The number of independent subsets and the energy of trees

by

Eric Ould Dadah Andriantiana

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Department of Mathematics,
University of Stellenbosch,
Private Bag X1, Matieland 7602, South Africa.

Supervisor: Prof. Stephan Wagner

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Signature: ....
E. O. D. Andriantiana

Date: ....2010/09/27.................

Abstract

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E. O. D. Andriantiana

Department of Mathematics,
University of Stellenbosch,
Private Bag X1, Matieland 7602, South Africa.

Thesis: MSc

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The Merrifield-Simmons index σ, defined as the total number of independent vertex subsets, the Hosoya index Z, defined similarly as the total number of independent edge subsets, and the energy En of a graph, which is the sum of the absolute values of its eigenvalues, are among the most popular parameters studied in chemical graph theory. For molecular graphs (in particular trees), they are known to be correlated to some physico-chemical properties of the corresponding compounds.

In this thesis, we first introduce the three parameters together with some of their basic properties. Then we discuss certain techniques to characterize the trees for which the maximum/minimum of σ, Z and En are reached. We also study several special classes of trees, such as trees with prescribed diameter or maximum degree, and provide additional results on trees with large Hosoya index or small Merrifield-Simmons index.

Finally, in the main part of this thesis, we study the three graph invariants for the class $\mathbb{T}_{1,d}$ of trees whose vertex degrees are restricted to either 1 or d (for some $d \geq 3$), which is a natural restriction in the chemical context. We find that the minimum of the Merrifield-Simmons index and the maximum of the Hosoya index are both attained for path-like trees which is followed by sequences of what we call generalized tripods. Other types of trees only appear much later in a list sorted with respect to the two graph invariants σ and Z. Elements of $\mathbb{T}_{1,d}$ with maximum Merrifield-Simmons index and with minimum Hosoya index are described as well, and similar results are also found for the energy. Comparing the behaviours of the three parameters for the set of all trees without restriction and the set $\mathbb{T}_{1,d}$ shows some interesting analogies.

Opsomming

Die aantal onafhanklike deelversamelings en die energie van bome

("The number of independent subsets and the energy of trees")

E. O. D. Andriantiana

Departement Wiskunde,
Universiteit van Stellenbosch,
Privaatsak X1, Matieland 7602, Suid Afrika.

Tesis: MSc

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Die Merrifield-Simmons indeks σ, wat as die aantal onafhanklike puntversamelings gedefinieer word, die Hosoya indeks Z, wat soortgelyk as die aantal onafhanklike lynversamelings gedefinieer word, en die energie En van 'n grafiek – die som van die absolute waardes van sy eiewaardes – is drie van die gewildste parameters wat in chemiese grafiekteorie bestudeer word. Dit is bekend dat hierdie drie parameters vir molekulêre grafieke (in die besonder bome) baie goed korreleer met sekere fisies-chemiese eienskappe van die ooreenstemmende verbindings.

Hierdie tesis begin met 'n voorstelling van die drie parameters en sommige van hul elementêre eienskappe. Ons gaan voort deur sekere tegnieke te behandel wat gebruik word om dié bome te karakteriseer wat die grootste/kleinste waardes van σ, Z en En lewer. Ons bestudeer ook sommige spesiale klasse van bome, soos bome met gegewe deursnee of maksimum graad, en gee addisionele resultate oor bome met groot Hosoya indeks of klein Merrifield-Simmons indeks.

In die hoofdeel van die tesis word die versameling $\mathbb{T}_{1,d}$ van alle bome beskou waarvan die grade almal 1 of d moet wees (vir 'n sekere $d \geq 3$). Hierdie beperking is 'n natuurlike vereiste in die chemiese konteks. Ons vind dat die minimum van die Merrifield-Simmons indeks en die maksimum van die Hosoya index vir bome verkry word wat soortgelyk aan paaie is. Hierdie bome word gevolg deur rye van sogenaamde veralgemeende driepote. Ander tipes bome kom eers baie later as 'n mens 'n lys beskou wat volgens die twee parameters σ en Z gesorteer word. Die elemente van $\mathbb{T}_{1,d}$ met die grootste Merrifield-

Simmons indeks en die kleinste Hosoya indeks word ook beskryf, en soortgelyke resultate word ook vir die energie bewys. Ons vind baie interessante ooreenkomste tussen die versameling van alle bome sonder beperkings en die versameling $\mathbb{T}_{1,d}$.

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I heartily thank all the members of my family for their continuous encouragement and support from the very beginning of my studies.

... by God's grace I am what I am, ... *Cor. I* 15:10

Dedications

To my dearest mother Rasoanirina J. Oberline, on occasion of her 53^{rd} *birthday.*

Contents

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Nomenclature

Symbols	**Definitions**
$\mathbb{N}$	the set of natural numbers
$\mathbb{Z}$	the set of integers
$\mathbb{R}$	the set of real numbers
$\lceil x \rceil$	the smallest integer greater or equal to x
$\lfloor x \rfloor$	the greatest integer smaller or equal to x
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 the vertex v in a graph G
$\mathrm{diam}(G)$	the diameter of a graph G
$\sigma(G)$	the number of independent vertex subsets of a graph G
$\mathrm{m}(G,k)$	the number of independent vertex subsets of order k of a a graph G
$\mathrm{Z}(G)$	the number of independent edge subsets of a graph G
$A(G)$	an adjacency matrix of a graph G
$\phi(G,x)$	the characteristic polynomial of a graph G
$\mathrm{En}(G)$	the energy of a graph G
P_n	the n vertex path
S_n	the n vertex star
C_n	the n vertex cycle
C_n^d	the $(\underbrace{d,\dots,d}_{n \text{ times}})$ -caterpillar
$C_n'^d$	the $(d-1,\underbrace{d,\dots,d}_{n-1 \text{ times}})$ -caterpillar
$C_n''^d$	the $(d-1,\underbrace{d,\dots,d,}_{n-2 \text{ times}}d-1)$ -caterpillar

$T(i,j,k)$	the tripod whose three branches are P_i, P_j and P_k
$T_d(i,j,k)$	the d-tripod whose three branches are $C_i'^d, C_j'^d$ and $C_k'^d$
D_h^d	the complete $(d-1)$-ary tree of height $h-1$
ς_n^d	the number of independent vertex subsets of $C_n'^d$
ζ_n^d	the number of independent edge subsets of $C_n'^d$

Chapter 1

Introduction

In 1941 Turán published a description of the graph of order n with maximum number of edges which does not contain a complete graph of order k, for some fixed k. This result [Tur41] is known to be the pioneer of a new branch of graph theory called *extremal graph theory.* Paul Erdős has made considerable and multiple contributions strengthening the field, see for instance [Erd65, Erd67, EH80].

Usually, problems in extremal graph theory consist of finding graphs, in a specific class of graphs, which minimize or maximize some graph invariants such as order, size, minimum or maximum degree, number of independent subsets or diameter. In this work, we are interested in graph-theoretical parameters which are important both in pure graph theory and in chemistry:

i) The *Hosoya index* [Hos71], denoted by Z, was first introduced by the Japanese chemist Haruo Hosoya under the name *topological index.* For a graph G, $\mathrm{Z}(G)$ is the number of ways in which one can select an arbitrary number (including zero) of mutually independent edges, i.e., no two chosen edges have a common end.

ii) The *Merrifield-Simmons index* [MS89], denoted by σ, has a very similar definition as Z. If G is a graph, then $\sigma(G)$ is the number of ways to form a set (possibly empty) of pairwise independent vertices of G, in other words, no two vertices in the set are joined by an edge. Its study was initiated by the American chemists Richard E. Merrifield and Howard E. Simmons.

iii) The *energy* $\mathrm{En}(G)$ of a graph is the sum of the absolute values of its eigenvalues [Gut01].

More about definitions and basic notions will be provided in Chapter 2.

The main motivation for studying these parameters is to predict physico-chemical properties of compounds, such as boiling point or heat of formation, from their structure that can be modeled as a graph. A wealth of theoretical results has been obtained in recent years, in particular regarding σ and Z of trees and tree-like structures (such as unicyclic graphs [Ou09, PV05]). Upper and lower bounds are known under various restrictions, such as diameter [YY05], number of leaves [YL07] or number of cut edges [Hua09]. In Chapter 3, we describe the extremal trees with respect to the three parameters and also discuss some closely related results, e.g., concerning trees with given diameter or maximum degree.

Degree restrictions are particularly natural in the chemical context; trees whose maximum degree is at most 4 are also known as *chemical trees* [FGH$^+$02]. Chapter 4 forms the main part of this thesis, since it comprises mostly original research; a shortened version was submitted for publication [AW10]. The chapter is devoted to results on a natural type of degree restriction: we consider trees whose vertex degrees are all either 1 or d; the set of all such trees will be denoted by $\mathbb{T}_{1,d}$. Note in particular that for $d = 4$, we obtain trees that represent saturated hydrocarbons (alkanes); the main results is characterisation of the extremal trees in $\mathbb{T}_{1,d}$ with respect to the three parameters σ, Z and En .

There is a striking similarity to the behaviour observed for trees without any restrictions as emphasized in the last chapter.

Chapter 2

Basic notions

2.1 Introduction

We describe in this chapter selected terminology that will be used in the other chapters. Some of them will be illustrated by some properties or examples.

Definition 2.1.1 A *simple undirected* graph G is defined by an ordered pair of sets $G = (V(G), E(G))$, where the elements of $V(G)$ are called *vertices* of G and the elements of $E(G)$ which consist of two-element subsets of $V(G)$ are called *edges* of G. $|V(G)|$ is the *order* of G and $|E(G)|$ its *size.*

Definition 2.1.2 A simple undirected graph G is *complete* if and only if for all vertices v and u of G we always have $vu \in E(G)$. Such a graph is denoted by K_n if it has n vertices.

For simplicity an edge $\{u, v\}$ will be denoted by uv. A graphical representation or diagram of a graph is obtained by using points as vertices and lines joining two vertices as edges, see Figure 2.1. The properties of being simple and undirected for a graph G refer to the fact that its graphical representation does not contain two vertices joined by multiple lines nor a vertex joined to itself and lines do not have directions. All graphs considered in the rest of this document are assumed to be simple and undirected.

For two graphs G and G' to be identical, one must have $V(G) = V(G')$ and $E(G) = E(G')$. But there are graphs that are so similar that they can be represented by the same diagram. In such a case the graphs are called isomorphic, formally defined as follows:

Definition 2.1.3 Two graphs G and G' are *isomorphic* if and only if there is a bijective function $f : V(G) \longrightarrow V(G')$ such that $uv \in E(G)$ if and only if $f(v)f(v) \in E(G')$.

We identify any two isomorphic graphs.

Definition 2.1.4 A graph of the form

$$(\{v_1, v_2, \cdots, v_k\}, \{v_1v_2, \cdots, v_{k-1}v_k\}),$$

where $k \geq 1$ and $v_i \neq v_j$ if $i \neq j$, is called a *path* and denoted by $v_1v_2 \cdots v_k$ or simply P_k if there is no risk of confusion. The two vertices v_1 and v_k are called its *ends*. The size of a path is also called its *length*.

Note that P_1 is an isolated vertex. It is convenient to denote by P_0 the empty graph.

Definition 2.1.5 Let v be a vertex in G. The set $\{w \in V(G) | vw \in E(G)\}$ is called the *neighbourhood* of v, denoted by $N_G(v)$. $|N_G(v)|$ is called the *degree* of v.

Example 2.1.6 In the path $P_3 = v_1v_2v_3$ we have $N_{P_3}(v_2) = \{v_1, v_3\}$. For $P_1 = w$, $N_{P_1}(w) = \varnothing$.

Definition 2.1.7 Let $k \geq 3$ be an integer and $(V, E) = v_1v_2 \cdots v_k$ be a path. The graph $(V, E \cup \{v_kv_1\})$ is called a *cycle*. It will be denoted by $v_1v_2 \cdots v_kv_1$ or simply C_k if there is no risk of confusion.

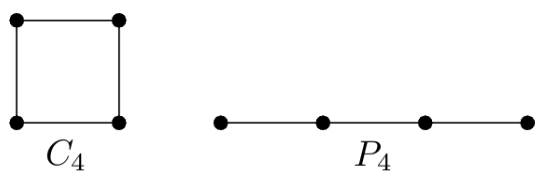


Figure 2.1: Examples of graphs described in Definitions 2.1.4 and 2.1.7

Definition 2.1.8 Let u and v be vertices of a graph G. The length of the shortest path in G joining the two vertices is called the *distance* between u and v.

Definition 2.1.9 For a graph G, the *diameter*, denoted by $\mathrm{diam}(G)$, is the largest distance between two vertices of G. The diameter of graphs with less than two vertices is set to be zero.

Definition 2.1.10 An *acyclic* graph is a graph which does not contain cycles, it is also called a *forest*. A connected forest is called a *tree*. A vertex with degree one in a tree is called a *leaf*.

Definition 2.1.11 A graph which contains exactly one cycle is called a *unicyclic* graph. Similarly, a *bicyclic* graph is a graph which has exactly two cycles.

Definition 2.1.12 Let G and G' be two graphs such that $V(G) \subseteq V(G')$ and $E(G') \subseteq E(G)$. Then G' is called a *subgraph* of G; if in particular $V(G) = V(G')$, then G' is called a *spanning* subgraph of G.

Clearly any connected graph has a spanning subgraph which is a tree, it is called a *spanning tree.*

Let $\{v_1, v_2, \cdots, v_k\}$ be a subset of the set of vertices of a graph G. The graph which result from G after deletion of the vertices $v_1, v_2, \cdots, v_k$ along with edges containing them will be denoted by

$$G - \{v_1, v_2, \cdots, v_k\}. \tag{2.1.1}$$

For $k = 1$, we simply write $G - v_1$ instead of $G - \{v_1\}$.

2.2 Number of independent subsets

In a graph G, two disjoint edges are called *independent* and two vertices u and v are called independent if and only if $uv \notin E(G)$. Vertices or edges that are not independent are called *adjacent.*

Definition 2.2.1 Let G be a graph. A subset of $V(G)$ is an *independent vertex subset* of G if and only if it does not contain adjacent vertices. We denote by $\sigma(G)$ the number of independent vertex subsets of G.

Similarly, a subset of $E(G)$ is called an *independent edge subset* or *matching* of G if and only if it does not contain adjacent edges. The number of independent edge subsets of cardinality k in G is denoted by $\mathrm{m}(G, k)$. The total number of matchings is then

$$\mathrm{Z}(G) = \sum_{k \geq 0} \mathrm{m}(G, k). \tag{2.2.1}$$

Since the empty set is an independent vertex subset and an independent edge subset of any graph, for all graphs G we have $\sigma(G) \geq 1$ and $\mathrm{Z}(G) \geq 1$.

The graph invariant Z was introduced by Haruo Hosoya in his paper [Hos71], which is why it was later named Hosoya topological index or simply *Hosoya index.* Also for historical reasons σ is called *Merrifield-Simmons index*: it was introduced by Richard E. Merrifield and Howard E. Simmons. Some authors call them Z-index and σ-index.

It is clear that removal of an edge vu from a graph G creates at least one new independent vertex subset (namely $\{v, u\}$) and destroys at least one independent edge subset (namely $\{vu\}$). This implies that among all graphs of order n, the edgeless graph D_n has maximum Merrifield-Simmons index $\sigma(D_n) = 2^n$ and minimum Hosoya index $\mathrm{Z}(D_n) = 1$, and the maximum Hosoya index as well as the minimum Merrifield-Simmons index are attained by the complete graph K_n, namely

$$\sigma(K_n) = n + 1 \tag{2.2.2}$$

and

$$\begin{aligned} \mathrm{Z}(K_n) &= \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(2k)!}{2^k k!} \binom{n}{2k} \\ &= \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n!}{2^k k! (n-2k)!}. \end{aligned} \tag{2.2.3}$$

The problem becomes more interesting when further restrictions are added. For instance, as we will see in the next chapter, it is less obvious that stars maximize σ and minimize Z among all connected graphs.

Remark 2.2.2 It occurs very often that a certain graph is extremal with respect to both σ and Z within a given class of graphs. Throughout the survey [WG10] one can see that in most classes of graphs that have been studied the graph that minimizes the Merrifield-Simmons index is also the one that maximizes the Hosoya index, and vice versa.

One of the rare exceptions to this remark is the result of Deng in [Den08, Den09] showing that the bicyclic graph that maximizes the Hosoya index is different from the bicyclic graph that minimizes the Merrifield-Simmons index. The former (Figure 2.2a) is a graph obtained by identifying two edges of a cycle of length 4 and a cycle of length $n-2$ and the latter (Figure 2.2b) is a graph which results from connecting two triangles (3-cycles) by a path of length $n-5$.

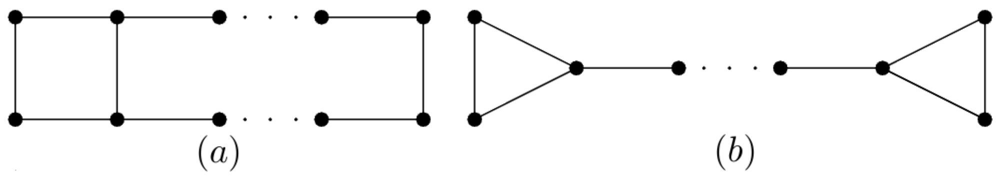


Figure 2.2: Among all bicyclic graphs (a) minimizes σ and (b) maximizes Z.

Usually, as the order and the size of the graph increase, the number of independent subsets grows fast and it quickly becomes not practical to enumerate them all. An alternative way to determine σ or Z for a big graph consists of reducing the problem to smaller graphs. The following lemma gives the necessary formulas for this purpose.

Lemma 2.2.3 *If G and G' are two disjoint graphs, then*

$$\mathrm{Z}(G \cup G') = \mathrm{Z}(G)\,\mathrm{Z}(G'), \tag{2.2.4}$$

$$\sigma(G \cup G') = \sigma(G)\sigma(G'). \tag{2.2.5}$$

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

$$\mathrm{Z}(G) = \mathrm{Z}(G-v) + \sum_{w \in N_G(v)} \mathrm{Z}(G - \{v, w\}), \tag{2.2.6}$$

$$\sigma(G) = \sigma(G-v) + \sigma(G - (\{v\} \cup N_G(v))). \tag{2.2.7}$$

Proof. Let G and G' be two disjoint graphs. Any independent edge subset $S \subseteq E(G \cup G')$ can be decomposed uniquely as

$$\begin{aligned} S &= S \cap (E(G \cup G')) \\ &= (S \cap E(G)) \cup (S \cap E(G')) \end{aligned} \tag{2.2.8}$$

and clearly, $S \cap E(G)$ and $S \cap E(G')$ are independent edge subsets of G and G', respectively. Conversely, if S and S' are respectively independent edge subsets in G and in G', then $S \cup S'$ is an independent edge subset of $G \cup G'$ since no edge in G is adjacent to an edge in G'. Therefore we have

$$\begin{aligned} \mathrm{Z}(G \cup G') &= \sum_{k \geq 0} \sum_{i+j=k} \mathrm{m}(G, i)\, \mathrm{m}(G', j) \\ &= \sum_{i \geq 0} \mathrm{m}(G, i) \sum_{j \geq 0} \mathrm{m}(G', j) \\ &= \mathrm{Z}(G)\, \mathrm{Z}(G') \end{aligned} \tag{2.2.9}$$

as in equation (2.2.4), the same idea applied to σ leads to equation (2.2.5).

In equation (2.2.6) the two terms on the right-hand side are respectively the number of independent edge subsets of G without edge incident to v and the number of those which contain an an edge incident to v, hence their sum gives $\mathrm{Z}(G)$. Similarly, in equation (2.2.7), $\sigma(G-v)$ corresponds to the number of independent vertex subsets of G which do not contain v and $\sigma(G - (\{v\} \cup N_G(v)))$ is the number of those which contain v. □

Example 2.2.4 As an example let us consider the case of an n-vertex path P_n. Trivially, we have $\sigma(P_0) = 1$, $\sigma(P_1) = 2$, $\mathrm{Z}(P_0) = 1$ and $\mathrm{Z}(P_1) = 1$. Applying Lemma 2.2.3 we have the relations

$$\sigma(P_{n+2}) = \sigma(P_{n+1}) + \sigma(P_n), \tag{2.2.10}$$

$$\mathrm{Z}(P_{n+2}) = \mathrm{Z}(P_{n+1}) + \mathrm{Z}(P_n), \tag{2.2.11}$$

for all $n \in \mathbb{N}$. Therefore, if we denote by F_k the k^{th} Fibonacci number, then

$$\sigma(P_n) = F_{n+1} = \frac{1}{\sqrt{5}} \left(\left(\frac{1+\sqrt{5}}{2} \right)^{n+2} - \left(\frac{1-\sqrt{5}}{2} \right)^{n+2} \right), \tag{2.2.12}$$

$$\mathrm{Z}(P_n) = F_n = \frac{1}{\sqrt{5}} \left(\left(\frac{1+\sqrt{5}}{2} \right)^{n+1} - \left(\frac{1-\sqrt{5}}{2} \right)^{n+1} \right). \tag{2.2.13}$$

2.3 Energy of graphs

Let us label the vertices of G by $v_1, \cdots, v_n$. We can then define a $n \times n$ matrix $A(G) = (a_{i,j})_{1 \le i,j \le n}$ where

$$a_{i,j} = \begin{cases} 1 \text{ if } v_i v_j \in E(G) \\ 0 \text{ otherwise.} \end{cases} \tag{2.3.1}$$

In particular, for all i and j in $\{1, \dots, n\}$, we have $a_{i,i} = 0$ and $a_{i,j} = a_{j,i}$, i.e. $A(G)$ is a symmetric matrix. $A(G)$ is called an *adjacency matrix* of G. A different way of numbering the vertices of G, say $v_{\pi(1)}, \cdots, v_{\pi(n)}$, may lead to a different adjacency matrix $A_\pi(G)$. More precisely, let $P_\pi = (p_{i,j})_{1 \le i,j \le n}$ be the permutation matrix corresponding to π in the sense that $p_{i,j} = 1$ if $\pi(i) = j$ and $p_{i,j} = 0$ otherwise. Then we have the relation

$$A_\pi(G) = P_\pi A(G) P_\pi^t \tag{2.3.2}$$

where P_π^t is the transpose of P_π. As a permutation matrix, P_π satisfies the identity $P_\pi^t = P_\pi^{-1}$. Furthermore, if we let I_n be the identity matrix of order n, then we have the relation

$$\begin{aligned} \phi(A_\pi(G), x) &= \det(xI_n - A_\pi(G)) \\ &= \det(xP_\pi I_n P_\pi^t - P_\pi A(G) P_\pi^t) \\ &= \det(P_\pi(xI_n - A(G))P_\pi^t) \\ &= \det(xI_n - A(G)) \\ &= \phi(A(G), x). \end{aligned} \tag{2.3.3}$$

Therefore it makes sense to define as *characteristic polynomial of* G the polynomial

$$\phi(G, x) = \phi(A(G), x). \tag{2.3.4}$$

Since $A(G)$ is symmetric, all the roots of $\phi(G, x)$ are real and they are called eigenvalues of the graph G.

Definition 2.3.1 Let G be a graph of order n and let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be its eigenvalues. The graph invariant

$$\mathrm{En}(G) = \sum_{k=1}^{n} |\lambda_k| \tag{2.3.5}$$

is called the *energy* of G.

In chemistry, the experimentally measured heats of formation for conjugated hydrocarbons are known to be closely related to their theoretically calculated total π-electron energies. Furthermore, within the framework of the

Hückel molecular orbital approximation [GP86], the calculation of the total π-energy of a conjugated hydrocarbon can be reduced to that of the energy of the corresponding molecular graph. These observations explain why the energy of graphs became a common interest of graph theoreticians and chemists.

Example 2.3.2 As an example let us consider the n-vertex cycle C_n. It has an adjacency matrix given by

$$A(C_n) = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & 1 & 0 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 & 0 & 1 \\ 1 & 0 & \cdots & 0 & 0 & 1 & 0 \end{bmatrix} \tag{2.3.6}$$

It is a type of square matrix called *circulant matrix* where the $(i+1)^{th}$ row can be obtained from a circular permutation of the i^{th} row for all $0 \leq i \leq n-1$. $A(C_n)$ can be decomposed into two simpler circulant matrices

$$A(C_n) = A_1 + A_2 \tag{2.3.7}$$

where

$$A_1 = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 0 & 1 \\ 1 & 0 & \cdots & 0 & 0 \end{bmatrix} \tag{2.3.8}$$

and

$$A_2 = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & 1 & 0 & 0 \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix} \tag{2.3.9}$$

Note that multiplying a matrix by A_1 has the same result as applying a one step circular permutation to each of its lines. In particular, this implies that $A_2 = A_1^{n-1}$. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of A_1 corresponding to the eigenvectors $V_1, V_2, \ldots, V_n$, respectively. Then for all $i \in \{1, 2, \ldots, n\}$ we have

$$A_1 V_i = \lambda_i V_i \tag{2.3.10}$$

which implies

$$A_2 V_i = A_1^{n-1} V_i = \lambda_i^{n-1} V_i \tag{2.3.11}$$

and

$$A(C_n)V_i = (A_1 + A_1^{n-1})V_i = (\lambda_i + \lambda_i^{n-1})V_i. \tag{2.3.12}$$

Therefore $\lambda_1 + \lambda_1^{n-1}, \lambda_2 + \lambda_2^{n-1}, \ldots, \lambda_n + \lambda_n^{n-1}$ are the eigenvalues of $A(C_n)$. Hence we only have to find out the eigenvalues of A_1 which are the roots of the following polynomial

$$P_1(x) = \begin{vmatrix} x & -1 & 0 & \cdots & 0 \\ 0 & x & -1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & x & -1 \\ -1 & 0 & \cdots & 0 & x \end{vmatrix}. \tag{2.3.13}$$

By determinant expansion with respect to the last row, we obtain

$$\begin{aligned} P_1(x) = (-1)^n &\begin{vmatrix} -1 & 0 & 0 & \cdots & 0 \\ x & -1 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & x & -1 & 0 \\ 0 & \cdots & 0 & x & -1 \end{vmatrix} + x \begin{vmatrix} x & -1 & 0 & \cdots & 0 \\ 0 & x & -1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & x & -1 \\ 0 & 0 & \cdots & 0 & x \end{vmatrix} \\ = x^n - 1, & \end{aligned} \tag{2.3.14}$$

thus the roots are

$$\lambda_k = e^{\frac{2i\pi}{n}k} \text{ for } k = 1, 2, \cdots, n. \tag{2.3.15}$$

Consequently, the eigenvalues of $A(C_n)$ are

$$\begin{aligned} e_k &= e^{\frac{2i\pi}{n}k} + \left(e^{\frac{2i\pi}{n}k}\right)^{n-1} \\ &= e^{\frac{2i\pi}{n}k} + e^{\frac{2(n-1)i\pi}{n}k} \\ &= 2\cos\frac{2\pi}{n}k \end{aligned} \tag{2.3.16}$$

where $k = 1, 2, \cdots, n$. Summing the geometric series one obtains (see Appendix C for details)

$$\mathrm{En}(C_n) = \begin{cases} 4\cot\frac{\pi}{n} \text{ if } n = 4l, \\ 2\csc\frac{\pi}{2n} \text{ if } n = 4l+1 \text{ or } n = 4l+3, \\ 4\csc\frac{\pi}{n} \text{ if } n = 4l+2. \end{cases} \tag{2.3.17}$$

In the same way, one can show that the eigenvalues of a path P_n are

$$2\cos\frac{k\pi}{n+1}, k \in \{1, 2, \ldots, n\}, \tag{2.3.18}$$

and thus

$$\mathrm{En}(P_n) = \begin{cases} 2\left(\csc\frac{\pi}{2n+2} - 1\right) \text{ if } n \text{ is even} \\ 2\left(\cot\frac{\pi}{2n+2} - 1\right) \text{ if } n \text{ is odd.} \end{cases} \tag{2.3.19}$$

Since the two following chapters are concerned with trees, the next theorems will be important when it comes to the study of the energy. First, we have a general expression of the characteristic polynomial of trees in terms of numbers of matchings.

Theorem 2.3.3 ([GP86]) *The characteristic polynomial of any tree T of order n is given by*

$$\phi(T,x) = \sum_{k \geq 0} (-1)^k \operatorname{m}(T,k) x^{n-2k}. \tag{2.3.20}$$

Proof. Let T be a tree whose set of vertices is $\{v_1, v_2, \cdots, v_n\}$, let $A(T)$ be an adjacency matrix of T and let $S(n)$ be the set of all permutations of $\{1, 2, \cdots, n\}$. By definition, the characteristic polynomial of T is

$$\begin{aligned} \phi(T,x) &= \det(xI_n - A(T)) \\ &= \sum_{\sigma \in S(n)} \operatorname{sgn}(\sigma) \prod_{i=1}^{n} b_{i,\sigma(i)}, \end{aligned} \tag{2.3.21}$$

where $b_{i,j}$ denotes the entry of the matrix $xI_n - A(T)$ at the crossing of the i^{th} row and the j^{th} column. Since

$$b_{i,\sigma(i)} = \begin{cases} x \text{ if } i = \sigma(i) \\ -1 \text{ if } v_i v_{\sigma(i)} \in E(T) \\ 0 \text{ otherwise} \end{cases} \tag{2.3.22}$$

the product

$$\prod_{i=1}^{n} b_{i,\sigma(i)} \tag{2.3.23}$$

is non-zero if and only if the decomposition of σ into disjoint cycles contains only 2-cycles and 1-cycles, say $\sigma = (i_1 j_1)(i_2 j_2) \ldots (i_k j_k)$, and such that for all $h \in \{1, 2, \cdots, k\}$ we have $v_{i_h} v_{j_h} \in E(T)$. If these conditions are satisfied then we have

$$\prod_{i=1}^{n} b_{i,\sigma(i)} = (-1)^{2k} x^{n-2k} \tag{2.3.24}$$

and $\operatorname{sgn}(\sigma) = (-1)^k$. Because the 2-cycles in the decomposition of σ are pairwise disjoint, the corresponding edges $v_{i_1} v_{j_1}, v_{i_2} v_{j_2}, \ldots, v_{i_k} v_{j_k}$ are pairwise independent and clearly the process can be reversed to start from an independent edge subset of order k and obtain a permutation which satisfies equation (2.3.24). Therefore, equation (2.3.21) is equivalent to

$$\phi(T,x) = \sum_{k \geq 0} (-1)^k \operatorname{m}(T,k) x^{n-2k}. \tag{2.3.25}$$

□

Furthermore, the following alternative formula for the energy of trees allows the computation of the energy of a given tree without knowing its eigenvalues. It is usually preferred when studying the energy in a subclass of trees.

Theorem 2.3.4 ([GP86]) *If T is a tree with n vertices, then*

$$\mathrm{En}(T) = \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log\left(\sum_{k\geq 0}\mathrm{m}(T,k)x^{2k}\right). \tag{2.3.26}$$

Proof. Let T be a tree with n vertices and let $Q(x) = \sum_{k\geq 0}\mathrm{m}(T,k)x^{2k}$. From Theorem 2.3.3, the characteristic polynomial of T is

$$\phi(T,x) = \sum_{k\geq 0}(-1)^k\,\mathrm{m}(T,k)x^{n-2k}. \tag{2.3.27}$$

Let i be the imaginary unit; ϕ and Q are related as follows

$$\begin{aligned}\phi(T,ix^{-1}) &= \sum_{k\geq 0}(-1)^k\,\mathrm{m}(T,k)i^n(-1)^k x^{2k-n}\\ &= i^n x^{-n}\sum_{k\geq 0}\mathrm{m}(T,k)x^{2k}\\ &= i^n x^{-n}Q(x).\end{aligned} \tag{2.3.28}$$

Note that $\phi(T,x)$ is a polynomial which is either even or odd depending on the parity of n, this means that its roots are symmetric with respect to 0. Let $\lambda_1,\lambda_2,\cdots,\lambda_m$ be all its positive roots, then equation (2.3.28) implies

$$\begin{aligned}Q(x) &= i^{-n}x^n(ix^{-1})^{n-2m}\prod_{j=1}^m(ix^{-1}-\lambda_j)(ix^{-1}+\lambda_j)\\ &= \prod_{j=1}^m(1+ix\lambda_j)(1-ix\lambda_j)\\ &= \prod_{j=1}^m(1+x^2\lambda_j^2)\end{aligned} \tag{2.3.29}$$

which allows us to write the integral as

$$\begin{aligned}\frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log Q(x) &= \frac{2}{\pi}\sum_{j=1}^m \int_0^\infty \frac{dx}{x^2}\log(1+x^2\lambda_j^2)\\ &= \frac{2}{\pi}\sum_{j=1}^m \left(\left[-\frac{\log(1+x^2\lambda_j^2)}{x}\right]_{x=0}^{x\to\infty} + \int_0^\infty \frac{dx}{x}\frac{2x\lambda_j^2}{1+x^2\lambda_j^2}\right)\\ &= \frac{2}{\pi}\sum_{j=1}^m [2\lambda_j \arctan \lambda_j x]_{x=0}^{x\to\infty}\\ &= 2\sum_{j=1}^m \lambda_j\\ &= \mathrm{En}(T). \end{aligned} \tag{2.3.30}$$

□

In fact Theorem 2.3.4 is a particular case of the so-called Coulson integral formula for the energy of any graph G with n vertices given by

$$\begin{aligned}\mathrm{En}(G) = \frac{1}{2\pi}\int_{-\infty}^\infty \frac{dx}{x^2}\log\Bigg[&\left(\sum_{j=0}^{\lfloor n/2\rfloor}(-1)^j a_{2j}x^{2j}\right)^2\\ &+\left(\sum_{j=0}^{\lfloor n/2\rfloor}(-1)^j a_{2j+1}x^{2j+1}\right)^2\Bigg]\end{aligned} \tag{2.3.31}$$

where $a_0, a_1, \cdots, a_n$ are the coefficients of the characteristic polynomial of G written in the form

$$\phi(G,x) = \sum_{i=0}^n a_i x^{n-i}. \tag{2.3.32}$$

In view of the expression in (2.3.26), we are going to introduce another graph theoretical parameter μ which is closely related to the energy for trees and has the advantage of being easier to study.

Definition 2.3.5 For any graph G and any positive real number x, we define $\mu(G,x)$ by

$$\mu(G,x) = \sum_{k\geq 0} \mathrm{m}(G,k)x^{2k}. \tag{2.3.33}$$

It has the Hosoya index as a special case because

$$\mu(G,1) = \mathrm{Z}(G) \tag{2.3.34}$$

for all graphs G. In terms of μ, the energy of a tree T is given by

$$\mathrm{En}(T) = \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2}\log\mu(T,x), \tag{2.3.35}$$

see Theorem 2.3.4. In particular for an isolated vertex P_1 and the empty graph P_0 we have $\mu(P_1, x) = \mu(P_0, x) = 1$. This is because $\mathrm{m}(P_1, k) = \mathrm{m}(P_0, k) = 0$ if $k \geq 1$ and $\mathrm{m}(P_1, 0) = \mathrm{m}(P_0, 0) = 1$.

Remark 2.3.6 From equation (2.3.35), we deduce that if T and T' are trees and $\mu(T, x) \leq \mu(T', x)$ for all positive real numbers x, then $\mathrm{En}(T) \leq \mathrm{En}(T')$. If furthermore, there exists a real number $x > 0$ such that $\mu(T, x) < \mu(T', x)$, then we have $\mathrm{En}(T) < \mathrm{En}(T')$.

By similar reasoning as we used to justify equations (2.2.4) and (2.2.6) we can also show for any integer $k \geq 1$ and any vertex v of a graph G that

$$\mathrm{m}(G, k) = \mathrm{m}(G - v, k) + \sum_{w \in N_G(v)} \mathrm{m}(G - \{v, w\}, k - 1). \tag{2.3.36}$$

Moreover if G and G' are two disjoint graphs and $k \in \mathbb{N}$, then

$$\mathrm{m}(G \cup G', k) = \sum_{\substack{i+j=k \\ i,j \geq 0}} \mathrm{m}(G, i)\,\mathrm{m}(G', j). \tag{2.3.37}$$

Equations (2.3.36) and (2.3.37) lead to a lemma providing an expression for $\mu(G, x)$ in terms of $\mu(., x)$ of some smaller graphs.

