and w are fixed in their original positions in G). If $\deg(v) \leq \deg(w^{'})$ and $M(H - v, x) < M(H - w^{'}, x)$, then swap d and $d^{'} + 1$, remove the edge $w^{'}w''$ and then add the edge vw''. Then, by Lemmas 3.31 and 3.40, we must have $M(G, x) > M(G^{'}, x)$ and the degree sequence of $G^{'}$ is Y_1. Hence, by Theorem 3.35,

$$M(\mathcal{S}(Y), x) > M(G, x) > M(G^{'}, x) \geq M(\mathcal{S}(Y_1), x).$$

Note that the degree sequence of G is not Y_1 and not Y.

If $Y_1 = D$, then we are done. Otherwise, we iterate the process. We set $Y = Y_0$, and if k is a positive integer and $Y_k \neq D$, then we construct Y_{k+1} in exactly the same way as Y_1 was constructed from Y. After a finite number $J = \dfrac{1}{2}\sum_{i \in \mathbb{I}} |d_i - y_i|$ of iterations, we will get the chain

$$Y = Y_0 \prec Y_1 \prec \cdots \prec Y_{J-1} \prec Y_J = D.$$

For any $k \in \{1, \ldots, J-1\}$, we can apply Lemmas 3.31, 3.38 and 3.40, with Theorem 3.35 to $\mathcal{S}(Y_k)$ as we did above, to deduce that there exists a caterpillar G_{k+1} with degree sequence Y_{k+1} such that

$$M(\mathcal{S}(Y_k), x) > M(G_{k+1}, x) \geq M(\mathcal{S}(Y_{k+1}), x).$$

Hence

$$M(\mathcal{S}(Y), x) > M(\mathcal{S}(Y_1), x) > \cdots > M(\mathcal{S}(Y_J), x) = M(\mathcal{S}(D), x).$$

□

Since $Z(T) = M(T, 1)$ and $En(T) = \frac{2}{\pi}\int_0^{\infty} \frac{dx}{x^2} \log M(T, x^2)$, for some tree T of order n Then, If T is minimal with respect to $M(., x)$, then T is also minimal with respect to $Z(T)$ and $En(T)$.

Corollary 3.42 *For any caterpillar C of order n and diameter $m(\leq n-1)$, we have*

$$M(C,x) \geq M(\mathcal{S}(d,\underbrace{2,\ldots,2}_{m-2}),x), \text{ for all positive } x \in \mathbb{R}$$

and hence

$$Z(C) \geq Z(\mathcal{S}(d,\underbrace{2,\ldots,2}_{m-2}))$$

and

$$En(C) \geq En(\mathcal{S}(d,\underbrace{2,\ldots,2}_{m-2})),$$

with equality if and only if $C \cong \mathcal{S}(d,\underbrace{2,\ldots,2}_{m-2})$, *where* $d = n-m+1$.

Remark 3.43 Let

$$D = (\underbrace{d,\ldots,d}_{k},\underbrace{r,2,\ldots,2}_{m-k-1}) = \begin{cases} (\underbrace{d,\ldots,d}_{k},\underbrace{r,2\ldots,2}_{m-k-1}), & \text{if } d > r \geq 2 \\ (\underbrace{d,\ldots,d}_{k},\underbrace{2,\ldots,2}_{m-k-1}), & \text{if } d > 1 \geq r \end{cases}$$

be a reduced degree sequence of a caterpillar G, with diameter m and order n. Then,

$$\begin{aligned} n &= \begin{cases} kd + 2(m-k-1) + r - 2 - (m-3), & \text{if } d > r \geq 2 \\ kd + 2(m-k-1) - (m-3), & \text{if } d > 1 \geq r \end{cases} \\ &= kd + 2(m-k-1) + \max\{r-2,0\} - (m-3) \\ &= kd + 2m - 2k - 2 + \max\{r-2,0\} - m + 3 \\ &= kd + m - 2k + 1 + \max\{r-2,0\} \\ &= k(d-2) + m + \max\{r-1,1\}. \end{aligned}$$

Therefore,

$$n = k(d-2) + m + \max\{r-1,1\} = \begin{cases} k(d-2) + m + r - 1, & \text{if } r \geq 2 \\ k(d-2) + m + 1, & \text{if } r \leq 1. \end{cases}$$

Then,

$$\begin{aligned} k &= \frac{n-m-\max\{r-1,1\}}{d-2} = \frac{n-m-1-\max\{r-2,0\}}{d-2} \\ &= \frac{n-m-1}{d-2} - \frac{\max\{r-2,0\}}{d-2} = \left\lfloor \frac{n-m-1}{d-2} \right\rfloor, \end{aligned}$$

since k is a whole number and $\max\{r-2,0\} < d-2$. Hence,

$$k = \begin{cases} \frac{n-m-1}{d-2}, & \text{if } r \leq 1 \\ \left\lfloor \frac{n-m-1}{d-2} \right\rfloor, & \text{otherwise.} \end{cases}$$

Then,

$$\begin{aligned} r &= \begin{cases} n+(m-3)-kd-2(m-k-1), & \text{if } k = \frac{n-m-1}{d-2} \\ n+(m-3)-kd-2(m-k-2), & \text{otherwise} \end{cases} \\ &= \begin{cases} 0, & \text{if } k = \frac{n-m-1}{d-2} \\ n-m-k(d-2)+1, & \text{otherwise} \end{cases} \\ &= \begin{cases} 0, & \text{if } k = \frac{n-m-1}{d-2} \\ n-m-\left\lfloor \frac{n-m-1}{d-2} \right\rfloor (d-2)+1, & \text{otherwise.} \end{cases} \end{aligned}$$

Therefore, $k = \left\lfloor \frac{n-m-1}{d-2} \right\rfloor$ and

$$r = \begin{cases} 0, & \text{if } k = \frac{n-m-1}{d-2} \\ n-m-\left\lfloor \frac{n-m-1}{d-2} \right\rfloor (d-2)+1, & \text{otherwise.} \end{cases}$$

Corollary 3.44 *For any caterpillar C of order n, diameter $m(\leq n-1)$ and vertex degree at most $d \leq n-m+1$, we have*

$$M(C,x) \geq M(\mathcal{S}(\underbrace{d,\ldots,d}_{k},\underbrace{r,2,\ldots,2}_{m-k-1}),x), \text{ for all positive } x \in \mathbb{R}$$

and hence

$$En(C) \geq En(\mathcal{S}(\underbrace{d,\ldots,d}_{k},\underbrace{r,2,\ldots,2}_{m-k-1}))$$

and

$$Z(C) \geq Z(\mathcal{S}(\underbrace{d,\ldots,d}_{k},\underbrace{r,2,\ldots,2}_{m-k-1})),$$

with equality if and only if $C \cong \mathcal{S}(\underbrace{d,\ldots,d}_{k},\underbrace{r,2,\ldots,2}_{m-k-1})$, *where* $k = \left\lfloor \frac{n-m-1}{d-2} \right\rfloor$ *and* $r = \begin{cases} 0, & \text{if } k = \frac{n-m-1}{d-2} \\ n-m-\left\lfloor \frac{n-m-1}{d-2} \right\rfloor (d-2)+1, & \text{otherwise.} \end{cases}$

Remark 3.45 Let

$$D = (\underbrace{d, \dots, d}_{k}, r) = \begin{cases} (\underbrace{d, \dots, d}_{k}), & \text{if } d > 1 \geq r \\ (\underbrace{d, \dots, d}_{k}, r), & \text{if } d > r \geq 2 \end{cases}$$

be a reduced degree sequence of a caterpillar G, with order n. Then,

$$n = \begin{cases} kd - (k-2), & \text{if } r < 2 \\ kd + r - (k-1), & \text{otherwise} \end{cases} = \begin{cases} k(d-1) + 2, & \text{if } r < 2 \\ k(d-1) + r + 1, & \text{otherwise} \end{cases}$$
$$= k(d-1) + \max\{2, r+1\}.$$

Therefore, $n = k(d-1) + \max\{2, r+1\}$. Then,

$$k = \frac{n - \max\{2, r+1\}}{d-1} = \frac{n - 2 - \max\{0, r-1\}}{d-1} = \frac{n-2}{d-1} - \frac{\max\{0, r-1\}}{d-1}$$
$$= \left\lfloor \frac{n-2}{d-1} \right\rfloor,$$

since $d - 1 > \max\{0, r-1\}$ and k is a whole number. Hence, $k = \left\lfloor \frac{n-2}{d-1} \right\rfloor$ and

$$r = \begin{cases} 0, & \text{if } k = \frac{n-2}{d-1} \\ n - k(d-1) - 1, & \text{otherwise} \end{cases} = \begin{cases} 0, & \text{if } k = \frac{n-2}{d-1} \\ n - \left\lfloor \frac{n-2}{d-1} \right\rfloor (d-1) - 1, & \text{otherwise.} \end{cases}$$

Corollary 3.46 *For any caterpillar C of order n and vertex degree of at most $d \leq n - m + 1$, we have*

$$M(C, x) \geq M(\mathcal{S}(\underbrace{d, \dots, d}_{k}, r), x), \text{ for all positive } x \in \mathbb{R}$$

and hence

$$En(C) \geq En(\mathcal{S}(\underbrace{d, \dots, d}_{k}, r))$$

and

$$Z(C) \geq Z(\mathcal{S}(\underbrace{d, \dots, d}_{k}, r)),$$

with equality if and only if $C \cong \mathcal{S}(\underbrace{d, \dots, d}_{k}, r)$, where $k = \left\lfloor \frac{n-2}{d-1} \right\rfloor$ and

$$r = \begin{cases} 0, & \text{if } k = \frac{n-2}{d-1} \in \mathbb{Z} \\ n - \left\lfloor \frac{n-2}{d-1} \right\rfloor (d-1) - 1, & \text{otherwise.} \end{cases}$$

4 Extremal caterpillars with respect to the Merrifield-Simmons index

Let G be a graph of order n and $\mu(G, k)$ the number of independent vertex subsets of order k in G. Recall that $\sigma(G, x)$ is defined to be

$$\sigma(G, x) = \sum_{k \geq 0} \mu(G, k) x^k, \text{ for all positive } x \in \mathbb{R}$$

and

$$\sigma(G) = \sigma(G, 1).$$

In this chapter, we derive a formula for the auxiliary invarinat $\sigma(G, x)$ of a caterpillar G, and this formula is used to characterize extremal caterpillars relative to $\sigma(., x)$ and Merrifield-Simmons index.

