On the Wiener index of bicyclic graphs and graphs with fixed segment sequence

by

Xhanti Sinoxolo

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Department of Mathematics (Pure and Applied)
Rhodes University, PO Box 94
6140 Grahamstown, South Africa

Promoter: Dr. Eric O. D. Andriantiana

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Declaration

I declare that the work in the dissertation entitled "On the Wiener index of bicyclic graphs and graphs with fixed segment sequence" which I hereby submit for the degree, Master of Science at Rhodes University, is my own work. I also declare that this research has not been submitted by me for a degree at this or any other tertiary institution and that all the sources that I have used or quoted have been indicated and acknowledged by means of complete references.

S.

S. Xhanti

Date signed

August 4, 2021

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Abstract

On the Wiener index of bicyclic graphs and graphs with fixed segment sequence

S. Xhanti

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Wiener index is defined as the sum of the distances between all unordered pairs of vertices in a graph. The study of the Wiener index is motivated by its application in chemistry. This thesis focuses on finding extremal bicyclic graphs relative to Wiener index under various conditions such as fixed circumference (length of the longest cycle) or fixed size of the core (maximal subgraph with no degree less than 2). A segment of a graph G is either a path whose end vertices have degree 1 or at least 3 in G and all the internal vertices have degree 2 in G, or a cycle where all the vertices have degree 2 in G except possibly one. The lengths of all the segments of G form it segment sequence. We also discuss extremal graphs with given segment sequence.

Acknowledgement

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1 | Introduction

A graph G is an ordered pair of sets $G = (V(G), E(G))$, where each element of $E(G)$ is a 2-element subset of $V(G)$. We call the elements of the sets $V(G)$ and $E(G)$ vertices and edges respectively. The total number of vertices in a graph G will be represented by n_G or the usual $|V(G)|$. In a drawing of a graph, the vertices are usually represented with dots while the edges are represented with lines joining the dots. See Figure 1.1 for an example.

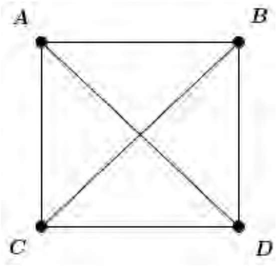

Figure 1.1: The graph ({A,B,C,D},{{A,B},{A,C},{A,D},{B,C},{B,D},{C,D}})

There are many applications of graph theory. One example of such applications would be modelling molecules as graphs. In this example, vertices are atoms and edges usually represent chemical bonds between atoms.

Every graph in this thesis is finite simple and undirected. That is, the total number of vertices and edges in a graph is finite, each pair of vertices in G is connected by at most one edge, and all the edges in G are not directed.

In a graph, two vertices are said to be adjacent if there is an edge connecting them, and two edges are said to be adjacent if they share a common vertex. A vertex is said to be incident to the edge if it is one of the end points of that edge.

Definition 1.1 A path is a graph representation of an alternating sequence $v_1, e_1, v_2, e_2, \ldots, v_k, e_k, v_{k+1}$ of distinct vertices and edges, where the edge e_i is incident to v_i and v_{i+1} for all i. A path with n vertices is denoted by P_n, see Figure 1.2 for P_5. $P_G(u,v)$ is the set of all paths from u to v in a graph G.

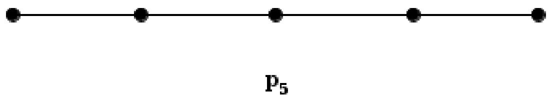

Figure 1.2: Path with 5 vertices

Definition 1.2 The length $l(P_n)$ of a path P_n is defined as the number of edges in it. Also the length of a path with n vertces is defined as the number of edges in it.

Definition 1.3 A graph is said to be connected if there is a path between every two vertices in the graph. That is, G is connected if $P_G(u,v) \neq \emptyset$ for any $u, v \in V(G)$.

Definition 1.4 A cycle is a graph obtained by adding an edge that joins the two ends of a path with at least 3 vertices. A cycle with n vertices is denoted by C_n, see Figure 1.3 for cycles with 4, 5 and 6 vertices. The length of a cycle is the number of edges in it. A unicyclic graph is a connected graph containing exactly one cycle.