Lemma 2.3.7 *Let G and G' be two disjoint graphs and let $x > 0$ be a real number. Then we have*

$$\mu(G \cup G', x) = \mu(G, x)\mu(G', x); \tag{2.3.38}$$

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

$$\mu(G, x) = \mu(G - v, x) + x^2 \sum_{w \in N_G(v)} \mu(G - \{v, w\}, x). \tag{2.3.39}$$

Proof. Let G, G', v and x be as described in the statement of the lemma. By definition we have

$$\mu(G \cup G', x) = \sum_{k \geq 0} \mathrm{m}(G \cup G', k) x^{2k} \tag{2.3.40}$$

and using (2.3.37) we find

$$\begin{aligned} \mu(G \cup G', x) &= \sum_{k \geq 0} \sum_{\substack{i+j=k \\ i,j \geq 0}} \mathrm{m}(G, i)\,\mathrm{m}(G', j) x^{2i+2j} \\ &= \sum_{i \geq 0} \mathrm{m}(G, i) x^{2i} \sum_{j \geq 0} \mathrm{m}(G', i) x^{2j} \\ &= \mu(G, x)\mu(G', x). \end{aligned} \tag{2.3.41}$$

Use of equation (2.3.36) leads to

$$
\begin{aligned}
\mu(G,x) &= \sum_{k\geq 0} \mathrm{m}(G,k)x^{2k} \\
&= \sum_{k\geq 0} \mathrm{m}(G-v,k)x^{2k} + \sum_{k\geq 0}\sum_{w\in N_G(v)} \mathrm{m}(G-\{v,w\},k-1)x^{2k} \\
&= \mu(G-v,x) + x^2 \sum_{w\in N_G(v)} \mu(G-\{v,w\},x). \qquad (2.3.42)
\end{aligned}
$$

□

Chapter 3

Extremal trees and closely related results

3.1 Introduction

Among all connected graphs with a given number of vertices, trees are the graphs with fewest edges and they always contain vertices of degree one. These are advantages that simplify the study of their independent subsets or their energy. Therefore it is not too surprising that the characterization of the extremal trees is among the earliest results obtained for each of the three parameters. For instance, short inductive proofs [PT82] can show that among all trees of order n the path P_n and the star S_n are the extremal trees with respect to each of σ, Z and En. In this chapter, these results will be proven using different approach involving graph transformations. The approach is slightly more complicated but it has an advantage of enabling us to obtain stronger results such as the description of the trees which follow the path as minimizer of σ and maximizer of Z and En .

Let us define two classes of trees that will play important roles.

Definition 3.1.1 A tree is called a *tripod* if and only if it has exactly three leaves.We denote by $T(i, j, k), 1 \leq i \leq j \leq k$ (Figure 3.1) a tripod whose three branches have lengths i, j and k, respectively.

Definition 3.1.2 Let e, d_{ij} be positive integers where $i, j \in \{1, 2\}$. We call a tree a *quadripod* if it has exactly four leaves. It is denoted by $H(e, d_{11}, d_{12}, d_{21}, d_{22})$ for $e, d_{11}, d_{12}, d_{21}$ and d_{22} as defined in Figure 3.1.

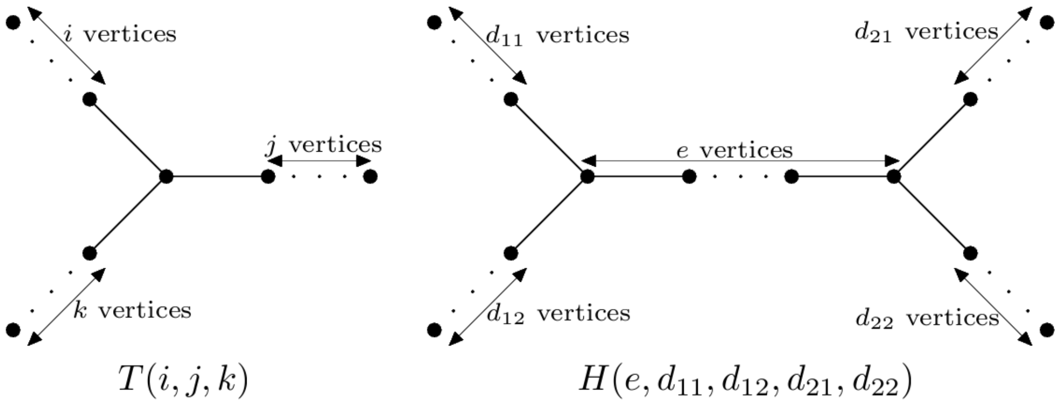


Figure 3.1: Tripod and quadripod

3.2 Minimal trees with respect to σ and maximal trees with respect to Z and En

We shall need the following simple yet crucial lemma not only in this chapter but also in the following one.

Lemma 3.2.1 *For all non-negative integers k and n such that $n \geq 3$ and real numbers $a \in (0, 1)$, the function defined on $I_n = \{1, \ldots, \lfloor \frac{n-1}{2} \rfloor\}$ by*

$$\begin{aligned} f_{a,k} : & I_n \longrightarrow \mathbb{R} \\ & i \longmapsto a^i + (-1)^k a^{n-i} \end{aligned}$$

is positive and decreasing on I_n.

Proof. For all $i \in I_n$ we know that $i < n - i$, and since $a \in (0, 1)$ it is clear that $a^i > |(-1)^k a^{n-i}|$, therefore $f_{a,k}(i) > 0$ for all $i \in I_n$.

Next, let us show that $f_{a,k}$ is decreasing. For all $i \in I_n \backslash \{\lfloor \frac{n-1}{2} \rfloor\}$ we have

$$\begin{aligned} f_{a,k}(i+1) - f_{a,k}(i) &= a^{i+1} + (-1)^k a^{n-(i+1)} - a^i - (-1)^k a^{n-i} && (3.2.1) \\ &= (a-1)(a^i - (-1)^k a^{n-i-1}) && (3.2.2) \end{aligned}$$

and

$$\begin{aligned} 0 \leq i < \frac{n-1}{2} &\Rightarrow 0 \leq 2i < n-1 \\ &\Rightarrow 0 \leq i < n-i-1 \\ &\Rightarrow a^i > a^{n-i-1} > 0 \\ &\Rightarrow a^i - (-1)^k a^{n-i-1} > 0. && (3.2.3) \end{aligned}$$

Hence equation (3.2.2) gives $f_{a,k}(i+1) < f_{a,k}(i)$ which means that $f_{a,k}$ is decreasing on I_n. $\square$

In addition to the explicit expressions for $\sigma(P_n)$ and $\mathrm{Z}(P_n)$ that we have seen in equations (2.2.12) and (2.2.13), we need a formula for $\mu(P_n, x)$ in terms of n and x. Let $n \geq 2$ be an integer and let v be an end vertex of the path P_n. The second equation in Lemma 2.3.7 leads to

$$\begin{aligned}\mu(P_n, x) &= \mu(P_n - v, x) + x^2 \sum_{w \in N_{P_n}(v)} \mu(P_n - \{v, w\}, x) \\ &= \mu(P_{n-1}, x) + x^2 \mu(P_{n-2}, x). \end{aligned} \tag{3.2.4}$$

This means that the sequence $(\mu(P_n, x))_{n \geq 0}$ satisfies a linear recurrence relation with characteristic equation $t^2 - t - x^2 = 0$ which has roots

$$X(x) = \frac{1 + \sqrt{1 + 4x^2}}{2} \tag{3.2.5}$$

and

$$\widetilde{X}(x) = \frac{1 - \sqrt{1 + 4x^2}}{2}. \tag{3.2.6}$$

Thus, $\mu(P_n, x)$ can be written in the form

$$\mu(P_n, x) = A(x) X^n(x) + B(x) \widetilde{X}^n(x), \tag{3.2.7}$$

where $A(x)$ and $B(x)$ are such that

$$\begin{cases} \mu(P_0, x) = A(x) + B(x) = 1, \\ \mu(P_1, x) = A(x) X(x) + B(x) \widetilde{X}(x) = 1. \end{cases} \tag{3.2.8}$$

After some calculation we have

$$A(x) = \frac{X(x)}{X(x) - \widetilde{X}(x)}, \tag{3.2.9}$$

$$B(x) = -\frac{\widetilde{X}(x)}{X(x) - \widetilde{X}(x)} \tag{3.2.10}$$

and therefore

$$\mu(P_n, x) = \frac{X^{n+1}(x) - \widetilde{X}^{n+1}(x)}{X(x) - \widetilde{X}(x)}. \tag{3.2.11}$$

Notation 3.2.2 Let G be a connected graph with at least two vertices, and let v be a vertex of G. Let $n \geq k$ be integers. We denote by $P(n, k, G, v)$ the graph which results from identifying v with the vertex v_k of a path $v_1, \cdots, v_n$ as in Figure 3.2.

Any tree with at least 3 vertices can be written in the form $P(n, k, G, v)$ for some n, k, G and v appropriately chosen. Without loss of generality we can restrict our attention to $P(n, k, G, v)$ for $\lfloor \frac{n}{2} \rfloor \geq k \geq 1$ only since

$$P(n, k, G, v) = P(n, n + 1 - k, G, v) \tag{3.2.12}$$

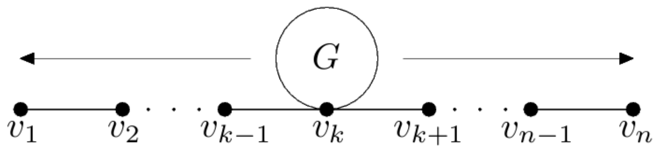


Figure 3.2: $P(n, k, G, v)$

for all $n \geq k \geq 1$.

The next lemma describes the behaviour of $\sigma(P(n, k, G, v))$, $\mathrm{Z}(P(n, k, G, v))$ and $\mathrm{En}(P(n, k, G, v))$ as a function of k. It is a useful tool to compare the number of independent subsets and energy of different trees.

Lemma 3.2.3 ([ZL06, Wag07]) *Let n be a positive integer, and write it as $n = 4m + h$, for some $h \in \{1, 2, 3, 4\}$ and for some $m \in \mathbb{N}$. Then the following inequalities hold*

$$\begin{aligned} &\sigma(P(n, 2, G, v)) > \sigma(P(n, 4, G, v)) > \cdots > \sigma(P(n, 2m + 2l, G, v)) \\ &> \sigma(P(n, 2m + 1, G, v)) > \cdots > \sigma(P(n, 3, G, v)) > \sigma(P(n, 1, G, v)), \end{aligned}$$

$$\begin{aligned} &\mathrm{Z}(P(n, 2, G, v)) < \mathrm{Z}(P(n, 4, G, v)) < \cdots < \mathrm{Z}(P(n, 2m + 2l, G, v)) \\ &< \mathrm{Z}(P(n, 2m + 1, G, v)) < \cdots < \mathrm{Z}(P(n, 3, G, v)) < \mathrm{Z}(P(n, 1, G, v)) \end{aligned}$$

and

$$\begin{aligned} &\mathrm{En}(P(n, 2, G, v)) < \mathrm{En}(P(n, 4, G, v)) < \cdots < \mathrm{En}(P(n, 2m + 2l, G, v)) \\ &< \mathrm{En}(P(n, 2m + 1, G, v)) < \cdots < \mathrm{En}(P(n, 3, G, v)) < \mathrm{En}(P(n, 1, G, v)) \end{aligned}$$

where $l = \lfloor \frac{h-1}{2} \rfloor$.

Before we prove the lemma, it is worth to be pointed out that varying k in $P(n, k, G, v)$ amounts to "sliding" the subgraph G along the path to which it is attached. This explains why the lemma is also called "Sliding along a path" in [WG10]. The lemma means that if we consider only even positions of G in $P(n, k, G, v)$, then increasing k will increase Z and En but decrease σ, and for odd positions of G it is the other way around.

Proof. Let n, i, and j be non-negative integers such that $i \in \{0, \ldots, \lfloor \frac{n-2}{2} \rfloor\}$ and $i + j = n - 1$. Let $C = \sigma(G - v)$ and $D = \sigma(G - (\{v\} \cup N_G(v)))$. Since G is connected and contains at least two vertices, $N_G(v)$ is not empty and consequently $C - D > 0$. Lemma 2.2.3 applied to $P(n, i + 1, G, v)$ gives

$$\begin{aligned} \sigma(P(n, i + 1, G, v)) &= \sigma(P(n, i + 1, G, v) - v) \\ &\quad + \sigma(P(n, i + 1, G, v) - (\{v\} \cup N_{P(n,i+1,G,v)}(v))) \\ &= C\sigma(P_i)\sigma(P_j) + D\sigma(P_{i-1})\sigma(P_{j-1}). \end{aligned} \tag{3.2.13}$$

The formula is still valid even for $i = 0$ by taking $\sigma(P_{-1}) = F_0 = 1$ which agrees with equation (2.2.12).

Let $X = \frac{1+\sqrt{5}}{2}$ and $\widetilde{X} = \frac{1-\sqrt{5}}{2}$, then by equation (2.2.12) we have

$$\begin{aligned}
&\sigma(P(n, i+1, G, v)) \\
&\quad = \frac{C}{5}(X^{i+2} - \widetilde{X}^{i+2})(X^{j+2} - \widetilde{X}^{j+2}) + \frac{D}{5}(X^{i+1} - \widetilde{X}^{i+1})(X^{j+1} - \widetilde{X}^{j+1}) \\
&\quad = \frac{1}{5}(C(X^{i+j+4} + \widetilde{X}^{i+j+4}) + D(X^{i+j+2} + \widetilde{X}^{i+j+2})) \\
&\qquad\qquad + \frac{(-1)^{i+1}(C-D)}{5}(X^{j-i} + \widetilde{X}^{j-i}). \qquad (3.2.14)
\end{aligned}$$

Since

$$\begin{aligned}
X^{j-i} + \widetilde{X}^{j-i} &= X^{i+j}\left(\left(\frac{1}{X^2}\right)^i + \left(\frac{\widetilde{X}}{X}\right)^{i+j}\left(\frac{1}{\widetilde{X}^2}\right)^i\right) \\
&= X^{i+j}\left(\left(\frac{1}{X^2}\right)^i + \left(\frac{-1}{X^2}\right)^{i+j}\left(\frac{1}{\widetilde{X}^2}\right)^i\right) \\
&= X^{i+j}\left(\left(\frac{1}{X^2}\right)^i + (-1)^{i+j}\left(\frac{1}{X^2}\right)^j\right), \qquad (3.2.15)
\end{aligned}$$

we have

$$\begin{aligned}
\sigma(P(n, i+1, G, v)) &= F(n) + \frac{(-1)^{i+1}(C-D)}{5}X^{i+j}\left(\left(\frac{1}{X^2}\right)^i + (-1)^{i+j}\left(\frac{1}{X^2}\right)^j\right) \\
&= F(n) + \frac{(-1)^{i+1}(C-D)}{5}X^{n-1}f_{X^{-2},n-1}(i) \qquad (3.2.16)
\end{aligned}$$

where

$$F(n) = \frac{1}{5}(C(X^{n+3} + \widetilde{X}^{n+3}) + D(X^{n+1} + \widetilde{X}^{n+1})) \qquad (3.2.17)$$

and $f_{X^{-2},n-1}$ is as in Lemma 3.2.1. $f_{X^{-2},n-1}$ is, then, positive valued and decreasing on $\{0, 1, \ldots, \lfloor \frac{n-2}{2} \rfloor\}$ which is exactly the set of values of i that we are interested in.

If we only consider even positions of G which correspond to odd values of i, equation (3.2.16) shows that $\sigma(P(n, i+1, G, v))$ is greater than $F(n)$ and it decreases with i just as $f_{X^{-2},n-1}$ does. In the other hand, for odd positions of G we have to restrict to even i and then $\sigma(P(n, i+1, G, v))$ is less than $F(n)$ and it increases as a function of i. This proves the first part of the lemma.

Next, we prove the following inequalities with respect to $\mu(., x)$

$$\begin{aligned}
&\mu(P(n, 2, G, v), x) < \mu(P(n, 4, G, v), x) < \cdots < \mu(P(n, 2m+2l, G, v), x) \\
&< \mu(P(n, 2m+1, G, v), x) < \cdots < \mu(P(n, 3, G, v), x) < \mu(P(n, 1, G, v), x)
\end{aligned}$$

for all real numbers $x > 0$, and the inequalities with respect to Z and the inequalities with respect to En in the rest of the lemma will follow by equation (2.3.34) and Remark 2.3.6.

We keep the notations i, j, n and the relation $n-1 = i+j$. From equation (2.3.39) in Lemma 2.3.7 we obtain

$$\mu(P(n, i+1, G, v), x) = \left(\mu(G-v, x) + x^2 \sum_{w \in N_G(v)} \mu(G - \{v, w\}, x)\right) \mu(P_i, x)\mu(P_j, x)$$
$$+ x^2\mu(G-v, x)(\mu(P_{i-1}, x)\mu(P_j, x) + \mu(P_i, x)\mu(P_{j-1}, x)). \tag{3.2.18}$$

Using the notations in the explicit expression (3.2.11) we have

$$X(x)\widetilde{X}(x) = -x^2 \tag{3.2.19}$$

and

$$\begin{aligned}
\mu(P_i, x)\mu(P_j, x) &= \frac{X^{i+1}(x) - \widetilde{X}^{i+1}(x)}{X(x) - \widetilde{X}(x)} \times \frac{X^{j+1}(x) - \widetilde{X}^{j+1}(x)}{X(x) - \widetilde{X}(x)} \\
&= \frac{X^{i+j+2}(x) + \widetilde{X}^{i+j+2}(x) - (-x^2)^{i+1}(X^{j-i}(x) + \widetilde{X}^{j-i}(x))}{(X(x) - \widetilde{X}(x))^2} \\
&= \frac{X^{i+j+2}(x) + \widetilde{X}^{i+j+2}(x)}{(X(x) - \widetilde{X}(x))^2} \\
&\quad - \frac{(-x^2)^{i+1}X^{i+j}(x)}{(X(x) - \widetilde{X}(x))^2}\left(X^{-2i}(x) + \frac{\widetilde{X}^{i+j}(x)}{X^{i+j}(x)}\widetilde{X}^{-2i}(x)\right).
\end{aligned} \tag{3.2.20}$$

Since

$$\begin{aligned}
X^{-2i}(x) + \frac{\widetilde{X}^{i+j}(x)}{X^{i+j}(x)}\widetilde{X}^{-2i}(x) &= \left(\frac{1}{X^2(x)}\right)^i + \left(\frac{\widetilde{X}(x)}{X(x)}\right)^{i+j}\left(\frac{1}{\widetilde{X}^2(x)}\right)^i \\
&= \left(\frac{1}{X^2(x)}\right)^i + \left(\frac{-x^2}{X^2(x)}\right)^{i+j}\left(\frac{1}{\widetilde{X}^2(x)}\right)^i \\
&= \left(\frac{1}{X^2(x)}\right)^i \\
&\quad + (-1)^{i+j}\left(\frac{1}{x^2}\right)^i\left(\frac{x^2}{X^2(x)}\right)^j,
\end{aligned} \tag{3.2.21}$$

it follows that

$$\begin{aligned}
\mu(P_i, x)\mu(P_j, x) &= \frac{X^{i+j+2}(x) + \widetilde{X}^{i+j+2}(x)}{(X(x) - \widetilde{X}(x))^2} \\
&\quad + \frac{(-1)^i x^2 X^{i+j}(x)}{(X(x) - \widetilde{X}(x))^2}\left(\left(\frac{x^2}{X^2(x)}\right)^i + (-1)^{i+j}\left(\frac{x^2}{X^2(x)}\right)^j\right).
\end{aligned} \tag{3.2.22}$$

Replacing i by $i-1$ we have

$$\mu(P_{i-1},x)\mu(P_j,x) = \frac{X^{i+j+1}(x)+\widetilde{X}^{i+j+1}(x)}{(X(x)-\widetilde{X}(x))^2} - \frac{(-1)^i X^{i+j+1}(x)}{(X(x)-\widetilde{X}(x))^2}\left(\left(\frac{x^2}{X^2(x)}\right)^i + (-1)^{i+j-1}\left(\frac{x^2}{X^2(x)}\right)^{j+1}\right), \quad (3.2.23)$$

while replacement of j by $j-1$ leads to

$$\mu(P_i,x)\mu(P_{j-1},x) = \frac{X^{i+j+1}(x)+\widetilde{X}^{i+j+1}(x)}{(X(x)-\widetilde{X}(x))^2} + \frac{(-1)^i X^{i+j+1}(x)}{(X(x)-\widetilde{X}(x))^2}\left(\left(\frac{x^2}{X^2(x)}\right)^{i+1} + (-1)^{i+j-1}\left(\frac{x^2}{X^2(x)}\right)^{j}\right). \quad (3.2.24)$$

Adding (3.2.23) to (3.2.24) gives

$$\mu(P_{i-1},x)\mu(P_j,x)+\mu(P_i,x)\mu(P_{j-1},x) = \frac{2X^{i+j+1}(x)+2\widetilde{X}^{i+j+1}(x)}{(X(x)-\widetilde{X}(x))^2} + \frac{(-1)^i X^{i+j-1}(x)(x^2-X^2(x))}{(X(x)-\widetilde{X}(x))^2}\left(\left(\frac{x^2}{X^2(x)}\right)^{i} + (-1)^{i+j}\left(\frac{x^2}{X^2(x)}\right)^{j}\right). \quad (3.2.25)$$

If we let

$$C_1 = \frac{(X^{n+1}(x)+\widetilde{X}^{n+1}(x))\left(\mu(G-v,x)+x^2\sum_{w\in N_G(v)}\mu(G-\{v,w\},x)\right)}{(X(x)-\widetilde{X}(x))^2} + \frac{(2X^n(x)+2\widetilde{X}^n(x))x^2\mu(G-v,x)}{(X(x)-\widetilde{X}(x))^2} \quad (3.2.26)$$

and

$$\begin{aligned} C_2 &= \frac{x^2X^{n-1}(x)\left(\mu(G-v,x)+x^2\sum_{w\in N_G(v)}\mu(G-\{v,w\},x)\right)}{(X(x)-\widetilde{X}(x))^2} + \frac{X^{n-2}(x)(x^2-X^2(x))x^2\mu(G-v,x)}{(X(x)-\widetilde{X}(x))^2} \\ &= \frac{x^4X^{n-1}(x)\sum_{w\in N_G(v)}\mu(G-\{v,w\},x)}{(X(x)-\widetilde{X}(x))^2} + \frac{x^2X^{n-2}(x)(-X^2(x)+X(x)+x^2)\mu(G-v,x)}{(X(x)-\widetilde{X}(x))^2} \\ &= \frac{x^4X^{n-1}(x)\sum_{w\in N_G(v)}\mu(G-\{v,w\},x)}{(X(x)-\widetilde{X}(x))^2} \end{aligned} \quad (3.2.27)$$

then we have

$$\mu(P(n,i+1,G,v),x) = C_1 + (-1)^i C_2 \left(\left(\frac{x^2}{X^2(x)} \right)^i + (-1)^{i+j} \left(\frac{x^2}{X^2(x)} \right)^j \right)$$
$$= C_1 + (-1)^i C_2 f_{\frac{x^2}{X^2(x)},n-1}(i) \qquad (3.2.28)$$

where the function $f_{\frac{x^2}{X^2(x)},n-1}$ is as described in Lemma 3.2.1, hence it is decreasing for $i \in \{0, 1, \ldots, \lfloor \frac{n-1}{2} \rfloor\}$. C_1 and C_2 are positive because $|X(x)| > |\widetilde{X}(x)|$. Knowing this we can conclude that

- if we only consider even values of i, then $\mu(P(n,i+1,G,v),x)$ is decreasing as a function of i and $\mu(P(n,i+1,G,v),x) > C_1$
- and on the contrary if we restrict ourselves to odd values of i, then $\mu(P(n,i+1,G,v),x)$ increases with i and $\mu(P(n,i+1,G,v),x) < C_1$.

This finally proves the claim. □

Remark 3.2.4 If G is a tree, $P(n,k,G,v)$ is also a tree and for all $k \geq 2$ it is clear that $P(n,k,G,v)$ has one more leaf than $P(n,1,G,v)$. Hence, if a tree T has more than two leaves, then there is a tree T' with the same order as T and fewer leaves than T such that $\sigma(T) > \sigma(T')$, $\mathrm{Z}(T) < \mathrm{Z}(T')$ and $\mathrm{En}(T) < \mathrm{En}(T')$. T' can be obtained by the transformation illustrated in Figure 3.3.

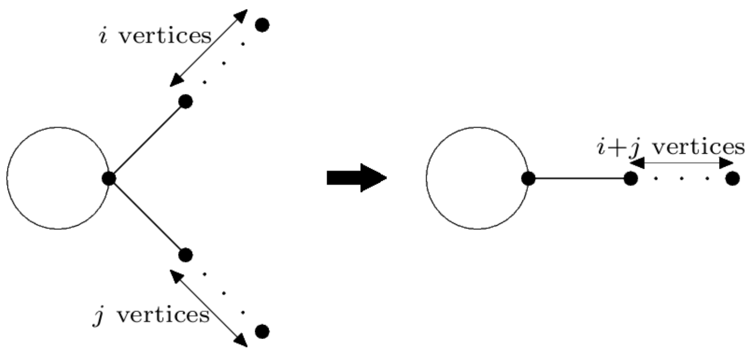


Figure 3.3: Transformation of subtrees

Therefore, the minimal tree with respect to σ, the maximal tree with respect to Z and the maximal tree with respect to En must have the smallest number of leaves. Thus the next theorem follows easily.

Theorem 3.2.5 *P_n is the tree with order n which is minimal with respect to σ, maximal with respect to* Z *and maximal with respect to* En.

Proof. Given a fixed order n, P_n is clearly the unique tree with minimum number of leaves. Hence, by Remark 3.2.4, P_n is the unique minimal tree with respect to σ, the unique tree with maximum Z and the unique tree with maximum En. $\square$

Furthermore, by Remark 3.2.4 we know that if all trees are put in increasing order with respect to σ or in decreasing order with respect to Z and En, P_n is followed by the tripod with smallest σ and greatest Z and En. One can easily obtain from Lemma 3.2.3 that this tripod is $T(2,2,n-5)$.

Note that by Lemma 3.2.3, we can compare any two tripods of the same order which have branches of the same length. In [Wag07], a complete ordering of all tripods with respect to the Merrifield-Simmons index and the Hosoya index is obtained. Only a few additional inequalities have to be proven by another approach. Furthermore, the following theorem is also proven in the same article.

Theorem 3.2.6 *For $n \geq 13$ we have*

$$\begin{array}{lllll}
\sigma(P_n) & & & & \\
<\sigma(T(2,2,n-5)) & <\sigma(T(2,4,n-7)) & <\cdots & <\sigma(T(2,5,n-8)) & <\sigma(T(2,3,n-6)) \\
<\sigma(T(4,4,n-9)) & <\sigma(T(4,6,n-11)) & <\cdots & <\sigma(T(4,7,n-12)) & <\sigma(T(4,5,n-10)) \\
\quad\vdots & \quad\vdots & \quad\vdots & \quad\vdots & \quad\vdots \\
<\sigma(T(3,4,n-8)) & <\sigma(T(3,6,n-10)) & <\cdots & <\sigma(T(3,5,n-9)) & <\sigma(T(3,3,n-7)) \\
<\sigma(T(1,2,n-4)) & <\sigma(T(1,4,n-6)) & <\cdots & <\sigma(T(1,3,n-5)) & <\sigma(H(2,2,2,2,n-8))
\end{array}$$

and for any tree T not in the above list we have $\sigma(H(2,2,2,2,n-8)) < \sigma(T)$. On the other hand we also have

$$\begin{array}{lllll}
\mathrm{Z}(P_n) & & & & \\
>\mathrm{Z}(T(2,2,n-5)) & >\mathrm{Z}(T(2,4,n-7)) & >\cdots & >\mathrm{Z}(T(2,5,n-8)) & >\mathrm{Z}(T(2,3,n-6)) \\
>\mathrm{Z}(T(4,4,n-9)) & >\mathrm{Z}(T(4,6,n-11)) & >\cdots & >\mathrm{Z}(T(4,7,n-12)) & >\mathrm{Z}(T(4,5,n-10)) \\
\quad\vdots & \quad\vdots & \quad\vdots & \quad\vdots & \quad\vdots \\
>\mathrm{Z}(T(3,4,n-8)) & >\mathrm{Z}(T(3,6,n-10)) & >\cdots & >\mathrm{Z}(T(3,5,n-9)) & >\mathrm{Z}(T(3,3,n-7)) \\
>\mathrm{Z}(T(1,2,n-4)) & >\mathrm{Z}(T(1,4,n-6)) & >\cdots & >\mathrm{Z}(T(1,5,n-7)) & >\mathrm{Z}(H(2,2,2,2,n-8)) \\
=\mathrm{Z}(H(n-8,2,2,2,2)), & & & &
\end{array}$$

and any tree T not mentioned in this list satisfies $\mathrm{Z}(H(n-8,2,2,2,2)) > \mathrm{Z}(T)$.

The lists are very similar except that $H(n-8,2,2,2,2)$ appears one position earlier in the second list compared to the first one.

Proof. The main idea of the proof is almost exactly the same as that of the proof Theorems 4.3.4 and 4.4.4 given in Chapter 4: First, find out the tree of order n whose number of leaves is more than three and such that it has minimum σ and maximum Z, then compare it to tripods. We refer the reader to [Wag07] for details. $\square$

The tree with minimum Merrifield-Simmons index and maximum Hosoya index among all elements of order n in any subclass of trees which contains tripods other than $T(1,1,n-3)$ and $T(1,3,n-4)$ can be obtained with the help of Theorem 3.2.6. For instance in the following corollary, we have a partial result for the class of trees of a given diameter.

Corollary 3.2.7 *Let $n \geq 6$ and c be positive integers such that*

$$\frac{2n}{3} \leq c \leq n-2. \tag{3.2.29}$$

Then among all trees of order n and of diameter c, the tree with minimum Merrifield-Simmons index and maximum Hosoya index is

$$Tr(c,n) = T\left(n-1-c, 2\left\lceil \frac{n-1-c}{2} \right\rceil, c-2\left\lceil \frac{n-1-c}{2} \right\rceil\right). \tag{3.2.30}$$

Proof. Let $\mathcal{D}_n^c$ be the set of all trees of order n and diameter c. Assume that c and n satisfy the condition (3.2.29), and let $M(c,n)$ be an element of $\mathcal{D}_n^c$ with minimum Merrifield-Simmons index (or maximum Hosoya index). Then $\mathcal{D}_n^c$ does not contain the path P_n (whose diameter is $n-1$). Since

$$2\left\lceil \frac{n-1-c}{2} \right\rceil \geq n-1-c \tag{3.2.31}$$

and (recall that $2n \leq 3c$)

$$\begin{aligned} c-2\left\lceil \frac{n-1-c}{2} \right\rceil &\geq c-(n-c) \\ &\geq 2c-n+2n-3c \\ &= n-c \\ &\geq 2\left\lceil \frac{n-1-c}{2} \right\rceil, \end{aligned} \tag{3.2.32}$$

we have

$$\operatorname{diam}(Tr(c,n)) = 2\left\lceil \frac{n-1-c}{2} \right\rceil + c - 2\left\lceil \frac{n-1-c}{2} \right\rceil = c \tag{3.2.33}$$

meaning that $\mathcal{D}_c^n$ contains at least a tripod, namely $Tr(c,n)$. Furthermore, knowing that the second shortest branch of $Tr(c,n)$ is of even length, we deduce that $Tr(c,n)$ is different from $T(1,1,n-3)$ and $T(1,3,n-5)$. Now, we can deduce from Theorem 3.2.6 that $M(c,n)$ exists and it is a tripod, say $M(c,n) = T(i,j,c-j)$.

All tripods of order n and diameter c have a shortest branch of length $i = n-1-c$. Considering the shortest branch as a “sliding” branch, we deduce from Lemma 3.2.3 that j must be the smallest even number greater or equal to i, this leads to

$$M(c,n) = Tr(c,n). \tag{3.2.34}$$

□

Not much is known about trees with small diameter: for results on trees with diameter at most 5, see [KTWZ07] for Merrifield-Simmons index and [Ou08] for Hosoya index.

If we restrict ourselves to the class of trees whose maximum degree is fixed, then we can still use Lemma 3.2.3 to obtain the following theorem.

Theorem 3.2.8 ([Wag07]) *Let $1 \le c_1 \le c_2 \le \cdots \le c_k$ be integers and let $S(c_1, c_2, \ldots, c_k)$ be the graph which is obtained by merging an end vertex from each of the paths $P_{c_1+1}, P_{c_2+1}, \ldots, P_{c_k+1}$. For a given number of vertices n and given maximum degree d, the tree with minimum Merrifield-Simmons index, maximum Hosoya index and maximum energy is $S(c_1, c_2, \ldots, c_d)$, where*

$$\begin{cases} c_1 = \cdots = c_{2d-n+1} = 1 \text{ and } c_{2d-n+2} = \cdots = c_d = 2 & \text{if } d > \frac{n-1}{2}, \\ c_1 = \cdots = c_{d-1} = 2 \text{ and } c_d = n+1-2d & \text{if } d \le \frac{n-1}{2}. \end{cases} \tag{3.2.35}$$

Proof. Let T be a tree with n vertices and with maximum degree d. Let us consider a vertex v of degree d in T. Assume that T is minimal with respect to σ, then necessarily all the branches of v are paths, otherwise we can apply the process in Figure 3.3 to reduce the number of leaves in a branch which is not yet a path and contradict the minimality of $\sigma(T)$. This means that $T = S(c_1, c_2, \ldots, c_d)$ for some positive integers $1 \le c_1 \le c_2 \le \cdots \le c_d$.

If $c_d = 2$ then we are done. Otherwise $c_d > 2$, and we claim that $c_1 = c_2 = \cdots = c_{d-1} = 2$. If this is not the case, then there are two possibilities:

- There is $i \in \{1, 2, \ldots, d-1\}$ such that $c_i = 1$, but then by taking

  $$G = S(c_1, \ldots, c_{i-1}, c_{i+1}, \ldots, c_{d-1}) \tag{3.2.36}$$

  we could apply Lemma 3.2.3 and have

  $$\begin{aligned} \sigma(T) &= \sigma(P(c_d+2, 2, G, v)) \\ &> \sigma(P(c_d+2, 3, G, v)) \\ &= \sigma(S(c_1, \ldots, c_{i-1}, 2, c_{i+1}, \ldots, c_d - 1)) \end{aligned} \tag{3.2.37}$$

  which contradicts the minimality of $\sigma(T)$ since the maximum degree of $S(c_1, \ldots, c_{i-1}, 2, c_{i-1}, \ldots, c_d - 1)$ is also d.

- There is $i \in \{1, 2, \ldots, d-1\}$ such that $c_i \ge 3$. By considering again

  $$G = S(c_1, \ldots, c_{i-1}, c_{i+1}, \ldots, c_{d-1}) \tag{3.2.38}$$

and by applying Lemma 3.2.3 we obtain

$$\begin{aligned}\sigma(T) &= \sigma(P(c_d + c_i + 1, c_i + 1, G, v)) \\ &> \sigma(P(c_d + c_i + 1, 3, G, v)) \\ &= \sigma(S(c_1, \dots, c_{i-1}, 2, c_{i+1}, \dots, c_d + c_i - 2)), \qquad (3.2.39)\end{aligned}$$

which contradicts again the minimality of $\sigma(T)$.

For the case of Z and En, one has to repeat exactly the same process and use the corresponding inequalities in Lemma 3.2.3. □

3.3 Maximal trees with respect to σ and minimal trees with respect to Z and En

In 1982 Prodinger and Tichy [PT82] showed that among all trees with n vertices the star S_n maximizes the Merrifield-Simmons index. By an approach using a graph transformation, as in Lemma 3.3.3, we can reprove the same result and some others related to it.

Definition 3.3.1 We call a tree a *star* if it has a vertex v, called the *centre*, adjacent to all other vertices. A star with n vertices will be denoted by S_n, see Figure 3.4 for an example.

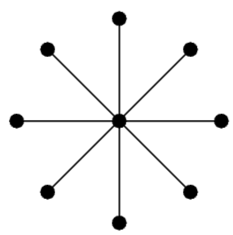


Figure 3.4: S_9

For convenience, we set $S_1 = P_1$ and $S_0 = P_0$.

Definition 3.3.2 Let $k \geq 3$ be an integer, and let G be a graph and v one of its vertices. $S(k, G, v)$ is the graph obtained by identifying the centre of S_k and the vertex v. $S'(k, G, v)$ is the graph obtained by identifying a leaf of S_k and the vertex v. See Figure 3.5 for examples.