4.1 A formula for the auxiliary invarinat $\sigma(G, x)$ of a caterpillar G

Let G be a caterpillar and be decomposed as in Figure 3.1. Let v' be a neighbor of v in H. Let w' be a neighbor of w in H. Then, using Lemma 2.7 iteratively, we have

$$\begin{aligned}
&\sigma(G, x) \\
&= \sigma(G - v, x) + x\sigma(G - N[v], x) \\
&= \sigma(G - v, x) + x\sigma(G - \{v, v_1, v_2, \ldots, v_d, v', r(B)\}, x) \\
&= \sigma(G - v - w, x) + x\sigma(G - v - N[w], x) \\
&\qquad + x\sigma(G - \{v, v_1, v_2, \ldots, v_d, v', r(B)\}, x) \\
&= \sigma(G - \{v, w\}, x) + x\sigma(G - \{v, w, w_1, w_2, \ldots, w_{d'}, w', r(B')\}, x) \\
&\qquad + x\sigma(G - \{v, v_1, v_2, \ldots, v_d, v', r(B)\}, x)
\end{aligned}$$

$$
\begin{aligned}
&= \sigma(G-\{v,w\},x) + x\sigma(G-\{v,w,w_1,w_2,\dots,w_{d'},w^{'},r(B^{'})\},x) \\
&\quad + x\left(\sigma(G-\{v,v_1,v_2,\dots,v_d,v^{'},r(B)\}-w,x) + x\sigma(G-N[v]\cup N[w],x)\right) \\
&= \sigma(G-\{v,w\},x) + x\sigma(G-\{v,w,w_1,w_2,\dots,w_{d'},w^{'},r(B^{'})\},x) \\
&\qquad + x\sigma(G-\{v,w,v_1,v_2,\dots,v_d,v^{'},r(B)\},x) \\
&+ x^2\sigma(G-\{v,v_1,v_2,\dots,v_d,v^{'},r(B),w,w_1,w_2,\dots,w_{d'},w^{'},r(B^{'})\},x) \\
&= \sigma(B,x)\sigma(B^{'},x)\sigma(H-\{v,w\},x)\sigma(v_1,x)\dots\sigma(v_d,x)\sigma(w_1,x)\dots\sigma(w_{d'},x) \\
&\quad + x\sigma(B,x)\sigma(B^{'}-r(B^{'}),x)\sigma(H-\{v,w,w^{'}\},x)\sigma(v_1,x)\sigma(v_2,x)\dots\sigma(v_d,x) \\
&+ x\sigma(B-r(B),x)\sigma(B^{'},x)\sigma(H-\{v,v^{'},w\},x)\sigma(w_1,x)\sigma(w_2,x)\dots\sigma(w_{d'},x) \\
&\qquad + x^2\sigma(B-r(B),x)\sigma(B^{'}-r(B^{'}),x)\sigma(H-\{v,v^{'},w,w^{'}\},x).
\end{aligned}
$$

Since $\sigma(v_1,x) = \sigma(v_2,x) = \cdots = \sigma(v_d,x) = \sigma(w_1,x) = \sigma(w_2,x) = \cdots = \sigma(w_{d'},x) = 1+x$, then

$$
\begin{aligned}
&\sigma(G,x) \\
&= \sigma(B,x)\sigma(B^{'},x)\sigma(H-\{v,w\},x)(1+x)^{d+d^{'}} \\
&\qquad + x\sigma(B,x)\sigma(B^{'}-r(B^{'}),x)\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d} \\
&+ x\sigma(B-r(B),x)\sigma(B^{'},x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}} \\
&\qquad + x^2\sigma(B-r(B),x)\sigma(B^{'}-r(B^{'}),x)\sigma(H-\{v,v^{'},w,w^{'}\},x) \\
&= \sigma(B,x)\sigma(B^{'},x)\Big[\sigma(H-\{v,w\},x)(1+x)^{d+d^{'}} \\
&\qquad + x\frac{\sigma(B^{'}-r(B^{'}),x)}{\sigma(B^{'},x)}\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d} \\
&+ x\frac{\sigma(B-r(B),x)}{\sigma(B,x)}\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}} \\
&\qquad + x^2\frac{\sigma(B-r(B),x)}{\sigma(B,x)}\frac{\sigma(B^{'}-r(B^{'}),x)}{\sigma(B^{'},x)}\sigma(H-\{v,v^{'},w,w^{'}\},x)\Big] \\
&= \sigma(B,x)\sigma(B^{'},x)\Big[\sigma(H-\{v,w\},x)(1+x)^{d+d^{'}} \\
&\qquad + x\rho(B^{'},x)\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d} \\
&+ x\rho(B,x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}} \\
&\qquad + x^2\rho(B,x)\rho(B^{'},x)\sigma(H-\{v,v^{'},w,w^{'}\},x)\Big].
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
&\sigma(G,x) \\
&= \sigma(B,x)\sigma(B^{'},x)\Big[\sigma(H-\{v,w\},x)(1+x)^{d+d^{'}}
\end{aligned}
$$

$$+ x\rho(B', x)\sigma(H - \{v, w, w'\}, x)(1 + x)^{d}$$
$$+ x\rho(B, x)\sigma(H - \{v, v', w\}, x)(1 + x)^{d'}$$
$$+ x^2\rho(B, x)\rho(B', x)\sigma(H - \{v, v', w, w'\}, x)\Big]. \quad (4.1)$$

Definition 4.1 Let G be a caterpillar and be decomposed as in Figure 3.1, v' the neighbor of v and w' the neighbor of w. Then, define

$$\sigma_v^w(G, x) = x\left[\rho(B', x)\sigma(H - \{v, w, w'\}, x)(1 + x)^{d} + \rho(B, x)\sigma(H - \{v, v', w\}, x)(1 + x)^{d'}\right].$$

Then,

$$\sigma(G, x) = \sigma(B, x)\sigma(B', x)\Big[\sigma(H - \{v, w\}, x)(1 + x)^{d+d'} + \sigma_v^w(G, x) + x^2\rho(B, x)\rho(B', x)\sigma(H - \{v, v', w, w'\}, x)\Big]. \quad (4.2)$$

4.2 Caterpillar with given degree sequence and maximum $\sigma(G, x)$

Let G be a graph of order n and $\mu(G, k)$ the number of independent vertex subsets of order k in G. Recall that $\sigma(G, x)$ is defined to be

$$\sigma(G, x) = \sum_{k \geq 0} \mu(G, k)x^k, \text{ for all positive } x \in \mathbb{R}$$

and

$$\sigma(G) = \sigma(G, 1).$$

In this section we prove that caterpillar $\mathcal{S}(D)$ also has maximum $\sigma(., x)$ and hence maximum Merrifield-Simmons index σ, among all caterpi-llars with degree sequence D. Then, we compare the two caterpillars $\mathcal{S}(D)$ and $\mathcal{S}(Y)$ i.e. $\sigma(\mathcal{S}(D), x)$ with $\sigma(\mathcal{S}(Y), x)$ and $\sigma(\mathcal{S}(D))$ with $\sigma(\mathcal{S}(Y))$, where the degree sequence Y is majorized by the degree sequence D. We say G is maximal with regard to an invariant $F(G)$, if and only if $F(G) = \max\{F(C) : C \in \mathbb{C}_D\}$, where D is a degree sequence of G.

The following simple technical lemma will play central role as we try to find out what exchange of branches increases $\sigma(., x)$.