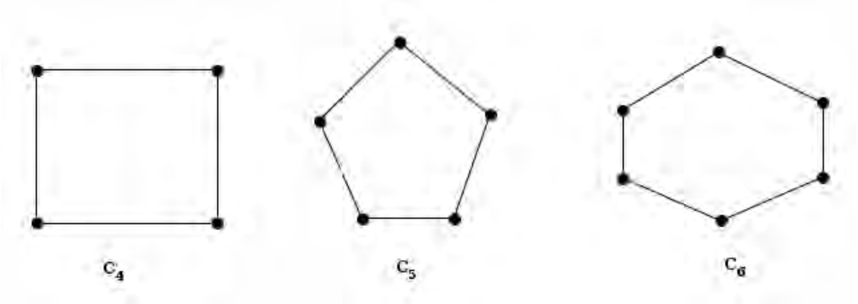

Figure 1.3: Cycles with 4, 5, and 6 vertices

Definition 1.5 Let G and H be simple graphs, H is called a subgraph of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$.

Definition 1.6 An acyclic graph is a graph without a cycle as a subgraph. A tree is a connected acyclic graph, see Figure 1.4 for an example. A star is a special n-vertex tree with $n-1$ leaves (vertices of degree at most 1). A star with n vertices is denoted by S_n, see Figure 1.5 for stars with 4, 5, 6, and 7 vertices.

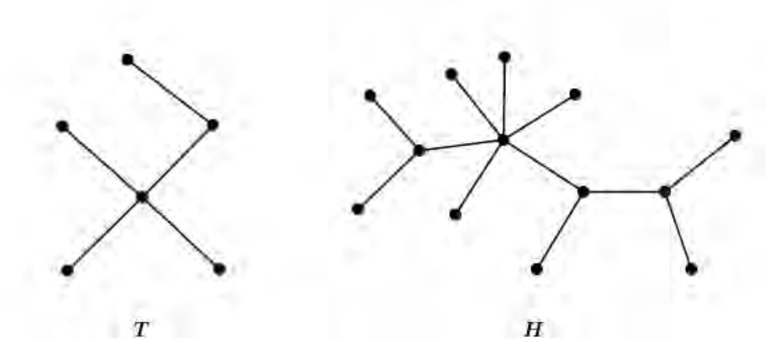

Figure 1.4: Trees T and H

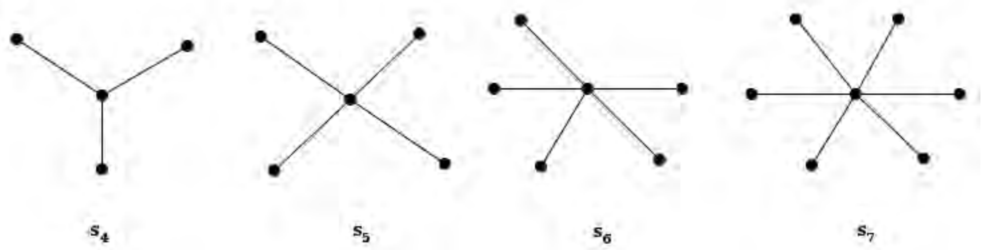

Figure 1.5: Star graphs

Definition 1.7 A bicyclic graph $B = (V, E)$ is a connected graph such that $|E| = |V| + 1$. A strictly bicyclic graph is a bicyclic graph with an additional property that it contains exactly two cycles.

The graph in Figure 1.6 (a) is not a strictly bicyclic graph since it contains three cycles: the pentagon, the square and the triangle. But the graph in Figure 1.6 (b) is a stricly bicyclic graph because it contains exactly two cycles.