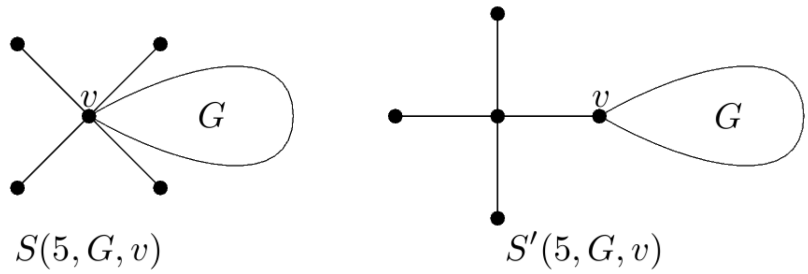


Figure 3.5: Examples of graphs described in Definition 3.3.2

Lemma 3.3.3 *Let v be a vertex in a graph G such that $N_G(v) \neq \varnothing$. Then the relations*

$$\sigma(S(k,G,v)) > \sigma(S'(k,G,v)), \tag{3.3.1}$$

$$\mu(S(k,G,v),x) < \mu(S'(k,G,v),x) \tag{3.3.2}$$

for all real numbers $x > 0$,

$$\mathrm{Z}(S(k,G,v)) < \mathrm{Z}(S'(k,G,v)) \tag{3.3.3}$$

and

$$\mathrm{En}(S(k,G,v)) < \mathrm{En}(S'(k,G,v)) \tag{3.3.4}$$

hold for all integers $k \geq 3$.

Proof. First, for inequality (3.3.1), we know that

$$\sigma(S(k,G,v)) = 2^{k-1}\sigma(G-v) + \sigma(G - (\{v\} \cup N_G(v))) \tag{3.3.5}$$

and

$$\sigma(S'(k,G,v)) = (2^{k-2}+1)\sigma(G-v) + 2^{k-2}\sigma(G - (\{v\} \cup N_G(v))). \tag{3.3.6}$$

Hence,

$$\begin{aligned}\sigma(S(k,G,v)) &- \sigma(S'(k,G,v)) \\ &= (2^{k-2}-1)(\sigma(G-v) - \sigma(G - (\{v\} \cup N_G(v)))),\end{aligned} \tag{3.3.7}$$

and the difference is clearly positive for $k \geq 3$, so we can conclude (3.3.1).

We only have to prove inequality (3.3.2) for all real numbers $x > 0$, and the two inequalities (3.3.3) and (3.3.4) follow by the relation (2.3.34) and by Remark 2.3.6. For this, let u be the centre of the star that is attached to G to form $S'(k, G, v)$. Use of equation (2.3.39) gives

$$\begin{aligned}
\mu(S'(k,G,v),x) &= \mu(S'(k,G,v)-u,x) + x^2 \sum_{w \in N_{S'(k,G,v)}(u)} \mu(S'(k,G,v)-\{u,w\},x) \\
&= \mu(G,x) + (k-2)x^2\mu(G,x) + x^2\mu(G-v,x) \\
&= \mu(G-v,x) + x^2 \sum_{w \in N_G(v)} \mu(G-\{w,v\}) \\
&\qquad + (k-2)x^2\mu(G,x) + x^2\mu(G-v,x) \\
&> (1+(k-1)x^2)\mu(G-v,x) + x^2 \sum_{w \in N_G(v)} \mu(G-\{w,v\}) \\
&= \mu(S(k,G,v),x). \qquad (3.3.8)
\end{aligned}$$

□

A more crucial lemma follows from Lemma 3.3.3.

Lemma 3.3.4 *If T is a tree with diameter $d \geq 3$, then there is a tree T' of diameter $d-1$ such that*

$$\sigma(T') > \sigma(T), \qquad (3.3.9)$$
$$\mathrm{Z}(T') < \mathrm{Z}(T) \qquad (3.3.10)$$

and

$$\mathrm{En}(T') < \mathrm{En}(T). \qquad (3.3.11)$$

Proof. We restrict ourselves to $d-1 \geq 2$ because it is impossible for a tree with more than two vertices to have diameter 1.

Let T be a tree such that $\mathrm{diam}(T) = d \geq 3$. Let P_{d+1} be a path of maximum length in T, thus the length of P_{d+1} is d, and let v_1, v_2, v_3, v_4 be the first four vertices of P_{d+1}. Then all the neighbours of v_2 are leaves except v_3 because otherwise we could find a path of length $d+1$ in T which is impossible. Let $k = |N_T(v_2)| + 1$, so that we have

$$T = S'(k, T - (N_{T-v_3}(v_2) \cup \{v_2\}), v_3), \qquad (3.3.12)$$

see Figure 3.6. If we take

$$T_1 = S(k, T - (N_{T-v_3}(v_2) \cup \{v_2\}), v_3), \qquad (3.3.13)$$

then $\mathrm{diam}(T_1) \leq \mathrm{diam}(T)$ and Lemma 3.3.3 shows that $\sigma(T_1) > \sigma(T)$, $\mathrm{Z}(T_1) < \mathrm{Z}(T)$ and $\mathrm{En}(T_1) < \mathrm{En}(T)$.

If $\mathrm{diam}(T_1) = \mathrm{diam}(T) - 1$, then we are done, otherwise $\mathrm{diam}(T_1) = \mathrm{diam}(T)$, and we apply the same process again to T_1 to obtain T_2. Since

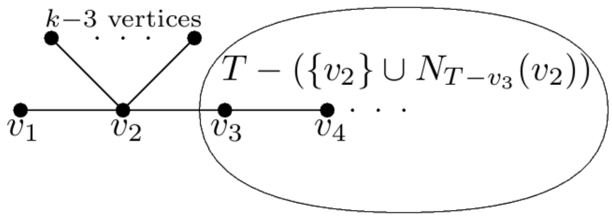


Figure 3.6: $S'(k, T - (\{v_2\} \cup N_{T-v_3}(v_2)), v_3)$

T is a finite graph, there must be an integer i such that iterating the process i times leads to a tree T_i such that $\mathrm{diam}(T_i) = \mathrm{diam}(T) - 1$,

$$\sigma(T_i) > \cdots > \sigma(T_1) > \sigma(T), \tag{3.3.14}$$
$$\mathrm{Z}(T_i) < \cdots < \mathrm{Z}(T_1) < \mathrm{Z}(T) \tag{3.3.15}$$

and

$$\mathrm{En}(T_i) < \cdots < \mathrm{En}(T_1) < \mathrm{En}(T). \tag{3.3.16}$$

□

Via this lemma, we can now prove the well known fact that the star S_n has maximum Merrifield-Simmons index, minimum Hosoya index and minimum energy among all trees of order $n \in \mathbb{N}$.

Theorem 3.3.5 *For any tree T with n vertices, we have either $\sigma(S_n) > \sigma(T)$, $\mathrm{Z}(S_n) < \mathrm{Z}(T)$ and $\mathrm{En}(S_n) < \mathrm{En}(T)$ or $T = S_n$.*

Proof. For the cases $n = 1, 2, 3$ the theorem is trivial, since there is only one tree corresponding to each value of n. For $n \geq 4$, it is impossible to have a tree of order n and diameter 1. Thus, from Lemma 3.3.4 we deduce that the maximal tree with respect to σ and the minimal tree with respect to Z and En must have diameter 2. Hence, there is no other choice than S_n which is the only tree of order n with diameter 2. □

The Merrifield-Simmons index and the Hosoya index of $S_n, n \geq 1$, are respectively

$$\sigma(S_n) = 2^{n-1} + 1 \tag{3.3.17}$$

and

$$\mathrm{Z}(S_n) = n. \tag{3.3.18}$$

For all positive real numbers x and positive integers n, we have

$$\mu(S_n, x) = 1 + x^2(n-1), \tag{3.3.19}$$

hence

$$\begin{aligned}
\mathrm{En}(S_n) &= \frac{2}{\pi}\int_0^{+\infty}\frac{dx}{x^2}\log(1+x^2(n-1)) \\
&= -\frac{2}{\pi}\left[\frac{\log(1+x^2(n-1))}{x}\right]_{x\to 0}^{x\to+\infty} + \frac{4(n-1)}{\pi}\int_0^{+\infty} dx\frac{1}{1+x^2(n-1)} \\
&= \frac{4\sqrt{n-1}}{\pi}\left[\arctan x\sqrt{n-1}\right]_{x\to 0}^{x\to+\infty} \\
&= 2\sqrt{n-1}. \qquad (3.3.20)
\end{aligned}$$

For σ and Z, Theorem 3.3.5 can be extended to a stronger corollary.

Corollary 3.3.6 *Among all graphs of order n which do not have isolated vertices, the star S_n has maximum Merrifield-Simmons index and minimum Hosoya index.*

Proof. Let G be a graph of order n which does not have isolated vertices, and let $G_1, \cdots, G_k$ be its connected components with orders $n_1, \cdots, n_k$ respectively. For each $i \in \{1, \cdots, k\}$, let T_i be a spanning tree of G_i. From Theorem 3.3.5 we have

$$\sigma(G_i) \le \sigma(T_i) \le \sigma(S_{n_i}) \qquad (3.3.21)$$

and

$$\mathrm{Z}(S_{n_i}) \le \mathrm{Z}(T_i) \le \mathrm{Z}(G_i). \qquad (3.3.22)$$

We are left to prove that for all positive integers $k, l \ge 2$ we have

$$\sigma(S_k \cup S_l) \le \sigma(S_{k+l}) \qquad (3.3.23)$$

and

$$\mathrm{Z}(S_{k+l}) \le \mathrm{Z}(S_k \cup S_l). \qquad (3.3.24)$$

These can be seen as follows:

$$\begin{aligned}
\sigma(S_k \cup S_l) &= (2^{k-1}+1)(2^{l-1}+1) \\
&= 2^{k+l-2} + 2^{k-1} + 2^{l-1} + 1 \\
&= 2^{k+l-2} + 2^{k+l-2}(2^{1-k} + 2^{1-l}) + 1 \\
&\le 2^{k+l-2} + 2^{k+l-2} + 1 \\
&= 2^{k+l-1} + 1 \\
&= \sigma(S_{k+l}). \qquad (3.3.25)
\end{aligned}$$

and

$$\begin{aligned}\mathrm{Z}(S_k \cup S_l) &= kl \\ &= k + l + (k-1)(l-1) - 1 \\ &\geq k + l \\ &= \mathrm{Z}(S_{k+l}). \end{aligned} \tag{3.3.26}$$

□

Interested readers are referred to [LL95] for descriptions of all n-vertex forests with Merrifield-Simmons index at least $2^{n-1} + 1$.

Lemma 3.3.4 was very useful for studying the class of all trees. In order to find the trees of a given diameter with maximum σ or minimum Z and En we have to use Lemma 3.3.3 in a different way.

Remark 3.3.7 Iterative applications of Lemma 3.3.3 show that replacing a non-leaf branch of a vertex in a tree by a star of the same order (see Figure 3.7), increases σ, decreases $\mu(., x)$ for all real numbers $x > 0$, and consequently decreases Z and En.

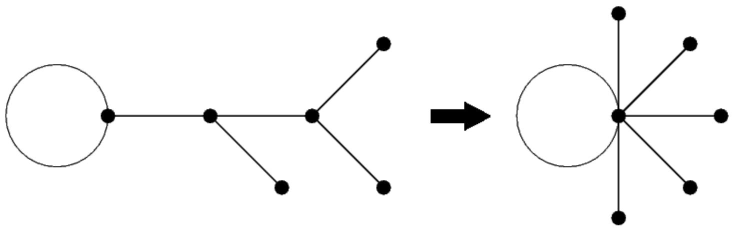


Figure 3.7: Example of the graph transformation described in Remark 3.3.7

Definition 3.3.8 For $n \geq 1$, let $c_1, \ldots, c_n$ be non-negative integers such that c_1 and c_n are positive. The tree which is obtained from the path $v_1 v_2 \ldots v_n$ by attaching c_i new leaves to v_i, for $1 \leq i \leq n$, is called a $(c_1, \ldots, c_n)$-*caterpillar* (Figure 3.8).

Definition 3.3.9 The tree which results from attaching k leaves to an end of a path P_n is called a *broom* (Figure 3.9), and it is denoted by B^k_{n+k}.

For all integers $n \geq 2$, the star S_n and the path P_n can be viewed as brooms:

$$S_n = B^{n-2}_n \tag{3.3.27}$$

and

$$P_n = B^1_n. \tag{3.3.28}$$

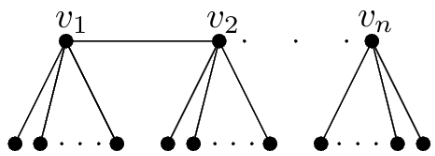


Figure 3.8: Caterpillar

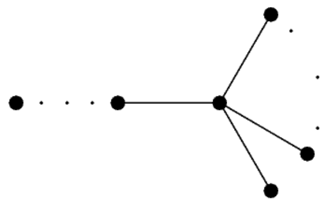


Figure 3.9: Broom

If we denote by v the vertex of B_n^k which is adjacent to k leaves, then it follows that

$$\begin{aligned}\sigma(B_n^k) &= \sigma(B_n^k - v) + \sigma(B_n^k - (\{v\} \cup N_{B_n^k}(v))) \\ &= 2^k \sigma(P_{n-k-1}) + \sigma(P_{n-k-2}) \\ &= 2^k F_{n-k} + F_{n-k-1} \end{aligned} \tag{3.3.29}$$

and for all real numbers $x > 0$

$$\begin{aligned}\mu(B_n^k, x) &= \mu(B_n^k - v, x) + x^2 \sum_{w \in N_{B_n^k}(v)} \mu(B_n^k - \{w, v\}, x) \\ &= (kx^2 + 1)\mu(P_{n-k-1}, x) + x^2 \mu(P_{n-k-2}, x). \end{aligned} \tag{3.3.30}$$

Theorem 3.3.10 ([LZG05, CW07, YY05]) *Let n and d be integers such that $n - 1 \geq d \geq 2$. The broom B_n^{n-d} is the tree of order n and diameter d which has maximum Merrifield-Simmons index, minimum Hosoya index and minimum energy.*

Proof. Let x be a positive real number, and let T_n^d be a tree of order n and diameter d which has maximum σ or minimum $\mu(., x)$. We will show that $T_n^d = B_n^d$ and the theorem follows by relation (2.3.34) and by Remark 2.3.6.

Consider a path $P_{d+1} = v_1 v_2 \dots v_{d+1}$ of length d in T_n^d. If there is an element i of $\{1, 2, \dots, d+1\}$ such that v_i has a non-leaf branch that is disjoint to P_{d+1}, then we can apply the graph transformation described in Remark 3.3.7 to obtain a $T_n'^d$ of order n which satisfies

$$\sigma(T_n^d) < \sigma(T_n'^d) \tag{3.3.31}$$

and

$$\mu(T_n^d, x) > \mu(T_n'^d, x) \tag{3.3.32}$$

for all real number $x > 0$. These inequalities would contradict the maximality of $\sigma(T_n^d)$ as well as the minimality of $\mu(T_n^d, x)$. Hence, T_n^d is necessarily a $(c_1, c_2, \ldots, c_{d-1})$-caterpillar, for some non-negative integers $c_1, c_2, \ldots, c_{d-1}$.

To show that $T_n^d = B_n^{n-d}$ we reason by induction with respect to the diameter d. If $d = 2$, then $B_n^{n-d} = B_n^{n-2} = S_n$. Therefore, from Theorem 3.3.5 we obtain $T_n^2 = B_n^{n-2}$. Assume that $T_n^d = B_n^{n-d}$ for all $n \geq d+1$, and for some $d \geq 2$. Now, let us show by induction with respect to n that $T_n^{d+1} = B_n^{n-(d+1)}$ for all $n \geq d+2$. If $n = d+2$, then $n-(d+1) = 1$ and $P_n = B_n^1$ is the only caterpillar of order n which has diameter $d+1$, hence, $T_{d+2}^{d+1} = B_{d+2}^1$. Assume that $T_n^{d+1} = B_n^{n-d-1}$, where n is at least equal to $d+2$. Let T be a $(c_1, c_2, \ldots, c_d)$-caterpillar of order $n+1$ and diameter $d+1$.

Case 1: Assume that $c_1 = 1$. Let w be the vertex corresponding to c_1 and let w' be the single leaf attached to w. Then, we have

$$\begin{aligned}\sigma(T) &= \sigma(T - w') + \sigma(T - (\{w'\} \cup N_T(w'))) \\ &= \sigma(T - w') + \sigma(T - \{w, w'\}) \end{aligned} \tag{3.3.33}$$

and for all real numbers $x > 0$ we have

$$\begin{aligned}\mu(T, x) &= \mu(T - w', x) + x^2 \sum_{u \in N_T(w')} \mu(T - \{w', u\}, x) \\ &= \mu(T - w', x) + x^2 \mu(T - \{w, w'\}, x). \end{aligned} \tag{3.3.34}$$

From the induction hypothesis with respect to d we know that if $B_n^{n-d} \neq T - w'$, then the inequalities

$$\sigma(T - w') < \sigma(B_n^{n-d}) \tag{3.3.35}$$

and

$$\mu(T - w', x) > \mu(B_n^{n-d}, x), \tag{3.3.36}$$

hold. Similarly, if $B_{n-1}^{n-d} \neq T - \{w, w'\}$, then we get

$$\sigma(T - \{w, w'\}) < \sigma(B_{n-1}^{n-d}) \tag{3.3.37}$$

and

$$\mu(T - \{w, w'\}, x) > \mu(B_{n-1}^{n-d}, x). \tag{3.3.38}$$

Note that $\mathrm{diam}(T - \{w, w'\})$ is either d or $d-1$, but in each case, (3.3.37) and (3.3.38) always hold because, by Lemma 3.3.3, we know that

$$\sigma(B_{n-1}^{n-d}) < \sigma(B_{n-1}^{n-d+1}) \tag{3.3.39}$$

and

$$\mu(B_{n-1}^{n-d}, x) > \mu(B_{n-1}^{n-d+1}, x). \tag{3.3.40}$$

If $T \neq B_{n+1}^{n-d-1}$, then it follows from equation (3.3.33) that

$$\begin{aligned} \sigma(T) &< \sigma(B_n^{n-d}) + \sigma(B_{n-1}^{n-d}) \\ &= \sigma(B_{n+1}^{n-d}), \end{aligned} \tag{3.3.41}$$

and from equation (3.3.34) we obtain

$$\begin{aligned} \mu(T,x) &> \mu(B_n^{n-d},x) + x^2\mu(B_{n-1}^{n-d},x) \\ &= \mu(B_{n+1}^{n-d},x). \end{aligned} \tag{3.3.42}$$

Case 2: Assume that $n-d \geq c_1 > 1$. The integer c_1 cannot be greater than $n-d$ otherwise T would have more than $n+1$ vertices. We keep the above notations where w' is one of the c_1 leaves attached to w. Let w'' be the non-leaf vertex that is adjacent to w. Then, we obtain

$$\begin{aligned} \sigma(T) &= \sigma(T-w') + \sigma(T - (\{w'\} \cup N_T(w'))) \\ &= \sigma(T-w') + 2^{c_1-1}\sigma(T - (\{w\} \cup N_T(w) - \{w''\})) \end{aligned} \tag{3.3.43}$$

and

$$\begin{aligned} \mu(T,x) &= \mu(T-w',x) + x^2 \sum_{u \in N_T(w')} \mu(T - \{u,w'\},x) \\ &= \mu(T-w',x) + x^2\mu(T - (\{w\} \cup N_T(w) - \{w''\}),x). \end{aligned} \tag{3.3.44}$$

$T - (\{w\} \cup N_T(w) - \{w''\})$ is either the $(c_2, c_3, \ldots, c_d)$-caterpillar (if $c_2 \geq 1$) or the $(c_3+1, c_4, \ldots, c_d)$-caterpillar (if $c_2 = 0$). In any case, $T - (\{w\} \cup N_T(w) - \{w''\})$ has $n - c_1$ vertices and its diameter is at least $d-1$. Since it contains the path P_d as subgraph, the following inequalities hold:

$$\sigma(T - (\{w\} \cup N_T(w) - \{w''\})) \leq 2^{n-c_1-d}\sigma(P_d) \tag{3.3.45}$$

and

$$\mu(T - (\{w\} \cup N_T(w) - \{w''\}),x) \geq \mu(P_d,x). \tag{3.3.46}$$

On the other hand, if $T \neq B_{n+1}^{n-d-1}$, then $n-d > c_1$, and using the induction hypothesis with respect to n we have

$$\sigma(T-w') < \sigma(B_n^{n-d-1}) \tag{3.3.47}$$

and

$$\mu(T-w',x) > \mu(B_n^{n-d-1},x). \tag{3.3.48}$$

Using inequalities (3.3.45) and (3.3.47), it follows from equation (3.3.43) that

$$\begin{aligned}\sigma(T) &< \sigma(B_n^{n-d-1}) + 2^{c_1-1}2^{n-c_1-d}\sigma(P_d)\\ &= \sigma(B_n^{n-d-1}) + 2^{n-d-1}\sigma(P_d)\\ &= \sigma(B_{n+1}^{n-d}). \end{aligned} \tag{3.3.49}$$

Similarly, by the inequalities (3.3.46) and (3.3.48), we deduce from equation (3.3.44) that

$$\begin{aligned}\mu(T,x) &> \mu(B_n^{n-d-1},x) + x^2\mu(P_d,x)\\ &= \mu(B_{n+1}^{n-d},x). \end{aligned} \tag{3.3.50}$$

This shows that $T_{n+1}^{d+1} = B_{n+1}^{n+1-(d+1)}$.

□

In the next chapter, among other results, we will see how σ, Z and En behave if we allow a subgraph to "slide" along a certain caterpillar. Then, for a class of trees including those which are used to represent saturated hydrocarbons, we deduce similar results as we have established from the lemma on "Sliding along a path".

Chapter 4

Trees with restricted degrees

4.1 Introduction

In this chapter we study the Merrifield-Simmons index, Hosoya index and energy for the set $\mathbb{T}_{1,d}$ of all trees whose vertices are either of degree 1 or d where d is a non-negative integer. For $d \in \{0,1\}$ we cannot form an element of $\mathbb{T}_{1,d}$ with more than two vertices and $\mathbb{T}_{1,2}$ is exactly the set of all paths, these are trivial cases. Throughout the rest of the chapter we assume d to be at least 3.

Each element of $\mathbb{T}_{1,d}$ can be constructed by starting from the path P_2 and progressively attach $d-1$ new leaves to an appropriately chosen existing leaf, hence the order of such a graph is of the form $(d-1)n+2$ where $n \in \mathbb{N}$. For all $n \in \mathbb{N}$, we denote by $\mathbb{T}_{1,d}^n$ the subset of $\mathbb{T}_{1,d}$ which contains all elements of order $(d-1)n+2$.

A special type of vertices which always exist in any element of $\mathbb{T}_{1,d} - \{P_2\}$ is described in the next definition, it is useful for describing some subclasses that will be of particular interest.

Definition 4.1.1 Let $G \in \mathbb{T}_{1,d}$. A vertex v in G is called a *pseudo-leaf* if and only if it is not a leaf and the number of vertices of degree d in its neighbourhood $N_G(v)$ is at most one. For example in Figure 4.1, u is a pseudo-leaf, but not v.

Notation 4.1.2 For any positive integer n and $d \geq 3$, we write C_n^d for the $(c_1, \ldots, c_n)$-caterpillar with $c_1 = c_n = d-1$ and $c_2 = \cdots = c_{n-1} = d-2$, $C_n'^d$ for the $(c_1, \ldots, c_n)$-caterpillar with $c_1 = d-1$ and $c_2 = \cdots = c_n = d-2$ and $C_n''^d$ for the $(c_1, \ldots, c_n)$-caterpillar with $c_1 = c_2 = \cdots = c_n = d-2$. $C_0^d, C_0'^d$ and $C_0''^d$ are set to be equal to P_2, P_1 and P_0, respectively.

For simplicity, it is convenient to abbreviate $\sigma(C_n'^d)$ and $\mathrm{Z}(C_n'^d)$ by ς_n^d and ζ_n^d, respectively.

For all $n \in \mathbb{N}$ we have $C_n^d \in \mathbb{T}_{1,d}$, $C_n'^d \notin \mathbb{T}_{1,d}$ and $C_n''^d \notin \mathbb{T}_{1,d}$.

Definition 4.1.3 We call an element of $\mathbb{T}_{1,d}$ a *d-tripod*, respectively *d-quadripod*, if and only if its number of pseudo-leaves is exactly 3, respectively, exactly 4. They are denoted, respectively, by $T_d(i,j,k)$ and by $H_d(e, d_{11}, d_{12}, d_{21}, d_{22})$ where the positive integers i, j, k are as described in Figure 4.1 and such that $i \leq j \leq k$ and the positive integers $e, d_{11}, d_{12}, d_{21}, d_{22}$ are as explained in Figure 4.2.

In a d-tripod, the unique vertex which is adjacent to three vertices of degree d is called the *centre*. A subgraph of $T_d(i,j,k)$ is called a *caterpillar branch* of $T_d(i,j,k)$ if and only if it is a caterpillar, it does not contain the centre and it is maximal with respect to the order.

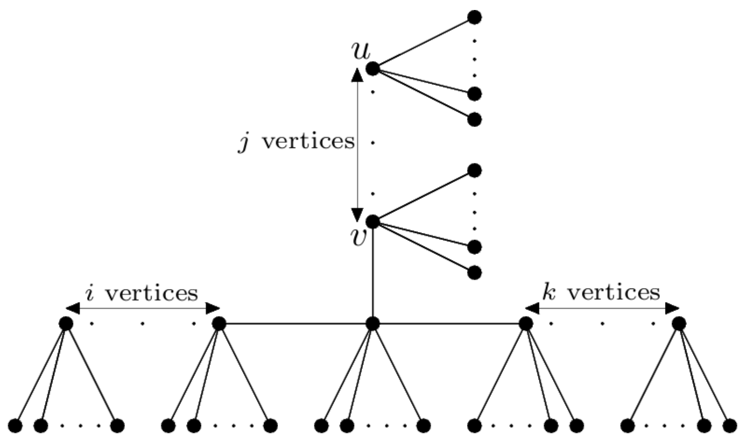


Figure 4.1: d-tripod $T_d(i,j,k)$

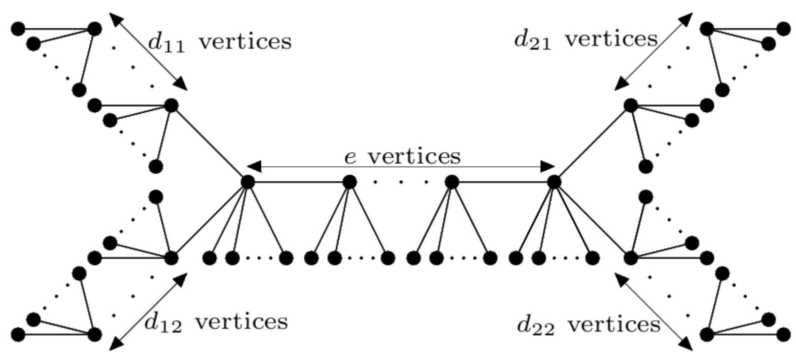


Figure 4.2: d-quadripod $H_d(e, d_{11}, d_{12}, d_{21}, d_{22})$

Note that Definition 4.1.3 allows multiple notations for a d-quadripod. In $H_d(e, d_{11}, d_{12}, d_{21}, d_{22})$, we still have the same d-quadripod if we swap d_{11} and d_{12} or d_{21} and d_{22}. This flexibility simplifies the formulation of some results in Section 4.4.

Since $\mathbb{T}_{1,d}$ is a subclass of trees, we can use again the expression for the energy given in equation (2.3.35) and $\mu(T, x)$ as defined in (2.3.33). The following recurrence relation follows by applying Lemma 2.2.3 to $C_n'^d$. Let v be a pseudo-leaf of $C_n'^d$. Then we have

$$\begin{aligned}\varsigma_n^d &= \sigma(C_n'^d - v) + \sigma(C_n'^d - (\{v\} \cup N_{C_n'^d}(v))) \\ &= 2^{d-2}\varsigma_{n-1}^d + 2^{d-2}\varsigma_{n-2}^d \end{aligned} \tag{4.1.1}$$

and

$$\begin{aligned}\zeta_n^d &= \mathrm{Z}(C_n'^d - v) + \sum_{w \in N_{C_n'^d}(v)} \mathrm{Z}(C_n'^d - \{vw\}) \\ &= \zeta_{n-1}^d + (d-2)\zeta_{n-1}^d + \zeta_{n-2}^d \\ &= (d-1)\zeta_{n-1}^d + \zeta_{n-2}^d, \end{aligned} \tag{4.1.2}$$

where $n \geq 2$. Similarly, it follows by Lemma 2.3.7 that for all integers $n \geq 2$ and for all real numbers $x > 0$ we have

$$\begin{aligned}\mu(C_n'^d, x) &= \mu(C_n'^d - v, x) + x^2 \sum_{w \in N_{C_n'^d}(v)} \mu(C_n'^d - \{v, w\}, x) \\ &= \mu(C_{n-1}'^d, x) + x^2(d-2)\mu(C_{n-1}'^d, x) + x^2\mu(C_{n-2}'^d, x) \\ &= (1 + x^2(d-2))\mu(C_{n-1}'^d, x) + x^2\mu(C_{n-2}'^d, x). \end{aligned} \tag{4.1.3}$$

Obviously $(\sigma(C_n''^d))_{n\in\mathbb{N}}$, $(\mathrm{Z}(C_n''^d))_{n\in\mathbb{N}}$ and $(\mu(C_n''^d, x))_{n\in\mathbb{N}}$ also satisfy the recurrence relations (4.1.1), (4.1.2) and (4.1.3), respectively.

In the next section, we study a similar situation as in Lemma 3.2.3. This time, the subgraph G "slides" along a caterpillar instead of a path.

4.2 Sliding along a caterpillar

Definition 4.2.1 Let G be a connected graph with a vertex v of degree at most $d-2$ and assume that G is not isomorphic to the star S_{d-1} with the centre at v. Let us label the vertices of degree d in C_n^d by $v_1, \ldots, v_n$. We define $C_d(n, k, G, v)$ to be the graph obtained by removing the $d-2$ leaves attached to v_k in C_n^d and by identifying v_k with the vertex v of G (see Figure 4.3).

4.2.1 Sliding along a caterpillar with respect to the Merrifield-Simmons index

First we need an explicit expression for $\sigma(C_n^d)$ as a function of n. The sequence $(\varsigma_n^d)_{n\in\mathbb{N}}$ satisfies a linear recurrence relation as described in equation (4.1.1) which has characteristic equation

$$P(t) = t^2 - 2^{d-2}t - 2^{d-2} = 0. \tag{4.2.1}$$

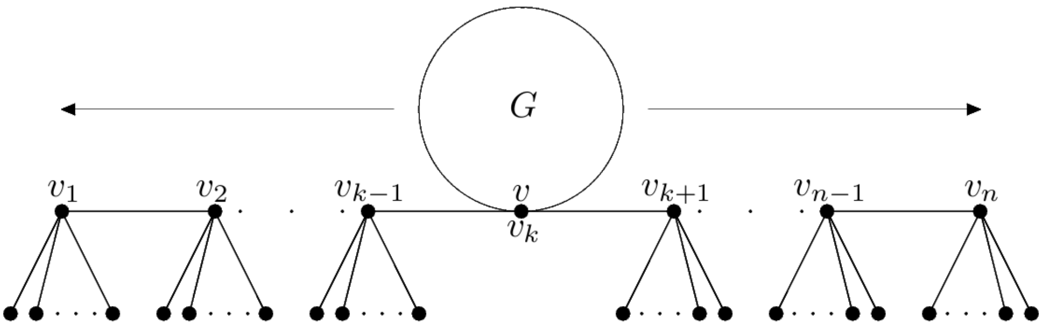


Figure 4.3: $C_d(n,k,G,v)$

$P(t)$ has two real roots

$$Y = 2^{d-3} + \sqrt{2^{2d-6} + 2^{d-2}} \tag{4.2.2}$$

and

$$\widetilde{Y} = 2^{d-3} - \sqrt{2^{2d-6} + 2^{d-2}}. \tag{4.2.3}$$

Therefore, for all $n \in \mathbb{N}$, ς_n^d can be expressed as

$$\varsigma_n^d = QY^n + R\widetilde{Y}^n \tag{4.2.4}$$

where Q and R satisfy the system of equations

$$\begin{cases} Q + R = \varsigma_0^d = 2 \\ QY + R\widetilde{Y} = \varsigma_1^d = 2^{d-1} + 1. \end{cases} \tag{4.2.5}$$

Easy calculations give

$$Q = \frac{2Y+1}{Y-\widetilde{Y}} \tag{4.2.6}$$

and

$$R = -\frac{2\widetilde{Y}+1}{Y-\widetilde{Y}} \tag{4.2.7}$$

leading to

$$\varsigma_n^d = \frac{2Y+1}{Y-\widetilde{Y}}Y^n - \frac{2\widetilde{Y}+1}{Y-\widetilde{Y}}\widetilde{Y}^n. \tag{4.2.8}$$

The next lemma provides information on the behaviour of the number of independent vertex subsets of $C_d(n,k,G,v)$ as k varies in $\{1, 2, \dots, \lfloor \frac{n}{2} \rfloor\}$.