Lemma 4.2 *Let x_1, x_2, y_1, y_2, z_1 and z_2 be nonnegative real numbers such that $x_1 \leq x_2$, $y_1 \leq y_2$ and $z_1 \leq z_2$. Then,*

$$x_1y_1z_1 + x_2y_2z_2 \geq \max\{x_1y_1z_2 + x_2y_2z_1, x_1y_2z_1 + x_2y_1z_2, x_1y_2z_2 + x_2y_1z_1\}.$$

Proof. Since $x_1 \leq x_2, y_1 \leq y_2$ and $z_1 \leq z_2$, then

(i) $$\begin{aligned} x_1y_1z_1 + x_2y_2z_2 - (x_1y_1z_2 + x_2y_2z_1) &= x_1y_1(z_1 - z_2) + x_2y_2(z_2 - z_1) \\ &= -x_1y_1(z_2 - z_1) + x_2y_2(z_2 - z_1) \\ &= (z_2 - z_1)(x_2y_2 - x_1y_1) \geq 0, \end{aligned}$$

(ii) $$\begin{aligned} x_1y_1z_1 + x_2y_2z_2 - (x_1y_2z_1 + x_2y_1z_2) &= x_1z_1(y_1 - y_2) + x_2z_2(y_2 - y_1) \\ &= -x_1z_1(y_2 - y_1) + x_2z_2(y_2 - y_1) \\ &= (y_2 - y_1)(x_2z_2 - x_1z_1) \geq 0, \end{aligned}$$

and

(iii) $$\begin{aligned} x_1y_1z_1 + x_2y_2z_2 - (x_1y_2z_2 + x_2y_1z_1) &= x_1(y_1z_1 - y_2z_2) + x_2(y_2z_2 - y_1z_1) \\ &= -x_1(y_2z_2 - y_1z_1) + x_2(y_2z_2 - y_1z_1) \\ &= (x_2 - x_1)(y_2z_2 - y_1z_1) \geq 0. \end{aligned}$$

Hence,

$$x_1y_1z_1 + x_2y_2z_2 \geq \max\{x_1y_1z_2 + x_2y_2z_1, x_1y_2z_1 + x_2y_1z_2, x_1y_2z_2 + x_2y_1z_1\}.$$

□

Lemma 4.3 *Let G be a caterpillar and be decomposed as in Figure 3.1, with both B and B' non-empty. Let v' be a neighbor of v in H and w' be a neighbor of w in H. If G is maximal with respect to $\sigma(., x)$ and $\rho(B', x) > \rho(B, x)$, then $\sigma(H - \{v, w, w'\}, x) \geq \sigma(H - \{v, v', w\}, x)$ and $d' \leq d$.*

Proof. Let G be a caterpillar and be decomposed as in Figure 3.1, with both B and B' non-empty. Let v' be a neighbor of v in H and w' be a neighbor of w in H. Suppose G is maximal with respect to $\sigma(., x)$. In particular, $\sigma(G, x)$ has the largest value among all the possible swappings of branches and flippings of H in G. That is, the swapping of B and B', the swapping of d and d', and/or the flipping of H in G.

Suppose $\rho(B', x) > \rho(B, x)$. Equation (4.2) suggests that the swapping of B and B', the swapping of d and d' and/or the flipping of H in G

only affect $\sigma_v^w(G,x)$ in $\sigma(G,x)$. This implies that the maximality of $\sigma_v^w(G,x)$ implies the maximality of $\sigma(G,x)$. Since $\rho(B',x) > \rho(B,x)$ and

$$\sigma_v^w(G,x) =$$
$$x\left[\rho(B',x)\sigma(H-\{v,w,w'\},x)(1+x)^d + \rho(B,x)\sigma(H-\{v,v',w\},x)(1+x)^{d'}\right],$$

then by Lemma 4.2, $\sigma_v^w(G,x)$ is maximal if and only if

$$\sigma(H-\{v,w,w'\},x) \geq \sigma(H-\{v,v',w\},x)$$

and $d \geq d'$. □

Lemma 4.4 *Let G be a caterpillar. Label all the non-leaf vertices in G from left to right as $u_1, u_2, \ldots, u_\ell$. If G is maximal with respect to $\sigma(.,x)$, then u_1 and u_ℓ have the largest degrees in G.*

Proof. If $\ell = 1$, then G is a star and has only one non-leaf vertex, which is of highest degree. If $\ell = 2$, then G has two non-leaf vertices and they have the largest degrees in G. If $\ell \geq 3$, then decompose G as in Figure 3.1 with B a leaf adjacent to u_1 and B' a complete branch of G such that B' contains neither u_1 nor u_2 and the root of B' is u_i for $3 \leq i \leq \ell$. Then, B' is neither empty nor a leaf. Since B is a leaf and B' is neither empty nor a leaf, then by Lemma 2.9 and Remark 2.10,

$$\rho(B,x) = \frac{1}{1+x} < \rho(B',x).$$

Since $\rho(B,x) < \rho(B',x)$, then by Lemma 4.3, $\deg(u_1) \geq \deg(u_{i-1})$. Hence $\deg(u_1) \geq \max\{\deg(u_i) : 2 \leq i \leq \ell-1\}$. Same reasoning leads to $\deg(u_\ell) \geq \max\{\deg(u_i) : 2 \leq i \leq \ell-1\}$. □

Lemma 4.5 *Let B and B' be complete branches of a caterpillar G, $h(B)$ and $h(B')$ their respective heights. If $h(B) = h(B')$, then $\rho(B,x) = \rho(B',x)$ if and only if $B \approx_r B'$.*

Proof. It is clear that $B \approx_r B'$ implies $\rho(B,x) = \rho(B',x)$. We only need to show that $\rho(B,x) = \rho(B',x)$ implies $B \approx_r B'$. Let $r(B)$ and $r(B')$ be the roots of B and B', respectively. Then, B and B' can be decomposed as in Figure 3.2. Suppose $h(B) = h(B') = h$. If $h = 1$ and $\rho(B,x) = \rho(B',x)$, then

$$\rho(B,x) = \frac{1}{1+x\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B)}} = \frac{1}{1+x\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B')}} = \rho(B',x).$$

Then, $1+x\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B)} = 1+x\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B^{'})}$. Since $x > 0$, then $\mathrm{rd}(B) = \mathrm{rd}(B^{'})$ and thus $B \approx_r B^{'}$. Suppose that for $h = k \geq 1$, $\rho(B,x) = \rho(B^{'},x)$ implies $B \approx_r B^{'}$. Then, for $h = k+1$ we have

$$\rho(B,x) = \frac{1}{1+x\prod_{i=1}^{\mathrm{rd}(B)}\rho(B_i,x)} = \frac{1}{1+x\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B)-1}\rho(B_1,x)}$$

and

$$\rho(B^{'},x) = \frac{1}{1+x\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B^{'})-1}\rho(B_1^{'},x)}.$$

Then, suppose $\rho(B,x) = \rho(B^{'},x)$. Then,

$$1+x\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B)-1}\rho(B_1,x) = 1+x\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B^{'})-1}\rho(B_1^{'},x).$$

Since $x > 0$, then

$$\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B)-1}\rho(B_1,x) = \left(\frac{1}{1+x}\right)^{\mathrm{rd}(B^{'})-1}\rho(B_1^{'},x)$$

and hence

$$\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B)}\rho(B_1,x) = \left(\frac{1}{1+x}\right)^{\mathrm{rd}(B^{'})}\rho(B_1^{'},x). \tag{4.3}$$

Suppose that $\mathrm{rd}(B) \neq \mathrm{rd}(B^{'})$, without loss of generality assume $\mathrm{rd}(B) > \mathrm{rd}(B^{'})$. Then, $\mathrm{rd}(B) \geq \mathrm{rd}(B^{'})+1$. Since B and $B^{'}$ are non-empty and $h \geq 2$, then B_1 and $B_1^{'}$ are non-empty and by Lemma 2.9, we must have

$$\frac{1}{1+x} \leq \rho(B_1,x), \rho(B_1^{'},x) \leq \frac{1}{1+x\left(\frac{1}{1+x}\right)^{\max\{\mathrm{rd}(B_1),\mathrm{rd}(B_1^{'})\}}} < 1. \tag{4.4}$$

With $\mathrm{rd}(B) \geq \mathrm{rd}(B^{'})+1$ and Equation (4.4) we have,

$$\begin{aligned}\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B)}\rho(B_1,x) &< \left(\frac{1}{1+x}\right)^{\mathrm{rd}(B)} \leq \left(\frac{1}{1+x}\right)^{\mathrm{rd}(B^{'})+1} \\ &= \left(\frac{1}{1+x}\right)^{\mathrm{rd}(B^{'})}\left(\frac{1}{1+x}\right) \leq \left(\frac{1}{1+x}\right)^{\mathrm{rd}(B^{'})}\rho(B_1^{'},x).\end{aligned}$$

Therefore,

$$\left(\frac{1}{1+x}\right)^{\mathrm{rd}(B)}\rho(B_1,x) < \left(\frac{1}{1+x}\right)^{\mathrm{rd}(B^{'})}\rho(B_1^{'},x). \tag{4.5}$$

Which is a contradiction to Equation (4.3), hence $\mathrm{rd}(B) = \mathrm{rd}(B')$. With $\mathrm{rd}(B) = \mathrm{rd}(B')$ and Equation (4.3) we must have $\rho(B_1, x) = \rho(B_1', x)$. So $\mathrm{rd}(B) = \mathrm{rd}(B')$ and $\rho(B_1, x) = \rho(B_1', x)$, then $B_1 \approx_r B_1'$ and thus $B \approx_r B'$. □

Theorem 4.6 *Let $\mathbb{C}_D$ be the set of all caterpillars with reduced degree sequence D. Then, $\sigma(\mathcal{S}(D), x) \geq \sigma(H, x)$ for all $H \in \mathbb{C}_D$.*

Proof. Let H be a caterpillar with reduced degree sequence $D = (d_1, d_2, \ldots, d_n)$. Suppose H is maximal with respect to $\sigma(., x)$. Label all the non-leaf vertices in H from left to right as $u_1, u_2, \ldots, u_n$.