Definition 1.8 The distance $d_G(u, v)$ between two vertices u and v in a graph G is defined to be the length of the shortest path between u and v. That is, $d_G(u, v) = \min\{l(P) : P \in P_G(u, v)\}$. When there can be no confusion, we simply write $d(u, v)$ instead. In Figure 1.6 (a)

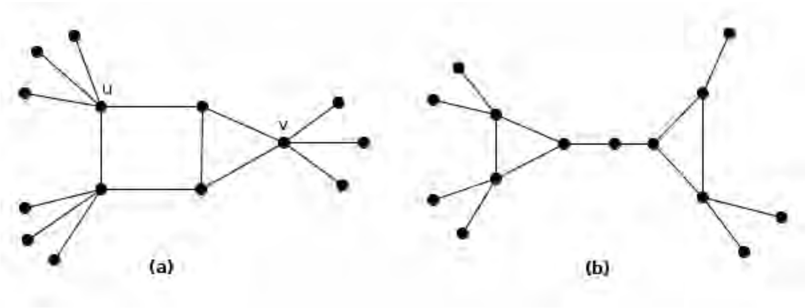

Figure 1.6: A bicyclic graph and a strictly bicyclic graph

the shortest path between vertices u and v consists of just two edges hence $d(u, v) = 2$.

We are now ready to define the Wiener index of a graph.

Definition 1.9 The Wiener index of a graph G, is defined to be

$$W(G) = \sum_{u,v \in V(G)} d_G(u, v),$$

where the sum goes over all the unordered pair of vertices.

Harold Wiener discovered that this Wiener index can actually be used to describe physico-chemical properties of substances. To be more precise, around 1947 he published a paper [18] titled “structural determination of paraffin boiling points”. In that paper he was able to find the correlation between the boiling points of paraffin and the structure of molecules.

Since that discovery mathematicians have been studying Wiener index. The study of Wiener index has grown beyond the molecular structures that were initially studied. Mathematicians have pushed the study to graphs that cannot represent a molecular structure. Most of these works consist of finding graphs with minimum (resp. maximum) Wiener index in a given set of graphs; we call such a graph a minimal (resp. maximal) graph.

The Wiener index of trees and unicyclic graphs have been studied extensively, see [4] and [19] for example. It is already known that, if we only consider the family of trees with fixed order n, the maximum and minimum Wiener index is attained by the path P_n and the star S_n respectively, see [4], specifically Equation 3. Let $L_{n,k}$ be the graph obtained by identifying a vertex of C_k with one end vertex of P_{n-k+1}. Let $H_{n,k}$ be the graph obtained from C_k by adding $n-k$ pendent vertices to a vertex of C_k. Now if we consider the set $U_{n,k}$ of unicyclic graphs with cycle of length k and order n then $L_{n,k}$ and $H_{n,k}$ are found to be extremal relative to Wiener index, see Theorem 1.1 in [19]. See also [3, 6–8, 12–14] for cases dealing with various other conditions imposed.

Researchers started to show interest in the Wiener index of bicyclic graphs. Let G be a connected graph with vertex set $V(G)$ and edge set $E(G)$. Two edges in $E(G)$ are independent if they are not adjacent in G. A matching of G is a set of pairwise independent edges, while a maximum matching of G is a matching with maximum cardinality and the matching number of G is the cardinality of a maximum matching. Let $v \in V(G)$ and M be a matching of G. If v is incident to an edge in M, then v is called saturated by M. If each vertex in $V(G)$ is saturated by M, then M is called a perfect matching of G.

Let a, s and q be postive integers such that $a, q \geq 3$. Let P_{a+2}, P_{s+2} and P_{q+2} be paths of length $a+2$, $s+2$ and $q+2$, respectively. Let $u, u^{'} \in V(P_{a+2})$, $v, v^{'} \in V(P_{s+2})$ and $w, w^{'} \in V(P_{q+2})$ such that $\deg(u) = \deg(u^{'}) = \deg(v) = \deg(v^{'}) = \deg(w) = \deg(w^{'}) = 1$. Then $B_1(a, s, q)$ is a graph formed by merging u with v and w and then merging $u^{'}$ with $v^{'}$ and $w^{'}$. Let C_a, C_q and P_s be cycles and path of length a, q and s, respectively. Let $x \in V(C_a)$, $x^{'} \in V(C_q)$ and $y, y^{'} \in V(P_s)$ such that $\deg(y) = \deg(y^{'}) = 1$. $B_2(a, s, q)$ is a graph formed by merging x with y and $x^{'}$ with $y^{'}$. The core of a bicyclic graph G is the minimal bicyclic subgraph of G. For $k \geq 5$, write