Lemma 4.2.2 ([AW10]) *Let m be a non-negative integer, $n = 4m + h$, $h \in \{1, 2, 3, 4\}$, and let l be the integer part of $\frac{h-1}{2}$. Then for all integers $d \geq 3$ we have*

$$\sigma(C_d(n,2,G,v)) > \sigma(C_d(n,4,G,v)) > \cdots > \sigma(C_d(n,2m+2l,G,v))$$
$$> \sigma(C_d(n,2m+1,G,v)) > \cdots > \sigma(C_d(n,3,G,v)) > \sigma(C_d(n,1,G,v)).$$

Proof. We keep the notations $Y, \widetilde{Y}, Q, R$ in equations (4.2.2), (4.2.3), (4.2.6), (4.2.7), respectively. We have

$$\begin{aligned} Y\widetilde{Y} &= \left(2^{d-3} + \sqrt{2^{2d-6} + 2^{d-2}}\right)\left(2^{d-3} - \sqrt{2^{2d-6} + 2^{d-2}}\right) \\ &= -2^{d-2}, \end{aligned} \tag{4.2.9}$$

hence

$$\frac{\widetilde{Y}}{Y} = \frac{\widetilde{Y}Y}{Y^2} = -\frac{2^{d-2}}{Y^2} \tag{4.2.10}$$

and

$$\begin{aligned} QR &= -\frac{(2Y+1)(2\widetilde{Y}+1)}{(Y-\widetilde{Y})^2} \\ &= -\frac{4Y\widetilde{Y} + 2(Y+\widetilde{Y}) + 1}{(Y-\widetilde{Y})^2} \\ &= -\frac{-2^d + 2^{d-1} + 1}{(Y-\widetilde{Y})^2} \\ &= \frac{2^{d-1} - 1}{(Y-\widetilde{Y})^2} > 0 \text{ since } d \geq 3. \end{aligned} \tag{4.2.11}$$

Furthermore, for all non-negative integers m and l we have

$$\begin{aligned} \varsigma_m^d \varsigma_l^d &= (QY^m + R\widetilde{Y}^m)(QY^l + R\widetilde{Y}^l) \\ &= Q^2 Y^{m+l} + R^2 \widetilde{Y}^{m+l} + QR(Y\widetilde{Y})^m (Y^{l-m} + \widetilde{Y}^{l-m}) \\ &= Q^2 Y^{m+l} + R^2 \widetilde{Y}^{m+l} + \frac{2^{d-1}-1}{(Y-\widetilde{Y})^2}(-2^{d-2})^m (Y^{l-m} + \widetilde{Y}^{l-m}). \end{aligned} \tag{4.2.12}$$

Now, if we apply the relation (2.2.7) to $C_d(n, i+1, G, v)$, then we obtain the following (note that in $C_d(n, i+1, G, v)$, v_{i+1} and v coincide)

$$\begin{aligned} &\sigma(C_d(n, i+1, G, v)) \\ &= \sigma(C_d(n, i+1, G, v) - v) + \sigma(C_d(n, i+1, G, v) - (\{v\} \cup N_{C_d(n,i+1,G,v)}(v))) \\ &= \varsigma_i^d \varsigma_j^d \sigma(G - v) + 2^{2d-4} \varsigma_{i-1}^d \varsigma_{j-1}^d \sigma(G - (\{v\} \cup N_G(v))), \end{aligned} \tag{4.2.13}$$

where $j = n - i - 1$. Replacing $\varsigma_i^d \varsigma_j^d$ and $\varsigma_{i-1}^d \varsigma_{j-1}^d$ by the corresponding expressions using equation (4.2.12) we have

$$\begin{aligned}
&\sigma(C_d(n,i+1,G,v)) \\
&= \left(Q^2Y^{i+j} + R^2\widetilde{Y}^{i+j} + \frac{2^{d-1}-1}{(Y-\widetilde{Y})^2}(-2^{d-2})^i(Y^{j-i}+\widetilde{Y}^{j-i})\right)\sigma(G-v) \\
&+ 2^{2d-4}\left(Q^2Y^{i+j-2} + R^2\widetilde{Y}^{i+j-2} + \frac{2^{d-1}-1}{(Y-\widetilde{Y})^2}(-2^{d-2})^{i-1}(Y^{j-i}+\widetilde{Y}^{j-i})\right) \\
&\qquad\qquad \sigma(G-(\{v\}\cup N_G(v))) \\
&= (Q^2Y^{i+j} + R^2\widetilde{Y}^{i+j})\sigma(G-v) \\
&+ 2^{2d-4}(Q^2Y^{i+j-2} + R^2\widetilde{Y}^{i+j-2})\sigma(G-(\{v\}\cup N_G(v))) + \frac{2^{d-1}-1}{(Y-\widetilde{Y})^2} \\
&(-2^{d-2})^i(Y^{j-i}+\widetilde{Y}^{j-i})(\sigma(G-v) - 2^{d-2}\sigma(G-(\{v\}\cup N_G(v)))). \qquad (4.2.14)
\end{aligned}$$

Using the relation $i+j=n-1$ and $j-i=n-1-2i$ we can define

$$\begin{aligned}
C(n) = (Q^2Y^{n-1} + R^2\widetilde{Y}^{n-1})\sigma(G-v) \\
+ 2^{2d-4}(Q^2Y^{n-3} + R^2\widetilde{Y}^{n-3})\sigma(G-(\{v\}\cup N_G(v))) \quad (4.2.15)
\end{aligned}$$

to get

$$\begin{aligned}
&\sigma(C_d(n,i+1,G,v)) \\
&= C(n) + \frac{2^{d-1}-1}{(Y-\widetilde{Y})^2}(-2^{d-2})^i(Y^{n-1-2i}+\widetilde{Y}^{n-1-2i}) \\
&\qquad (\sigma(G-v) - 2^{d-2}\sigma(G-(\{v\}\cup N_G(v)))) \\
&= C(n) + \frac{2^{d-1}-1}{(Y-\widetilde{Y})^2}(-1)^i\left(Y^{n-1}\left(\frac{2^{d-2}}{Y^2}\right)^i + \widetilde{Y}^{n-1}\left(\frac{2^{d-2}}{\widetilde{Y}^2}\right)^i\right) \\
&\qquad (\sigma(G-v) - 2^{d-2}\sigma(G-(\{v\}\cup N_G(v)))) \\
&= C(n) + \frac{Y^{n-1}(2^{d-1}-1)}{(Y-\widetilde{Y})^2}(-1)^i\left(\left(\frac{2^{d-2}}{Y^2}\right)^i + \left(\frac{\widetilde{Y}}{Y}\right)^{n-1}\left(\frac{2^{d-2}}{\widetilde{Y}^2}\right)^i\right) \\
&\qquad (\sigma(G-v) - 2^{d-2}\sigma(G-(\{v\}\cup N_G(v)))). \qquad (4.2.16)
\end{aligned}$$

Using relation (4.2.10) we obtain

$$\begin{aligned}
&\sigma(C_d(n,i+1,G,v)) \\
&= C(n) + \frac{Y^{n-1}(2^{d-1}-1)}{(Y-\widetilde{Y})^2}(-1)^i\left(\left(\frac{2^{d-2}}{Y^2}\right)^i + \left(\frac{-2^{d-2}}{Y^2}\right)^{n-1}\left(\frac{2^{d-2}}{\widetilde{Y}^2}\right)^i\right) \\
&\qquad (\sigma(G-v) - 2^{d-2}\sigma(G-(\{v\}\cup N_G(v)))) \qquad (4.2.17)
\end{aligned}$$

which leads to

$$\begin{aligned}&\sigma(C_d(n, i+1, G, v))\\&= C(n) + \frac{Y^{n-1}(2^{d-1}-1)}{(Y-\widetilde{Y})^2}(-1)^i \left(\left(\frac{2^{d-2}}{Y^2}\right)^i + (-1)^{n-1}\left(\frac{2^{d-2}}{Y^2}\right)^j\right)\\&\qquad (\sigma(G-v) - 2^{d-2}\sigma(G-(\{v\}\cup N_G(v)))). \quad (4.2.18)\end{aligned}$$

If we let

$$D(n) = \frac{Y^{n-1}(2^{d-1}-1)\left(2^{d-2}\sigma(G-(\{v\}\cup N_G(v)) - \sigma(G-v)\right)}{(Y-\widetilde{Y})^2}, \quad (4.2.19)$$

then

$$\sigma(C_d(n, i+1, G, v)) = C(n) + D(n)(-1)^{i+1} f_{\frac{2^{d-2}}{Y^2}, n-1}(i) \quad (4.2.20)$$

where $f_{\frac{2^{d-2}}{Y^2}, n-1}$ is as in Lemma 3.2.1.

The cases of small $n \in \{1, 2\}$ are not interesting, since they correspond to the single possibility $C_d(n, 1, G, v)$, thus there is no comparison to be done. Furthermore, knowing that the degree of the vertex v in G is at most $d-2$ we deduce that

$$\begin{aligned}\sigma(G-v) &\leq 2^{|N_G(v)|}\sigma((G-v) - N_G(v))\\&\leq 2^{d-2}\sigma(G-(\{v\}\cup N_G(v))). \quad (4.2.21)\end{aligned}$$

Equality occurs only when $G = S_{d-1}$ and v is the centre, but this case is excluded by definition of $C_d(n, i+1, G, v)$. Therefore we obtain $D(n) > 0$ for all integers n. From Lemma 3.2.1 we know that $f_{\frac{2^{d-2}}{Y^2}, n-1}$ is positive and decreasing on $I_n = \{0, 1, \ldots, \lfloor\frac{n-2}{2}\rfloor\}$ which is exactly the set of values of i that we are interested in.

Let k be an integer such that $2k+1 \in I_n$. Equation (4.2.20) gives

$$\sigma(C_d(n, (2k+1)+1, G, v)) = C(n) + D(n) f_{\frac{2^{d-2}}{Y^2}, n-1}(2k+1) > C(n) \quad (4.2.22)$$

showing that $\sigma(C_d(n, 2k+2, G, v))$ is a decreasing function of k just as $f_{\frac{2^{d-2}}{Y^2}, n-1}$. This describes the even positions of G.

On the other hand, if we let k be an integer such that $2k \in I_n$, then what we obtain from equation (4.2.20) is an increasing function of k:

$$\sigma(C_d(n, 2k+1, G, v)) = C(n) - D(n) f_{\frac{2^{d-2}}{Y^2}, n-1}(2k) < C(n), \quad (4.2.23)$$

which corresponds to the odd positions of G.

Hence the lemma follows. □

4.2.2 Sliding along a caterpillar with respect to the Hosoya index and with respect to the energy

In addition to the relations between $\mu(.,x)$ and the energy, we have also seen a correspondence between $\mu(.,x)$ and the Hosoya index in equation (2.3.34). Therefore, we only have to establish a lemma of "sliding along a caterpillar" with respect to $\mu(.,x)$ and the cases of the energy and the Hosoya index will follow trivially. To do this, we need an explicit expression for $\mu(C_n^{\prime\prime d},x)$.

A linear recurrence relation for the sequence $(\mu(C_n^{\prime\prime d},x))_{n\in\mathbb{N}}$ is given in equation (4.1.3) for arbitrary positive real numbers x, and it has characteristic equation

$$P(t) = t^2 - (1 + x^2(d-2))t - x^2 = 0, \tag{4.2.24}$$

which has the two roots

$$Y(x) = \frac{1 + (d-2)x^2 + \sqrt{1 + 2dx^2 + (d-2)^2x^4}}{2} \tag{4.2.25}$$

and

$$\widetilde{Y}(x) = \frac{1 + (d-2)x^2 - \sqrt{1 + 2dx^2 + (d-2)^2x^4}}{2}. \tag{4.2.26}$$

Therefore the explicit expression for $\mu(C_n^{\prime\prime d},x)$ is of the form

$$\mu(C_n^{\prime\prime d},x) = Q(x)Y^n(x) + R(x)\widetilde{Y}^n(x), \tag{4.2.27}$$

where $Q(x)$ and $R(x)$ satisfy the system of equations

$$\begin{cases} \mu(C_0^{\prime\prime d},x) = Q(x) + R(x) = 1, \\ \mu(C_1^{\prime\prime d},x) = Q(x)Y + B(x)\widetilde{Y} = 1 + (d-1)x^2. \end{cases} \tag{4.2.28}$$

Solving the system using the relation

$$Y(x) + \widetilde{Y}(x) = 1 + (d-2)x^2, \tag{4.2.29}$$

we find

$$\begin{aligned} Q(x) &= \frac{1 + (d-1)x^2 - \widetilde{Y}(x)}{Y(x) - \widetilde{Y}(x)} \\ &= \frac{Y(x) + x^2}{Y(x) - \widetilde{Y}(x)}, \end{aligned} \tag{4.2.30}$$

$$\begin{aligned} R(x) &= \frac{Y(x) - 1 - (d-1)x^2}{Y(x) - \widetilde{Y}(x)} \\ &= -\frac{\widetilde{Y}(x) + x^2}{Y(x) - \widetilde{Y}(x)}, \end{aligned} \tag{4.2.31}$$

and therefore we have

$$\mu(C_n^{\prime\prime d},x) = \frac{Y(x) + x^2}{Y(x) - \widetilde{Y}(x)}Y^n(x) - \frac{\widetilde{Y}(x) + x^2}{Y(x) - \widetilde{Y}(x)}\widetilde{Y}^n(x). \tag{4.2.32}$$

Remark 4.2.3 In fact $C_n'^d$ is not defined for negative n. But whenever values of ς_n^d and $\mu(C_n'^d, x)$ for negative n will be needed we use the expression in (4.2.8) and the expression in (4.2.32), respectively, to determine them. The fact that $Y, \widetilde{Y}, Y(x)$ and $\widetilde{Y}(x)$ are non-zero makes this possible.

As described in the following lemma, the order of $C_d(n,k,G,v)$ with respect to $\mu(.,x)$ is exactly the opposite of the order with respect to σ seen in Lemma 4.2.2.

Lemma 4.2.4 ([AW10]) *Let m be a non-negative integer, $n = 4m+t$, $t \in \{1,2,3,4\}$, and let l be the integer part of $\frac{t-1}{2}$. Then for all integers $d \geq 3$ and all positive real numbers x we have*

$$\mu(C_d(n,2,G,v),x) < \mu(C_d(n,4,G,v),x) < \cdots < \mu(C_d(n,2m+2l,G,v),x)$$
$$< \mu(C_d(n,2m+1,G,v),x) < \cdots < \mu(C_d(n,3,G,v),x) < \mu(C_d(n,1,G,v),x).$$

Proof. Let d and n be integers at least equal to 3 and let $x > 0$ be a real number. Note that the relation

$$\begin{aligned} Y(x)\widetilde{Y}(x) &= \frac{(1+(d-2)x^2)^2 - (1+2dx^2+(d-2)^2x^4)}{4} \\ &= -x^2 \end{aligned} \tag{4.2.33}$$

will often be used.

We can apply Lemma (2.3.7) to $C_d(n,i+1,G,v)$ and have the following (with $j = n-1-i$):

$$\begin{aligned} &\mu(C_d(n,i+1,G,v),x) \\ &= \mu(C_d(n,i+1,G,v)-v,x) \\ &\qquad + x^2 \sum_{w \in N_{C_d(n,i+1,G,v)}(v)} \mu(C_d(n,i+1,G,v)-\{v,w\},x) \\ &= x^2(\mu(C_{i-1}'^d,x)\mu(C_j'^d,x) + \mu(C_i'^d,x)\mu(C_{j-1}'^d,x))\mu(G-v,x) \\ &+ \mu(C_i'^d,x)\mu(C_j'^d,x)\left(\mu(G-v,x) + x^2 \sum_{w \in N_G(v)} \mu(G-\{v,w\},x)\right) \end{aligned} \tag{4.2.34}$$

Using the explicit expression for $\mu(C_n'^d, x)$ we have

$$\begin{aligned} \mu(C_i'^d,x)\mu(C_j'^d,x) &= (Q(x)Y^i(x) + R(x)\widetilde{Y}^i(x))(Q(x)Y^j(x) + R(x)\widetilde{Y}^j(x)) \\ &= Q^2(x)Y^{i+j}(x) + R^2(x)\widetilde{Y}^{i+j}(x) \\ &+ Q(x)R(x)(Y(x)\widetilde{Y}(x))^i(Y^{j-i}(x) + \widetilde{Y}^{j-i}(x)) \end{aligned} \tag{4.2.35}$$

where

$$\begin{aligned}
Y^{j-i}(x)+\widetilde{Y}^{j-i}(x) &= Y^{j+i-2i}(x)+\widetilde{Y}^{j+i-2i}(x)\\
&= Y^{j+i}(x)\left(\left(\frac{1}{Y^2(x)}\right)^i+\left(\frac{\widetilde{Y}(x)}{Y(x)}\right)^{i+j}\left(\frac{1}{\widetilde{Y}^2(x)}\right)^i\right)\\
&= Y^{j+i}(x)\left(\left(\frac{1}{Y^2(x)}\right)^i+\left(-\frac{x^2}{Y^2(x)}\right)^{i+j}\left(\frac{1}{\widetilde{Y}^2(x)}\right)^i\right)\\
&= Y^{j+i}(x)\left(\left(\frac{1}{Y^2(x)}\right)^i+(-1)^{i+j}\left(\frac{1}{x^2}\right)^i\left(\frac{x^2}{Y^2(x)}\right)^j\right) \qquad (4.2.36)
\end{aligned}$$

and

$$\begin{aligned}
Q(x)R(x)(Y(x)\widetilde{Y}(x))^i &= -\frac{(Y(x)+x^2)(\widetilde{Y}(x)+x^2)(-x^2)^i}{(Y(x)-\widetilde{Y}(x))^2}\\
&= (-1)^{i+1}\frac{(d-1)x^{2i+4}}{(Y(x)-\widetilde{Y}(x))^2}. \qquad (4.2.37)
\end{aligned}$$

Hence equation (4.2.35) can be rewritten as

$$\begin{aligned}
&\mu(C_i'^d,x)\mu(C_j'^d,x) = Q^2(x)Y^{i+j}(x)+R^2(x)\widetilde{Y}^{i+j}(x)\\
&+(-1)^{i+1}\frac{(d-1)Y^{j+i}(x)x^4}{(Y(x)-\widetilde{Y}(x))^2}\left(\left(\frac{x^2}{Y^2(x)}\right)^i+(-1)^{i+j}\left(\frac{x^2}{Y^2(x)}\right)^j\right). \qquad (4.2.38)
\end{aligned}$$

If we replace i by $i-1$ in the above equation, then we obtain

$$\begin{aligned}
&\mu(C_{i-1}'^d,x)\mu(C_j'^d,x)\\
&= Q^2(x)Y^{i+j-1}(x)+R^2(x)\widetilde{Y}^{i+j-1}(x)+(-1)^i\frac{(d-1)Y^{i+j-1}(x)x^4}{(Y(x)-\widetilde{Y}(x))^2}\\
&\qquad\left(\left(\frac{x^2}{Y^2(x)}\right)^{i-1}+(-1)^{i+j-1}\left(\frac{x^2}{Y^2(x)}\right)^j\right)\\
&= Q^2(x)Y^{i+j-1}(x)+R^2(x)\widetilde{Y}^{i+j-1}(x)+(-1)^i\frac{(d-1)Y^{i+j+1}(x)x^2}{(Y(x)-\widetilde{Y}(x))^2}\\
&\qquad\left(\left(\frac{x^2}{Y^2(x)}\right)^{i}+(-1)^{i+j-1}\left(\frac{x^2}{Y^2(x)}\right)^{j+1}\right). \qquad (4.2.39)
\end{aligned}$$

Similarly, replacement of j by $j-1$ in equation (4.2.38) gives

$$\begin{aligned}&\mu(C_i'^d,x)\mu(C_{j-1}'^d,x)\\&=Q^2(x)Y^{i+j-1}(x)+R^2(x)\widetilde{Y}^{i+j-1}(x)+(-1)^{i+1}\frac{(d-1)Y^{i+j+1}(x)x^2}{(Y(x)-\widetilde{Y}(x))^2}\\&\qquad\left(\left(\frac{x^2}{Y^2(x)}\right)^{i+1}+(-1)^{i+j-1}\left(\frac{x^2}{Y^2(x)}\right)^{j}\right).\end{aligned}\tag{4.2.40}$$

The sum of (4.2.39) and (4.2.40) is

$$\begin{aligned}&\mu(C_{i-1}'^d,x)\mu(C_j'^d,x)+\mu(C_i'^d,x)\mu(C_{j-1}'^d,x)\\&=2Q^2(x)Y^{i+j-1}(x)+2R^2(x)\widetilde{Y}^{i+j-1}(x)+(-1)^i\frac{(d-1)x^2Y^{i+j-1}(x)(Y^2(x)-x^2)}{(Y(x)-\widetilde{Y}(x))^2}\\&\qquad\left(\left(\frac{x^2}{Y^2(x)}\right)^{i}+(-1)^{i+j}\left(\frac{x^2}{Y^2(x)}\right)^{j}\right).\end{aligned}\tag{4.2.41}$$

If we write (note that $i+j=n-1$)

$$\begin{aligned}F(n)&=(2Q^2(x)Y^{n-2}(x)+2R^2(x)\widetilde{Y}^{n-2}(x))x^2\mu(G-v,x)+(Q^2(x)Y^{n-1}(x)\\&\quad+R^2(x)\widetilde{Y}^{n-1}(x))\left(\mu(G-v,x)+x^2\sum_{w\in N_G(v)}\mu(G-\{v,w\},x)\right)\end{aligned}\tag{4.2.42}$$

and

$$\begin{aligned}K(n)&=-\frac{(d-1)x^4Y^{n-1}(x)}{(Y(x)-\widetilde{Y}(x))^2}\\&\left(\frac{x^2+Y(x)-Y^2(x)}{Y(x)}\mu(G-v,x)+x^2\sum_{w\in N_G(v)}\mu(G-\{v,w\},x)\right),\end{aligned}\tag{4.2.43}$$

then equation (4.2.34) becomes

$$\mu(C_d(n,i+1,G,v),x)=F(n)+K(n)(-1)^i f_{\frac{x^2}{Y^2(x)},n-1}(i),\tag{4.2.44}$$

where the function $f_{\frac{x^2}{Y^2(x)},n-1}$ is as defined in Lemma 3.2.1.

Knowing that $d\geq 3$, we can deduce from equations (4.2.25) and (4.2.26) that

$$|\widetilde{Y}(x)|<Y(x)\tag{4.2.45}$$

and this implies that

$$|R(x)|<Q(x).\tag{4.2.46}$$

Combining (4.2.45) and (4.2.46), we find that $F(n) > 0$ for all n. By definition of $C_d(n,k,G,v)$, $|N_G(v)| \leq d-2$ and if $|N_G(v)| = d-2$ then there must be some $w \in N_G(v)$ such that $\mu(G-\{v,w\},x) < \mu(G-v,x)$, since otherwise $G = S_{d-1}$ which is in contradiction to Definition 4.2.1. Therefore

$$\sum_{w \in N_G(v)} \mu(G-\{v,w\},x) < (d-2)\mu(G-v,x), \tag{4.2.47}$$

and equation (4.2.43) gives

$$\begin{aligned} K(n) &> -\frac{(d-1)x^4Y^{n-1}(x)}{(Y(x)-\widetilde{Y}(x))^2} \\ &\qquad \left(\frac{x^2+Y(x)-Y^2(x)}{Y(x)}\mu(G-v,x) + x^2(d-2)\mu(G-v,x)\right) \\ &= -\frac{(d-1)x^4Y^{n-1}(x)}{(Y(x)-\widetilde{Y}(x))^2} \times \frac{x^2+(1+(d-2)x^2)Y(x)-Y^2(x)}{Y(x)}\mu(G-v,x) \\ &= 0 \end{aligned} \tag{4.2.48}$$

because $Y(x)$ is a solution of equation (4.2.24).

It is easy to see from equation (4.2.25) that $0 < \frac{x^2}{Y^2(x)} < 1$, thus $f_{\frac{x^2}{Y^2(x)},n-1}$ is as in Lemma 3.2.1.

Finally, comparing equations (4.2.20) and (4.2.44) shows that as a function of i, $\mu(C_d(n,i+1,G,v))$ behaves in the opposite way as $\sigma(C_d(n,i+1,G,v))$, so we conclude the lemma. □

4.2.3 Application

Let v be a vertex in a graph G such that $C_d(n,k,G,v) \in \mathbb{T}_{1,d}$ for some positive integers $n \geq k \geq 1$ and $d \geq 3$. If $n > k \geq 2$, then $C_d(n,k,G,v)$ has one more pseudo-leaf (namely v_1) compared to $C_d(n,1,G,v)$. Therefore the following is a consequence of Lemma 4.2.2 and Lemma 4.2.4: if an element T in $\mathbb{T}_{1,d}$ has more than 3 pseudo-leaves, by choosing an appropriate C_k^d to "slide", we can form a new graph T' of the same size and order as T but with one pseudo-leave less, and such that $\sigma(T') < \sigma(T)$ and $\mu(T',x) > \mu(T,x)$ for all real numbers $x > 0$. In other words, for a fixed order $(d-1)n+2$, the element of $\mathbb{T}_{1,d}$ which has the fewest pseudo-leaves has also minimum Merrifield-Simmons index, maximum Hosoya index and maximum energy. In the following theorem, we state this more precisely.

Theorem 4.2.5 ([AW10]) *Let n and $d \geq 3$ be positive integers. The element of $\mathbb{T}_{1,d}^n$ which has the minimum Merrifield-Simmons index, the maximum Hosoya index and the maximum energy is C_n^d, and it is followed by*

- $T_d(1,1,1)$ *if* $n = 4$,

- $T_d(1,1,2)$ *if* $n=5$,
- $T_d(1,2,2)$ *if* $n=6$,
- $T_d(2,2,n-5)$ *if* $n \geq 7$.

For all real $x>0$ *we have*

$$\sigma(C_n) = \frac{3Y+2^{d-2}+1}{Y-\widetilde{Y}}Y^n - \frac{3\widetilde{Y}+2^{d-2}+1}{Y-\widetilde{Y}}\widetilde{Y}^n, \tag{4.2.49}$$

$$\mu(C_n,x) = \frac{(Y(x)+x^2)^2}{Y(x)-\widetilde{Y}(x)}Y^{n-1}(x) - \frac{(\widetilde{Y}(x)+x^2)^2}{Y(x)-\widetilde{Y}(x)}\widetilde{Y}^{n-1}(x), \tag{4.2.50}$$

where $Y, \widetilde{Y}, Y(x)$ *and* $\widetilde{Y}(x)$ *are as in equations* (4.2.2),(4.2.3) (4.2.25) *and* (4.2.26)*, respectively.*

Proof. There is no element in $\mathbb{T}^n_{1,d}$ whose number of pseudo-leaves is less than 3 except for the caterpillar C^d_n. Hence the first part of the theorem follows.

Since C^d_n is the unique caterpillar in $\mathbb{T}^n_{1,d}$, the non-caterpillar element of $\mathbb{T}^n_{1,d}$ with minimum Merrifield-Simmons index, maximum Hosoya index and maximum energy is a d-tripod, say $T_d(i,j,n-1-i-j)$ for some positive integer i and j. The cases corresponding to $n \in \{4,5\}$ are trivial since there is only one possible d-tripod of order $(d-1)n+2$ and it is as described in the statement of the theorem. The two possible d-tripods corresponding to $n=6$ are $T_d(1,2,2)$ and $T_d(1,1,3)$. However, we have

$$\sigma(T_d(1,2,2)) < \sigma(T_d(1,1,3)) \tag{4.2.51}$$

and

$$\mu(T_d(1,2,2),x) > \mu(T_d(1,1,3),x) \tag{4.2.52}$$

for every $x>0$; the inequalities follow from Lemma 4.2.2 and Lemma 4.2.4 respectively. For $n \geq 7$, one among the three caterpillar branches of T must be C''^d_2. Otherwise, we can choose the shortest of its caterpillar branches as a "sliding" subgraph and apply Lemma 4.2.2 to get,

$$\sigma(T_d(i,2,n-3-i)) < \sigma(T_d(i,j,n-1-i-j)) \text{ if } i \leq 2 \tag{4.2.53}$$

or

$$\sigma(T_d(2,i,n-3-i)) < \sigma(T_d(i,j,n-1-i-j)) \text{ if } i > 2, \tag{4.2.54}$$

which contradict the minimality of $\sigma(T_d(i,j,n-1-i-j))$ and we can also apply Lemma 4.2.4 to get for any real number $x>0$ that

$$\mu(T_d(i,2,n-3-i),x) > \mu(T_d(i,j,n-1-i-j),x) \text{ if } i \leq 2 \tag{4.2.55}$$

or

$$\mu(T_d(2,i,n-3-i),x) > \mu(T_d(i,j,n-1-i-j),x) \text{ if } i>2, \qquad (4.2.56)$$

contradicting the maximality of $\mathrm{Z}(T_d(i,j,n-1-i-j))$ and $\mathrm{En}(T_d(i,j,n-1-i-j))$. By repeating the same argument, but this time choosing the $C_2'^d$ branch as a "sliding" subgraph, we will have again a contradiction if one of i and j is not equal to 2. Therefore

$$T_d(i,j,n-1-i-j) = T_d(2,2,n-5) \text{ if } n \geq 7. \qquad (4.2.57)$$

Let v be a leaf attached to one of the pseudo-leaves v_1 of C_n^d. We can apply relation (2.2.7) to C_n^d to get (recall that $Y + \widetilde{Y} = 2^{d-2}$)

$$\begin{aligned}
\sigma(C_n^d) &= \sigma(C_n^d - v) + \sigma(C_n^d - \{v, v_1\}) \\
&= \varsigma_n^d + 2^{d-2}\varsigma_{n-1}^d \\
&= \frac{2Y+1}{Y-\widetilde{Y}}Y^n - \frac{2\widetilde{Y}+1}{Y-\widetilde{Y}}\widetilde{Y}^n + \frac{2^{d-2}(2Y+1)}{Y-\widetilde{Y}}Y^{n-1} - \frac{2^{d-2}(2\widetilde{Y}+1)}{Y-\widetilde{Y}}\widetilde{Y}^{n-1} \\
&= \frac{2Y+1-\widetilde{Y}(2Y+1)}{Y-\widetilde{Y}}Y^n - \frac{2\widetilde{Y}+1-Y(2\widetilde{Y}+1)}{Y-\widetilde{Y}}\widetilde{Y}^n \\
&= \frac{2Y+1+2^{d-1}-\widetilde{Y}}{Y-\widetilde{Y}}Y^n - \frac{2\widetilde{Y}+1+2^{d-1}-Y}{Y-\widetilde{Y}}\widetilde{Y}^n \\
&= \frac{3Y+2^{d-2}+1}{Y-\widetilde{Y}}Y^n - \frac{3\widetilde{Y}+2^{d-2}+1}{Y-\widetilde{Y}}\widetilde{Y}^n \qquad (4.2.58)
\end{aligned}$$

and similarly with the help of equation (2.3.39) one obtains

$$\begin{aligned}
\mu(C_n^d,x) &= \mu(C_n^d - v, x) + x^2\mu(C_n^d - \{v,v_1\}, x) \\
&= \mu(C_n'^d, x) + x^2\mu(C_{n-1}'^d, x) \\
&= \frac{Y(x)+x^2}{Y(x)-\widetilde{Y}(x)}Y^n(x) - \frac{\widetilde{Y}(x)+x^2}{Y(x)-\widetilde{Y}(x)}\widetilde{Y}^n(x) \\
&\qquad + \frac{x^2(Y(x)+x^2)}{Y(x)-\widetilde{Y}(x)}Y^{n-1}(x) - \frac{x^2(\widetilde{Y}(x)+x^2)}{Y(x)-\widetilde{Y}(x)}\widetilde{Y}^{n-1}(x) \\
&= \frac{(Y(x)+x^2)^2}{Y(x)-\widetilde{Y}(x)}Y^{n-1}(x) - \frac{(\widetilde{Y}(x)+x^2)^2}{Y(x)-\widetilde{Y}(x)}\widetilde{Y}^{n-1}(x). \qquad (4.2.59)
\end{aligned}$$

□

Definition 4.2.6 Let v be a vertex of a graph G, and let k be a positive integer. The cardinality of the set $\{u \in N_G(v) | \deg(u) = k\}$ is called the *k-degree* of v, it is denoted by $\deg_k(v)$.

The value of the d-degree of a vertex of a tree in $\mathbb{T}_{1,d}$ ranges from 0 to d.

Definition 4.2.7 Let $k, j, d, c_1, c_2, \ldots, c_k$ be integers such that $1 \leq k$, $1 \leq j$, $3 \leq d$ and $1 \leq c_1 \leq c_2 \leq \cdots \leq c_k$. We denote by $S_d(j, c_1, c_2, \ldots, c_k)$ the tree which is obtained by merging into a vertex v the centre of the star S_j and a leaf attached to a pseudo-leaf from each of the caterpillars $C^d_{c_1}, C^d_{c_2}, \ldots, C^d_{c_k}$. The vertex v is called the *centre* of $S_d(j, c_1, c_2, \ldots, c_k)$.

$S_d(j, c_1, c_2, \ldots, c_k)$ is an element of $\mathbb{T}_{1,d}$ if and only if $j = d-k+1$. In particular $S_d(d-2, c_1, c_2, c_3)$ is a d-tripod.

By considering the set of all elements of $\mathbb{T}_{1,d}$ which have a given maximum d-degree we obtain a theorem of the same type as Theorem 3.2.8:

Theorem 4.2.8 *Let $1 \leq k$ and $3 \leq d$ be integers such that $k \leq d$. Among all elements of $\mathbb{T}^n_{1,d}$ which have maximum d-degree k, the tree which has minimum Merrifield-Simmons index, maximum Hosoya index and maximum energy is $S_d(d-k+1, c_1, c_2, \ldots, c_k)$, where*

$$\begin{cases} c_1 = \cdots = c_{2k-n+1} = 1 \text{ and } c_{2k-n+2} = \cdots = c_k = 2 & \text{if } k > \frac{n-1}{2}, \\ c_1 = \cdots = c_{k-1} = 2 \text{ and } c_k = n+1-2k & \text{if } k \leq \frac{n-1}{2}. \end{cases} \tag{4.2.60}$$

Proof. We start by proving that the tree $S_d(d-k+1, c_1, c_2, \ldots, c_k)$, as in the statement of the theorem, is the unique element of $\mathbb{T}^n_{1,d}$ that has maximum Z and maximum En. This will be done by showing that it is the one which has maximum $\mu(., x)$ for all real numbers $x > 0$.

Let T be an element of $\mathbb{T}^n_{1,d}$ with maximum d-degree k. Let x be a positive real number. Assume that T is maximal with respect to $\mu(., x)$. Let us consider a vertex v of d-degree k in T. All the branches of v are caterpillars, otherwise by Lemma 4.2.4 we can replace a non-caterpillar branch of v by a caterpillar to obtain another element T' of $\mathbb{T}^n_{1,d}$ with maximum d-degree k such that

$$\mu(T, x) < \mu(T', x). \tag{4.2.61}$$

But this contradicts the maximality of $\mu(T, x)$. Therefore we deduce that $T = S_d(d-k+1, c_1, c_2, \ldots, c_k)$ for some positive integers $1 \leq c_1 \leq c_2 \leq \cdots \leq c_k$.

If $c_k = 2$ or if $c_k > 2$ and $c_1 = c_2 = \cdots = c_{k-1} = 2$, then we are done. Otherwise, we have the following cases:

- There is $i \in \{1, 2, \ldots, k-1\}$ such that $c_i = 1$, but then by taking

  $$G = S_d(d-k-1, c_1, \ldots, c_{i-1}, c_{i+1}, \ldots, c_{k-1}) \tag{4.2.62}$$

  we could apply Lemma 4.2.4 and have

  $$\begin{aligned} \mu(T, x) &= \mu(P_d(c_d + 2, 2, G, v), x) \\ &< \mu(P_d(c_d + 2, 3, G, v), x) \\ &= \mu(S_d(d-k+1, c_1, \ldots, c_{i-1}, 2, c_{i+1}, \ldots, c_k), x) \end{aligned} \tag{4.2.63}$$

which contradicts the maximality of $\sigma(T)$ since the maximum d-degree in $S_d(d-k+1, c_1, \ldots, c_{i-1}, 2, c_{i-1}, \ldots, c_k)$ is also k.

- There is $i \in \{1, 2, \ldots, k-1\}$ such that $c_i \geq 3$. By considering again

$$G = S_d(d-k-1, c_1, \ldots, c_{i-1}, c_{i+1}, \ldots, c_{k-1}) \tag{4.2.64}$$

and by applying Lemma 4.2.4 we obtain

$$\begin{aligned}\mu(T, x) &= \mu(P_d(c_d + c_i + 1, c_i + 1, G, v), x) \\ &< \mu(P_d(c_d + c_i + 1, 3, G, v), x) \\ &= \mu(S_d(d-k+1, c_1, \ldots, c_{i-1}, 2, c_{i+1}, \ldots, c_k + c_i - 2)),\end{aligned} \tag{4.2.65}$$

which contradicts again the minimality of $\mu(T, x)$.

For the case of σ, one has to repeat exactly the same proof, replacing $\mu(., x)$ by σ, reversing all inequalities and use Lemma 4.2.2 instead of Lemma 4.2.4. □

In the next section, we establish a complete ordering of all d-tripods in $\mathbb{T}^n_{1,d}$, with respect to σ and then with respect to Z. This will pave the way to obtain the successors of $T_d(2, 2, n-5)$ in the list of elements of $\mathbb{T}^n_{1,d}$ sorted by increasing Merrifield-Simmons index and decreasing Hosoya index.

4.3 Complete ordering of all d-tripods

The lemmas on “sliding along a caterpillar” allow us to compare Merrifield-Simmons index, Hosoya index and energy of any two d-tripods $T_d(i, j, k)$ and $T_d(i', j', k')$ whenever

$$\{i, j, k\} \cap \{i', j', k'\} \neq \varnothing. \tag{4.3.1}$$

Some comparisons of d-tripods require multiple applications to different subgraphs. For instance, in order to compare $\sigma(T_d(1, 4, 4))$ to $\sigma(T_d(2, 2, 5))$ we have to slide successively different branches: by moving a C'^d_1 branch we have

$$\sigma(T_d(1, 4, 4)) > \sigma(T_d(1, 2, 6)), \tag{4.3.2}$$

and moving a C'^d_2 branch will give

$$\sigma(T_d(1, 2, 6)) > \sigma(T_d(2, 2, 5)). \tag{4.3.3}$$

The two inequalities imply the desired relation

$$\sigma(T_d(1, 4, 4)) > \sigma(T_d(2, 2, 5)). \tag{4.3.4}$$

Some d-tripods cannot be compared by this “sliding” method, and these cases can be grouped in three. In the next two subsections we will solve these “stubborn” cases for the Merrifield-Simmons index and for the Hosoya index. Since the proofs are very long, we only state the results and give the proofs in Appendix A and Appendix B respectively.

4.3.1 Ordering d-tripods with respect to their Merrifield-Simmons index

Selected inequalities between tripods that cannot be obtained by the method of "sliding" subgraphs are provided in the next lemma.

Lemma 4.3.1 *Let n, k, l, m, k', l', m' be integers such that $n \geq 7$,*

$$1 \leq k' \leq l' \leq m' \tag{4.3.5}$$
$$2 \leq k \leq l \leq m \tag{4.3.6}$$
$$k + l + m = k' + l' + m' = n - 1 \tag{4.3.7}$$

and such that k is even and k' is odd. Then we have

$$\sigma(T_d(k, l, m)) < \sigma(T_d(k', l', m')). \tag{4.3.8}$$

For all positive integers t such that $2 \leq t \leq \frac{n-1}{6}$ we have

$$\sigma(T_d(2t, 2t, n - 1 - 4t)) > \sigma(T_d(2t - 2, 2t - 1, n - 4t + 2)), \tag{4.3.9}$$

For all positive integers t such that $1 \leq t \leq \frac{n-4}{6}$ we have

$$\sigma(T_d(2t - 1, 2t, n - 4t)) > \sigma(T_d(2t + 1, 2t + 1, n - 4t - 3)). \tag{4.3.10}$$

Proof. The proof consists of computing the difference for each of the given pairs of d-tripods and showing that it is positive. The reader is referred to Appendix A for details. □

The two Lemmas 4.2.2 and 4.3.1 are enough to construct the complete "tower" of d-tripods with respect to the Merrifield-Simmons index.