(i) If $n = 1$, then H is a star and $H = C(d_1) = C_L^1(d_1)$. Hence $H = \mathcal{S}(D)$, with $C_R^1(d_1) = ()$.

(ii) If $n = 2$, then $H = C(d_1, d_2)$. $C(d_1, d_2)$ can be viewed as a caterpillar obtained by joining the roots of $C(d_1 - 1) = C_L^1(d_1, d_2)$ and $C(d_2 - 1) = C_R^1(d_1, d_2)$. Hence $H = C(d_1, d_2) = \mathcal{S}(D)$.

(iii) If $n = 3$, then by Lemma 4.4, u_1 and u_3 attain the largest degrees in H. Assume $\deg(u_1) \geq \deg(u_3)$. Then, H is the caterpillar of Figure 3.24 (a), which can be viewed as in Figure 3.24 (b), with $C_L^2(d_1, d_2, d_3) = C(d_1, d_3 - 1)$ and $C_R^2(d_1, d_2, d_3) = C(d_2 - 1)$. This is just $\mathcal{S}(D)$ hence $H \cong \mathcal{S}(D)$.

(iv) If $n = 4$, then by Lemma 4.4, u_1 and u_4 must have the largest degrees in H. Assume $\deg(u_1) \geq \deg(u_4)$. And since $x > 0$, then

$$\left(\frac{1}{1+x}\right)^{\deg(u_1)-1} \leq \left(\frac{1}{1+x}\right)^{\deg(u_4)-1}$$

and

$$\rho(B_L^{u_1}, x) = \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_1)-1}} \geq \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_4)-1}} = \rho(B_R^{u_4}, x),$$

with equality if and only if $\deg(u_1) = \deg(u_4)$. If $\rho(B_L^{u_1}, x) = \rho(B_R^{u_4}, x)$, then we choose $\deg(u_2) \leq \deg(u_3)$. Otherwise $\rho(B_L^{u_1}, x) > \rho(B_R^{u_4}, x)$ and by Lemma 4.3, we get that $\deg(u_2) \leq \deg(u_3)$. Hence we always have $\deg(u_2) \leq \deg(u_3)$ in all cases. Then, H is the caterpillar of Figure 3.25 (a), which can be viewed as in Figure 3.25 (b). This is just $\mathcal{S}(D)$ and hence $H \cong \mathcal{S}(D)$.

(v) Suppose $n \geq 5$. Note that it is enough to show that for all integers j in $1 \leq j \leq n$, if j is odd, then

$$\rho(B_L^{u_{j-1}}, x) \leq \rho(B_R^{u_{n-j+2}}, x) < \rho(B_L^{u_{i-2}}, x), \text{ for all } i \text{ in } j + 2 \leq i \leq n - j - 1$$

and

$$\deg(u_j) \geq \deg(u_{n-j+1}) \geq \max\{\deg(u_{j+1}), \ldots, \deg(u_{n-j})\}.$$

And if j is even, then

$$\rho(B_L^{u_{j-1}}, x) \geq \rho(B_R^{u_{n-j+2}}, x) > \rho(B_L^{u_{i-2}}, x), \text{ for all } i \text{ where } j+2 \leq i \leq n-j-1$$

and

$$\deg(u_j) \leq \deg(u_{n-j+1}) \leq \min\{\deg(u_{j+1}), \ldots, \deg(u_{n-j})\}.$$

As the former characterizes the caterpillar $\mathcal{S}(D)$.

Base case: By Lemma 4.4, u_1 and u_n must have the largest degrees in H. Without loss of generality we can assume $\deg(u_1) \geq \deg(u_n)$. Then

$$\deg(u_1) \geq \deg(u_n) \geq \max\{\deg(u_2), \ldots, \deg(u_{n-1})\}. \tag{4.6}$$

Then,

$$\left(\frac{1}{1+x}\right)^{\deg(u_1)-1} \leq \left(\frac{1}{1+x}\right)^{\deg(u_n)-1}$$

and

$$\rho(B_L^{u_1}, x) = \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_1)-1}} \geq \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_n)-1}} = \rho(B_R^{u_n}, x), \tag{4.7}$$

with equality if and only if $\deg(u_1) = \deg(u_n)$. If $\rho(B_L^{u_1}, x) = \rho(B_R^{u_n}, x)$, we then choose $\deg(u_2) \leq \deg(u_{n-1})$. Otherwise, $\rho(B_L^{u_1}, x) > \rho(B_R^{u_n}, x)$ and by Lemma 4.3, we get that $\deg(u_2) \leq \deg(u_{n-1})$. Hence

$$\deg(u_2) \leq \deg(u_{n-1}). \tag{4.8}$$

From (4.6) $\deg(u_n) \geq \max\{\deg(u_i) : 2 \leq i \leq n-1\}$. Since $n \geq 5$, then for $2 \leq i \leq n-1$, the complete branch $B_L^{u_i}$ is neither empty nor a leaf nor a pseudo leaf branch. By Lemma 2.9 and Remark 2.10, we have

$$\rho(B_R^{u_n}, x) = \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_n)-1}} > \rho(B_L^{u_i}, x) > \frac{1}{1+x}, \tag{4.9}$$

for all i in $2 \leq i \leq n-1$. By Lemma 4.3,

$$\deg(u_{n-1}) \leq \deg(u_{i+1}), \text{ for all } i \text{ in } 2 \leq i \leq n-3. \tag{4.10}$$

From (4.8) and (4.10) we get that $\deg(u_2) \leq \deg(u_{n-1}) \leq \deg(u_{i+1})$, for all i in $2 \leq i \leq n-3$. Therefore

$$\deg(u_2) \leq \deg(u_{n-1}) \leq \min\{\deg(u_3), \ldots, \deg(u_{n-2})\}. \tag{4.11}$$

From (4.7) we have $\rho(B_L^{u_1},x) \geq \rho(B_R^{u_n},x)$, with equality if and only if $\deg(u_1) = \deg(u_n)$. From (4.11) we get that $\deg(u_2) \leq \deg(u_{n-1})$. Since $\deg(u_2) \leq \deg(u_{n-1})$ and $\rho(B_L^{u_1},x) \geq \rho(B_R^{u_n},x)$, then

$$\rho(B_L^{u_2},x) = \frac{1}{1+x\left(\frac{1}{1+x}\right)^{\deg(u_2)-2}\rho(B_L^{u_1},x)} \leq \frac{1}{1+x\left(\frac{1}{1+x}\right)^{\deg(u_{n-1})-2}\rho(B_R^{u_n},x)}$$
$$= \rho(B_R^{u_{n-1}},x).$$

The inequality above becomes equality if and only if $\deg(u_2) = \deg(u_{n-1})$ and $\rho(B_L^{u_1},x) = \rho(B_R^{u_n},x)$. Note that since

$$\deg(u_2) \leq \deg(u_{n-1}),$$

then

$$\left(\frac{1}{1+x}\right)^{\deg(u_2)-2} \geq \left(\frac{1}{1+x}\right)^{\deg(u_{n-1})-2}.$$

Therefore,

$$\rho(B_L^{u_2},x) \leq \rho(B_R^{u_{n-1}},x). \tag{4.12}$$

If $\rho(B_L^{u_2},x) = \rho(B_R^{u_{n-1}},x)$ and thus $B_L^{u_2} \approx_r B_R^{u_{n-1}}$, then choose $\deg(u_3) \geq \deg(u_{n-2})$. Otherwise $\rho(B_L^{u_2},x) < \rho(B_R^{u_{n-1}},x)$ and by Lemma 4.3, we get $\deg(u_3) \geq \deg(u_{n-2})$. Hence, we always have

$$\deg(u_3) \geq \deg(u_{n-2}). \tag{4.13}$$

For any i with $3 \leq i \leq n-2$, the complete branch $B_L^{u_{i-1}}$ is neither empty nor a leaf nor a pseudo leaf branch. By Lemma 2.9 and Remark 2.10, we get

$$\rho(B_R^{u_n},x) = \frac{1}{1+x\left(\frac{1}{1+x}\right)^{\deg(u_n)-2}} > \rho(B_L^{u_{i-1}},x) > \frac{1}{1+x}, \tag{4.14}$$

For any i with $3 \leq i \leq n-2$. From (4.11) and (4.14) we get

$$\rho(B_R^{u_{n-1}},x) = \frac{1}{1+x\left(\frac{1}{1+x}\right)^{\deg(u_{n-1})-2}\rho(B_R^{u_n},x)}$$
$$< \frac{1}{1+x\left(\frac{1}{1+x}\right)^{\deg(u_i)-2}\rho(B_L^{u_{i-1}},x)} = \rho(B_L^{u_i},x).$$

Note that since $\deg(u_{n-1}) \leq \deg(u_i)$, then $\left(\frac{1}{1+x}\right)^{\deg(u_{n-1})-2} \geq \left(\frac{1}{1+x}\right)^{\deg(u_i)-2}$. Therefore

$$\rho(B_R^{u_{n-1}},x) < \rho(B_R^{u_i},x), \text{ for any } i \text{ in } 3 \leq i \leq n-2. \tag{4.15}$$