$$J(k) = \{B_1(a, s, q) : a \geq q \geq s, aq \neq 0, a + q + s + 2 = k\}.$$

Let $\theta(m)$ denote the set of all bicyclic graphs with $2m$ vertices and perfect matching. $C_{n,m,r}$ is a graph formed from r C_3's, $m - r - 1$ P_3's and $n - 2m + 1$ P_2's as follows: Identify a vertex in each of the $3-$vertex cycles, identify one vertex of degree one in each of the paths then merge all the identified vertices.

Tan showed in [11] that if $k \geq 5$, then $B_1\left(\left\lceil \frac{k-2}{3} \right\rceil, \left\lfloor \frac{k-2}{3} \right\rfloor, k - 2 - \left\lceil \frac{k-2}{3} \right\rceil - \left\lfloor \frac{k-2}{3} \right\rfloor\right)$ and $B_1\left(\frac{k+1}{3}, \frac{k-5}{3}, \frac{k-2}{3}\right)$ with $k \equiv 2 \pmod 3$ are all graphs with minimum Wiener index in $J(k)$. In the same paper [11], it is also known that: (i) $C_{6,3,2}$ and $B_1(2, 1, 1)$ are all graphs with minimum Wiener index in $\theta(3)$. (ii) $C_{8,4,2}$ and $C_{n,m,r}$ are all graphs with minimum Wiener index in $\theta(4)$. (iii) $C_{2m,m,2}$ is the unique graph with the minimum Wiener index in $\theta(m)$ for $m \geq 5$. For more on this, see [11]. For more results on Wiener index of bicyclic graphs, one can also see [5, 9, 16]. We decided to put our focus on bicyclic graphs, for which not many results have been reported yet.

We will first present preliminaries chapter dedicated to lemmas from other articles that we need for the other chapters. The main work starts in Section 3.1, where we will be studying bicyclic graphs with given circumference. We will first find a graph in that set that minimizes the Wiener index. Then we try to find a graph that maximizes the Wiener index in that set. We will then proceed to Section 3.2, where we will be studying the set of graphs under the condition that the core size is fixed. In that section we will only find the graph that maximizes the Wiener index. Finally, in Chapter 4 we will focus on finding extremal graphs with given segment sequence. We will first study graphs of long segments (graphs with all segments of length at least 3) seperately and later study graphs of short segments (graphs with all segments of length less than or equal 2). This chapter does not only contain results on bicyclic graphs but also results on graphs in general.

In most cases, we iterate selected graph transformations. Then we find explicit expressions of the Wiener indices of graphs for which the transformation cannot be applied. Extremal graphs are found after comparison of these expressions.

2 Preliminaries

In this chapter we present known lemmas that will be useful for us.

The following two lemmas are well-known and will be playing a huge role in this thesis.

Lemma 2.1 *[1] Let $a, d \in \mathbb{R}$. Let (a_n) be the arithmetic sequence defined by $a_i = a + (i-1)d$. Then*

$$\sum_{i=1}^{n} a_i = \frac{n}{2}[2a + (n-1)d].$$

Lemma 2.2 *[1] For all positive integers n we have $\sum_{j=1}^{n} j^2 = \frac{n(n+1)(2n+1)}{6}$.*

The formulas in Lemmas 2.3 and 2.4 will be needed to get explicit formulas of more complicated graphs.

Lemma 2.3 *[2] The Wiener index of a path P_n is given by:*

$$W(P_n) = \binom{n+1}{3} = \frac{(n+1)!}{3!(n-2)!} = \frac{n^3 - n}{6}. \tag{2.1}$$