Theorem 4.3.2 *For all positive integers $n \geq 19$ (for smaller n, remove all impossible d-tripods from the list below) we have*

$$\begin{array}{lllll}
\sigma(T_d(2,2,n-5)) & < \sigma(T_d(2,4,n-7)) & < \cdots & < \sigma(T_d(2,5,n-8)) & < \sigma(T_d(2,3,n-6)) \\
< \sigma(T_d(4,4,n-9)) & < \sigma(T_d(4,6,n-11)) & < \cdots & < \sigma(T_d(4,7,n-12)) & < \sigma(T_d(4,5,n-10)) \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
< \sigma(T_d(3,4,n-8)) & < \sigma(T_d(3,6,n-10)) & < \cdots & < \sigma(T_d(3,5,n-9)) & < \sigma(T_d(3,3,n-7)) \\
< \sigma(T_d(1,2,n-4)) & < \sigma(T_d(1,4,n-6)) & < \cdots & < \sigma(T_d(1,3,n-5)) & < \sigma(T_d(1,1,n-3)).
\end{array}$$

Proof. d-tripods in a line have the same shortest caterpillar branches. Considering these shortest caterpillar branches as "sliding" subgraphs, the order in each line follows easily from Lemma 4.2.2.

When it comes to comparing the number of independent vertex subsets of a d-tripod at the end of a line with that of the first one in the following line, we use Lemma 4.3.1. Say $T_d(i, j, k)$ and $T_d(i', j', k')$ are two such a d-tripods, then we have the following three cases:

- If i and i' do not have the same parity, then we use inequality (4.3.8).
- If i and i' are both even, then the corresponding relation follows from inequality (4.3.9).
- If i and i' are both odd, then the corresponding relation comes from inequality (4.3.10).

□

A similar result also holds for the Hosoya index, as shown in the following:

4.3.2 Ordering d-tripods with respect to their Hosoya index

The method is comparable to that of the previous subsection.

Lemma 4.3.3 *Let n, k, l, m, k', l', m' be integers such that $n \geq 7$*

$$\begin{aligned} k &\leq l \leq m \\ k' &\leq l' \leq m' \\ k + l + m &= k' + l' + m' = n - 1 \end{aligned}$$

and such that k is even and k' is odd. Then we have

$$\mathrm{Z}(T_d(k, l, m)) > \mathrm{Z}(T_d(k', l', m')) \tag{4.3.11}$$

For all positive integers t such that $2 \leq t \leq \frac{n-1}{6}$ we have

$$\mathrm{Z}(T_d(2t, 2t, n - 1 - 4t)) < \mathrm{Z}(T_d(2t - 2, 2t - 1, n - 4t + 2)). \tag{4.3.12}$$

For all positive integers t such that $1 \leq t \leq \frac{n-4}{6}$ we have

$$\mathrm{Z}(T_d(2t - 1, 2t, n - 4l)) < \mathrm{Z}(T_d(2t + 1, 2t + 1, n - 4t - 3)). \tag{4.3.13}$$

Proof. The proof is similar to that of Lemma 4.3.1, it is transferred to Appendix B. □

Now it becomes clear that the list of d-tripods in decreasing order with respect to the Hosoya index is exactly the same as the list with respect to increasing Merrifield-Simmons index.

Theorem 4.3.4 *For all positive integers $n \geq 19$ (for smaller n, remove all impossible d-tripods from the list below) we have*

$$\begin{array}{lllll} \mathrm{Z}(T_d(2,2,n-5)) & > \mathrm{Z}(T_d(2,4,n-7)) & > \cdots & > \mathrm{Z}(T_d(2,5,n-8)) & > \mathrm{Z}(T_d(2,3,n-6)) \\ > \mathrm{Z}(T_d(4,4,n-9)) & > \mathrm{Z}(T_d(4,6,n-11)) & > \cdots & > \mathrm{Z}(T_d(4,7,n-12)) & > \mathrm{Z}(T_d(4,5,n-10)) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ > \mathrm{Z}(T_d(3,4,n-8)) & > \mathrm{Z}(T_d(3,6,n-10)) & > \cdots & > \mathrm{Z}(T_d(3,5,n-9)) & > \mathrm{Z}(T_d(3,3,n-7)) \\ > \mathrm{Z}(T_d(1,2,n-4)) & > \mathrm{Z}(T_d(1,4,n-6)) & > \cdots & > \mathrm{Z}(T_d(1,3,n-5)) & > \mathrm{Z}(T_d(1,1,n-3)) \end{array}$$

Proof. Exactly the same as the proof of Theorem 4.3.2, except that Lemmas 4.2.2 and 4.3.1 are replaced by Lemmas 4.2.4 and 4.3.3, respectively. □

Now that we have a good understanding of the behaviour of the graph invariants σ and Z on the set of d-tripods, the next section will use these results to extend Theorem 4.2.5 greatly.

4.4 First appearance of a non-d-tripod

This section consists of two parts: one for the Merrifield-Simmons index, one for the Hosoya index. But the methods used in the two subsections are essentially the same. First we ignore all caterpillars and d-tripods and we denote the corresponding subset of $\mathbb{T}^n_{1,d}$ by $\mathbb{T}'^n_{1,d}$. Then we determine the graph with minimum Merrifield-Simmons index or maximum Hosoya index in $\mathbb{T}'^n_{1,d}$. The last step consists of comparing it to d-tripods in order to be able to place it in the known list of d-tripods.

4.4.1 Merrifield-Simmons index

If an element of $\mathbb{T}'^n_{1,d}$ contains more than four pseudo-leaves, then via Lemma 4.2.2 we can always form a new tree with smaller number of pseudo-leaves and smaller Merrifield-Simmons index that is still an element of $\mathbb{T}'^n_{1,d}$. Hence, it is clear that the minimal element in $\mathbb{T}'^n_{1,d}$ with respect to the Merrifield-Simmons index must have exactly four pseudo-leaves, this means that it is of the type $H_d(e, d_{11}, d_{12}, d_{21}, d_{22})$. The Merrifield-Simmons index of such a graph can be expressed as

$$\begin{aligned}
&\sigma(H_d(e, d_{11}, d_{12}, d_{21}, d_{22})) \\
&= 2^{d-3}\varsigma^d_{d_{12}}\varsigma^d_{d_{11}}\left(2^{d-3}\varsigma^d_{d_{21}}\varsigma^d_{d_{22}}\sigma(C''^d_{e-2}) + 2^{3(d-2)}\varsigma^d_{d_{21}-1}\varsigma^d_{d_{22}-1}\sigma(C''^d_{e-3})\right) \\
&\qquad + 2^{3(d-2)}\varsigma^d_{d_{12}-1}\varsigma^d_{d_{11}-1}\left(2^{d-3}\varsigma^d_{d_{21}}\varsigma^d_{d_{22}}\sigma(C''^d_{e-3}) + 2^{3(d-2)}\varsigma^d_{d_{21}-1}\varsigma^d_{d_{22}-1}\sigma(C''^d_{e-4})\right) \\
&= 2^{2(d-3)}\sigma(C''^d_{e-2})\prod_{\substack{1\le i\le 2\\1\le j\le 2}}\varsigma^d_{d_{ij}} + 2^{6(d-2)}\sigma(C''^d_{e-4})\prod_{\substack{1\le i\le 2\\1\le j\le 2}}\varsigma^d_{d_{ij}-1} \\
&\qquad\qquad + 2^{4(d-2)-1}\sigma(C''^d_{e-3})\left(\prod_{\substack{1\le i\le 2\\1\le j\le 2}}\varsigma^d_{d_{ij}-i+1} + \prod_{\substack{1\le i\le 2\\1\le j\le 2}}\varsigma^d_{d_{ij}+i-2}\right).
\end{aligned} \tag{4.4.1}$$

With the values $\sigma(C''^d_{-1}) = 2^{2-d}$, $\sigma(C''^d_{-2}) = 0$, $\sigma(C''^d_{-3}) = 2^{4-2d}$ which are obtained by respecting the recurrence relation for $\sigma(C''^d_n)$, the formula (4.4.1) even holds for $e \in \{1, 2, 3\}$. As a consequence of the recurrence relations for $\sigma(C''^d_n)$ and ς^d_n, however, we can deduce from equation (4.4.1) relations for

d-quadripods of different orders:

$$\begin{aligned}
&\sigma(H_d(e, d_{11}, d_{12}, d_{21}, d_{22})) \\
&= 2^{d-2}(\sigma(H_d(e-1, d_{11}, d_{21}, d_{12}, d_{22})) + \sigma(H_d(e-2, d_{11}, d_{21}, d_{12}, d_{22}))) \\
&= 2^{d-2}(\sigma(H_d(e, d_{11}-1, d_{21}, d_{12}, d_{22})) + \sigma(H_d(e, d_{11}-2, d_{21}, d_{12}, d_{22}))). \quad (4.4.2)
\end{aligned}$$

Moreover, from the general formula for the Merrifield-Simmons index of d-tripods given by

$$\sigma(T_d(k, l, m)) = 2^{d-3}\varsigma_k^d \varsigma_m^d \varsigma_l^d + 2^{3d-6}\varsigma_{k-1}^d \varsigma_{m-1}^d \varsigma_{l-1}^d, \quad (4.4.3)$$

we deduce that

$$\sigma(T_d(k, l, m+2)) = 2^{d-2}\sigma(T_d(k, l, m+1)) + 2^{d-2}\sigma(T_d(k, l, m)) \quad (4.4.4)$$

for all triples (k, l, m) of positive integers. These allow us to prove the next theorem on minimal trees in $\mathbb{T}'^n_{1,d}$ with respect to σ by induction.

Theorem 4.4.1 *Let $n \geq 9$ and $d \geq 3$ be integers. Among all elements of $\mathbb{T}'^n_{1,d}$, the tree which has the minimum Merrifield-Simmons index is*

$$H_d(2, 2, 2, 2, n-8). \quad (4.4.5)$$

Proof. By Lemma 4.2.2, it is clear that the element in $\mathbb{T}'^n_{1,d}$ which has minimum Merrifield-Simmons index must have one of the forms shown in Figure 4.4, i.e., of the form $H_d(n-4, 1, 1, 1, 1)$, $H_d(n-5, 1, 1, 1, 2)$, $H_d(n-6, 1, 2, 1, 2)$, $H_d(n-d_{22}-5, 1, 2, 2, d_{22})$ or $H_d(n-d_{12}-d_{22}-4, 2, d_{12}, 2, d_{22})$ where d_{12} and d_{22} are at least 2.

Let us reason by induction with respect to the number n of vertices of degree d in the tree. The two first cases can be checked directly:

- For $n = 9$, nine elements of $\mathbb{T}'^n_{1,d}$ match the forms described in Figure 4.4 and their Merrifield-Simmons indices satisfy

$$\begin{aligned}
\sigma(H_d(1,1,1,2,4)) - \sigma(H_d(2,1,2,2,2)) &= (2^d-2)^2(2^d+2)(2^d+12)2^{4d-14} \\
\sigma(H_d(1,1,2,2,3)) - \sigma(H_d(2,1,2,2,2)) &= (2^d-2)^2(2^d+2)(2^d+6)2^{4d-14} \\
\sigma(H_d(1,2,2,2,2)) - \sigma(H_d(2,1,2,2,2)) &= (2^d-2)^3(2^d+4)2^{4d-14} \\
\sigma(H_d(2,1,1,2,3)) - \sigma(H_d(2,1,2,2,2)) &= (2^d-2)^2(2^d+6)2^{4d-13} \\
\sigma(H_d(3,1,1,2,2)) - \sigma(H_d(2,1,2,2,2)) &= (2^d-2)^2(3 \cdot 2^d+10)2^{4d-13} \\
\sigma(H_d(3,1,2,1,2)) - \sigma(H_d(2,1,2,2,2)) &= 3(2^d-2)^2(2^d+2)2^{4d-13} \\
\sigma(H_d(4,1,1,1,2)) - \sigma(H_d(2,1,2,2,2)) &= (2^d-2)^2(2^d+2)2^{4d-11} \\
\sigma(H_d(5,1,1,1,1)) - \sigma(H_d(2,1,2,2,2)) &= (2^d-2)^2(5 \cdot 2^{2d}+9 \cdot 2^{d+1}+8)2^{3d-13}
\end{aligned}$$

This shows that $\sigma(H_d(2,1,2,2,2))$ is the minimum.

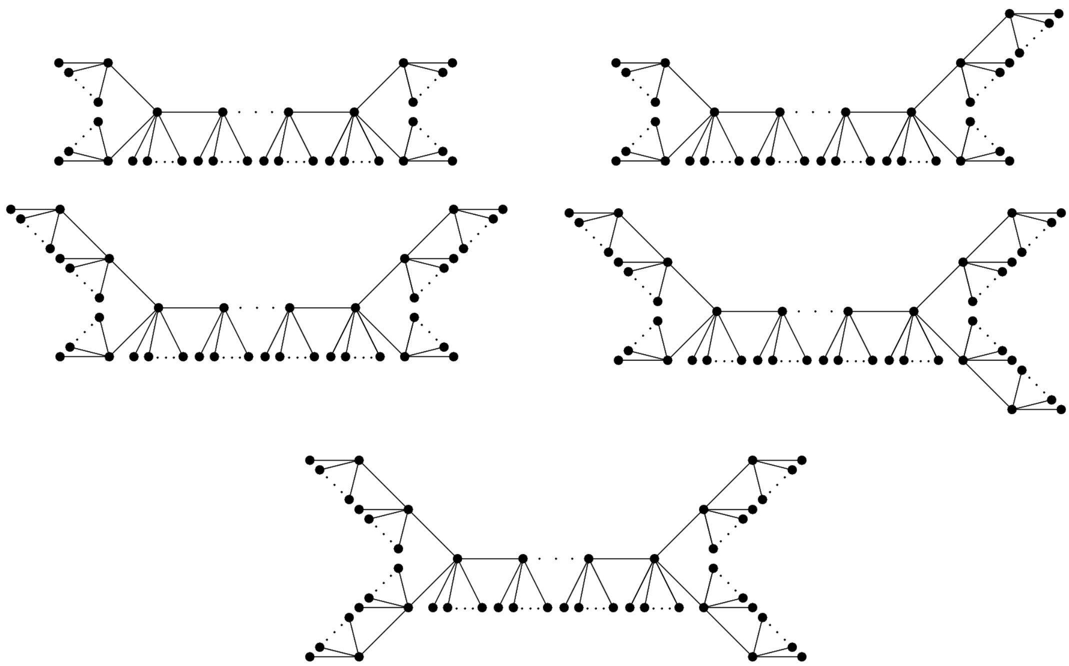


Figure 4.4:

- If $n = 10$ the twelve trees which are of the form in Figure 4.4 satisfy

$$\begin{aligned}
\sigma(H_d(1,1,1,2,5)) - \sigma(H_d(2,2,2,2,2)) =& 2^{4d-16}(2^d-2)^2 \\
& (5\cdot 2^{2d+2} + 2^{3d} + 17\cdot 2^{d+2} + 48) \\
\sigma(H_d(1,1,2,2,4)) - \sigma(H_d(2,2,2,2,2)) =& 2^{5d-14}(2^{d-1}-1)^2(2^{2d} + 7\cdot 2^{d+1} + 32) \\
\sigma(H_d(1,2,2,2,3)) - \sigma(H_d(2,2,2,2,2)) =& 2^{5d-14}(2^{d-1}-1)^2(2^d+2)(2^d+6) \\
\sigma(H_d(2,1,1,2,4)) - \sigma(H_d(2,2,2,2,2)) =& (2^d-2)^2(2^d+2)(2^d+4)2^{4d-14} \\
\sigma(H_d(2,1,2,2,3)) - \sigma(H_d(2,2,2,2,2)) =& 2^{5d-15}(2^d-2)(2^d+6) \\
\sigma(H_d(3,1,1,2,3)) - \sigma(H_d(2,2,2,2,2)) =& (2^d-2)^2(2^d+1)(2^d+6)2^{4d-13} \\
\sigma(H_d(3,1,2,2,2)) - \sigma(H_d(2,2,2,2,2)) =& 2^{5d-15}(2^d-2)^2(3\cdot 2^d+10) \\
\sigma(H_d(4,1,1,2,2)) - \sigma(H_d(2,2,2,2,2)) =& (2^d-2)^2(2^d+2)^2 2^{4d-13} \\
\sigma(H_d(4,1,2,1,2)) - \sigma(H_d(2,2,2,2,2)) =& 2^{5d-13}(2^d-2)^2(2^d+3) \\
\sigma(H_d(5,1,1,1,2)) - \sigma(H_d(2,2,2,2,2)) =& (2^d-2)^2(2^d+4)(5\cdot 2^d+6)2^{4d-15} \\
\sigma(H_d(6,1,1,1,1)) - \sigma(H_d(2,2,2,2,2)) =& (2^d-2)^2(2^d+6)(3\cdot 2^d+2)2^{4d-14}
\end{aligned}$$

  which shows again that $\sigma(H_d(2,2,2,2,2))$ is the minimum.

Assume that $H_d(2,2,2,2,(n-1)-8)$ and $H_d(2,2,2,2,n-8)$ are the trees which have the minimum Merrifield-Simmons index among all elements in $\mathbb{T}'^{n-1}_{1,d}$ and in $\mathbb{T}'^{n}_{1,d}$, respectively. Let $H_d(e, d_{11}, d_{12}, d_{21}, d_{22})$ be an element of $\mathbb{T}'^{n+1}_{1,d}$. Without loss of generality we can assume that $d_{22} = \max(\{d_{11}, d_{12}, d_{21}, d_{22}\})$.

- If $d_{22} \geq 3$, then use of the recurrence relation (4.4.2) leads to

$$\begin{aligned}&\sigma(H_d(e, d_{11}, d_{12}, d_{21}, d_{22}))\\&= 2^{d-2}\sigma(H_d(e, d_{11}, d_{12}, d_{21}, d_{22} - 1)) + 2^{d-2}\sigma(H_d(e, d_{11}, d_{12}, d_{21}, d_{22} - 2)),\end{aligned}$$

and from the induction hypothesis we know that

$$\sigma(H_d(e, d_{11}, d_{12}, d_{21}, d_{22} - 1)) \geq \sigma(H_d(2, 2, 2, 2, n - 8)) \tag{4.4.6}$$
$$\sigma(H_d(e, d_{11}, d_{12}, d_{21}, d_{22} - 2)) \geq \sigma(H_d(2, 2, 2, 2, (n - 1) - 8)). \tag{4.4.7}$$

Therefore

$$\begin{aligned}&\sigma(H_d(e, d_{11}, d_{12}, d_{21}, d_{22}))\\&\geq 2^{d-2}\sigma(H_d(2, 2, 2, 2, n - 8)) + 2^{d-2}\sigma(H_d(2, 2, 2, 2, (n - 1) - 8))\\&= \sigma(H_d(2, 2, 2, 2, n + 1 - 8)).\end{aligned} \tag{4.4.8}$$

- If $d_{22} < 3$, then necessarily

$$\begin{aligned}e &= n + 1 - d_{11} - d_{12} - d_{21} - d_{22}\\&\geq n + 1 - 8\\&\geq 3 \text{ since } n \geq 10.\end{aligned} \tag{4.4.9}$$

As

$$\begin{aligned}&\sigma(H_d(e, d_{11}, d_{12}, d_{21}, d_{22}))\\&= 2^{d-2}\sigma(H_d(e - 1, d_{11}, d_{12}, d_{21}, d_{22})) + 2^{d-2}\sigma(H_d(e - 2, d_{11}, d_{12}, d_{21}, d_{22}))\end{aligned}$$

we can apply the induction hypothesis to obtain

$$\begin{aligned}&\sigma(H_d(e, d_{11}, d_{12}, d_{21}, d_{22}))\\&\geq 2^{d-2}\sigma(H_d(2, 2, 2, 2, n - 8)) + 2^{d-2}\sigma(H_d(2, 2, 2, 2, (n - 1) - 8))\\&= \sigma(H_d(2, 2, 2, 2, n + 1 - 8)).\end{aligned} \tag{4.4.10}$$

These show that $H_d(2, 2, 2, 2, n + 1 - 8)$ has actually the minimum Merrifield-Simmons index among all elements of $\mathbb{T}'^{n+1}_{1,d}$ and the lemma follows. □

The next lemma tells us where $\sigma(H_d(2, 2, 2, 2, n + 1 - 8))$ must be placed in the list of d-tripods of order $n(d - 1) + 2$ sorted by decreasing Merrifield-Simmons index.

Lemma 4.4.2 *For all integers $n \geq 10$ we have*

- *for $d = 3$*

$$\sigma(T_d(1, 1, n - 3)) > \sigma(H_d(2, 2, 2, 2, n - 8)) > \sigma(T_d(1, 3, n - 5)) \tag{4.4.11}$$

- *and for $d \geq 4$*

$$\sigma(H_d(2,2,2,2,n-8)) > \sigma(T_d(1,1,n-3)). \tag{4.4.12}$$

Proof. The proof is by induction with respect to n.

- For $n = 10$ we have

$$\begin{aligned}&\sigma(H_d(2,2,2,2,2)) - \sigma(T_d(1,3,5)) \\ &\qquad = 2^{4d-12}(2^{d-1}-1)^2(2^{d-1}+1)(2^{2d-2}-8),\end{aligned} \tag{4.4.13}$$

which is clearly positive for $d \geq 3$ and

$$\begin{aligned}&\sigma(H_d(2,2,2,2,2)) - \sigma(T_d(1,1,7)) \\ &= 2^{4d-12}(2^{d-1}-1)^2(64 \cdot 2^{3d-9} - 16 \cdot 2^{2d-6} - 64 \cdot 2^{d-3} - 8) \qquad (4.4.14) \\ &= 2^{4d-12}(2^{d-1}-1)^2(512 \cdot 2^{3d-12} - 64 \cdot 2^{2d-8} - 128 \cdot 2^{d-4} - 8) \qquad (4.4.15)\end{aligned}$$

the expression in (4.4.14) shows that the difference is negative for $d = 3$, but as it can be seen clearly in (4.4.15) the difference is positive for all $d \geq 4$. Together with (4.4.13), these imply

$$\sigma(T_d(1,1,7)) > \sigma(H_d(2,2,2,2,2)) > \sigma(T_d(1,3,5)) \tag{4.4.16}$$

for $d = 3$ and

$$\sigma(H_d(2,2,2,2,2)) > \sigma(T_d(1,1,7)) \tag{4.4.17}$$

for $d \geq 4$, and these agree with the statement of the lemma.

- For $n = 11$ we have

$$\begin{aligned}&\sigma(H_d(2,2,2,2,3)) - \sigma(T_d(1,3,6)) \\ &= 2^{5d-15}(2^{d-1}-1)^2(2^{d-1}+2)(2^{2d}+2^{d+1}-32),\end{aligned} \tag{4.4.18}$$

which is positive since $d \geq 3$, and

$$\begin{aligned}&\sigma(H_d(2,2,2,2,3)) - \sigma(T_d(1,1,8)) \\ &= 2^{5d-14}(2^{d-1}-1)^2(2^{d-3}+1)(64 \cdot 2^{2d-6} - 48 \cdot 2^{d-3} - 24) \\ &= 2^{5d-14}(2^{d-1}-1)^2(2^{d-3}+1)(256 \cdot 2^{2d-8} - 96 \cdot 2^{d-4} - 24)\end{aligned} \tag{4.4.19}$$

is negative for $d = 3$ and positive for all $d \geq 4$. Therefore, we have

$$\sigma(T_d(1,1,8)) > \sigma(H_d(2,2,2,2,2)) > \sigma(T_d(1,3,6)) \tag{4.4.20}$$

for $d = 3$ and

$$\sigma(H_d(2,2,2,2,2)) > \sigma(T_d(1,1,8)) \tag{4.4.21}$$

for $d \geq 4$, which still agrees with the lemma.

Assume that for $n \in \{k, k-1\}$ ($11 \le k \in \mathbb{N}$) the inequality (4.4.11) is satisfied for $d = 3$ and the inequality (4.4.12) holds for $d \ge 4$. We can apply equation (4.4.2) to obtain

$$\sigma(H_d(2,2,2,2,k+1-8)) = 2^{d-2}\sigma(H_d(2,2,2,2,k-8)) + 2^{d-2}\sigma(H_d(2,2,2,2,k-1-8)). \quad (4.4.22)$$

For $d = 3$, the induction hypothesis tells us that

$$\sigma(T_d(1,1,(k-1)-3)) > \sigma(H_d(2,2,2,2,(k-1)-8)) > \sigma(T_d(1,3,(k-1)-5)) \quad (4.4.23)$$

and

$$\sigma(T_d(1,1,k-3)) > \sigma(H_d(2,2,2,2,k-8)) > \sigma(T_d(1,3,k-5)). \quad (4.4.24)$$

Therefore it follows that

$$2^{d-2}\sigma(T_d(1,1,k-3)) + 2^{d-2}\sigma(T_d(1,1,k-1-3)) > \sigma(H_d(2,2,2,2,k+1-8)) > 2^{d-2}\sigma(T_d(1,3,k-5)) + 2^{d-2}\sigma(T_d(1,3,(k-1)-5)) \quad (4.4.25)$$

and by (4.4.4) this implies

$$\sigma(T_d(1,1,(k+1)-3)) > \sigma(H_d(2,2,2,2,(k+1)-8)) > \sigma(T_d(1,3,(k+1)-5)). \quad (4.4.26)$$

For $d \ge 4$, the induction hypothesis gives

$$\sigma(H_d(2,2,2,2,(k-1)-8)) > \sigma(T_d(1,1,(k-1)-3)) \quad (4.4.27)$$

and

$$\sigma(H_d(2,2,2,2,k-8)) > \sigma(T_d(1,1,k-3)). \quad (4.4.28)$$

Therefore equation (4.4.22) implies

$$\sigma(H_d(2,2,2,2,(k+1)-8)) > 2^{d-2}\sigma(T_d(1,1,k-3)) + 2^{d-2}\sigma(T_d(1,1,(k-1)-3)) \quad (4.4.29)$$

and thus

$$\sigma(H_d(2,2,2,2,(k+1)-8)) > \sigma(T_d(1,1,(k+1)-3)). \quad (4.4.30)$$

(4.4.26) and (4.4.30) show that the desired inequalities still hold for $n = k+1$. $\square$

Remark 4.4.3 For the particular case of $n = 9$ we have

$$\begin{aligned}
&\sigma(H_d(2,1,2,2,2)) - \sigma(T_d(1,1,6)) \\
&\qquad = 2^{4d-12}(2^{d-1}-1)^2((2^{d-1}-1)2^d - 16) > 0 \quad (4.4.31)
\end{aligned}$$

which implies that for all $d \geq 3$ we always have $\sigma(H_d(2,1,2,2,2)) > \sigma(T_d(1,1,6))$.

The following theorem is a summary of the previous results about the σ-index. It gives a list of minimal trees in $\mathbb{T}^n_{1,d}$ up until the first appearance of a non d-tripod tree. If we replace all the d-tripods $T_d(i,j,k)$ by the corresponding tripods $T(i,k,j)$ and replace the d-quadripod $H_d(2,2,2,2,n-8)$ by the corresponding quadripod $H(2,2,2,2,n-8)$, then we almost obtain the first list in Theorem 3.2.6 except a one step delay in the appearance of $H(2,2,2,2,n-8)$ for $d = 3$ and a two step delay if $d \geq 4$.

Theorem 4.4.4 *The list of all trees in $\mathbb{T}^n_{1,d}$, sorted by increasing Merrifield-Simmons index reads up until the first non-d-tripod, as follows:*

- *for $d = 3$,*

$$\begin{array}{lllll}
\sigma(C^d_n) & & & & \\
<\sigma(T_d(2,2,n-5)) & <\sigma(T_d(2,4,n-7)) & <\cdots & <\sigma(T_d(2,5,n-8)) & <\sigma(T_d(2,3,n-6)) \\
<\sigma(T_d(4,4,n-9)) & <\sigma(T_d(4,6,n-11)) & <\cdots & <\sigma(T_d(4,7,n-12)) & <\sigma(T_d(4,5,n-10)) \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
<\sigma(T_d(3,4,n-8)) & <\sigma(T_d(3,6,n-10)) & <\cdots & <\sigma(T_d(3,5,n-9)) & <\sigma(T_d(3,3,n-7)) \\
<\sigma(T_d(1,2,n-4)) & <\sigma(T_d(1,4,n-6)) & <\cdots & <\sigma(T_d(1,5,n-5)) & <\sigma(T_d(1,3,n-3)) \\
 & & & & <\sigma(H_d(2,2,2,2,n-8)),
\end{array}$$

- *for $d \geq 4$,*

$$\begin{array}{lllll}
\sigma(C^d_n) & & & & \\
<\sigma(T_d(2,2,n-5)) & <\sigma(T_d(2,4,n-7)) & <\cdots & <\sigma(T_d(2,5,n-8)) & <\sigma(T_d(2,3,n-6)) \\
<\sigma(T_d(4,4,n-9)) & <\sigma(T_d(4,6,n-11)) & <\cdots & <\sigma(T_d(4,7,n-12)) & <\sigma(T_d(4,5,n-10)) \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
<\sigma(T_d(3,4,n-8)) & <\sigma(T_d(3,6,n-10)) & <\cdots & <\sigma(T_d(3,5,n-9)) & <\sigma(T_d(3,3,n-7)) \\
<\sigma(T_d(1,2,n-4)) & <\sigma(T_d(1,4,n-6)) & <\cdots & <\sigma(T_d(1,3,n-5)) & <\sigma(T_d(1,1,n-3)) \\
 & & & & <\sigma(H_d(2,2,2,2,n-8))
\end{array}$$

4.4.2 Hosoya index

The Hosoya index of any d-quadripod $H_d(e, d_{11}, d_{12}, d_{21}, d_{22})$ can be written as

$$
\begin{aligned}
&\mathrm{Z}(H_d(e, d_{11}, d_{12}, d_{21}, d_{22})) \\
&= [(d-2)\zeta^d_{d_{11}}\zeta^d_{d_{12}} + \zeta^d_{d_{11}-1}\zeta^d_{d_{12}} + \zeta^d_{d_{11}}\zeta^d_{d_{12}-1}][(d-2)\zeta^d_{d_{21}}\zeta^d_{d_{22}}\,\mathrm{Z}(C''^d_{e-2}) \\
&\qquad + \zeta^d_{d_{21}-1}\zeta^d_{d_{22}}\,\mathrm{Z}(C''^d_{e-2}) + \zeta^d_{d_{21}}\zeta^d_{d_{22}-1}\,\mathrm{Z}(C''^d_{e-2}) + \zeta^d_{d_{21}}\zeta^d_{d_{22}}\,\mathrm{Z}(C''^d_{e-3})] \\
&+ \zeta^d_{d_{11}}\zeta^d_{d_{12}}[(d-2)\zeta^d_{d_{21}}\zeta^d_{d_{22}}\,\mathrm{Z}(C''^d_{e-3}) + \zeta^d_{d_{21}-1}\zeta^d_{d_{22}}\,\mathrm{Z}(C''^d_{e-3}) \\
&\qquad + \zeta^d_{d_{21}}\zeta^d_{d_{22}-1}\,\mathrm{Z}(C''^d_{e-3}) + \zeta^d_{d_{21}}\zeta^d_{d_{22}}\,\mathrm{Z}(C''^d_{e-4})] \\
&= (d-2)\,\mathrm{Z}(C''^d_{e-2}) \prod_{1\le i,j\le 2} \zeta^d_{d_{ij}} \left((d-2) + \sum_{1\le i,j\le 2} \frac{\zeta^d_{d_{ij}-1}}{\zeta^d_{d_{ij}}} + \frac{1}{d-2} \sum_{1\le i,j\le 2} \frac{\zeta^d_{d_{1i}-1}\zeta^d_{d_{2j}-1}}{\zeta^d_{d_{1i}}\zeta^d_{d_{2j}}} \right) \\
&\quad + \prod_{1\le i,j\le 2} \zeta^d_{d_{ij}} \left(\mathrm{Z}(C''^d_{e-3}) \left(2(d-2) + \sum_{1\le i,j\le 2} \frac{\zeta^d_{d_{ij}-1}}{\zeta^d_{d_{ij}}} \right) + \mathrm{Z}(C''^d_{e-4}) \right). \qquad (4.4.32)
\end{aligned}
$$

For the cases where $e \in \{1, 2, 3\}$ we use the values $\mathrm{Z}(C''^d_{-1}) = 0$, $\mathrm{Z}(C''^d_{-2}) = 1$ and $\mathrm{Z}(C''^d_{-3}) = 1 - d$. In the above form we can see that the following relations are consequences of the recurrence relations for $(\zeta^d_n)_{n\ge -2}$ and for $(\mathrm{Z}(C''^d_n))_{n\ge -2}$:

$$
\begin{aligned}
&\mathrm{Z}(H_d(e, d_{11}, d_{12}, d_{21}, d_{22})) \\
&= (d-1)\,\mathrm{Z}(H_d(e-1, d_{11}, d_{21}, d_{12}, d_{22})) \\
&\qquad + \mathrm{Z}(H_d(e-2, d_{11}, d_{21}, d_{12}, d_{22})) \qquad (4.4.33) \\
&= (d-1)\,\mathrm{Z}(H_d(e, d_{11}, d_{21}, d_{12}, d_{22}-1)) \\
&\qquad + \mathrm{Z}(H_d(e, d_{11}, d_{21}, d_{12}, d_{22}-2)). \qquad (4.4.34)
\end{aligned}
$$

Now, we are able to describe the maximal trees in $\mathbb{T}'^n_{1,d}$ with respect to the Hosoya index:

Theorem 4.4.5 *Let $n \ge 9$ and $d \ge 3$ be integers. Among all elements of $\mathbb{T}'^n_{1,d}$, the tree with maximum Hosoya index is $H_d(2, 2, 2, 2, n-8)$.*

Proof. Similar reasoning as in the proof of Theorem 4.4.1 shows that the tree with maximum Hosoya index in $\mathbb{T}'^n_{1,d}$ must have one of the forms shown in Figure 4.4. This reduces as before considerably the size of the set where we have to look for the maximal tree.

Let us reason by induction with respect to the number n of vertices of degree d in the trees.

For $n = 9$ we have

$$
\begin{aligned}
\mathrm{Z}(H_d(2,1,2,2,2)) - \mathrm{Z}(H_d(1,1,1,2,4)) &= (d-1)^3(d^3(d-2) + 5d^2 - 4d + 2) \\
\mathrm{Z}(H_d(2,1,2,2,2)) - \mathrm{Z}(H_d(1,1,2,2,3)) &= (d-1)^3(d^2 - d + 1)^2 \\
\mathrm{Z}(H_d(2,1,2,2,2)) - \mathrm{Z}(H_d(1,2,2,2,2)) &= (d-1)^3(d^2 - d - 1)(d^2 - d + 1) \\
\mathrm{Z}(H_d(2,1,2,2,2)) - \mathrm{Z}(H_d(2,1,1,2,3)) &= (d-1)^3(d(d-2) + 2) \\
\mathrm{Z}(H_d(2,1,2,2,2)) - \mathrm{Z}(H_d(3,1,1,2,2)) &= 2(d-1)^3(d^2 - d + 1)
\end{aligned}
$$

$$\begin{aligned}
\mathrm{Z}(H_d(2,1,2,2,2)) - \mathrm{Z}(H_d(3,1,2,1,2)) &= (d-1)^3(2d^2-2d+1)\\
\mathrm{Z}(H_d(2,1,2,2,2)) - \mathrm{Z}(H_d(4,1,1,1,2)) &= (d-1)^3(d(3d-4)+2)\\
\mathrm{Z}(H_d(2,1,2,2,2)) - \mathrm{Z}(H_d(5,1,1,1,1)) &= 2(d-1)^2(d^2(2d-5)+5d-1).
\end{aligned}$$

We see that $\mathrm{Z}(H_d(2,1,2,2,2))$ is maximal for this case.

For $n = 10$ we have

$$\begin{aligned}
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(1,1,1,2,5)) &= (d-1)^2\\
&\qquad (d^4(d-2)^2 + d^3(8d-22) + 25d^2 - 16d + 5)\\
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(1,1,2,2,4)) &= (d-1)^4(d^2-d+1)(d^2-d+3)\\
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(1,2,2,2,3)) &= (d-1)^4(d^2-d+1)^2\\
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(2,1,2,2,3)) &= (d-1)^4(d^2-2d+2)\\
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(2,1,2,2,3)) &= (d-1)^2\\
&\qquad (2d^2(d-2)^2 + 6d(d-2) + 5)\\
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(3,1,1,2,3)) &= (d-1)^2\\
&\qquad (3d^2(d-2)^2 + 2d^3 + d(5d-14) + 5)\\
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(3,1,2,2,2)) &= 2(d-1)^4(d^2-d+1)\\
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(4,1,1,2,2)) &= (d-1)^2(d^2-d+1)(d(3d-7)+5)\\
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(4,1,2,1,2)) &= (d-1)^4(3d^2-4d+3)\\
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(5,1,1,1,2)) &= (d-1)^2\\
&\qquad (4d^2(d-2)^2 + 2d^3 + d(6d-16) + 5)\\
\mathrm{Z}(H_d(2,2,2,2,2)) - \mathrm{Z}(H_d(6,1,1,1,1)) &= (d-1)^3((5d-13)d^2 + 17d - 5)
\end{aligned}$$

This shows that $H_d(2,2,2,2,2)$ has the greatest Hosoya index in this case.