By Lemma 4.3, we get that $\deg(u_{n-2}) \geq \deg(u_{i+1})$, for any i in $3 \leq i \leq n-4$. Hence,

$$\deg(u_{n-2}) \geq \max\{\deg(u_4), \ldots, \deg(u_{n-3})\}. \tag{4.16}$$

From (4.13) and (4.16) we get that

$$\deg(u_3) \geq \deg(u_{n-2}) \geq \max\{\deg(u_4), \ldots, \deg(u_{n-3})\}. \tag{4.17}$$

Hence, from (4.6) we have

$$\deg(u_1) \geq \deg(u_n) \geq \max\{\deg(u_2), \ldots, \deg(u_{n-1})\}.$$

From (4.7) and (4.9) we have

$$\rho(B_L^{u_1}, x) \geq \rho(B_R^{u_n}, x) > \rho(B_L^{u_{i-2}}, x),$$

for any i in $4 \leq i \leq n-3$, and from (4.11) we have

$$\deg(u_2) \leq \deg(u_{n-1}) \leq \min\{\deg(u_3), \ldots, \deg(u_{n-2})\}.$$

From (4.12) and (4.15) we have

$$\rho(B_L^{u_2}, x) \leq \rho(B_R^{u_{n-1}}, x) < \rho(B_L^{u_{i-2}}, x),$$

for any i in $5 \leq i \leq n-4$, and from (4.17) we have

$$\deg(u_3) \geq \deg(u_{n-2}) \geq \max\{\deg(u_4), \ldots, \deg(u_{n-3})\}.$$

Suppose that for some integers j in $1 \leq j \leq n$ we have the following.
(a) If j is odd, then for any i in $j+2 \leq i \leq n-j-1$

$$\rho(B_L^{u_{j-1}}, x) \leq \rho(B_R^{u_{n-j+2}}, x) < \rho(B_L^{u_{i-2}}, x), \tag{4.18}$$

and

$$\deg(u_j) \geq \deg(u_{n-j+1}) \geq \max\{\deg(u_{j+1}), \ldots, \deg(u_{n-j})\}. \tag{4.19}$$

(b) If j is even, then for any i in $j+2 \leq i \leq n-j-1$

$$\rho(B_L^{u_{j-1}}, x) \geq \rho(B_R^{u_{n-j+2}}, x) > \rho(B_L^{u_{i-2}}, x), \tag{4.20}$$

and

$$\deg(u_j) \leq \deg(u_{n-j+1}) \leq \max\{\deg(u_{j+1}), \ldots, \deg(u_{n-j})\}. \tag{4.21}$$

(i) Suppose j is odd. From (4.18) and (4.19) we have $\rho(B_L^{u_{j-1}}, x) \leq \rho(B_R^{u_{n-j+2}}, x)$ and $\deg(u_j) \geq \deg(u_{n-j+1})$. Hence

$$\begin{aligned}\rho(B_L^{u_j}, x) &= \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_j)-2}\rho(B_L^{u_{j-1}}, x)} \\ &\geq \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_{n-j+1})-2}\rho(B_R^{u_{n-j+2}}, x)} = \rho(B_R^{u_{n-j+1}}, x),\end{aligned}$$

with equality if and only if $\deg(u_j) = \deg(u_{n-j+1})$ and $\rho(B_L^{u_{j-1}}, x) = \rho(B_R^{u_{n-j+2}}, x)$. Note that since $\deg(u_j) \geq \deg(u_{n-j+1})$, then

$$\left(\frac{1}{1+x}\right)^{\deg(u_j)-2} \leq \left(\frac{1}{1+x}\right)^{\deg(u_{n-j+1})-2}.$$

Therefore,

$$\rho(B_L^{u_j}, x) \geq \rho(B_R^{u_{n-j+1}}, x). \tag{4.22}$$

If $\rho(B_L^{u_j}, x) = \rho(B_R^{u_{n-j+1}}, x)$ and thus $B_L^{u_j} \approx_r B_R^{u_{n-j+1}}$, then we choose $\deg(u_{j+1}) \leq \deg(u_{n-j})$. Otherwise $\rho(B_L^{u_j}, x) > \rho(B_R^{u_{n-j+1}}, x)$ and by Lemma 4.3, we must have $\deg(u_{j+1}) \leq \deg(u_{n-j})$. In all the cases we have

$$\deg(u_{j+1}) \leq \deg(u_{n-j}). \tag{4.23}$$

From (4.18), we have $\rho(B_R^{u_{n-j+2}}, x) < \rho(B_L^{u_{i-2}}, x)$, for any i in $j+2 \leq i \leq n-j-1$. By Lemma 4.3, we must have $\deg(u_{n-j+1}) \geq \deg(u_{i-1})$ and hence,

$$\begin{aligned}\rho(B_R^{u_{n-j+1}}, x) &= \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_{n-j+1})-2}\rho(B_R^{u_{n-j+2}}, x)} \\ &> \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_{i-1})-2}\rho(B_L^{u_{i-2}}, x)} = \rho(B_L^{u_{i-1}}, x).\end{aligned}$$

Note that since $\deg(u_{n-j+1}) \geq \deg(u_{i-1})$, then

$$\left(\frac{1}{1+x}\right)^{\deg(u_{n-j+1})-2} \leq \left(\frac{1}{1+x}\right)^{\deg(u_{i-1})-2}.$$

Therefore, for any i in $j+2 \leq i \leq n-j-1$ we have

$$\rho(B_R^{u_{n-j+1}}, x) > \rho(B_L^{u_{i-1}}, x). \tag{4.24}$$

Hence, from (4.22) and (4.24) we get

$$\rho(B_L^{u_j}, x) \geq \rho(B_R^{u_{n-j+1}}, x) > \rho(B_L^{u_{i-1}}, x), \tag{4.25}$$

for any i in $j+2 \le i \le n-j-1$. From (4.25) we have, $\rho(B_R^{u_{n-j+1}}, x) > \rho(B_L^{u_{i-1}}, x)$ for any i in $j+2 \le i \le n-j-1$. By Lemma 4.3, we must have $\deg(u_{n-j}) \le \deg(u_i)$. Hence

$$\deg(u_{n-j}) \le \min\{\deg(u_{j+2}), \ldots, \deg(u_{n-j-1})\}. \tag{4.26}$$

Therefore, from (4.23) and (4.26) we must have

$$\deg(u_{j+1}) \le \deg(u_{n-j}) \le \min\{\deg(u_{j+2}), \ldots, \deg(u_{n-j-1})\}. \tag{4.27}$$

Hence from (4.25) and (4.27) if j is odd, then

$$\rho(B_L^{u_j}, x) \ge \rho(B_R^{u_{n-j+1}}, x) > \rho(B_L^{u_{i-1}}, x),$$

for any i in $j+2 \le i \le n-j-1$, and

$$\deg(u_{j+1}) \le \deg(u_{n-j}) \le \min\{\deg(u_{j+2}), \ldots, \deg(u_{n-j-1})\}.$$

(ii) Suppose j is even. From (4.20) and (4.21) we have $\rho(B_L^{u_{j-1}}, x) \ge \rho(B_R^{u_{n-j+2}}, x)$ and $\deg(u_j) \le \deg(u_{n-j+1})$. Then,

$$\begin{aligned}\rho(B_L^{u_j}, x) &= \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_j)-2} \rho(B_L^{u_{j-1}}, x)} \\ &\le \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_{n-j+1})-2} \rho(B_R^{u_{n-j+2}}, x)} = \rho(B_R^{u_{n-j+1}}, x),\end{aligned}$$

with equality if and only if $\deg(u_{n-j+1}) = \deg(u_j)$ and $\rho(B_L^{u_{j-1}}, x) = \rho(B_R^{u_{n-j+2}}, x)$ and thus $B_L^{u_j} \approx_r B_R^{u_{n-j+1}}$. Note that since $\deg(u_j) \le \deg(u_{n-j+1})$, then

$$\left(\frac{1}{1+x}\right)^{\deg(u_j)-2} \ge \left(\frac{1}{1+x}\right)^{\deg(u_{n-j+1})-2}.$$

Therefore,

$$\rho(B_L^{u_j}, x) \le \rho(B_R^{u_{n-j+1}}, x). \tag{4.28}$$

If $\rho(B_L^{u_j}, x) = \rho(B_R^{u_{n-j+1}}, x)$ and thus $B_L^{u_j} \approx_r B_R^{u_{n-j+1}}$, then we choose $\deg(u_{j+1}) \ge \deg(u_{n-j})$. Otherwise $\rho(B_L^{u_j}, x) < \rho(B_R^{u_{n-j+1}}, x)$ and by Lemma 4.3, we must have $\deg(u_{j+1}) \ge \deg(u_{n-j})$. Hence, in all cases we have

$$\deg(u_{j+1}) \ge \deg(u_{n-j}). \tag{4.29}$$

From (4.20) we have $\rho(B_R^{u_{n-j+2}}, x) > \rho(B_L^{u_{i-2}}, x)$, for any i in $j+2 \le i \le n-j-1$. By Lemma 4.3, we must have $\deg(u_{n-j+1}) \le \deg(u_{i-1})$ and hence,

$$\rho(B_R^{u_{n-j+1}}) = \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_{n-j+1})-2} \rho(B_R^{u_{n-j+2}}, x)}$$

$$< \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(u_{i-1})-2} \rho(B_L^{u_{i-2}}, x)} = \rho(B_L^{u_{i-1}}, x).$$