And the Wiener index of a star with n vertices is given by:

$$W(S_n) = (n-1)^2. \tag{2.2}$$

Proof. To see why Equation (2.1) is true, first label vertices of a path from one end to the other end as $v_1, v_2, ..., v_n$. Then using Lemmas 2.1 and 2.2 we obtain

$$\begin{aligned} W(P_n) &= \sum_{u,v \in V(P_n)} d(u,v) = \sum_{j=1}^{n-1} \sum_{i=j+1}^{n} d(v_j, v_i) \\ &= \sum_{j=1}^{n-1} j + \sum_{j=1}^{n-2} j + \sum_{j=1}^{n-3} j + \cdots + \sum_{j=1}^{1} j \end{aligned}$$

$$
\begin{aligned}
&= \sum_{i=1}^{n-1}\sum_{j=1}^{i} j = \sum_{i=1}^{n-1}\left[\frac{i}{2}(i+1)\right] = \frac{1}{2}\left[\sum_{i=1}^{n-1} i^2 + \sum_{i=1}^{n-1} i\right] \\
&= \frac{1}{2}\left[\frac{(n-1)n(2(n-1)+1)}{6} + \frac{n-1}{2}[2+(n-2)(1)]\right] \\
&= \frac{n^3-n}{6},
\end{aligned}
$$

as in Equation (2.1).

For Equation (2.2) we note that there are $n-1$ leaves of distance 1 from the vertex in the center, plus $2\binom{n-1}{2}$ contribution of distances between leaves to give:

$$
\begin{aligned}
W(S_n) &= n-1+2\binom{n-1}{2} = n-1+(n-2)(n-1) \\
&= (n-1)(1+n-2) = (n-1)^2,
\end{aligned}
$$

which completes the proof. □

Lemma 2.4 ***[17]*** *The Wiener index of a cycle C_n is given by:*

$$
W(C_n) = \begin{cases} \frac{1}{8}n^3 & \text{if n is even,} \\ \frac{1}{8}n(n^2-1) & \text{if n is odd.} \end{cases}
$$

The following lemma on unicyclic graphs will be needed in Section 3.2.

Lemma 2.5 ***[17]*** *Let $C = C_3$ and $P = P_{n-2}$ where n is a natural number greater than or equal to 3. Let $u \in V(C)$, v be an end of P and H be a graph formed by merging u and v. Then among the set of all unicyclic graphs of order n, H attains maximum Wiener index.*

3 Bicyclic Graphs

We noted the papers [5, 9, 11, 16] that study Wiener index of bicyclic graphs. In this chapter we continue this line of research by investigating the Wiener index of bicyclic graphs with additional properties.

3.1 Fixed Circumference

Definition 3.1 Let G be a connected graph, the circumference of G is the length of the longest cycle in G. If G does not contain a cycle then the circumference is zero.

In this section we will be focussing on finding extremal bicyclic graph with given circumference and order, in other words the circumference and order are fixed and everything else is allowed to change. The first part will be based on finding minimal graph(s) then we proceed to finding maximal graph(s).

Definition 3.2 Suppose that each of H and F is a connected graph, $v \in V(H)$ and $w \in V(F)$. Then define $H_{vw}F$ as a graph formed by merging v and w. When it is neccessary to do so, we write $G = (H)_{vw}(F)$, $G = H_{vw}(F)$ or $G = (H)_{vw}F$ to mean that $G = H_{vw}F$.

We define

$$f_G(u) = \sum_{v \in V(G)} d_G(u, v) \text{ and } f_G(H, u) = \sum_{v \in V(H)} d_G(u, v),$$

for fixed vertex $u \in V(G)$ and fixed subgraph H of G.

The next lemma essentially means that moving branches of a graph G from a vertex w to another vertex u increases the Wiener index if $f_G(w)$ is smaller than $f_G(u)$.

Lemma 3.3 ***[15, Theorem 2.2]***
Suppose each of H, F and J is a connected graph with $v \in V(H)$, $u, w \in V(F)$ and $z \in V(J)$. If $f_F(w) \leq f_F(u)$ then

$$W(H_{vu}F_{wz}J) \geq W(H_{vw}F_{wz}J),$$

with strict inequality if $1 < n_J, n_H$ *and* $d_F(u,w) > 0$.