Let us assume that the lemma is satisfied for $n \in \{k, k-1\}$ (where $k \geq 10$) and let us show that it still holds for $n = k+1$. Let $H_d(e, d_{11}, d_{12}, d_{21}, d_{22})$ be an element of $\mathbb{T}'^{k+1}_{1,d}$. Without loss of generality we can assume that $d_{22} = \max\{d_{11}, d_{12}, d_{21}, d_{22}\}$.

- If $d_{22} \geq 3$, then by equation (4.4.34) we have

$$\begin{aligned}
&\mathrm{Z}(H_d(e, d_{11}, d_{12}, d_{21}, d_{22}))\\
&= (d-1)\,\mathrm{Z}(H_d(e, d_{11}, d_{12}, d_{21}, d_{22}-1))\\
&\qquad + \mathrm{Z}(H_d(e, d_{11}, d_{12}, d_{21}, d_{22}-2)). \qquad (4.4.35)
\end{aligned}$$

By the induction hypothesis we know that

$$\mathrm{Z}(H_d(e, d_{11}, d_{12}, d_{21}, d_{22}-1)) \leq \mathrm{Z}(H_d(2,2,2,2,n-8)) \qquad (4.4.36)$$

and

$$\mathrm{Z}(H_d(e, d_{11}, d_{12}, d_{21}, d_{22}-2)) \leq \mathrm{Z}(H_d(2,2,2,2,n-1-8)), \qquad (4.4.37)$$

therefore

$$\begin{aligned}
&\mathrm{Z}(H_d(e, d_{11}, d_{12}, d_{21}, d_{22})) \\
&\leq (d-1)\,\mathrm{Z}(H_d(2,2,2,2,n-8)) + \mathrm{Z}(H_d(2,2,2,2,n-1-8)) \\
&= \mathrm{Z}(2,2,2,2,n+1-8). \qquad (4.4.38)
\end{aligned}$$

- Otherwise we have $1 \leq d_{11}, d_{12}, d_{21}, d_{22} \leq 2$ and so $e \geq k+1-8 \geq 3$ (because $k \geq 10$). Using equation (4.4.33), we obtain

$$\begin{aligned}
&\mathrm{Z}(H_d(e, d_{11}, d_{12}, d_{21}, d_{22})) \\
&= (d-1)\,\mathrm{Z}(H_d(e-1, d_{11}, d_{12}, d_{21}, d_{22})) \\
&\qquad + \mathrm{Z}(H_d(e-2, d_{11}, d_{12}, d_{21}, d_{22})). \qquad (4.4.39)
\end{aligned}$$

Since the induction hypothesis gives

$$\mathrm{Z}(H_d(e-1, d_{11}, d_{12}, d_{21}, d_{22})) \leq \mathrm{Z}(H_d(2,2,2,2,n-8)) \qquad (4.4.40)$$

and

$$\mathrm{Z}(H_d(e-2, d_{11}, d_{12}, d_{21}, d_{22})) \leq \mathrm{Z}(H_d(2,2,2,2,n-1-8)). \qquad (4.4.41)$$

We finally obtain

$$\begin{aligned}
&\mathrm{Z}(H_d(e, d_{11}, d_{12}, d_{21}, d_{22})) \\
&\leq (d-1)\,\mathrm{Z}(H_d(2,2,2,2,n-8)) + \mathrm{Z}(H_d(2,2,2,2,n-1-8)) \\
&= \mathrm{Z}(H_d(2,2,2,2,n+1-8)), \qquad (4.4.42)
\end{aligned}$$

showing that $\mathrm{Z}(H_d(2,2,2,2,n+1-8))$ is indeed maximal.

□

The final theorem tells us about the first appearance of a non-d-tripod and non-caterpillar in the list of elements in $\mathbb{T}^n_{1,d}$ sorted by decreasing Hosoya index.

Theorem 4.4.6 *Let $n \geq 17$ and $d \geq 3$ be integers, the list of trees in $\mathbb{T}^n_{1,d}$, sorted by decreasing Hosoya index, starts as follows:*

$$\begin{array}{lllll}
\mathrm{Z}(C^d_n) & & & & \\
>\mathrm{Z}(T_d(2,2,n-5)) & >\mathrm{Z}(T_d(2,4,n-7)) & >\cdots & >\mathrm{Z}(T_d(2,5,n-8)) & >\mathrm{Z}(T_d(2,3,n-6)) \\
>\mathrm{Z}(T_d(4,4,n-9)) & >\mathrm{Z}(T_d(4,6,n-11)) & >\cdots & >\mathrm{Z}(T_d(4,7,n-12)) & >\mathrm{Z}(T_d(4,5,n-10)) \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
>\mathrm{Z}(T_d(3,4,n-8)) & >\mathrm{Z}(T_d(3,6,n-10)) & >\cdots & >\mathrm{Z}(T_d(3,5,n-9)) & >\mathrm{Z}(T_d(3,3,n-7)) \\
>\mathrm{Z}(T_d(1,2,n-4)) & >\mathrm{Z}(T_d(1,4,n-6)) & >\cdots & >\mathrm{Z}(T_d(1,3,n-5)) & >\mathrm{Z}(T_d(1,1,n-3)) \\
 & & & & >\mathrm{Z}(H_d(2,2,2,2,n-8)).
\end{array}$$

For smaller $n \leq 9$, remove all impossible d-tripods from the list.

Proof. The theorem is actually a direct consequence of Theorems 4.3.4 and 4.4.5. All we have left to prove is the inequality

$$\mathrm{Z}(T_d(1,1,n-3)) > \mathrm{Z}(H_d(2,2,2,2,n-8)) \tag{4.4.43}$$

for all integers $n \geq 10$, where d is an integer at least equal to 3. For this, we proceed by induction with respect to the number n of vertices of degree d.

For $n = 9$ we have

$$\begin{aligned} &\mathrm{Z}(T_d(1,1,6)) - \mathrm{Z}(H_d(2,1,2,2,2)) \\ &\qquad = (d-1)^3((d-2)d-1)((d-2)d+2) > 0. \end{aligned} \tag{4.4.44}$$

For $n = 10$ we have

$$\begin{aligned} &\mathrm{Z}(T_d(1,1,7)) - \mathrm{Z}(H_d(2,2,2,2,2)) \\ &\qquad = (d-1)^2((d-6)d^5 + (14d-16)d^3 + (5d+6)d - 5). \end{aligned} \tag{4.4.45}$$

The difference is clearly an increasing function of d for $d \geq 6$, its values at $d \in \{3,4,5,6\}$ are respectively $124, 5499, 60400, 372475$. Therefore we get the desired inequality for $d \geq 3$.

Now, assume that inequality (4.4.43) is satisfied for $n \in \{k, k-1\}$ (where k is at least 10) and let us show that it still holds for $n = k+1$.

By the induction hypothesis, we have

$$Z(T_d(1,1,(k-1)-3)) > Z(H_d(2,2,2,2,(k-1)-8)) \tag{4.4.46}$$

and

$$Z(T_d(1,1,k-3)) > Z(H_d(2,2,2,2,k-8)). \tag{4.4.47}$$

If we combine the two inequalities and make use of (4.4.34), we obtain

$$\begin{aligned} Z(T_d(1,1,(k+1)-3)) &= (d-1)Z(T_d(1,1,k-3)) + Z(T_d(1,1,(k-1)-3)) \\ &> Z(H_d(2,2,2,2,(k+1)-8)), \end{aligned} \tag{4.4.48}$$

which completes the induction. Therefore inequality (4.4.43) holds for all integers $n \geq 9$. $\square$

Especially for the case of $d \geq 4$ comparison between Theorem 4.4.6 and Theorem 4.4.4 confirms Remark 2.2.2 on a certain relation between σ and Z. But once again for $d = 3$ we encounter a situation which violates the remark exactly at the appearance of the first non-d-tripod, since we have

$$\sigma(H_3(2,2,2,2,n-8)) < \sigma(S_3(1,1,n-3)) \tag{4.4.49}$$

and

$$\mathrm{Z}(H_3(2,2,2,2,n-8)) < \mathrm{Z}(S_3(1,1,n-3)). \tag{4.4.50}$$

The next corollary follows trivially from Theorems 4.4.4 and 4.4.6.

Corollary 4.4.7 *Let $n > d \geq 3$ be integers. Let A be a subset of $\mathbb{T}^n_{1,d}$ such that A contains a d-tripod different from $T_d(1, 1, n-3)$. Then, there exists a unique element T in A which has minimum Merrifield-Simmons index and maximum Hosoya index among all elements of A. Furthermore, T is exactly the d-tripod in A which has minimum Merrifield-Simmons index and maximum Hosoya index.*

With the complete understanding of the behaviours of σ and Z in the set of d-tripods, the above corollary simplifies greatly the task of finding trees that minimize σ and maximize Z within a specified class of trees. Considering elements of $\mathbb{T}^n_{1,d}$ with a given diameter, the following corollary shows an example of such a class of trees.

Corollary 4.4.8 *Let $n \geq 6$ and c be two positive integers such that*

$$\frac{2(n+3)}{3} \leq c \leq n. \tag{4.4.51}$$

Then among all trees in $\mathbb{T}^n_{1,d}$ with diameter c, the tree with minimum Merrifield-Simmons index and maximum Hosoya index is

$$Tr(d, c, n) = T_d\left(n - c + 1, 2\left\lceil\frac{n+1-c}{2}\right\rceil, c - 2\left\lceil\frac{n+1-c}{2}\right\rceil - 2\right). \tag{4.4.52}$$

Proof. Let $\mathcal{D}(c, d, n)$ be the set of all trees in $\mathcal{T}^n_{1,d}$ of diameter c. Assume that c and n satisfy the condition (4.4.51), and let $M(c, d, n)$ be an element of $\mathcal{D}(c, d, n)$ with minimum Merrifield-Simmons index and maximum Hosoya index. Then $\mathcal{D}(c, d, n)$ does not contain the caterpillar C^d_n (whose diameter is $n + 1$).

Note that $\operatorname{diam}(T_d(i, j, k)) = j + k + 2$ for all positive integers i, j and k. Since

$$2\left\lceil\frac{n+1-c}{2}\right\rceil \geq n + 1 - c \tag{4.4.53}$$

and (recall that $2n + 6 \leq 3c$)

$$\begin{aligned} c - 2\left\lceil\frac{n+1-c}{2}\right\rceil - 2 &\geq c - (n + 2 - c) - 2 \\ &\geq 2c - n - 4 + 2n + 6 - 3c \\ &\geq n + 2 - c \\ &\geq 2\left\lceil\frac{n+1-c}{2}\right\rceil, \end{aligned} \tag{4.4.54}$$

we have

$$\operatorname{diam}(Tr(c, d, n)) = 2\left\lceil\frac{n+1-c}{2}\right\rceil + c - 2\left\lceil\frac{n+1-c}{2}\right\rceil - 2 + 2 = c \tag{4.4.55}$$

meaning that $\mathcal{D}(c,d,n)$ contains at least a tripod, namely $Tr(c,d,n)$. Furthermore, knowing that the second shortest branch of $Tr(c,d,n)$ is of even length, we deduce that $Tr(c,d,n)$ is different from $T_d(1,1,n-3)$. Now, we can deduce from Corollary 4.4.7 that $M(c,d,n)$ is a d-tripod. Therefore it is of the form $M(c,d,n) = T_d(i,j,c-j-2)$, for some positive integers i and j. Since $M(c,d,n)$ is an element of $\mathcal{T}^n_{1,d}$, the integers i and j must satisfy the relation $i+j+c-j-2 = n-1$ which implies

$$i = n+1-c. \tag{4.4.56}$$

By Theorems 4.3.2 and 4.3.4, we know that j must be the smallest even number greater than i. Therefore we have

$$M(c,d,n) = Tr(c,d,n). \tag{4.4.57}$$

□

Having seen which graph has minimum Merrifield-Simmons index, maximum Hosoya index and maximum energy in $\mathbb{T}^n_{1,d}$, it is natural to start asking about what kind of graph has maximum σ, minimum Z and minimum En in the same set. This will be answered in the next section.

4.5 The element of $\mathbb{T}^n_{1,d}$ that maximizes the Merrifield-Simmons index and minimizes Hosoya index and energy

For trees with given maximum degree d and given order n, it has been shown [HW08, HW09] that the maximum Merrifield-Simmons index, the minimum Hosoya index and the minimum energy are reached by a unique tree $T_{n,d}$. On the other hand, we know that the order of elements in $\mathbb{T}_{1,d}$ is of the form $(d-1)n+2$ for some $n \in \mathbb{N}$. In this section we show that for all non-negative integers n we have $T_{(d-1)n+2,d} \in \mathbb{T}_{1,d}$.

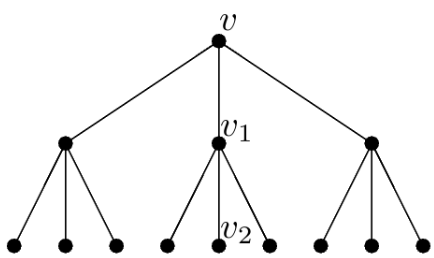
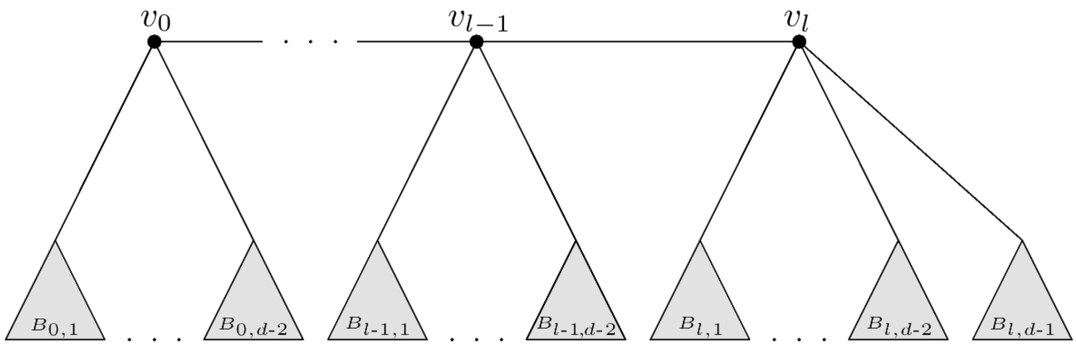


Figure 4.5: D^4_3 with root v, v_2 is a child of v_1

In a non-empty tree T one can choose a vertex $v \in V(T)$ as "special" and call it *root*. A tree with a fixed root is called a *rooted tree*. In a rooted tree

T with root v, if w is a vertex adjacent to u and the distance between v and w is greater than the distance between v and u, then w is called a *child* of u (see Figure 4.5). The length of a longest path starting from the root of a rooted tree T is called the *height* of T. A *d-ary tree* is a rooted tree where every vertex has 0 or d children. A *complete d-ary tree* is a d-ary tree where all leaves are at the same distance from the root. We denote by D_h^{d+1} a complete d-ary tree of height $h-1$ and we set D_0^{d+1} to be the empty graph.

Definition 4.5.1 Let $n > d \geq 3$ be integers. $\mathcal{T}_{n,d}$ is the set of trees with n vertices that can be decomposed as



with $B_{k,1}, \ldots, B_{k,d-2} \in \{D_k^d, D_{k+2}^d\}$ for $0 \leq k < l$ and either $B_{l,1} = \cdots = B_{l,d-1} = D_{l-1}^d$ or $B_{l,1} = \cdots = B_{l,d-1} = D_l^d$ or $B_{l,1}, \cdots, B_{l,d-1} \in \{D_l^d, D_{l+1}^d, D_{l+2}^d\}$, where at least two of $B_{l,1}, \cdots, B_{l,d-1}$ are equal to D_{l+1}^d.

Let $\mathbb{T}_d^n$ denote the set of all trees of order n whose maximum vertex degree is at most d. For all $d+1 \leq n \in \mathbb{N}$ we clearly have

$$\mathbb{T}_{1,d}^n \subset \mathbb{T}_d^{(d-1)n+2}. \tag{4.5.1}$$

The following theorem combines two very recent results. We refer the reader to [HW08, HW09] for the proof.

Theorem 4.5.2 ([HW08, HW09]) *Let $n > d \geq 3$ be integers. The set $\mathcal{T}_{n,d}$ only contains a single element. Among all trees in $\mathbb{T}_d^n$, the element of $\mathcal{T}_{n,d}$ is the tree which maximizes the Merrifield-Simmons index and minimizes the Hosoya index and energy.*

We are interested in the following corollary, which provides the solution to the problem described at the beginning of this section. We denote by $T_{n,d}$ the unique element of $\mathcal{T}_{n,d}$.

Corollary 4.5.3 *Let $d \geq 3$ and n be non-negative integers. Among all trees in $\mathbb{T}_{1,d}^n$, $T_{(d-1)n+2,d}$ is the tree which maximizes the Merrifield-Simmons index and minimizes Hosoya index and energy.*

Proof. From Theorem 4.5.2 and inclusion (4.5.1) it follows that for all trees $T \in \mathbb{T}^n_{1,d}$ if $T \neq T_{(d-1)n+2,d}$ then

$$\sigma(T) < \sigma(T_{(d-1)n+2,d}), \tag{4.5.2}$$
$$\mathrm{Z}(T) > \mathrm{Z}(T_{(d-1)n+2,d}) \tag{4.5.3}$$

and

$$\mathrm{En}(T) > \mathrm{En}(T_{(d-1)n+2,d}). \tag{4.5.4}$$

Next, we claim that $T_{(d-1)n+2,d} \in \mathbb{T}_{1,d}$ for all $n \in \mathbb{N}$. Using the notation of Definition 4.5.1, v_0 is a vertex with degree at most $d-1$, furthermore it is the only vertex in $T_{(d-1)n+2,d}$ which can possibly have a degree not in $\{1, d\}$. Say d_0 is the degree of v_0. Reasoning by contradiction, assume that $T_{(d-1)n+2,d} \notin \mathbb{T}_{1,d}$, then $1 < d_0 < d$. By attaching $d - d_0$ new leaves to v_0 we would obtain an element of $\mathbb{T}_{1,d}$ of order $(d-1)n + 2 + (d - d_0)$, which is impossible since $0 < d - d_0 \leq d - 2$. Therefore d_0 has to be 1 and we conclude the claim. $\square$

For instance, let $k \geq 1$ be an integer and let D'^d_{k+1} be the tree which results from joining the root of D^d_{k+1} to the root of D^d_k by an edge, see Figure 4.6 for an example. Then for all integers $d \geq 3$ and $k \geq 2$ we have

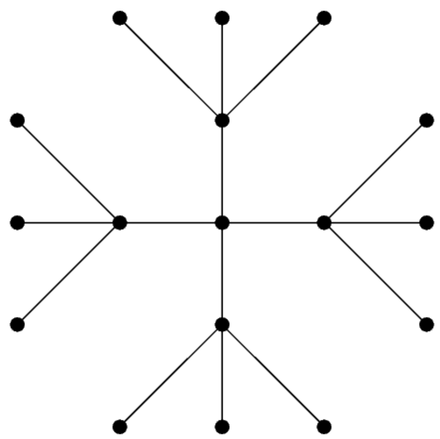


Figure 4.6: D'^4_3

$$T_{(d-1)\mathcal{N}_k+2,d} = D'^d_k \in \mathbb{T}_{1,d}, \tag{4.5.5}$$

where

$$\mathcal{N}_k = \begin{cases} 1 & \text{if } k = 2 \\ 1 + d\sum_{i=0}^{k-3}(d-1)^i & \text{if } k \geq 3. \end{cases} \tag{4.5.6}$$

According to the notation of Definition 4.5.1 it corresponds to $l = k - 1$,

$$B_{k,i} = D_k^d, \text{ for all } 0 \leq k \leq l, 1 \leq i \leq d-2, \tag{4.5.7}$$

and $B_{l,d-1} = D_l^d$.

Chapter 5

Conclusion

Our results do not only confirm the observed relations between the three graph invariants as mentioned in Remark 2.2.2 but they also show an interesting analogy between trees in the class $\mathbb{T}_{1,d}$ and general trees without degree restrictions:

- Minimum σ, maximum Z and maximum energy in $\mathbb{T}_{1,d}$ are both reached by the most path-like element C_n^d.
- The star-like element $D_n'^d$ has maximum σ, minimum Z and minimum energy among all elements in $\mathbb{T}_{1,d}$.

We also believe that our crucial Lemmas 4.2.2 and 4.2.4 can be applied to the study of unicyclic graphs or other tree-like structures with similar degree restrictions.

A natural problem for further study would be to consider trees with more general degree restrictions, such as prescribing the entire degree sequence. This might be a very hard problem, but partial results can possibly be obtained along the lines of this work.

Appendices

Appendix A

Detailed proof of Lemma 4.3.1

The following identity will often be used in this section. Let U, V, z, y be four constant real numbers and let $f : \mathbb{Z} \to \mathbb{R}$ be an function defined by $f(i) = Uz^i + Vy^i$ for all $i \in \mathbb{Z}$. Then the following holds, for all integers k, m, n

$$\begin{aligned}
f(k)f(l)f(m) &= (Uz^k + Vy^k)(Uz^m + Vy^m)(Uz^l + Vy^l) \\
&= U^3 z^{k+m+l} + U^2 V z^{l+k} y^m + U^2 V z^{m+k} y^l + UV^2 z^k y^{l+m} \\
&+ U^2 V z^{l+m} y^k + UV^2 z^l y^{m+k} + UV^2 z^m y^{l+k} + V^3 y^{k+m+l} \\
&= U^3 z^{k+m+l} + V^3 y^{k+m+l} + UV \big((zy)^k f(m+l-k) \\
&\qquad + (zy)^m f(k+l-m) + (zy)^l f(k+m-l) \big) . \qquad \text{(A.0.1)}
\end{aligned}$$

We also need the following auxiliary lemma which provides more relations between the values of ς_n^d for different n, in addition to the recurrence relation for $(\varsigma_n^d)_{n\in\mathbb{Z}}$ that we already know.

Lemma A.0.1 *For all integers $n \geq 1$ we have*

$$2^{(d-2)(n+1)+1} |\varsigma_{-n}^d| < \varsigma_n^d. \qquad \text{(A.0.2)}$$

For all integers $k \geq 1$ and $n \geq -1$ we have

$$2^{(d-1)k} \varsigma_n^d < \varsigma_{n+2k}^d \qquad \text{(A.0.3)}$$

Proof. We prove inequality (A.0.2) by induction.

- For $n = 1$ we have

$$\begin{aligned}
2^{2(d-2)+1} |\varsigma_{-1}^d| &= 2^{2d-3} 2^{2-d} \\
&= 2^{d-1} \\
&< 2^{d-1} + 1 = \varsigma_1^d, \qquad \text{(A.0.4)}
\end{aligned}$$

- and for $n = 2$ we have

$$\begin{aligned} 2^{3(d-2)+1}|\varsigma_{-2}^{d}| &= 2^{3d-5}2^{2-d} \\ &= 2^{2d-3} \\ &< 2^{2d-3} + 3 \cdot 2^{d-2} = \varsigma_{2}^{d}. \end{aligned} \tag{A.0.5}$$

Let us assume that for all $1 \leq k \leq n, n \geq 2$, we have

$$2^{(d-2)(k+1)+1}|\varsigma_{-k}^{d}| < \varsigma_{k}^{d}. \tag{A.0.6}$$

Then it follows that

$$\begin{aligned} 2^{(d-2)(n+2)+1}|\varsigma_{-(n+1)}^{d}| &= 2^{(d-2)(n+2)+1}|2^{2-d}\varsigma_{-(n-1)}^{d} - \varsigma_{-n}^{d}| \\ &\leq 2^{(d-2)(n+1)+1}|\varsigma_{-n+1}^{d}| + 2^{(d-2)(n+2)+1}|\varsigma_{-n}^{d}| \\ &< 2^{(d-2)}\varsigma_{n-1}^{d} + 2^{(d-2)}\varsigma_{n}^{d} \\ &= \varsigma_{n+1}^{d}. \end{aligned} \tag{A.0.7}$$

For inequality (A.0.3) we will use the fact that $\varsigma_n^d > 0$ for all $n \geq -1$ which is easy to check. Together with the recurrence relation (4.1.1) it shows that $\varsigma_{n+1}^d > \varsigma_n^d$ for all $n \geq -1$. Therefore we have the following for all integers $n \geq -1$:

$$\begin{aligned} \varsigma_{n+2}^{d} &= 2^{d-2}(\varsigma_{n+1}^{d} + \varsigma_{n}^{d}) \\ &> 2^{d-1}\varsigma_{n}^{d}. \end{aligned} \tag{A.0.8}$$

An iterative use of this clearly leads to inequality (A.0.3). □

Now, we are ready for the proof of Lemma 4.3.1. Let $Y, \widetilde{Y}, Q, R$ be as in equations (4.2.2), (4.2.3), (4.2.6), (4.2.7), respectively. Let d be an integer at least equal to 3. We know that for all non-negative integers k, l and m we have

$$\sigma(T_d(k,l,m)) = 2^{d-3}\varsigma_k^d\varsigma_m^d\varsigma_l^d + 2^{3d-6}\varsigma_{k-1}^d\varsigma_{m-1}^d\varsigma_{l-1}^d. \tag{A.0.9}$$

Now we can use equation (A.0.1) where the function f will be replaced by the explicit expression for ς_n^d to obtain

$$\begin{aligned} &\sigma(T_d(k,l,m)) \\ &= 2^{d-3}Q^3Y^{k+m+l-3}(Y^3 + 2^{2d-3}) + 2^{d-3}R^3\widetilde{Y}^{k+m+l-3}(\widetilde{Y}^3 + 2^{2d-3}) \\ &+ 2^{d-3}QR((Y\widetilde{Y})^k\varsigma_{m+l-k}^d + (Y\widetilde{Y})^m\varsigma_{l+k-m}^d + (Y\widetilde{Y})^l\varsigma_{m+k-l}^d) \\ &+ 2^{3d-6}QR((Y\widetilde{Y})^{k-1}\varsigma_{m+l-k-1}^d + (Y\widetilde{Y})^{m-1}\varsigma_{l+k-m-1}^d + (Y\widetilde{Y})^{l-1}\varsigma_{m+k-l-1}^d). \end{aligned} \tag{A.0.10}$$

With the fact that for all integers i, $\varsigma_i^d - 2^{d-2}\varsigma_{i-1}^d = 2^{d-2}\varsigma_{i-2}^d$ and $Y\widetilde{Y} = -2^{d-2}$ we deduce

$$\begin{aligned}
&\sigma(T_d(k,l,m))\\
&= 2^{d-3}Q^3Y^{k+m+l-3}(Y^3 + 2^{2d-3}) + 2^{d-3}R^3\widetilde{Y}^{k+m+l-3}(\widetilde{Y}^3 + 2^{2d-3})\\
&+ \frac{QR(Y\widetilde{Y})^2}{2}((Y\widetilde{Y})^k\varsigma_{m+l-k-2}^d + (Y\widetilde{Y})^l\varsigma_{m+k-l-2}^d + (Y\widetilde{Y})^m\varsigma_{l+k-m-2}^d)\\
&- \frac{QR(Y\widetilde{Y})^2}{2}((Y\widetilde{Y})^k\varsigma_{m+l-k-1}^d + (Y\widetilde{Y})^m\varsigma_{l+k-m-1}^d + (Y\widetilde{Y})^l\varsigma_{m+k-l-1}^d). \quad \text{(A.0.11)}
\end{aligned}$$

It follows that if $1 \le k \le l \le m$, $1 \le k' \le l' \le m'$, $4 \le n$ are integers such that $k + l + m = k' + l' + m' = n - 1$, then

$$\begin{aligned}
&\sigma(T_d(k,l,m)) - \sigma(T_d(k',l',m')) = \frac{QR(Y\widetilde{Y})^2}{2}\\
&\quad((Y\widetilde{Y})^k\varsigma_{m+l-k-2}^d + (Y\widetilde{Y})^l\varsigma_{m+k-l-2}^d + (Y\widetilde{Y})^m\varsigma_{l+k-m-2}^d\\
&\quad- (Y\widetilde{Y})^k\varsigma_{m+l-k-1}^d - (Y\widetilde{Y})^l\varsigma_{m+k-l-1}^d - (Y\widetilde{Y})^m\varsigma_{l+k-m-1}^d\\
&\quad- (Y\widetilde{Y})^{k'}\varsigma_{m'+l'-k'-2}^d - (Y\widetilde{Y})^{l'}\varsigma_{m'+k'-l'-2}^d - (Y\widetilde{Y})^{m'}\varsigma_{l'+k'-m'-2}^d\\
&\quad+ (Y\widetilde{Y})^{k'}\varsigma_{m'+l'-k'-1}^d + (Y\widetilde{Y})^{l'}\varsigma_{m'+k'-l'-1}^d + (Y\widetilde{Y})^{m'}\varsigma_{l'+k'-m'-1}^d) \quad \text{(A.0.12)}
\end{aligned}$$

If we set $j = m - l$, $j' = m' - l'$, $i = l - k$, $i' = l' - k'$ and

$$C = \frac{QR(Y\widetilde{Y})^2}{2} \quad \text{(A.0.13)}$$

then we have

$$\begin{aligned}
&\sigma(T_d(k,l,m)) - \sigma(T_d(k',l',m'))\\
&\quad= C(Y\widetilde{Y})^k(\varsigma_{k+2i+j-2}^d + (Y\widetilde{Y})^i\varsigma_{k+j-2}^d + (Y\widetilde{Y})^{i+j}\varsigma_{k-j-2}^d)\\
&\quad- C(Y\widetilde{Y})^k(\varsigma_{k+2i+j-1}^d + (Y\widetilde{Y})^i\varsigma_{k+j-1}^d + (Y\widetilde{Y})^{i+j}\varsigma_{k-j-1}^d)\\
&\quad+ C(Y\widetilde{Y})^{k'}(\varsigma_{k'+2i'+j'-1}^d + (Y\widetilde{Y})^{i'}\varsigma_{k'+j'-1}^d + (Y\widetilde{Y})^{i'+j'}\varsigma_{k'-j'-1}^d)\\
&\quad- C(Y\widetilde{Y})^{k'}(\varsigma_{k'+2i'+j'-2}^d + (Y\widetilde{Y})^{i'}\varsigma_{k'+j'-2}^d + (Y\widetilde{Y})^{i'+j'}\varsigma_{k'-j'-2}^d) \quad \text{(A.0.14)}
\end{aligned}$$

To prove inequality (4.3.8), let us assume that k is even and k' is odd (no assumption about l, m, l', m'). This implies that $(Y\widetilde{Y})^k = 2^{(d-2)k}$ and $(Y\widetilde{Y})^{k'} = -2^{(d-2)k'}$. Therefore, we can deduce from equation (A.0.14) that

$$\begin{aligned}
&\sigma(T_d(k,l,m)) - \sigma(T_d(k',l',m'))\\
&= C2^{(d-2)k}(\varsigma_{k+2i+j-2}^d - \varsigma_{k+2i+j-1}^d + (-2^{d-2})^i(\varsigma_{k+j-2}^d - \varsigma_{k+j-1}^d)\\
&\qquad\qquad + (-2^{d-2})^{i+j}(\varsigma_{k-j-2}^d - \varsigma_{k-j-1}^d))\\
&+ C2^{(d-2)k'}(\varsigma_{k'+2i'+j'-2}^d - \varsigma_{k'+2i'+j'-1}^d + (-2^{d-2})^{i'}(\varsigma_{k'+j'-2}^d - \varsigma_{k'+j'-1}^d)\\
&\qquad\qquad + 2^{(d-2)(i'+j')}(\varsigma_{k'-j'-2}^d - \varsigma_{k'-j'-1}^d))\\
&= h(i,j,k) + h(i',j',k'), \quad \text{(A.0.15)}
\end{aligned}$$

where the function h is defined by

$$\begin{aligned}h(x,y,z) = C2^{(d-2)z}((1-2^{d-2})\varsigma^d_{z+2x+y-2} - 2^{d-2}\varsigma^d_{z+2x+y-3}\\ + (-2^{d-2})^x((1-2^{d-2})\varsigma^d_{z+y-2} - 2^{d-2}\varsigma^d_{z+y-3})\\ + (-2^{d-2})^{x+y}((1-2^{d-2})\varsigma^d_{z-y-2} - 2^{d-2}\varsigma^d_{z-y-3})).\end{aligned} \tag{A.0.16}$$

The particular case $x = 0$ will be of interest, it corresponds to the expression

$$\begin{aligned}h(0,y,z) = C2^{(d-2)z}(2(1-2^{d-2})\varsigma^d_{z+y-2} - 2^{d-1}\varsigma^d_{z+y-3}\\ + (-2^{d-2})^y((1-2^{d-2})\varsigma^d_{z-y-2} - 2^{d-2}\varsigma^d_{z-y-3})),\end{aligned} \tag{A.0.17}$$

Note that $h(0,y,1)$ corresponds to the d-tripod $T_d(1, 1+0, 1+0+y)$. From Lemma 4.2.2 it is clear that $T_d(1,1,1+y)$ is the d-tripod which has the maximum Merrifield-Simmons index among all d-tripods of the same order. Hence, all cases of comparison involving such a type of d-tripod are trivial, and they agree with the statement of the lemma.

Now we are going to show that $h(x,y,z)$ is negative for all triples (x,y,z) of non-negative integers which are different from $(0,y,1)$. There are four cases to consider:

Case 1.a: If $z-y-3 \geq -1$ and $x \geq 1$, then $\varsigma^d_{z-y-2} > 0$, $\varsigma^d_{z-y-3} > 0$. Hence, we get from equation (A.0.16) that

$$\begin{aligned}h(x,y,z) \leq C2^{(d-2)z}((1-2^{d-2})\varsigma^d_{z+2x+y-2} - 2^{d-2}\varsigma^d_{z+2x+y-3}\\ + 2^{(d-2)x}((2^{d-2}-1)\varsigma^d_{z+y-2} + 2^{d-2}\varsigma^d_{z+y-3})\\ + 2^{(d-2)(x+y)}((2^{d-2}-1)\varsigma^d_{z-y-2} + 2^{d-2}\varsigma^d_{z-y-3})).\end{aligned} \tag{A.0.18}$$

By Lemma A.0.1 we know that for $t \in \{2,3\}$

$$2^{(d-2)x}\varsigma^d_{z+y-t} < \frac{\varsigma^d_{z+2x+y-t}}{2^x} \tag{A.0.19}$$

and

$$2^{(d-2)(x+y)}\varsigma^d_{z-y-t} < \frac{\varsigma^d_{z+2x+y-t}}{2^{x+y}}, \tag{A.0.20}$$

therefore (A.0.18) gives

$$\begin{aligned}h(x,y,z) < C2^{(d-2)z}((1-2^{d-2})\varsigma^d_{z+2x+y-2} - 2^{d-2}\varsigma^d_{z+2x+y-3})\\ + C2^{(d-2)z}\left((2^{d-2}-1)\frac{\varsigma^d_{z+2x+y-2}}{2^x} + 2^{d-2}\frac{\varsigma^d_{z+2x+y-3}}{2^x}\right)\\ + C2^{(d-2)z}\left((2^{d-2}-1)\frac{\varsigma^d_{z+2x+y-2}}{2^{x+y}} + 2^{d-2}\frac{\varsigma^d_{z+2x+y-3}}{2^{x+y}}\right)\end{aligned} \tag{A.0.21}$$

Since $x \geq 1$ and $y \geq 0$ we have $2^{x+y} \geq 2^x \geq 2$ and and we can deduce from (A.0.21) that $h(x, y, z) < 0$.