Note that since $\deg(u_{n-j+1}) \leq \deg(u_{i-1})$, then

$$\left(\frac{1}{1+x}\right)^{\deg(u_{n-j+1})-2} \geq \left(\frac{1}{1+x}\right)^{\deg(u_{i-1})-2}.$$

Therefore, for any i in $j+2 \leq i \leq n-j-1$

$$\rho(B_R^{u_{n-j+1}}, x) < \rho(B_L^{u_{i-1}}, x). \tag{4.30}$$

Thus from (4.28) and (4.30) we must have

$$\rho(B_L^{u_j}, x) \leq \rho(B_R^{u_{n-j+1}}, x) < \rho(B_L^{u_{i-1}}, x), \tag{4.31}$$

for any i in $j+2 \leq i \leq n-j-1$. From (4.31) we have $\rho(B_R^{u_{n-j+1}}, x) < \rho(B_L^{u_{i-1}}, x)$, for any i in $j+2 \leq i \leq n-j-1$. By Lemma 4.3, we must have $\deg(u_{n-j}) \geq \deg(u_i)$, for any i in $j+2 \leq i \leq n-j-1$. Hence

$$\deg(u_{n-j}) \geq \max\{\deg(u_{j+2}), \ldots, \deg(u_{n-j-1})\}. \tag{4.32}$$

From (4.29) and (4.32) we get

$$\deg(u_{j+1}) \geq \deg(u_{n-j}) \geq \max\{\deg(j+2), \ldots, \deg(u_{n-j-1})\}. \tag{4.33}$$

Hence from (4.31) and (4.33) if j is even, then for any i in $j+2 \leq i \leq n-j-1$

$$\rho(B_L^{u_j}, x) \leq \rho(B_R^{u_{n-j+1}}, x) < \rho(B_L^{u_{i-1}}, x)$$

and

$$\deg(u_{j+1}) \geq \deg(u_{n-j}) \geq \max\{\deg(u_{j+2}), \ldots, \deg(u_{n-j-1})\}.$$

□

Remark 4.7 Let G be a caterpillar. Suppose that whenever G is decomposed as in Figure 3.1, with B, B' and H non-empty we have that, if $\rho(B', x) \geq \rho(B, x)$ then $d' \leq d$. Then $G \cong \mathcal{S}(D)$, where D is the reduced degree sequence of G. This follows from the proof of Theorem 4.6.

Lemma 4.8 *Let i, j and n be positive integers such that $1 \leq i < j \leq n$. Let $D = (d_1, \ldots, d_i, \ldots, d_j, \ldots, d_n)$ be a reduced degree sequence of a caterpillar C, such that $d_i \geq d_j > 2$. Decompose $\mathcal{S}(D)$ as in Figure 3.26, with B, B' and H non-empty. Let v and w be vertices of $\mathcal{S}(D)$ such that $\deg(v) = d_i$ and $\deg(w) = d_j$. Let v' be a neighbor of v in H and let w' be a neighbor of w in H. Let w^* be a leaf adjacent to w. Let*

G be obtained from $\mathcal{S}(D)$ by removing the edge ww^* and then adding the edge vw^*. If either (i) $\rho(B', x) > \rho(B, x)$ or (ii) $\rho(B', x) = \rho(B, x)$, $\sigma(H - \{v, w, w'\}, x) \geq \sigma(H - \{v, v', w\}, x)$ and $d_i \geq d_j$, then

$$\sigma(\mathcal{S}(D), x) < \sigma(G, x) \leq \sigma(\mathcal{S}(D'), x),$$

where $D' = (d_1, \ldots, d_{i-1}, d_i + 1, d_{i+1}, \ldots, d_{j-1}, d_j - 1, d_{j+1}, \ldots, d_n)$.

Proof. Let $d = d_i - 2$ and $d' = d_j - 2$. Suppose $\deg(v) = d_i = d + 2$ and $\deg(w) = d_j = d' + 2$. Since $d_i \geq d_j > 2$, then $d \geq d' \geq 1$. Then, from Equation (4.2) we have

$$\begin{aligned}\sigma(\mathcal{S}(D), x) = \sigma(B, x)\sigma(B', x) \Big[\sigma(H - \{v, w\}, x)(1 + x)^{d+d'} + \sigma_v^w(\mathcal{S}(D), x) \\ + x^2\rho(B, x)\rho(B', x)\sigma(H - \{v, v', w, w'\}, x)\Big],\end{aligned} \tag{4.34}$$

where

$$\begin{aligned}\sigma_v^w(\mathcal{S}(D), x) = x \Big[\rho(B', x)\sigma(H - \{v, w, w'\}, x)(1 + x)^d \\ + \rho(B, x)\sigma(H - \{v, v', w\}, x)(1 + x)^{d'}\Big],\end{aligned} \tag{4.35}$$

and

$$\begin{aligned}\sigma(G, x) = \sigma(B, x)\sigma(B', x) \Big[\sigma(H - \{v, w\}, x)(1 + x)^{d+d'} + \sigma_v^w(G, x) \\ + x^2\rho(B, x)\rho(B', x)\sigma(H - \{v, v', w, w'\}, x)\Big],\end{aligned} \tag{4.36}$$

where

$$\begin{aligned}\sigma_v^w(G, x) = x \Big[\rho(B', x)\sigma(H - \{v, w, w'\}, x)(1 + x)^{d+1} \\ + \rho(B, x)\sigma(H - \{v, v', w\}, x)(1 + x)^{d'-1}\Big].\end{aligned} \tag{4.37}$$

Then,

$$\sigma(\mathcal{S}(D), x) - \sigma(G, x) = \sigma(B, x)\sigma(B', x) \left[\sigma_v^w(\mathcal{S}(D), x) - \sigma_v^w(G, x)\right].$$

But

$$\begin{aligned}&\sigma_v^w(\mathcal{S}(D), x) - \sigma_v^w(G, x) \\ &= x \Big[\rho(B', x)\sigma(H - \{v, w, w'\}, x) \left((1 + x)^d - (1 + x)^{d+1}\right) \\ &\qquad + \rho(B, x)\sigma(H - \{v, v', w\}, x) \left((1 + x)^{d'} - (1 + x)^{d'-1}\right)\Big] \\ &= x \Big[\rho(B', x)\sigma(H - \{v, w, w'\}, x)(1 + x)^d (1 - (1 + x))\end{aligned}$$

$$+ \rho(B,x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}-1}((1+x)-1)\Big]$$
$$= x^2\Big[-\rho(B^{'},x)\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d} + \rho(B,x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}-1}\Big].$$

Then,

$$\sigma(\mathcal{S}(D),x)-\sigma(G,x)$$
$$= x^2\sigma(B,x)\sigma(B^{'},x)\Big[-\rho(B^{'},x)\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d} + \rho(B,x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}-1}\Big] < 0,$$

if $\rho(B^{'},x) = \rho(B,x)$, $\sigma(H-\{v,w,w^{'}\},x) \geq \sigma(H-\{v,v^{'},w\},x)$ and $d \geq d^{'}$. Suppose $\rho(B^{'},x) > \rho(B,x)$. Then, by Lemma 4.3, we must have $\sigma(H-\{v,w,w^{'}\},x) \geq \sigma(H-\{v,v^{'},w\},x)$ and $d^{'} \leq d$. Again,

$$\sigma(\mathcal{S}(D),x)-\sigma(G,x)$$
$$= x^2\sigma(B,x)\sigma(B^{'},x)\Big[-\rho(B^{'},x)\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d} + \rho(B,x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}-1}\Big] < 0.$$

Therefore, $\sigma(\mathcal{S}(D),x) < \sigma(G,x)$. Since G and $\mathcal{S}(D^{'})$ have the same reduced degree sequence $D^{'}$ and are both caterpillars, then by Theorem 4.6

$$\sigma(\mathcal{S}(D),x) < \sigma(G,x) \leq \sigma(\mathcal{S}(D^{'}),x).$$

□

Lemma 4.9 *Let G be a caterpillar and be decomposed as in Figure 3.1, with B, $B^{'}$ and H non-empty. Let $v^{'}$ be the neighbor of v in H and let $w^{'}$ be the neighbor of w in H. Let $G^{'}$ be obtained from G by removing the edge $wr(B^{'})$ and then adding the edge $vr(B^{'})$. Suppose G is maximal with respect $\sigma(.,x)$. If either (i) $\rho(B^{'},x) > \rho(B,x)$ or (ii) $\sigma(H-\{v,w,w^{'}\},x) \geq \sigma(H-\{v,v^{'},w\},x)$ and $d^{'} \leq d$, then*

$$\sigma(G,x) < \sigma(G^{'},x).$$

Proof. Suppose G is a caterpillar and decomposed as in Figure 3.1, with B, $B^{'}$ and H non-empty. Then,

$$\sigma(G,x)$$
$$= \sigma(G-v,x) + x\sigma(G-N[v],x)$$
$$= \sigma(G-\{v,w\},x) + x\sigma(G-v-N[w],x) + x\sigma(G-N[v],x)$$

$$
\begin{aligned}
&= \sigma(G-\{v,w\},x) + x\sigma(G-v-N[w],x) + x\,[\sigma(G-w-N[v],x) \\
&\qquad\qquad + x\,\sigma(G-N[v]\cup N[w],x)] \\
&= \sigma(G-\{v,w\},x) + x\sigma(G-v-N[w],x) + x\sigma(G-w-N[v],x) \\
&\qquad\qquad + x^2\sigma(G-N[v]\cup N[w],x).
\end{aligned}
$$