Case 1.b: If $z - y - 3 \geq -1$ and $x = 0$, then we still have $\varsigma^d_{z-y-2} > 0$, $\varsigma^d_{z-y-3} > 0$. Hence, from equation (A.0.17) we have

$$\begin{aligned} h(x, y, z) \leq C2^{(d-2)z}(2(1 - 2^{d-2})\varsigma^d_{z+y-2} - 2^{d-1}\varsigma^d_{z+y-3} \\ + 2^{(d-2)y}((2^{d-2} - 1)\varsigma^d_{z-y-2} + 2^{d-2}\varsigma^d_{z-y-3})). \end{aligned} \tag{A.0.22}$$

By Lemma A.0.1 we know that for $t \in \{2, 3\}$

$$2^{(d-2)y}\varsigma^d_{z-y-t} < \frac{\varsigma^d_{z+y-t}}{2^y}, \tag{A.0.23}$$

therefore

$$\begin{aligned} h(x, y, z) &< C2^{(d-2)z}(2(1 - 2^{d-2})\varsigma^d_{z+y-2} - 2^{d-1}\varsigma^d_{z+y-3}) \\ &+ C2^{(d-2)z}\left((2^{d-2} - 1)\frac{\varsigma^d_{z+y-2}}{2^y} + 2^{d-2}\frac{\varsigma^d_{z+y-3}}{2^y}\right) \\ &< 0. \end{aligned} \tag{A.0.24}$$

Case 2.a: If $z - y - 2 < 0$ and $x \geq 1$, then we obtain from (A.0.16)

$$\begin{aligned} h(x, y, z) &\leq C2^{(d-2)z}((1 - 2^{d-2})\varsigma^d_{z+2x+y-2} - 2^{d-2}\varsigma^d_{z+2x+y-3}) \\ &+ C2^{(d-2)(z+x)}\left((2^{d-2} - 1)\varsigma^d_{z+y-2} + 2^{d-2}\varsigma^d_{z+y-3}\right) \\ &+ C2^{(d-2)(z+x+y-1)}|2^{d-2}\varsigma^d_{z-y-1} + 2^{d-2}\varsigma^d_{z-y-2} - 2^{d-1}\varsigma^d_{z-y-2}| \\ &\leq C2^{(d-2)z}((1 - 2^{d-2})\varsigma^d_{z+2x+y-2} - 2^{d-2}\varsigma^d_{z+2x+y-3}) \\ &+ C2^{(d-2)(z+1)}2^{(d-2)(x-1)}\left((2^{d-2} - 1)\varsigma^d_{z+y-2} + 2^{d-2}\varsigma^d_{z+y-3}\right) \\ &+ C2^{(d-2)(2z+x-4)}2^{(d-2)(y-z+3)}(|\varsigma^d_{z-y}| + 2^{d-1}|\varsigma^d_{z-y-2}|). \end{aligned} \tag{A.0.25}$$

Using Lemma A.0.1 we know that for $h \in \{1, 2\}$

$$\begin{aligned} 2^{(d-2)(x-1)}\varsigma^d_{z+y-h} &\leq \frac{\varsigma^d_{z+2(x-1)+y-h}}{2^{x-1}} \\ &\leq \varsigma^d_{z+2(x-1)+y-h} \end{aligned} \tag{A.0.26}$$

and for $h \in \{0, 2\}$ we have

$$2^{(d-2)(y-z+h+1)}|\varsigma^d_{z-y-h}| < \varsigma^d_{y-z+h}, \tag{A.0.27}$$

therefore we can deduce from (A.0.25) that

$$\begin{aligned} h(x, y, z) &< C2^{(d-2)z}((1 - 2^{d-2})\varsigma^d_{z+2x+y-2} - 2^{d-2}\varsigma^d_{z+2x+y-3}) \\ &+ C2^{(d-2)(z+1)}\left((2^{d-2} - 1)\varsigma^d_{z+2(x-1)+y-2} + 2^{d-2}\varsigma^d_{z+2(x-1)+y-3}\right) \\ &+ C2^{(d-2)(z+1)}2^{(d-2)(x+z-5)}(2^{2d-4}\varsigma^d_{y-z} + 2^{d-1}\varsigma^d_{y-z+2}). \end{aligned} \tag{A.0.28}$$

We can use Lemma A.0.1 again to get

$$\begin{aligned} 2^{(d-2)(x+z-3)}\varsigma^d_{y-z} &= 2^{(d-2)(x+z-3)}\varsigma^d_{z+2(x-1)+y-2-2(z+x-2)} \\ &\leq \frac{\varsigma^d_{z+2(x-1)+y-2}}{2^{d-2}} \end{aligned} \tag{A.0.29}$$

and

$$\begin{aligned} 2^{(d-2)(x+z-4)+1}\varsigma^d_{y-z+2} &< 2^{(d-2)(x+z-3)+1}\varsigma^d_{z+2(x-1)+y-2(z+x-2)} \\ &\leq 2\frac{\varsigma^d_{z+2(x-1)+y}}{2^{d-2}} \\ &\leq \varsigma^d_{z+2(x-1)+y}. \end{aligned} \tag{A.0.30}$$

Now (A.0.28) implies

$$\begin{aligned} h(x,y,z) &< C2^{(d-2)z}((1-2^{d-2})\varsigma^d_{z+2x+y-2} - 2^{d-2}\varsigma^d_{z+2x+y-3}) \\ &+ C2^{(d-2)(z+1)}\left((2^{d-2}-1)\varsigma^d_{z+2(x-1)+y-2} + 2^{d-2}\varsigma^d_{z+2(x-1)+y-3}\right) \\ &+ C2^{(d-2)(z+1)}\frac{\varsigma^d_{z+2(x-1)+y-2}}{2^{d-2}} + C2^{(d-2)z}\varsigma^d_{z+2(x-1)+y} \\ &= C2^{(d-2)z}((1-2^{d-2})\varsigma^d_{z+2x+y-2} - 2^{d-2}\varsigma^d_{z+2x+y-3}) \\ &+ C2^{(d-2)(z+1)}\left(\varsigma^d_{z+2x+y-3} - \varsigma^d_{z+2x+y-4}\right) \\ &+ C2^{(d-2)z}\varsigma^d_{z+2x+y-4} + C2^{(d-2)z}\varsigma^d_{z+2x+y-2} \\ &\leq C2^{(d-2)z}(2-2^{d-2})\varsigma^d_{z+2x+y-2} \leq 0. \end{aligned} \tag{A.0.31}$$

Case 2.b: If $z-y-2<0$ and $x=0$, then we have by equation (A.0.17)

$$\begin{aligned} h(x,y,z) &\leq C2^{(d-2)z}(2(1-2^{d-2})\varsigma^d_{z+y-2} - 2^{d-1}\varsigma^d_{z+y-3}) \\ &+ C2^{(d-2)(2z-3)}2^{(d-2)(y-z+3)}((2^{d-2}-1)|\varsigma^d_{z-y-2}| + 2^{d-2}|\varsigma^d_{z-y-3}|). \end{aligned} \tag{A.0.32}$$

Using Lemma A.0.1, we know that for $h \in \{2,3\}$

$$2^{(d-2)(y-z+h+1)}|\varsigma^d_{z-y-h}| < \varsigma^d_{y-z+h}, \tag{A.0.33}$$

hence

$$\begin{aligned} h(x,y,z) &< C2^{(d-2)z}((2-2^{d-1})\varsigma^d_{z+y-2} - 2^{d-1}\varsigma^d_{z+y-3}) \\ &\quad + C2^{(d-2)(2z-3)}((2^{d-2}-1)\varsigma^d_{y-z+2} + \varsigma^d_{y-z+3}). \end{aligned} \tag{A.0.34}$$

For $z \geq 3$ we have

$$\begin{aligned} h(x,y,z) &< C2^{(d-2)z}((2-2^{d-1})\varsigma^d_{z+y-2} - 2^{d-1}\varsigma^d_{z+y-3}) \\ &\quad + C2^{(d-2)(2z-3)}((2^{d-2}-1)\varsigma^d_{z+y-2-2(z-2)} + \varsigma^d_{z+y-3-2(z-3)}) \\ &< C2^{(d-2)z}(2(1-2^{d-2})\varsigma^d_{z+y-2} - 2^{d-1}\varsigma^d_{z+y-3}) \\ &\quad + C2^{(d-2)(z-1)}\left((2^{d-2}-1)\varsigma^d_{z+y-2} + 2^{d-2}\varsigma^d_{z+y-3}\right) \\ &< 0, \end{aligned} \tag{A.0.35}$$

and for $z = 2$ we have

$$\begin{aligned} h(x,y,z) &< C2^{2(d-2)}((2-2^{d-1})\varsigma_y^d - 2^{d-1}\varsigma_{y-1}^d + 2^{-(d-2)}((2^{d-2}-1)\varsigma_y^d + \varsigma_{y+1}^d)) \\ &< C2^{2(d-2)}((1-2^{d-2})\varsigma_y^d - 2^{d-1}\varsigma_{y-1}^d + 2^{-(d-2)}\varsigma_{y+1}^d) \\ &= C2^{2(d-2)}((2-2^{d-2})\varsigma_y^d + (1-2^{d-1})\varsigma_{y-1}^d) \\ &\leq 0. \end{aligned} \tag{A.0.36}$$

This completes the proof of (4.3.8).

To prove inequality (4.3.9), we consider equation (A.0.14) again for

$$T_d(k,l,m) = T_d(2t, 2t, n-4t-1) \tag{A.0.37}$$

and

$$T_d(k',l',m') = T_d(2t-2, 2t-1, n-4t+2) \tag{A.0.38}$$

which correspond to $i = 0, j = n-6t-1, i' = 1$ and $j' = n-6t+3$, where t is an integer such that $2 \leq t \leq \frac{n-1}{6}$. Then we have

$$\begin{aligned} &\sigma(T_d(k,l,m)) - \sigma(T_d(k',l',m')) \\ &\quad = C2^{(d-2)2t}(2\varsigma_{n-4t-3}^d - 2\varsigma_{n-4t-2}^d + (-2^{d-2})^{n-6t-1}(\varsigma_{8t-n-1}^d - \varsigma_{8t-n}^d)) \\ &\quad + C2^{(d-2)(2t-2)}(\varsigma_{n-4t+2}^d - \varsigma_{n-4t+1}^d + 2^{d-2}(\varsigma_{n-4t-1}^d - \varsigma_{n-4t}^d)) \\ &\quad + C2^{(d-2)(2t-2)}(-2^{d-2})^{n-6t+4}(\varsigma_{8t-n-6}^d - \varsigma_{8t-n-7}^d) \\ &\quad \geq C2^{(d-2)2t+1}((1-2^{d-2})\varsigma_{n-4t-3}^d - 2^{d-2}\varsigma_{n-4t-4}^d) \\ &\quad + C2^{(d-2)(2t-2)}((2^{d-2}-1)\varsigma_{n-4t+1}^d + 2^{d-2}\varsigma_{n-4t-1}^d) \\ &\quad + C2^{(d-2)(n-4t-1)}((1-2^{d-2})|\varsigma_{8t-n-1}^d| - 2^{d-2}|\varsigma_{8t-n-2}^d|) \\ &\quad + C2^{(d-2)(n-4t+2)}((1-2^{d-2})|\varsigma_{8t-n-7}^d| - 2^{d-2}|\varsigma_{8t-n-8}^d|). \end{aligned} \tag{A.0.39}$$

Using the second relation in Lemma A.0.1 we get

$$\begin{aligned} \varsigma_{n-4t+1}^d &= 2^{d-2}\varsigma_{n-4t}^d + 2^{d-2}\varsigma_{n-4t-1}^d \\ &> 2^{d-2}\varsigma_{n-4t}^d + 2\cdot 2^{2d-4}\varsigma_{n-4t-3}^d \end{aligned} \tag{A.0.40}$$

and

$$\begin{aligned} \varsigma_{n-4t-1}^d &= 2^{d-2}\varsigma_{n-4t-2}^d + 2^{d-2}\varsigma_{n-4t-3}^d \\ &> 2\cdot 2^{2d-4}\varsigma_{n-4t-4}^d + 2^{d-2}\varsigma_{n-4t-3}^d \end{aligned} \tag{A.0.41}$$

(note that since $n-6t-3 \geq -2, t \geq 2$ it follows that $n-4t-4 \geq 1$), which show that (A.0.39) implies

$$\begin{aligned} &\sigma(T_d(k,l,m)) - \sigma(T_d(k',l',m')) \\ &\quad > C2^{(d-2)(2t-1)}((2^{d-2}-1)\varsigma_{n-4t}^d + 2^{d-2}\varsigma_{n-4t-3}^d) \\ &\quad + C2^{(d-2)(n-4t-1)}((1-2^{d-2})|\varsigma_{8t-n-1}^d| - 2^{d-2}|\varsigma_{8t-n-2}^d|) \\ &\quad + C2^{(d-2)(n-4t+2)}((1-2^{d-2})|\varsigma_{8t-n-7}^d| - 2^{d-2}|\varsigma_{8t-n-8}^d|). \end{aligned} \tag{A.0.42}$$

To obtain a lower bound for the two last lines with the help of Lemma A.0.1 we have to consider two cases for each value of h in $\{0,3\}$:

Case 1: If $8t-n-1-2h \geq -1$, we have

$$\begin{aligned} 0 < 2^{(d-2)(n-4t-1+h)}\varsigma^d_{8t-n-1-2h} &= 2^{(d-2)(2t-1+n-6t+h)}\varsigma^d_{n-4t-1-2(n-6t+h)} \\ &< 2^{(d-2)(2t-1)}\frac{\varsigma^d_{n-4t-1}}{2^{n-6t+h}} \\ &\leq 2^{(d-2)(2t-1)}\frac{\varsigma^d_{n-4t-1}}{2} \\ &\leq 2^{(d-2)2t}\frac{\varsigma^d_{n-4t-1}}{4}. \end{aligned} \tag{A.0.43}$$

and

$$\begin{aligned} 0 < 2^{(d-2)(n-4t-1+h)}\varsigma^d_{8t-n-2-2h} &= 2^{(d-2)(2t-1+n-6t+h)}\varsigma^d_{n-4t-2-2(n-6t+h)} \\ &= 2^{(d-2)(2t-1)}2^{(d-1)(n-6t+h)}\frac{\varsigma^d_{n-4t-2-2(n-6t+h)}}{2^{n-6t+h}} \\ &< 2^{(d-2)(2t-1)}\frac{\varsigma^d_{n-4t-2}}{2^{n-6t+h}} \\ &\leq 2^{(d-2)(2t-1)}\frac{\varsigma^d_{n-4t-2}}{2}. \end{aligned} \tag{A.0.44}$$

Case 2: If $8t-n-1-2h < -1$, then we have (note that for $t \geq 2$ and $h \in \{0,3\}$, $2t-h-1 \geq 0$)

$$\begin{aligned} 2^{(d-2)(n-4t-1+h)}|\varsigma^d_{8t-n-1-2h}| &= 2^{(d-2)(4t-h-3+n-8t+2h+2)}|\varsigma^d_{8t-n-1-2h}| \\ &< 2^{(d-2)(4t-h-3)}\varsigma^d_{n-8t+1+2h} \\ &= 2^{(d-2)(2t-2+2t-h-1)}\varsigma^d_{n-4t-1-2(2t-h-1)} \\ &\leq 2^{(d-2)(2t-2)}\varsigma^d_{n-4t-1} \\ &\leq 2^{(d-2)2t}\frac{\varsigma^d_{n-4t-1}}{4} \end{aligned} \tag{A.0.45}$$

just as in inequality (A.0.43).

For the remaining inequalities, the two sub-cases for the different values of h must be considered separately:

- for $h=0$,

$$\begin{aligned} 2^{(d-2)(n-4t-1)}|\varsigma^d_{8t-n-2}| &= 2^{(d-2)(4t-4+n-8t+3)}|\varsigma^d_{8t-n-2}| \\ &\leq 2^{(d-2)(4t-4)}\varsigma^d_{n-8t+2} \\ &= 2^{(d-2)(2t-2+2t-2)}\varsigma^d_{n-4t-2-2(2t-2)} \\ &< 2^{(d-2)(2t-2)}\frac{\varsigma^d_{n-4t-2}}{2^{2t-2}} \\ &\leq 2^{(d-2)(2t-1)}\frac{\varsigma^d_{n-4t-2}}{8}. \end{aligned} \tag{A.0.46}$$

- For $h = 3$,

$$
\begin{aligned}
&2^{(d-2)(n-4t+2)}|\varsigma^d_{8t-n-8}| \\
&\qquad = 2^{(d-2)(n-4t+1)}|\varsigma^d_{8t-n-6} - 2^{d-2}\varsigma^d_{8t-n-7}| \\
&\qquad = 2^{(d-2)(n-4t+1)}|\varsigma^d_{8t-n-6} - \varsigma^d_{8t-n-5} + 2^{d-2}\varsigma^d_{8t-n-6}| \\
&\qquad \leq 2^{(d-2)(4t-6+n-8t+7)}((2^{d-2}+1)|\varsigma^d_{8t-n-6}| + |\varsigma^d_{8t-n-5}|) \\
&\qquad \leq 2^{(d-2)(4t-6)}((2^{d-2}+1)\varsigma^d_{n-8t+6} + 2^{d-2}\varsigma^d_{n-8t+5}) \\
&\qquad \leq 2^{(d-2)(2t-2+2t-4)}\left((2^{d-2}+1)\varsigma^d_{n-4t-2-2(2t-4)} + 2^{d-2}\varsigma^d_{n-4t-3-2(2t-4)}\right) \\
&\qquad \leq 2^{(d-2)(2t-2)}((2^{d-2}+1)\varsigma^d_{n-4t-2} + 2^{d-2}\varsigma^d_{n-4t-3}) \\
&\qquad \leq 2^{(d-2)(2t-1)}((1+2^{2-d})\varsigma^d_{n-4t-2} + \varsigma^d_{n-4t-3}) \\
&\qquad \leq 2^{(d-2)(2t-1)}\left(\frac{3}{2}\varsigma^d_{n-4t-2} + \varsigma^d_{n-4t-3}\right) \qquad \text{(A.0.47)}
\end{aligned}
$$

From inequalities (A.0.43) and (A.0.45) we have

$$
\begin{aligned}
&C(1-2^{d-2})(2^{(d-2)(n-4t-1)}|\varsigma^d_{8t-n-1}| + 2^{(d-2)(n-4t+2)}|\varsigma^d_{8t-n-7}|) \\
&\qquad\qquad \geq C(1-2^{d-2})2^{(d-2)2t}\frac{\varsigma^d_{n-4t-1}}{2} \qquad \text{(A.0.48)}
\end{aligned}
$$

and from inequalities (A.0.44), (A.0.46) and (A.0.47) we get

$$
\begin{aligned}
&C(-2^{d-2})(2^{(d-2)(n-4t-1)}|\varsigma^d_{8t-n-2}| + 2^{(d-2)(n-4t+2)}|\varsigma^d_{8t-n-8}|) \\
&\qquad\qquad \geq -C2^{(d-2)2t}(2\varsigma^d_{n-4t-2} + \varsigma^d_{n-4t-3}). \qquad \text{(A.0.49)}
\end{aligned}
$$

Combining the two inequalities we obtain

$$
\begin{aligned}
&C2^{(d-2)(n-4t-1)}((1-2^{d-2})|\varsigma^d_{8t-n-1}| - 2^{d-2}|\varsigma^d_{8t-n-2}|) \\
&\quad + C2^{(d-2)(n-4t+2)}((1-2^{d-2})|\varsigma^d_{8t-n-7}| - 2^{d-2}|\varsigma^d_{8t-n-8}|) \\
&\qquad \geq C(1-2^{d-2})2^{(d-2)2t}\frac{\varsigma^d_{n-4t-1}}{2} - C2^{(d-2)2t}(2\varsigma^d_{n-4t-2} + \varsigma^d_{n-4t-3}) \\
&\qquad \geq C2^{(d-2)2t}(1-2^{d-2})\varsigma^d_{n-4t-1} - C2^{(d-2)2t}\varsigma^d_{n-4t-2} - C2^{(d-2)2t}\varsigma^d_{n-4t-3} \\
&\qquad \geq C2^{(d-2)(2t-1)}((1-2^{d-2})\varsigma^d_{n-4t} - 2^{d-2}\varsigma^d_{n-4t-3}). \qquad \text{(A.0.50)}
\end{aligned}
$$

Hence we can deduce from inequality (A.0.42) that

$$\sigma(T_d(k,l,m)) - \sigma(T_d(k',l',m')) > 0 \qquad \text{(A.0.51)}$$

which means, by equations (A.0.37) and (A.0.38), that

$$\sigma(T_d(2t,2t,n-4t-1)) > \sigma(T_d(2t-2,2t-1,n-4t+2)). \qquad \text{(A.0.52)}$$

Finally, to prove (4.3.10), we consider

$$T_d(k,l,m) = T_d(2t-1,2t,n-4t) \qquad \text{(A.0.53)}$$

and

$$T_d(k',l',m') = T_d(2t+1, 2t+1, n-4t-3), \tag{A.0.54}$$

which correspond to $i=1, j=n-6t, i'=0$ and $j'=n-6t-4$ where the integer t is such that $1 \le t \le \frac{n-4}{6}$. With these new values for i, i', j, j', equation (A.0.14) becomes

$$\begin{aligned}
&\sigma(T_d(k,l,m)) - \sigma(T_d(k',l',m')) \\
&\quad = C2^{(d-2)(2t-1)}(\varsigma^d_{n-4t} - \varsigma^d_{n-4t-1} + 2^{d-2}(\varsigma^d_{n-4t-3} - \varsigma^d_{n-4t-2})) \\
&\quad + C2^{(d-2)(2t-1)}(-2^{d-2})^{n-6t+1}(\varsigma^d_{8t-n-2} - \varsigma^d_{8t-n-3}) \\
&\quad + C2^{(d-2)(2t+1)}(2\varsigma^d_{n-4t-5} - 2\varsigma^d_{n-4t-4}) \\
&\quad + C2^{(d-2)(2t+1)}(-2^{d-2})^{n-6t-4}(\varsigma^d_{8t-n+3} - \varsigma^d_{8t-n+4}) \\
&\quad \ge C2^{(d-2)2t}((2^{d-2}-1)\varsigma^d_{n-4t-2} + 2^{d-2}\varsigma^d_{n-4t-3}) \\
&\quad + C2^{(d-2)(n-4t)}((1-2^{d-2})|\varsigma^d_{8t-n-3}| - 2^{d-2}|\varsigma^d_{8t-n-4}|) \\
&\quad + C2^{(d-2)(2t+1)}(2(1-2^{d-2})\varsigma^d_{n-4t-5} - 2^{d-1}\varsigma^d_{n-4t-6}) \\
&\quad + C2^{(d-2)(n-4t-3)}((1-2^{d-2})|\varsigma^d_{8t-n+3}| - 2^{d-2}|\varsigma^d_{8t-n+2}|)
\end{aligned} \tag{A.0.55}$$

Using the relations

$$\begin{aligned}
\varsigma^d_{n-4t-3} &= 2^{d-2}\varsigma^d_{n-4t-4} + 2^{d-2}\varsigma^d_{n-4t-5} \\
&= 2^{2d-4}\varsigma^d_{n-4t-5} + 2^{2d-4}\varsigma^d_{n-4t-6} + 2^{d-2}\varsigma^d_{n-4t-5} \\
&= 2^{2d-4}\varsigma^d_{n-4t-6} + 2^{d-2}(2^{d-2}+1)\varsigma^d_{n-4t-5}
\end{aligned} \tag{A.0.56}$$

and

$$\begin{aligned}
\varsigma^d_{n-4t-2} &= 2^{d-2}\varsigma^d_{n-4t-3} + 2^{d-2}\varsigma^d_{n-4t-4} \\
&= 2^{2d-4}\varsigma^d_{n-4t-5} + 2^{d-2}(2^{d-2}+1)\varsigma^d_{n-4t-4}
\end{aligned} \tag{A.0.57}$$

we obtain

$$\begin{aligned}
&\sigma(T_d(k,l,m)) - \sigma(T_d(k',l',m')) \\
&\quad \ge C2^{(d-2)(2t+1)}((2^{d-2}-1)(2^{d-2}+1)\varsigma^d_{n-4t-4} + 2^{d-2}(2^{d-2}+1)\varsigma^d_{n-4t-5}) \\
&\quad + C2^{(d-2)(n-4t)}((1-2^{d-2})|\varsigma^d_{8t-n-3}| - 2^{d-2}|\varsigma^d_{8t-n-4}|) \\
&\quad + C2^{(d-2)(n-4t-3)}((1-2^{d-2})|\varsigma^d_{8t-n+3}| - 2^{d-2}|\varsigma^d_{8t-n+2}|) \\
&\quad = C2^{(d-2)(2t+1)}((2^{d-2}-1)\varsigma^d_{n-4t-4} + 2^{d-2}\varsigma^d_{n-4t-5}) \\
&\quad + C2^{(d-2)(2t+2)}((2^{d-2}-1)\varsigma^d_{n-4t-4} + 2^{d-2}\varsigma^d_{n-4t-5}) \\
&\quad + C2^{(d-2)(n-4t)}((1-2^{d-2})|\varsigma^d_{8t-n-3}| - 2^{d-2}|\varsigma^d_{8t-n-4}|) \\
&\quad + C2^{(d-2)(n-4t-3)}((1-2^{d-2})|\varsigma^d_{8t-n+3}| - 2^{d-2}|\varsigma^d_{8t-n+2}|)
\end{aligned} \tag{A.0.58}$$

Let $h \in \{0, 3\}$, and consider two cases depending on $8t-n+3-2h$:

Case 1: If $8t - n + 3 - 2h \geq -1$, then we have

$$\begin{aligned} 2^{(d-2)(n-4t-3+h)}\varsigma^d_{8t-n+3-2h} &= 2^{(d-2)(2t+1+n-6t-4+h)}\varsigma^d_{n-4t-5-2(n-6t-4+h)} \\ &< 2^{(d-2)(2t+1)}\varsigma^d_{n-4t-5} \\ &< 2^{(d-2)(2t+1)}\frac{\varsigma^d_{n-4t-4}}{2} \end{aligned} \tag{A.0.59}$$

and

$$\begin{aligned} 2^{(d-2)(n-4t-3+h)}\varsigma^d_{8t-n+2-2h} &= 2^{(d-2)(2t+1+n-6t-4+h)}\varsigma^d_{n-4t-6-2(n-6t-4+h)} \\ &< 2^{(d-2)(2t+1)}\varsigma^d_{n-4t-6} \\ &< 2^{(d-2)(2t+1)}\frac{\varsigma^d_{n-4t-5}}{2}. \end{aligned} \tag{A.0.60}$$

Case 2: If $8t - n + 3 - 2h < -1$, then we have the following sub-cases

- if $t \geq 3$, then

$$\begin{aligned} 2^{(d-2)(n-4t-3+h)}|\varsigma^d_{8t-n+3-2h}| &= 2^{(d-2)(4t-h-1+n-8t-2+2h)}|\varsigma^d_{8t-n+3-2h}| \\ &< 2^{(d-2)(4t-h-1)}\varsigma^d_{n-8t-3+2h} \\ &= 2^{(d-2)(2t+2t-h-1)}\varsigma^d_{n-4t-5-2(2t-h-1)} \\ &\leq 2^{(d-2)2t}\varsigma^d_{n-4t-5} \\ &< 2^{(d-2)(2t+1)}\frac{\varsigma^d_{n-4t-4}}{2} \end{aligned} \tag{A.0.61}$$

  and

$$\begin{aligned} 2^{(d-2)(n-4t-3+h)}|\varsigma^d_{8t-n+2-2h}| &= 2^{(d-2)(4t-h-2+n-8t-1+2h)}|\varsigma^d_{8t-n+2-2h}| \\ &< 2^{(d-2)(4t-h-2)}\varsigma^d_{n-8t-2+2h} \\ &= 2^{(d-2)(2t+2t-h-2)}\varsigma^d_{n-4t-6-2(2t-h-2)} \\ &\leq 2^{(d-2)2t}\varsigma^d_{n-4t-6} \\ &< 2^{(d-2)(2t+1)}\frac{\varsigma^d_{n-4t-5}}{2}. \end{aligned} \tag{A.0.62}$$

- if $t = 2$, then we still have inequality (A.0.61) valid and

$$\begin{aligned} 2^{(d-2)(n-4t-3+h)}|\varsigma^d_{8t-n+2-2h}| &= 2^{(d-2)(n-11+h)}|\varsigma^d_{18-n-2h}| \\ &= 2^{(d-2)(6-h+n-17+2h)}|\varsigma^d_{18-n-2h}| \\ &< 2^{(d-2)(6-h)}\frac{\varsigma^d_{n-18+2h}}{2} \\ &\leq 2^{(d-2)(7-h)}\varsigma^d_{n-19+2h} \\ &= 2^{(d-2)(4+3-h)}\varsigma^d_{n-8-5-2(3-h)} \\ &\leq 2^{(d-2)4}\varsigma^d_{n-8-5} \\ &\leq 2^{(d-2)(2t+1)}\frac{\varsigma^d_{n-4t-5}}{2}. \end{aligned} \tag{A.0.63}$$

Inequalities (A.0.59), (A.0.60), (A.0.61), (A.0.62) and (A.0.63) imply that, for $t \geq 2$

$$\begin{aligned} & C2^{(d-2)(2t+1)}((2^{d-2}-1)\varsigma^d_{n-4t-4} + 2^{d-2}\varsigma^d_{n-4t-5}) \\ & + C2^{(d-2)(2t+2)}((2^{d-2}-1)\varsigma^d_{n-4t-4} + 2^{d-2}\varsigma^d_{n-4t-5}) \\ & \qquad > C2^{(d-2)(n-4t)}((2^{d-2}-1)|\varsigma^d_{8t-n-3}| + 2^{d-2}|\varsigma^d_{8t-n-4}|) \\ & \qquad + C2^{(d-2)(n-4t-3)}((2^{d-2}-1)|\varsigma^d_{8t-n+3}| + 2^{d-2}|\varsigma^d_{8t-n+2}|) \end{aligned} \tag{A.0.64}$$

Hence we can conclude from inequality (A.0.58) that $\sigma(T_d(k,l,m)) > \sigma(T_d(k',l',m'))$, which means, in view of equations (A.0.53) and (A.0.54), that

$$\sigma(T_d(2t-1, 2t, n-4t)) > \sigma(T_d(2t+1, 2t+1, n-4t-3)). \tag{A.0.65}$$

In the particular case $t = 1$ which is left we proceed in a different way. It corresponds to the comparison between $\sigma(T_d(1,2,n-4))$ and $\sigma(T_d(3,3,n-7))$. Let $S'_d(1,2,n-4)$ denote the graph which results from deletion of a leaf attached to the pseudo-leaf in the C''^d_{n-4}-branch of $T_d(1,2,n-4)$, and similarly $S'_d(3,3,n-7)$ is the graph that we obtain by deleting a leaf adjacent to a pseudo-leaf of the C''^d_{n-7}-branch of $T_d(3,3,n-7)$. An easy calculation gives ($d \geq 3$)

$$\begin{aligned} \sigma(S'_d(1,2,5)) - \sigma(S'_d(3,3,2)) &= 2^{4d-9} + 2^{7d-14} - 3 \cdot 2^{6d-13} - 2^{5d-11} \\ &> 0 \end{aligned} \tag{A.0.66}$$

and

$$\begin{aligned} \sigma(S'_d(1,2,6)) - \sigma(S'_d(3,3,3)) &= 3 \cdot 2^{5d-11} + 2^{8d-16} - 2^{7d-15} - 2^{6d-12} - 2^{4d-9} \\ &> 0, \end{aligned} \tag{A.0.67}$$

which are the two first cases corresponding to $n = 9$ and $n = 10$, respectively. Since, for all $n \geq 11$, we have the recurrence relations

$$\begin{aligned} \sigma(S'_d(1,2,n-4)) = 2^{d-2}(&\sigma(S'_d(1,2,(n-1)-4)) \\ &+ \sigma(S'_d(1,2,(n-2)-4))) \end{aligned} \tag{A.0.68}$$

and

$$\begin{aligned} \sigma(S'_d(3,3,n-7)) = 2^{d-2}(&\sigma(S'_d(3,3,(n-1)-7)) \\ &+ \sigma(S'_d(3,3,(n-2)-7))) \end{aligned} \tag{A.0.69}$$

we can deduce from the two inequalities (A.0.66) and (A.0.67) that for all integers $n \geq 9$ the inequality

$$\sigma(S'_d(1,2,n-4)) > \sigma(S'_d(3,3,n-7)) \tag{A.0.70}$$

holds. Consequently, for all integers $n \geq 10$ we have

$$\begin{aligned}\sigma(T_d(1,2,n-4)) &= \sigma(S'_d(1,2,n-4)) + 2^{d-2}\sigma(S'_d(1,2,(n-1)-4)) \\ &> \sigma(S'_d(3,3,n-7)) + 2^{d-2}\sigma(S'_d(3,3,(n-1)-7)) \\ &= \sigma(T_d(3,3,n-7)). \end{aligned} \tag{A.0.71}$$

This finishes the proof of the lemma.

Appendix B

Detailed proof of Lemma 4.3.3

With the same approach as in Appendix A, we need the following auxiliary lemma.

Lemma B.0.2 *For all integers $n \geq 1$ we have*

$$d|\zeta_{-n}^d| \leq \zeta_n^d. \tag{B.0.1}$$

For all integers $k \geq 1$ and $n \geq -1$ we have

$$d^k \zeta_n^d \leq \zeta_{n+2k}^d, \tag{B.0.2}$$

where equality occurs only when $n = -1$ and $k = 1$.
For all positive integers k, l, m such that $m = k + 2l$ and $l \geq 1$, we have

$$d^{l+1}|\zeta_{-k}^d| < \zeta_m^d. \tag{B.0.3}$$

Proof. For equation (B.0.1) we proceed by induction. The base cases are

- for $n = 1$:
$$d|\zeta_{-1}^d| = d \leq d = \zeta_1^d \tag{B.0.4}$$

- for $n = 2$:

$$\begin{aligned} d|\zeta_{-2}^d| &= |2d - d^2| \\ &= d^2 - 2d \\ &\leq d^2 - d + 1 \\ &= \zeta_2^d. \end{aligned} \tag{B.0.5}$$

Now, assume that for all k such that $1 \leq k \leq n$ we have

$$d|\zeta_{-k}^d| \leq \zeta_k^d \tag{B.0.6}$$

and let us show that the inequality still holds for $n+1$:

$$\begin{aligned} d|\zeta^d_{-n-1}| &= d|\zeta^d_{-n+1} - (d-1)\zeta^d_{-n}| \\ &\leq d|\zeta^d_{-n+1}| + (d-1)d|\zeta^d_{-n}| \\ &\leq \zeta^d_{n-1} + (d-1)\zeta^d_n \\ &= \zeta^d_{n+1}. \end{aligned} \tag{B.0.7}$$

This completes the proof of inequality (B.0.1).

To prove inequality (B.0.2) we use the fact that for $n \geq 0$ we have

$$\zeta^d_{n+1} > \zeta^d_n > 0 \tag{B.0.8}$$

and $\zeta^d_0 = \zeta^d_{-1} = 1$. It implies that for all $n \geq 0$, we have

$$\begin{aligned} \zeta^d_{n+2} &= (d-1)\zeta^d_{n+1} + \zeta^d_n \\ &> d\zeta^d_n. \end{aligned} \tag{B.0.9}$$

and, since $\zeta^d_1 = d$,

$$\zeta^d_1 = d\zeta^d_{-1}. \tag{B.0.10}$$

An iterative application of inequality (B.0.9) and eventual use of equation (B.0.10) clearly lead to inequality (B.0.2).

Finally inequality (B.0.3) is a direct consequence of the two previous inequalities. □

The main proof of Lemma 4.3.3 starts from here. We will use again equation (A.0.1) for

$$f(i) = \mu(C'^d_i, 1) = \zeta^d_i = A'Y'^i + B'\widetilde{Y}'^i \tag{B.0.11}$$

where, using the notations of equations (4.2.25) and (4.2.26),

$$\begin{aligned} Y' = Y(1) &= \frac{d-1+\sqrt{1+2d+(d-2)^2}}{2}, \\ \widetilde{Y}' = \widetilde{Y}(1) &= \frac{d-1-\sqrt{1+2d+(d-2)^2}}{2}. \end{aligned} \tag{B.0.12}$$

We have seen in equations (4.2.30) and (4.2.31) that

$$A' = A(1) = \frac{Y'+1}{Y'-\widetilde{Y}'}, \tag{B.0.13}$$

$$B' = B(1) = -\frac{\widetilde{Y}'+1}{Y'-\widetilde{Y}'} \tag{B.0.14}$$

and thus

$$Y'\widetilde{Y}' = -1, \tag{B.0.15}$$

$$A'B' = \frac{1-d}{(Y'-\widetilde{Y}')^2}. \tag{B.0.16}$$

Therefore we have

$$\begin{aligned} f(k)f(l)f(m) &= \zeta_k^d \zeta_l^d \zeta_m^d \\ &= A'^3 Y'^{k+l+m} + B'^3 \widetilde{Y}'^{k+l+m} \\ &+ \frac{1-d}{(Y'-\widetilde{Y}')^2}((-1)^k \zeta_{m+l-k}^d + (-1)^l \zeta_{m+k-l}^d + (-1)^m \zeta_{l+k-m}^d) \\ &= A'^3 Y'^{k+l+m} + B'^3 \widetilde{Y}'^{k+l+m} \\ &+ \frac{1-d}{(Y'-\widetilde{Y}')^2}(-1)^k (\zeta_{k+2i+j}^d + (-1)^i \zeta_{k+j}^d + (-1)^{i+j} \zeta_{k-j}^d) \end{aligned} \tag{B.0.17}$$

where $i = l - k$ and $j = m - l$.