$G^{'}$ can be decomposed as in Figure 3.27. Then,

$$
\begin{aligned}
&\sigma(G^{'},x) \\
&= \sigma(G^{'}-v,x) + x\sigma(G^{'}-N[v],x) \\
&= \sigma(G^{'}-\{v,w\},x) + x\sigma(G^{'}-v-N[w],x) + x\sigma(G^{'}-N[v],x) \\
&= \sigma(G^{'}-\{v,w\},x) + x\sigma(G^{'}-v-N[w],x) + x\left[\sigma(G^{'}-w-N[v],x)\right. \\
&\qquad\qquad \left. + x\,\sigma(G^{'}-N[v]\cup N[w],x)\right] \\
&= \sigma(G-\{v,w\},x) + x\sigma(G^{'}-v-N[w],x) + x\left[\sigma(G^{'}-w-N[v],x)\right. \\
&\qquad\qquad + x\,\sigma(G-N[v]\cup N[w],x)] \\
&= \sigma(G-\{v,w\},x) + x\sigma(G^{'}-v-N[w],x) + x\,\sigma(G^{'}-w-N[v],x) \\
&\qquad\qquad + x^2\,\sigma(G-N[v]\cup N[w],x)\ .
\end{aligned}
$$

Then,

$$
\begin{aligned}
&\sigma(G,x)-\sigma(G^{'},x) \\
&= x\left[\sigma(G-v-N[w],x) + \sigma(G-w-N[v],x) - \sigma(G^{'}-v-N[w],x)\right. \\
&\qquad\qquad \left. - \sigma(G^{'}-w-N[v],x)\right] \\
&= x\left[\sigma(B,x)\sigma(B^{'}-r(B^{'}),x)\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d}\right. \\
&\qquad\qquad + \sigma(B^{'},x)\sigma(B-r(B),x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}} \\
&- \sigma(B,x)\sigma(B^{'},x)\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d} \\
&\qquad\qquad \left. - \sigma(B^{'}-r(B^{'}),x)\sigma(B-r(B),x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}}\right] \\
&= x\sigma(B,x)\sigma(B^{'},x)\left[\frac{\sigma(B^{'}-r(B^{'}),x)}{\sigma(B^{'},x)}\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d}\right. \\
&\qquad\qquad + \frac{\sigma(B-r(B),x)}{\sigma(B,x)}\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}} \\
&- \sigma(H-\{v,w,w^{'}\},x)(1+x)^{d} \\
&\qquad\qquad \left. - \frac{\sigma(B^{'}-r(B^{'}),x)}{\sigma(B^{'},x)}\frac{\sigma(B-r(B),x)}{\sigma(B,x)}\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}}\right] \\
&= x\sigma(B,x)\sigma(B^{'},x)\left[\rho(B^{'},x)\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d}\right.
\end{aligned}
$$

$$+ \rho(B,x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}} - \sigma(H-\{v,w,w^{'}\},x)(1+x)^{d}$$
$$- \rho(B^{'},x)\rho(B,x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}}\Big]$$
$$= x\sigma(B,x)\sigma(B^{'},x)\left[\left(\rho(B^{'},x)-1\right)\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d}\right.$$
$$\left. + \left(1-\rho(B^{'},x)\right)\rho(B,x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}}\right]$$
$$= x\sigma(B,x)\sigma(B^{'},x)\left(1-\rho(B^{'},x)\right)\left[-\sigma(H-\{v,w,w^{'}\},x)(1+x)^{d}\right.$$
$$\left. + \rho(B,x)\sigma(H-\{v,v^{'},w\},x)(1+x)^{d^{'}}\right].$$

Suppose G is maximal with respect to $\sigma(.,x)$. Suppose $\rho(B^{'},x) > \rho(B,x)$, then by Lemma 4.3, we must have $\sigma(H-\{v,w,w^{'}\},x) \geq \sigma(H-\{v,v^{'},w\},x)$ and $d^{'} \leq d$. Thus, in both cases (i) and (ii) we have $\sigma(H-\{v,w,w^{'}\},x) \geq \sigma(H-\{v,v^{'},w\},x)$ and $d^{'} \leq d$. Also, since $x > 0$, $\rho(B^{'},x) < 1$ ($B^{'}$ is not empty), $\sigma(B,x) > 0$ and $\sigma(B^{'},x) > 0$, then $\sigma(G,x) - \sigma(G^{'},x) < 0$. Hence

$$\sigma(G,x) < \sigma(G^{'},x).$$

□

Theorem 4.10 *Let* $(y_1,\ldots,y_n)$ *and* $(d_1,\ldots,d_n)$ *be two degree sequences of caterpillars. If* $(y_1,\ldots,y_n) \prec (d_1,\ldots,d_n)$ *and* $\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} d_i$*, then for all* $x > 0$ *we have*

$$\sigma(\mathcal{S}(y_1,\ldots,y_n),x) < \sigma(\mathcal{S}(d_1,\ldots,d_n),x).$$

Proof. Suppose $Y = (y_1,\ldots,y_n)$ and $D = (d_1,\ldots,d_n)$ are two degree sequences of caterpillars, $Y \prec D$ and $\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} d_i$. Then, there exits i_0, such that $d_{i_0} \neq y_{i_0}$. In fact, the set $\mathbb{I} = \{i : d_i \neq y_i\}$ must have at least two elements, otherwise $\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} d_i$ would be impossible. Let $l = \min\{i : d_i \neq y_i\}$ and $m = \max\{i : d_i \neq y_i\}$. Then, we must have $y_m > d_m \geq 1$. And since $y_l \geq y_m$, we must also have $d_l > y_l$. We define

$$Y_1 = (y_1,\ldots,y_{l-1},y_l+1,y_{l+1},\ldots,y_{m-1},y_m-1,y_{m+1},\ldots,y_n).$$

Note that Y_1 is still a valid degree sequence. If $l > 1$, then $y_{l-1} = d_{l-1} \geq d_l \geq y_l + 1 > d_m + 1 \geq 2$ and if $l = 1$, then $d_l \geq y_l + 1 > d_m + 1 \geq 2$. If $m < n$, then $y_m - 1 \geq d_m \geq d_{m+1} = y_{m+1} \geq 1$ and if $m = n$, then $y_m - 1 \geq d_m \geq 1$. It is clear that $Y \prec Y_1$. If $y_m > 2$, then by applying Lemma 4.8 to

$\mathcal{S}(Y)$, we know that there exists a caterpillar G with degree sequence Y_1 such that

$$\sigma(\mathcal{S}(Y), x) < \sigma(G, x) \leq \sigma(\mathcal{S}(Y_1), x).$$

Otherwise $y_m = 2$. In such case, decompose $\mathcal{S}(Y)$ as in Figure 3.28, with B not empty, $\deg(v) = y_l$ and $\deg(w) = y_m = 2$. Since the non-leaf vertices at the ends of $\mathcal{S}(Y)$ are of largest degrees, then without loss of generality we assume $\deg(r(B^{'})) \geq \deg(u^{'})$, for all non-leaf vertices $u^{'}$ in $\mathcal{S}(Y)$. Since $\deg(r(B^{'})) \geq \deg(u^{'})$, for all non-leaf vertices $u^{'}$ in $\mathcal{S}(Y)$, then by Lemma 2.9 and Remark 2.10, we must have

$$\rho(B^{'}, x) = \frac{1}{1 + x\left(\frac{1}{1+x}\right)^{\deg(r(B^{'}))-1}} \geq \rho(B_L^{u^{'}}, x), \rho(B, x),$$

with equality if and only if $B^{'} \approx_r B_L^{u^{'}}$. Let G be a caterpillar obtained from $\mathcal{S}(Y)$, by removing the edge $wr(B^{'})$ and then adding the edge $w^{'}r(B^{'})$. Since $\deg(w^{'}) \geq 2 = \deg(w)$ and $\sigma(H' - \{w^{'}, w^*, w\}, x) = \sigma(\emptyset, x) = 1$, for all vertices w^* (H' is the two vertex path with end vertices w and $w^{'}$), then by Lemma 4.9, we must have

$$\sigma(\mathcal{S}(Y), x) < \sigma(G, x).$$

Let $w^{''}$ be a leaf adjacent to $w^{'}$ in G. Let w^* be the neighbor of $w^{'}$ in H and v^* be the neighbor of v in H. Let $G^{'}$ be a caterpillar obtained from G as follows: If either

(i) $\rho(B^{'}, x) > \rho(B, x)$, or

(ii) $\rho(B^{'}, x) = \rho(B, x)$, $\sigma(H - \{v, w^{'}, w^*\}, x) \geq \sigma(H - \{v, v^*, w^{'}\}, x)$ and $\deg(v) \geq \deg(w^{'})$,

then remove the edge $w^{'}w^{''}$ and then add the edge $vw^{''}$. Otherwise

(i) $\rho(B^{'}, x) \geq \rho(B, x)$, $\sigma(H - \{v, w^{'}, w^*\}, x) < \sigma(H - \{v, v^*, w^{'}\}, x)$ and $\deg(v) \geq \deg(w^{'})$, or

(ii) $\rho(B^{'}, x) \geq \rho(B, x)$, $\sigma(H - \{v, w^{'}, w^*\}, x) \geq \sigma(H - \{v, v^*, w^{'}\}, x)$ and $\deg(v) < \deg(w^{'})$.