For simplicity, we let

$$C = \frac{1-d}{(Y'-\widetilde{Y}')^2}, \tag{B.0.18}$$

so that the number of independent edge subsets of a d-tripod $T_d(k, l, m)$ is given by

$$\begin{aligned} &\mathrm{Z}(T_d(k,l,m)) \\ &= (d-2)\zeta_k^d \zeta_l^d \zeta_m^d + \zeta_{k-1}^d \zeta_l^d \zeta_m^d + \zeta_k^d \zeta_{l-1}^d \zeta_m^d + \zeta_k^d \zeta_l^d \zeta_{m-1}^d \\ &= (d-2)(A'^3 Y'^{k+l+m} + B'^3 \widetilde{Y}'^{k+l+m}) + 3(A'^3 Y'^{k+l+m-1} + B'^3 \widetilde{Y}'^{k+l+m-1}) \\ &+ (d-2)C(-1)^k (\zeta_{k+2i+j}^d + (-1)^i \zeta_{k+j}^d + (-1)^{i+j} \zeta_{k-j}^d) \\ &+ C(-1)^{k-1} (\zeta_{k+2i+j+1}^d + (-1)^{i+1} \zeta_{k+j-1}^d + (-1)^{i+j+1} \zeta_{k-j-1}^d) \\ &+ C(-1)^k (\zeta_{k+2i+j-1}^d + (-1)^{i-1} \zeta_{k+j+1}^d + (-1)^{i+j} \zeta_{k-j-1}^d) \\ &+ C(-1)^k (\zeta_{k+2i+j-1}^d + (-1)^i \zeta_{k+j-1}^d + (-1)^{i+j-1} \zeta_{k-j+1}^d). \end{aligned} \tag{B.0.19}$$

After rearranging the terms we have

$$\begin{aligned} &\mathrm{Z}(T_d(k,l,m)) \\ &= (d-2)(A'^3 Y'^{k+l+m} + B'^3 \widetilde{Y}'^{k+l+m}) + 3(A'^3 Y'^{k+l+m-1} + B'^3 \widetilde{Y}'^{k+l+m-1}) \\ &+ (d-1)C(-1)^k (\zeta_{k+2i+j}^d + (-1)^i \zeta_{k+j}^d + (-1)^{i+j} \zeta_{k-j}^d) \\ &- C(-1)^k (\zeta_{k+2i+j}^d + (-1)^i \zeta_{k+j}^d + (-1)^{i+j} \zeta_{k-j}^d) \\ &+ C(-1)^k (\zeta_{k+2i+j-1}^d + (-1)^i \zeta_{k+j-1}^d + (-1)^{i+j} \zeta_{k-j-1}^d) \\ &+ C(-1)^{k-1} (\zeta_{k+2i+j+1}^d + (-1)^{i+1} \zeta_{k+j-1}^d + (-1)^{i+j+1} \zeta_{k-j-1}^d) \\ &+ C(-1)^k (\zeta_{k+2i+j-1}^d + (-1)^{i-1} \zeta_{k+j+1}^d + (-1)^{i+j-1} \zeta_{k-j+1}^d). \end{aligned} \tag{B.0.20}$$

We can merge the third and the fifth line by using the recurrence relation given in (4.1.2) and obtain

$$\begin{aligned}
&\mathrm{Z}(T_d(k,l,m)) \\
&= (d-2)(A'^3Y'^{k+l+m} + B'^3\widetilde{Y}'^{k+l+m}) + 3(A'^3Y'^{k+l+m-1} + B'^3\widetilde{Y}'^{k+l+m-1}) \\
&+ C(-1)^k(\zeta^d_{k+2i+j+1} + (-1)^i\zeta^d_{k+j+1} + (-1)^{i+j}\zeta^d_{k-j+1}) \\
&- C(-1)^k(\zeta^d_{k+2i+j} + (-1)^i\zeta^d_{k+j} + (-1)^{i+j}\zeta^d_{k-j}) \\
&+ C(-1)^{k-1}(\zeta^d_{k+2i+j+1} + (-1)^i\zeta^d_{k+j+1} + (-1)^{i+j}\zeta^d_{k-j+1}) \\
&+ C(-1)^k(\zeta^d_{k+2i+j-1} + (-1)^i\zeta^d_{k+j-1} + (-1)^{i+j}\zeta^d_{k-j-1}) \\
&= (d-2)(A'^3Y'^{k+l+m} + B'^3\widetilde{Y}'^{k+l+m}) + 3x^2(A'^3Y'^{k+l+m-1} + B'^3\widetilde{Y}'^{k+l+m-1}) \\
&- C(-1)^k(\zeta^d_{k+2i+j} + (-1)^i\zeta^d_{k+j} + (-1)^{i+j}\zeta^d_{k-j}) \\
&+ C(-1)^k(\zeta^d_{k+2i+j-1} + (-1)^i\zeta^d_{k+j-1} + (-1)^{i+j}\zeta^d_{k-j-1}).
\end{aligned} \tag{B.0.21}$$

Now, if we consider another d-tripod $T_d(k',l',m')$ with the same order as $T_d(k,l,m)$ and such that $i' = l' - k'$ and $j' = m' - l'$, then the difference of their Hosoya indices is

$$\begin{aligned}
&\mathrm{Z}(T_d(k,l,m)) - \mathrm{Z}(T_d(k',l',m')) \\
&\qquad = -C(-1)^k(\zeta^d_{k+2i+j} + (-1)^i\zeta^d_{k+j} + (-1)^{i+j}\zeta^d_{k-j}) \\
&\qquad + C(-1)^k(\zeta^d_{k+2i+j-1} + (-1)^i\zeta^d_{k+j-1} + (-1)^{i+j}\zeta^d_{k-j-1}) \\
&\qquad + C(-1)^{k'}(\zeta^d_{k'+2i'+j'} + (-1)^{i'}\zeta^d_{k'+j'} + (-1)^{i'+j'}\zeta^d_{k'-j'}) \\
&\qquad - C(-1)^{k'}(\zeta^d_{k'+2i'+j'-1} + (-1)^{i'}\zeta^d_{k'+j'-1} + (-1)^{i'+j'}\zeta^d_{k'-j'-1}).
\end{aligned} \tag{B.0.22}$$

To show inequality (4.3.11), we assume that k is even and k' is odd, so that equation (B.0.22) becomes

$$\mathrm{Z}(T_d(k,l,m)) - \mathrm{Z}(T_d(k',l',m')) = g(i,j,k) + g(i',j',k') \tag{B.0.23}$$

where the function g is defined by

$$\begin{aligned}
g(x,y,z) = -C(\zeta^d_{z+2x+y} + (-1)^x\zeta^d_{z+y} + (-1)^{x+y}\zeta^d_{z-y}) + \\
C(\zeta^d_{z+2x+y-1} + (-1)^x\zeta^d_{z+y-1} + (-1)^{x+y}\zeta^d_{z-y-1})
\end{aligned} \tag{B.0.24}$$

Next we show that $g(x,y,z) > 0$ for all non-negative integers x, y and $z \geq 1$. Remember that $C < 0$.

- If $x = y = 0$ we have

$$\begin{aligned}
g(0,0,z) &= -3C(\zeta^d_z - \zeta^d_{z-1}) \\
&> 0
\end{aligned}$$

- If $x \geq 1, y = 0$ we have

$$\begin{aligned} g(x,y,z) &= -C(\zeta^d_{z+2x} - \zeta^d_{z+2x-1} + 2(-1)^x(\zeta^d_z - \zeta^d_{z-1})) \\ &\geq -C(\zeta^d_{z+2x} - \zeta^d_{z+2x-1} + 2(\zeta^d_{z-1} - \zeta^d_z)) \\ &= -C((d-2)\zeta^d_{z+2x-1} + \zeta^d_{z+2x-2} + 2((2-d)\zeta^d_{z-1} - \zeta^d_{z-2})), \end{aligned} \tag{B.0.25}$$

  and using the second inequality in Lemma B.0.2 we have

$$\begin{aligned} g(x,y,z) &> -C(d^x(d-2)\zeta^d_{z-1} + d^x\zeta^d_{z-2} + 2((2-d)\zeta^d_{z-1} - \zeta^d_{z-2})) \\ &> 0 \text{ since } d \geq 3. \end{aligned} \tag{B.0.26}$$

- If $x = 0, y \geq 1$ we have

$$\begin{aligned} g(x,y,z) &= -C(2\zeta^d_{z+y} + (-1)^y\zeta^d_{z-y} - 2\zeta^d_{z+y-1} - (-1)^y\zeta^d_{z-y-1}) \\ &\geq -C(2(d-2)\zeta^d_{z+y-1} + 2\zeta^d_{z+y-2} - \zeta^d_{|z-y|} - \zeta^d_{|z-y-1|}). \end{aligned} \tag{B.0.27}$$

  Since $d \geq 3$, $z+y-1 \geq |z-y|$ and $z+y-1 \geq |z-y-1|$, we clearly have $g(x,y,z) > 0$.

- If $x \geq 1, y \geq 1$ we have

$$\begin{aligned} g(x,y,z) &\geq -C(\zeta^d_{z+2x+y} - \zeta^d_{z+2x+y-1} - \zeta^d_{z+y-1} - \zeta^d_{z+y} - \zeta^d_{|z-y-1|} - \zeta^d_{|z-y|}) \\ &= -C((d-2)\zeta^d_{z+2x+y-1} + \zeta^d_{z+2x+y-2} - \zeta^d_{z+y-1} \\ &\qquad - \zeta^d_{z+y} - \zeta^d_{|z-y-1|} - \zeta^d_{|z-y|}) \\ &\geq -C((d-2)\zeta^d_{z+2x+y-1} - \zeta^d_{z+y-1} - \zeta^d_{|z-y-1|} - \zeta^d_{|z-y|}). \end{aligned} \tag{B.0.28}$$

  Now we apply the second inequality in Lemma B.0.2 to obtain

$$g(x,y,z) \geq -C(d^x(d-2)\zeta^d_{z+y-1} - \zeta^d_{z+y-1} - \zeta^d_{|z-y-1|} - \zeta^d_{|z-y|}), \tag{B.0.29}$$

  and since $d \geq 3$, $z+y-1 > |z-y|$ and $z+y-1 \geq |z-y-1|$ we clearly have $g(x,y,z) > 0$.

We have seen that for all possible cases $g(x,y,z) > 0$, and in view of equation (B.0.23) this implies that

$$\mathrm{Z}(T_d(k,l,m)) > \mathrm{Z}(T_d(k',l',m')) \tag{B.0.30}$$

as in inequality (4.3.11).

To prove inequality (4.3.12) we can use again equation (B.0.22) for

$$T_d(k,l,m) = T_d(2t-2, 2t-1, n-4t+2) \tag{B.0.31}$$

and

$$T_d(k',l',m') = T_d(2t, 2t, n-4t-1), \tag{B.0.32}$$

where $2 \le t \le \frac{n-1}{6}$. These correspond to $i = 1$, $j = n - 6t + 3$, $i' = 0$ and $j' = n - 6t - 1$, therefore we have

$$\begin{aligned}
&T_d(2t-2, 2t-1, n-4t+2) - T_d(2t, 2t, n-4t-1)) \\
&= -C(\zeta^d_{n-4t+3} - \zeta^d_{n-4t+2} - \zeta^d_{n-4t+1} + \zeta^d_{n-4t} \\
&\qquad\qquad + (-1)^{n-6t+4}\zeta^d_{8t-n-5} - (-1)^{n-6t+4}\zeta^d_{8t-n-6}) \\
&+ C(\zeta^d_{n-4t-1} - \zeta^d_{n-4t-2} + \zeta^d_{n-4t-1} - \zeta^d_{n-4t-2} \\
&\qquad\qquad + (-1)^{n-6t-1}\zeta^d_{8t-n+1} - (-1)^{n-6t-1}\zeta^d_{8t-n})) \\
&= -C((d-2)\zeta^d_{n-4t+2} + \zeta^d_{n-4t} + (-1)^{n-6t+4}((d-2)\zeta^d_{8t-n-6} \\
&+ \zeta^d_{8t-n-7}) + 2(\zeta^d_{n-4t-2} - \zeta^d_{n-4t-1}) + (-1)^{n-6t-1}((2-d)\zeta^d_{8t-n} - \zeta^d_{8t-n-1})) \\
&\ge -C((d-2)\zeta^d_{n-4t+2} + (d-3)\zeta^d_{n-4t-1} + 3\zeta^d_{n-4t-2}) \\
&- C((2-d)|\zeta^d_{8t-n-6}| - |\zeta^d_{8t-n-7}| + (2-d)|\zeta^d_{8t-n}| - |\zeta^d_{8t-n-1}|)
\end{aligned} \tag{B.0.33}$$

Note that for $h \in \{0, 3\}$, the following inequalities hold by Lemma (B.0.2):

- if $8t - n - 2h \ge 0$, then

$$\begin{aligned}
\frac{\zeta^d_{n-4t+2}}{4} &> \frac{\zeta^d_{n-4t}}{2} \\
&= \frac{\zeta^d_{8t-n-2h+2(n-6t+h)}}{2} \\
&> \frac{d^{n-6t+h}\zeta^d_{8t-n-2h}}{2} \\
&> \zeta^d_{8t-n-2h}
\end{aligned} \tag{B.0.34}$$

  and

$$\begin{aligned}
\frac{\zeta^d_{n-4t+2}}{4} &> \frac{\zeta^d_{n-4t+1}}{2} \\
&= \frac{\zeta^d_{8t-n-1-2h+2(n-6t+1+h)}}{2} \\
&> \frac{d^{n-6t+1+h}\zeta^d_{8t-n-1-2h}}{2} \\
&> \zeta^d_{8t-n-1-2h}
\end{aligned} \tag{B.0.35}$$

- if $8t - n - 2h < 0, h \in \{0, 3\}$, then

$$\begin{aligned}
\frac{\zeta^d_{n-4t+2}}{4} &= \frac{\zeta^d_{n-8t+2h+2(2t+1-h)}}{4} \\
&\ge \frac{d^{2t+1-h}\zeta^d_{n-8t+2h}}{4} \\
&> |\zeta^d_{8t-n-2h}|
\end{aligned} \tag{B.0.36}$$

and

$$\begin{aligned}\frac{\zeta^d_{n-4t+2}}{4} &> \frac{\zeta^d_{n-4t+1}}{2}\\ &= \frac{\zeta^d_{n-8t+1+2h+2(2t-h)}}{2}\\ &\geq \frac{d^{2t-h}\zeta^d_{n-8t+1+2h}}{2}\\ &> |\zeta^d_{8t-n-1-2h}|. \end{aligned} \tag{B.0.37}$$

Hence, knowing that $d \geq 3$, inequality (B.0.33) implies

$$\begin{aligned} T_d(2t-2, 2t-1, n-4t+2) - T_d(2t, 2t, n-4t-1))\\ > -C((d-3)\zeta^d_{n-4t-1} + 3\zeta^d_{n-4t-2})\\ > 0, \end{aligned} \tag{B.0.38}$$

which completes the proof of inequality (4.3.12).

Finally, to prove inequality (4.3.13), we have to replace $T_d(k, l, m)$ and $T_d(k', l', m')$ in equation (B.0.22) by $T_d(2t+1, 2t+1, n-4t-3)$ and $T_d(2t-1, 2t, n-4t)$, respectively. This time, the integer t is such that $1 \leq t \leq \frac{n-4}{6}$. Note that with these new assignments we now have $i = 0$, $j = n-6t-4$, $i' = 1$ and $j' = n-6t$. The difference between their Hosoya indices then becomes

$$\begin{aligned} &T_d(2t+1, 2t+1, n-4t-3) - T_d(2t-1, 2t, n-4t)\\ &\geq -C(2\zeta^d_{n-4t-4} - 2\zeta^d_{n-4t-3} - |\zeta^d_{8t-n+5} - \zeta^d_{8t-n+4}|\\ &\qquad + \zeta^d_{n-4t+1} - \zeta^d_{n-4t} + \zeta^d_{n-4t-2} - \zeta^d_{n-4t-1} - |\zeta^d_{8t-n-1} - \zeta^d_{8t-n-2}|)\\ &= -C(2(2-d)\zeta^d_{n-4t-4} - 2\zeta^d_{n-4t-5} + (d-2)\zeta^d_{n-4t} + \zeta^d_{n-4t-1}\\ &+ (2-d)\zeta^d_{n-4t-2} - \zeta^d_{n-4t-3} - |\zeta^d_{8t-n+5} - \zeta^d_{8t-n+4}| - |\zeta^d_{8t-n-1} - \zeta^d_{8t-n-2}|)\\ &= -C(2(2-d)\zeta^d_{n-4t-4} - 2\zeta^d_{n-4t-5} + (d-2)(d-1)\zeta^d_{n-4t-1}\\ &\qquad + (d-1)\zeta^d_{n-4t-2} - |\zeta^d_{8t-n+5} - \zeta^d_{8t-n+4}| - |\zeta^d_{8t-n-1} - \zeta^d_{8t-n-2}|)\\ &\geq -C((d-2)(d-1)\zeta^d_{n-4t-1} + \zeta^d_{n-4t-4})\\ &- C(-(d-2)|\zeta^d_{8t-n+4}| - |\zeta^d_{8t-n+3}| - (d-2)|\zeta^d_{8t-n-2}| - |\zeta^d_{8t-n-3}|)). \end{aligned} \tag{B.0.39}$$

Let $h \in \{0, 3\}$, with the help of Lemma B.0.2 the following inequalities are easy to see (recall that $n-6t-4 \geq 0$):

- Since $|8t-n+3-2h| \leq n-4t-4+h$, we have

$$\zeta^d_{n-4t-4+h} \geq |\zeta^d_{8t-n+3-2h}|. \tag{B.0.40}$$

- If $8t-n-2+2h \geq 0$, then we have

$$\begin{aligned}\zeta^d_{n-4t-2} &= \zeta^d_{8t-n-2+2h+2(n-6t-h)}\\ &> \zeta^d_{8t-n-2+2h}, \end{aligned} \tag{B.0.41}$$

- and if $8t - n - 2 + 2h < 0$, then we get

$$\begin{aligned}
\zeta^d_{n-4t-2} &= \zeta^d_{n-8t+2-2h+2(2t-2+h)} \\
&> \zeta^d_{n-8t+2-2h} \\
&> |\zeta^d_{8t-n-2+2h}|. && \text{(B.0.42)}
\end{aligned}$$

These allow us to deduce from inequality (B.0.39) that

$$\begin{aligned}
&T_d(2t+1, 2t+1, n-4t-3) - T_d(2t-1, 2t, n-4t) \\
&\quad > -C((d-2)\zeta^d_{n-4t-1} + (d-2)^2(d-1)\zeta^d_{n-4t-2} + (d-2)^2\zeta^d_{n-4t-3}) \\
&\quad - C(\zeta^d_{n-4t-4} - \zeta^d_{n-4t-1} - 2(d-2)\zeta^d_{n-4t-2} - \zeta^d_{n-4t-4}) \\
&\quad > 0. && \text{(B.0.43)}
\end{aligned}$$

This completes the proof of the lemma.

Appendix C

Energy of a cycle C_n

Let n be a positive integer. Then, as we have seen in equation (2.3.16), the eigenvalues of the cycle C_n of order n are

$$e_k = 2\cos\frac{2i\pi}{n}k \tag{C.0.1}$$

where $k = 1, 2, \cdots, n$.

The following identity will be useful for the calculation of the energy $\mathrm{En}(C_n)$ of C_n.

For all integers $l \geq 0$, $m \geq 0$ and $n \geq 1$ we have

$$\begin{aligned}
S(l,m) &= 2\sum_{l\leq k\leq m}\cos\frac{2k\pi}{n} \qquad\qquad (\mathrm{C.0.2})\\
&= \sum_{l\leq k\leq m}\left(e^{\frac{i2k\pi}{n}} + e^{-\frac{i2k\pi}{n}}\right)\\
&= \frac{e^{\frac{i2(m+1)\pi}{n}} - e^{\frac{i2l\pi}{n}}}{e^{\frac{i2\pi}{n}} - 1} + \frac{e^{-\frac{i2(m+1)\pi}{n}} - e^{-\frac{i2l\pi}{n}}}{e^{-\frac{i2\pi}{n}} - 1}\\
&= \frac{e^{\frac{i2m\pi}{n}} - e^{-\frac{i2(l-1)\pi}{n}} - e^{\frac{i2(m+1)\pi}{n}} + e^{\frac{i2l\pi}{n}}}{1 - e^{\frac{i2\pi}{n}} - e^{-\frac{i2\pi}{n}} + 1}\\
&\qquad + \frac{e^{-\frac{i2m\pi}{n}} - e^{-\frac{i2(l-1)\pi}{n}} - e^{-\frac{i2(m+1)\pi}{n}} + e^{-\frac{i2l\pi}{n}}}{1 - e^{\frac{i2\pi}{n}} - e^{-\frac{i2\pi}{n}} + 1}\\
&= \frac{2\cos\frac{2m\pi}{n} - 2\cos\frac{2(l-1)\pi}{n} - 2\cos\frac{2(m+1)\pi}{n} + 2\cos\frac{2l\pi}{n}}{2 - 2\cos\frac{2\pi}{n}}. \qquad\qquad (\mathrm{C.0.3})
\end{aligned}$$

Using the relations

$$\cos\frac{2(m+1)\pi}{n} = \cos\frac{2m\pi}{n}\cos\frac{2\pi}{n} - \sin\frac{2m\pi}{n}\sin\frac{2\pi}{n} \tag{C.0.4}$$

and

$$\cos\frac{2l\pi}{n} = \cos\frac{2(l-1)\pi}{n}\cos\frac{2\pi}{n} - \sin\frac{2(l-1)\pi}{n}\sin\frac{2\pi}{n}, \tag{C.0.5}$$

equation (C.0.3) becomes

$$\begin{aligned}
S(l,m) &= \frac{\left(\sin\frac{2m\pi}{n} - \sin\frac{2(l-1)\pi}{n}\right)\sin\frac{2\pi}{n}}{1-\cos\frac{2\pi}{n}} + \cos\frac{2m\pi}{n} - \cos\frac{2(l-1)\pi}{n} \\
&= \frac{\left(\sin\frac{2m\pi}{n} - \sin\frac{2(l-1)\pi}{n}\right)2\cos\frac{\pi}{n}\sin\frac{\pi}{n}}{2\sin^2(\pi/n)} + \cos\frac{2m\pi}{n} - \cos\frac{2(l-1)\pi}{n} \\
&= \left(\sin\frac{2m\pi}{n} - \sin\frac{2(l-1)\pi}{n}\right)\cot\frac{\pi}{n} \\
&\qquad + \cos\frac{2m\pi}{n} - \cos\frac{2(l-1)\pi}{n}. \qquad \text{(C.0.6)}
\end{aligned}$$

All positive integers n can be written as $n = 4l + i$ where $i \in \{0, 1, 2, 3\}$ and $l \in \mathbb{N}$. Using the expressions for the eigenvalues of C_n in equation (C.0.1), the energy of C_n is given by

$$\begin{aligned}
\mathrm{En}(C_n) &= \sum_{k=1}^{n}\left|2\cos\frac{2k\pi}{4l+i}\right| \\
&= 2\sum_{0<2k\pi/n\le\frac{\pi}{2}}\cos\frac{2k\pi}{4l+i} - 2\sum_{\frac{\pi}{2}<2k\pi/n\le\frac{3\pi}{2}}\cos\frac{2k\pi}{4l+i} \\
&\qquad + 2\sum_{\frac{3\pi}{2}<2k\pi/n\le 2\pi}\cos\frac{2k\pi}{4l+i} \\
&= 2\sum_{1\le k\le l+\frac{i}{4}}\cos\frac{2k\pi}{4l+i} - 2\sum_{l+\frac{i}{4}<k\le 3l+\frac{3i}{4}}\cos\frac{2k\pi}{4l+i} \\
&\qquad + 2\sum_{3l+\frac{3i}{4}<k\le n}\cos\frac{2k\pi}{4l+i}. \qquad \text{(C.0.7)}
\end{aligned}$$

Next, we compute the energy $\mathrm{En}(C_{4l+i})$ corresponding to each value of i.

- For $i = 0$ corresponding to $n = 4l$, we have

$$\mathrm{En}(C_n) = 2\sum_{1\le k\le l}\cos\frac{2k\pi}{4l} - 2\sum_{l+1\le k\le 3l}\cos\frac{2k\pi}{4l} + 2\sum_{3l+1\le k\le n}\cos\frac{2k\pi}{4l}.$$

From equation (C.0.6) we get

$$\begin{aligned}
2\sum_{1\le k\le l}\cos\frac{2k\pi}{4l} &= \left(\sin\frac{2l\pi}{4l} - \sin\frac{2(1-1)\pi}{4l}\right)\cot\frac{\pi}{4l} \\
&\qquad + \cos\frac{2l\pi}{4l} - \cos\frac{2(1-1)\pi}{4l} \\
&= \sin\frac{\pi}{2}\cot\frac{\pi}{4l} + \cos\frac{\pi}{2} - 1 \qquad \text{(C.0.8)} \\
&= \cot\frac{\pi}{4l} - 1, \qquad \text{(C.0.9)}
\end{aligned}$$

$$
\begin{aligned}
2\sum_{l+1\le k\le 3l}\cos\frac{2k\pi}{4l} &= \left(\sin\frac{2\cdot 3l\pi}{4l}-\sin\frac{2(l+1-1)\pi}{4l}\right)\cot\frac{\pi}{4l}\\
&\qquad\qquad + \cos\frac{2\cdot 3l\pi}{4l}-\cos\frac{2(l+1-1)\pi}{4l}\\
&= \left(\sin\frac{3\pi}{2}-\sin\frac{\pi}{2}\right)\cot\frac{\pi}{4l}+\cos\frac{3\pi}{2}-\cos\frac{\pi}{2}\\
&= -2\cot\frac{\pi}{4l} \qquad\qquad (\text{C.0.10})
\end{aligned}
$$

and

$$
\begin{aligned}
2\sum_{3l+1\le k\le n}\cos\frac{2k\pi}{4l} &= \left(\sin\frac{2n\pi}{4l}-\sin\frac{2(3l+1-1)\pi}{4l}\right)\cot\frac{\pi}{4l}\\
&\qquad\qquad + \cos\frac{2n\pi}{4l}-\cos\frac{2(3l+1-1)\pi}{4l}\\
&= \left(\sin 2\pi-\sin\frac{3\pi}{2}\right)\cot\frac{\pi}{4l}+\cos 2\pi-\cos\frac{3\pi}{2}\\
&= \cot\frac{\pi}{4l}+1. \qquad\qquad (\text{C.0.11})
\end{aligned}
$$

Therefore

$$
\begin{aligned}
\mathrm{En}(C_n) &= \cot\frac{\pi}{4l}-1+2\cot\frac{\pi}{4l}+\cot\frac{\pi}{4l}+1\\
&= 4\cot\frac{\pi}{n}. \qquad\qquad (\text{C.0.12})
\end{aligned}
$$

- For $i = 1$ we have $n = 4l + 1$ and equation (C.0.7) becomes

$$
\mathrm{En}(C_n) = 2\sum_{1\le k\le l}\cos\frac{2k\pi}{4l+1}-2\sum_{l+1\le k\le 3l}\cos\frac{2k\pi}{4l+1}+2\sum_{3l+1\le k\le n}\cos\frac{2k\pi}{4l+1}.
$$

We can use equation (C.0.6) to obtain

$$
\begin{aligned}
2\sum_{1\le k\le l}\cos\frac{2k\pi}{4l+1} &= \left(\sin\frac{2l\pi}{4l+1}-\sin\frac{2(1-1)\pi}{4l+1}\right)\cot\frac{\pi}{4l+1}\\
&\qquad\qquad + \cos\frac{2l\pi}{4l+1}-\cos\frac{2(1-1)\pi}{4l+1}\\
&= \sin\frac{2l\pi}{4l+1}\cot\frac{\pi}{4l+1}+\cos\frac{2l\pi}{4l+1}-1 \qquad (\text{C.0.13})
\end{aligned}
$$

$$
\begin{aligned}
2\sum_{l+1\le k\le 3l}\cos\frac{2k\pi}{4l+1} &= \left(\sin\frac{2\cdot 3l\pi}{4l+1}-\sin\frac{2(l+1-1)\pi}{4l+1}\right)\cot\frac{\pi}{4l+1}\\
&\qquad +\cos\frac{2\cdot 3l\pi}{4l+1}-\cos\frac{2(l+1-1)\pi}{4l+1}\\
&= \left(\sin\frac{6l\pi}{4l+1}-\sin\frac{2l\pi}{4l+1}\right)\cot\frac{\pi}{4l+1}\\
&\qquad +\cos\frac{6l\pi}{4l+1}-\cos\frac{2l\pi}{4l+1}, \qquad (C.0.14)
\end{aligned}
$$

$$
\begin{aligned}
2\sum_{3l+1\le k\le n}\cos\frac{2k\pi}{4l+1} &= \left(\sin\frac{2n\pi}{4l+1}-\sin\frac{2(3l+1-1)\pi}{4l+1}\right)\cot\frac{\pi}{4l+1}\\
&\qquad +\cos\frac{2n\pi}{4l+1}-\cos\frac{2(3l+1-1)\pi}{4l+1}\\
&= -\sin\frac{6l\pi}{4l+1}\cot\frac{\pi}{4l+1}+1-\cos\frac{6l\pi}{4l+1}, \qquad (C.0.15)
\end{aligned}
$$

and in total we have

$$
\begin{aligned}
\mathrm{En}(C_n) &= \left(2\sin\frac{2l\pi}{4l+1}-2\sin\frac{6l\pi}{4l+1}\right)\cot\frac{\pi}{4l+1}+2\cos\frac{2l\pi}{4l+1}-2\cos\frac{6l\pi}{4l+1}\\
&= \frac{2\sin\left(\frac{2l\pi}{4l+1}+\frac{\pi}{4l+1}\right)-2\sin\left(\frac{6l\pi}{4l+1}+\frac{\pi}{4l+1}\right)}{\sin\frac{\pi}{4l+1}}\\
&= \frac{2\sin\left(\frac{4l\pi+1\pi}{8l+2}+\frac{\pi}{8l+2}\right)-2\sin\left(\frac{12l\pi+3\pi}{8l+2}-\frac{\pi}{8l+2}\right)}{\sin\frac{\pi}{4l+1}}\\
&= \frac{4\cos\frac{\pi}{8l+2}}{2\sin\frac{\pi}{8l+2}\cos\frac{\pi}{8l+2}}\\
&= 2\csc\frac{\pi}{2n}. \qquad (C.0.16)
\end{aligned}
$$

- For $i=2$ and thus $n=4l+2$, equation (C.0.7) becomes

  $$\mathrm{En}(C_n) = 2\sum_{1\le k\le l}\cos\frac{2k\pi}{4l+2}-2\sum_{l+1\le k\le 3l+1}\cos\frac{2k\pi}{4l+2}+2\sum_{3l+2\le k\le n}\cos\frac{2k\pi}{4l+2}.$$

  Exactly in the same way as for equation (C.0.8) we get

  $$2\sum_{1\le k\le l}\cos\frac{2k\pi}{4l+2} = \sin\frac{2l\pi}{4l+2}\cot\frac{\pi}{4l+2}+\cos\frac{2l\pi}{4l+2}-1. \qquad (C.0.17)$$

By equation (C.0.6) we have

$$\begin{aligned}
2\sum_{l+1\le k\le 3l+1}\cos\frac{2k\pi}{4l+2} &= \left(\sin\frac{2\cdot(3l+1)\pi}{4l+2}-\sin\frac{2(l+1-1)\pi}{4l+2}\right)\cot\frac{\pi}{4l+2}\\
&\quad+\cos\frac{2\cdot(3l+1)\pi}{4l+2}-\cos\frac{2(l+1-1)\pi}{4l+2}\\
&=\left(\sin\frac{(6l+2)\pi}{4l+2}-\sin\frac{2l\pi}{4l+2}\right)\cot\frac{\pi}{4l+2}\\
&\quad+\cos\frac{(6l+2)\pi}{4l+2}-\cos\frac{2l\pi}{4l+2},
\end{aligned}\tag{C.0.18}$$

$$\begin{aligned}
2\sum_{3l+2\le k\le n}\cos\frac{2k\pi}{4l+2} &= \left(\sin\frac{2n\pi}{4l+2}-\sin\frac{2(3l+2-1)\pi}{4l+2}\right)\cot\frac{\pi}{4l+2}\\
&\quad+\cos\frac{2n\pi}{4l+2}-\cos\frac{2(3l+2-1)\pi}{4l+2}\\
&=-\sin\frac{(6l+2)\pi}{4l+2}\cot\frac{\pi}{4l+2}\\
&\quad+1-\cos\frac{(6l+2)\pi}{4l+2},
\end{aligned}\tag{C.0.19}$$

and consequently

$$\begin{aligned}
\mathrm{En}(C_n) &= \left(2\sin\frac{2l\pi}{4l+2}-2\sin\frac{(6l+2)\pi}{4l+2}\right)\cot\frac{\pi}{4l+2}\\
&\quad-2\cos\left(\frac{(6l+2)\pi}{4l+2}\right)+2\cos\left(\frac{2l\pi}{4l+2}\right)\\
&=\left(2\sin\left(\frac{\pi}{2}-\frac{\pi}{4l+2}\right)-2\sin\left(\frac{3\pi}{2}-\frac{\pi}{4l+2}\right)\right)\cot\frac{\pi}{4l+2}\\
&\quad-2\cos\left(\frac{3\pi}{2}-\frac{\pi}{4l+2}\right)+2\cos\left(\frac{\pi}{2}-\frac{\pi}{4l+2}\right)\\
&=\frac{4\cos^2\frac{\pi}{4l+2}}{\sin\frac{\pi}{4l+2}}+4\sin\frac{\pi}{4l+2}\\
&=4\csc\frac{\pi}{n}.
\end{aligned}\tag{C.0.20}$$

- For $i=3$ we have $n=4l+3$, and equation (C.0.7) gives

$$\mathrm{En}(C_n)=2\sum_{1\le k\le l}\cos\frac{2k\pi}{4l+3}-2\sum_{l+1\le k\le 3l+2}\cos\frac{2k\pi}{4l+3}+2\sum_{3l+3\le k\le n}\cos\frac{2k\pi}{4l+3}$$

where

$$2\sum_{1\le k\le l}\cos\frac{2k\pi}{4l+3}=\sin\frac{2l\pi}{4l+3}\cot\frac{\pi}{4l+3}+\cos\frac{2l\pi}{4l+3}-1, \quad \text{(C.0.21)}$$

$$\begin{aligned}2\sum_{l+1\le k\le 3l+2}\cos\frac{2k\pi}{4l+3}&=\left(\sin\frac{(6l+4)\pi}{4l+3}-\sin\frac{2l\pi}{4l+3}\right)\cot\frac{\pi}{4l+3}\\&\quad+\cos\frac{(6l+4)\pi}{4l+3}-\cos\frac{2l\pi}{4l+3}, \quad \text{(C.0.22)}\end{aligned}$$

and

$$\begin{aligned}2\sum_{3l+3\le k\le n}\cos\frac{2k\pi}{4l+3}&=-\sin\frac{(6l+4)\pi}{4l+3}\cot\frac{\pi}{4l+3}\\&\quad+1-\cos\frac{(6l+4)\pi}{4l+3}. \quad \text{(C.0.23)}\end{aligned}$$

Hence

$$\begin{aligned}\mathrm{En}(C_n)&=\left(2\sin\frac{2l\pi}{4l+3}-2\sin\frac{(6l+4)\pi}{4l+3}\right)\cot\frac{\pi}{4l+3}\\&\quad+2\cos\frac{2l\pi}{4l+3}-2\cos\frac{(6l+4)\pi}{4l+3}\\&=\frac{2\sin\left(\frac{2l\pi}{4l+3}+\frac{\pi}{4l+3}\right)-2\sin\left(\frac{(6l+4)\pi}{4l+3}+\frac{\pi}{4l+3}\right)}{\sin\frac{\pi}{4l+3}}\\&=\frac{2\sin\left(\frac{\pi}{2}-\frac{\pi}{8l+6}\right)-2\sin\left(\frac{3\pi}{2}+\frac{\pi}{8l+6}\right)}{\sin\frac{\pi}{4l+3}}\\&=\frac{4\cos\frac{\pi}{8l+6}}{2\sin\frac{\pi}{8l+6}\cos\frac{\pi}{8l+6}}\\&=2\csc\frac{\pi}{2n}. \quad \text{(C.0.24)}\end{aligned}$$

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