If (i), then flip H, remove the edge $w^{'}w^{''}$ and then add the edge $vw^{''}$ (note that when flipping H, we assume v and w' are fixed in their original positions in G). If (ii), then swap d and $d^{'} + 1$, remove the edge $w^{'}w^{''}$ and then add the edge $vw^{''}$. Then, by Lemma 4.8, we must have $\sigma(G, x) < \sigma(G^{'}, x)$ and the degree sequence of $G^{'}$ is Y_1. Hence, By Theorem 4.6,

$$\sigma(\mathcal{S}(Y), x) < \sigma(G, x) < \sigma(G^{'}, x) \leq \sigma(\mathcal{S}(Y_1), x).$$

Note that the degree sequence of G' is Y_1. If $Y_1 = D$, then we are done. Otherwise, we iterate the process. We set $Y = Y_0$, and if k is a positive integer and $Y_k \neq D$, then we construct Y_{k+1} in exactly the same way Y_1 was constructed from Y. After a finite number $J = \frac{1}{2}\sum_{i\in\mathbb{I}} |d_i - y_i|$ of iterations, we will get the chain

$$Y = Y_0 \prec Y_1 \prec \cdots \prec Y_{J-1} \prec Y_J = D.$$

For any $k \in \{1, \ldots, J-1\}$, we can apply Lemmas 4.8 and 4.9 with Theorem 4.6 to $\mathcal{S}(Y_k)$ as we did above, to deduce that there exists a caterpillar G_{k+1} with degree sequence Y_{k+1} such that

$$\sigma(\mathcal{S}(Y_k), x) < \sigma(G_{k+1}, x) \leq \sigma(\mathcal{S}(Y_{k+1}), x).$$

Hence,

$$\sigma(\mathcal{S}(Y), x) < \sigma(\mathcal{S}(Y_1), x) < \ldots, < \sigma(\mathcal{S}(Y_J), x) = \sigma(\mathcal{S}(D), x).$$

□

Corollary 4.11 *For any caterpillar C of order n and diameter $m(\leq n-1)$, we have*

$$\sigma(C, x) \leq \sigma(\mathcal{S}(d, \underbrace{2, \ldots, 2}_{m-2}), x), \text{ for all positive } x \in \mathbb{R}$$

with equality if and only if $C \cong \mathcal{S}(d, \underbrace{2, \ldots, 2})$, where $d = n - m + 1$.

Corollary 4.12 *For any caterpillar C of order n, diameter $m(\leq n-1)$ and vertex degree at most $d(\leq n-m+1)$, we have*

$$\sigma(C, x) \leq \sigma(\mathcal{S}(\underbrace{d, \ldots, d}_{k}, \underbrace{r, 2, \ldots, 2}_{m-k-1}), x), \text{ for all positive } x \in \mathbb{R}$$

with equality if and only if $C \cong \mathcal{S}(\underbrace{d, \ldots, d}_{k}, \underbrace{r, 2, \ldots, 2}_{m-k-1})$, where $k = \left\lfloor \frac{n-m-1}{d-2} \right\rfloor$

and $r = \begin{cases} 0, & \text{if } k = \frac{n-m-1}{d-2}, \\ n - m - \left\lfloor \frac{n-m-1}{d-2} \right\rfloor (d-2) + 1, & \text{otherwise.} \end{cases}$

Corollary 4.13 *For any caterpillar C of order n and vertex degree of at most $d(\leq n-m+1)$, we have*

$$\sigma(C, x) \leq \sigma(\mathcal{S}(\underbrace{d, \ldots, d}_{k}, r), x), \text{ for all positive } x \in \mathbb{R}$$

with equality if and only if $C \cong \mathcal{S}(\underbrace{d, \ldots, d}_{k}, r)$, *where* $k = \left\lfloor \frac{n-2}{d-1} \right\rfloor$ *and*

$$r = \begin{cases} 0, & \textit{if } k = \frac{n-2}{d-1} \in \mathbb{Z}, \\ n - \left\lfloor \frac{n-2}{d-1} \right\rfloor (d-1) - 1, & \textit{otherwise.} \end{cases}$$

5 Conclusion

In this thesis, it is shown that: among all caterpillars with reduced degree sequence D, $\mathcal{X}(D)$ maximizes the auxiliary invariant $M(., x)$, for all positive $x \in \mathbb{R}$, the Hosoya index Z and the energy En. Among all caterpillars with reduced degree sequence D, $\mathcal{S}(D)$ minimizes $M(., x)$, for all positive $x \in \mathbb{R}$, the Hosoya index Z and the energy En. The caterpillar $\mathcal{S}(D)$ was also found to be maximizing the auxiliary invariant $\sigma(., x)$, for all positive $x \in \mathbb{R}$, and hence the Merrifield-Simmons index σ. Furthermore, we show that, if $(b_1, \ldots, b_n)$ and $(d_1, \ldots, d_n)$ are two degree sequences of caterpillars, such that $(b_1, \ldots, b_n) \prec (d_1, \ldots, d_n)$ and

$$\sum_{i=1}^{n} b_i = \sum_{i=1}^{n} d_i,$$

then

$$\begin{aligned}
M(\mathcal{X}(d_1, \ldots, d_n), x) &< M(\mathcal{X}(b_1, \ldots, b_n), x), \\
M(\mathcal{S}(d_1, \ldots, d_n), x) &< M(\mathcal{S}(b_1, \ldots, b_n), x), \\
Z(\mathcal{X}(d_1, \ldots, d_n)) &< Z(\mathcal{X}(b_1, \ldots, b_n)), \\
Z(\mathcal{S}(d_1, \ldots, d_n)) &< Z(\mathcal{S}(b_1, \ldots, b_n)), \\
En(\mathcal{X}(d_1, \ldots, d_n)) &< En(\mathcal{X}(b_1, \ldots, b_n)), \\
En(\mathcal{S}(d_1, \ldots, d_n)) &< En(\mathcal{S}(b_1, \ldots, b_n)), \\
\sigma(\mathcal{S}(d_1, \ldots, d_n), x) &> \sigma(\mathcal{S}(b_1, \ldots, b_n), x),
\end{aligned}$$

and

$$\sigma(\mathcal{S}(d_1, \ldots, d_n)) > \sigma(\mathcal{S}(b_1, \ldots, b_n)),$$

for all positive $x \in \mathbb{R}$. From these results, one deduces that, among all caterpillars of order n and size m, the path graph P_n maximizes $M(., x)$, the energy and the Hosoya index, and minimizes $\sigma(., x)$ and hence the Merrifield-Simmons index. The star S_n minimizes $M(., x)$, the energy and the Hosoya index. This is to be expected, since the path graph and star in [38], were found to be extremal, when the family of trees with given order is considered. Since the family of caterpillars is within the class of trees, the path graph and star must also be extremal among all caterpillars. The broom $P_{n,2}$ turns out to be the caterpillar with order n and second largest $M(.,x)$, En and Z, and second smallest $\sigma(.,x)$ and hence σ. The double star $S_{n-3,3}$ is the caterpillar with order n and second smallest $M(.,x)$, En and Z. These also are to be expected, as the broom and double star are extremal among all trees of given order, see survey [135] for the Hosoya index and [88] for the graph energy. We used similar techniques used to characterize extremal caterpillars with regard to $M(.,x)$, to characterize caterpillars with given degree sequence maximizing $\sigma(.,x)$. Our attempt to use those techniques to characterize caterpillars with degree sequence D that minimize $\sigma(.,x)$ did not succeed. Our investigation suggests the following conjectures:

Conjecture 5.1 *Among all caterpillars of degree sequence D, $\mathcal{X}(D)$ minimizes the auxiliary invariant $\sigma(.,x)$, for all positive $x \in \mathbb{R}$, and hence the Merrifield-Simmons index.*

Conjecture 5.2 *Let $(b_1,\dots,b_n)$ and $(d_1,\dots,d_n)$ be two degree sequences of caterpillars. If $(b_1,\dots,b_n) \prec (d_1,\dots,d_n)$ and $\sum_{i=1}^{n} b_i = \sum_{i=1}^{n} d_i$, then for all positive $x \in \mathbb{R}$, we have*

$$\sigma(\mathcal{X}(d_1,\dots,d_n),x) > \sigma(\mathcal{X}(b_1,\dots,b_n),x)$$

and hence

$$\sigma(\mathcal{X}(d_1,\dots,d_n)) > \sigma(\mathcal{X}(b_1,\dots,b_n)).$$

Besides the aforementioned conjectures, we intend to study the number of independent subsets and the energy of caterpillars with given segment sequence. We also plan to find cospectral caterpillars. Last but not least of interest are also the connections between graph entropies and graph energy under degree restriction, or the average size of independent sets in caterpillars.

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