Proof. Let $n_F = |V(F)|, n_J = |V(J)|, n_H = |V(H)|$, $G = H_{vu}F_{wz}J$ and $G^* = H_{vw}F_{wz}J$, then

$$
\begin{aligned}
&W(G) - W(G^*) \\
&= \left[\sum_{\substack{v^{'} \in V(H) \\ u^{'} \in V(F)}} d_G(u^{'}, v^{'}) - \sum_{\substack{v^{'} \in V(H) \\ u^{'} \in V(F)}} d_{G^*}(u^{'}, v^{'}) \right] \\
&+ \left[\sum_{\substack{v^{'} \in V(H) \\ u^{'} \in V(J-z)}} d_G(u^{'}, v^{'}) - \sum_{\substack{v^{'} \in V(H) \\ u^{'} \in V(J-z)}} d_{G^*}(u^{'}, v^{'}) \right] \\
&= [(n_F - 1)f_H(v) + (n_H - 1)f_F(u) - ((n_F - 1)f_H(v) + (n_H - 1)f_F(w))] \\
&+ [(n_H - 1)f_J(z) + (n_J - 1)f_H(v) + (n_H - 1)(n_J - 1)d_G(u,w) \\
&\qquad\qquad - ((n_H - 1)f_J(z) + (n_J - 1)f_H(v))] \\
&= [(n_H - 1)(f_F(u) - f_F(w)) + (n_F - 1)(f_H(v) - f_H(v))] \\
&+ [(n_H - 1)(f_J(z) - f_J(z)) + (n_J - 1)(f_H(v) - f_H(v)) \\
&\qquad\qquad + (n_H - 1)(n_J - 1)d_G(u,w)] \\
&= (n_H - 1)(f_F(u) - f_F(w)) + (n_H - 1)(n_J - 1)d_G(u,w) \geq 0.
\end{aligned}
$$

If $n_J, n_H > 1$ and $d_F(u,w) > 0$ then the last term is positive, hence we get a strict inequality. ☐

Lemma 3.4 *Suppose each of* F, H *and* J *is a connected graph with* $u \in V(F)$, $v \in V(H)$ *and* $u^{'}, v^{'} \in V(J)$. *If* $f_J(u^{'}) \geq f_J(v^{'})$ *and* $n_F \geq n_H$ *then*

$$W(F_{uu^{'}}J_{v^{'}v}H) \geq W(H_{vu^{'}}J_{v^{'}u}F).$$

Proof. Let $d(u^{'}, v^{'}) = a$, then

$$
\begin{aligned}
&W(F_{uu^{'}}J_{v^{'}v}H) - W(F) - W(J) - W(H) && (3.1)\\
&= \sum_{\substack{u \in V(F) \\ v \in V(J) \\ u,v \neq u^{'}}} d(u,v) + \sum_{\substack{u \in V(F) \\ v \in V(H) \\ \{u,v\} \notin \{u^{'}, v^{'}\}}} d(u,v) + \sum_{\substack{u \in V(J) \\ v \in V(H) \\ u,v \neq v^{'}}} d(u,v) && (3.2)\\
&= (n_F - 1)f_J(u^{'}) + (n_J - 1)f_F(u) + (n_F - 1)f_H(v) \\
&+ (n_H - 1)\sum_{\substack{v \in V(F) \\ v \neq u^{'}}} d(v^{'}, v) + (n_J - 1)f_H(v) + (n_H - 1)f_J(v^{'})
\end{aligned}
$$

$$
\begin{aligned}
&= (n_F-1)f_J(u^{'}) + (n_J-1)f_F(u) + (n_F-1)f_H(v)\\
&+ (n_H-1)\sum_{\substack{v\in V(F)\\ v\neq u^{'}}}(d(u^{'},v)+a) + (n_J-1)f_H(v)\\
&+ (n_H-1)f_J(v^{'})\\
&= (n_F-1)f_J(u^{'}) + (n_J-1)f_F(u) + (n_F-1)f_H(v)\\
&+ (n_H-1)f_F(u) + (n_H-1)(n_F-1)a + (n_J-1)f_H(v)\\
&+ (n_H-1)f_J(v^{'}).
\end{aligned}
$$

Note that:
$(n_H-1)\sum_{\substack{v\in V(F)\\ v\neq u^{'}}}\Big(d(u^{'},v)+a\Big) = (n_H-1)f_F(u) + (n_H-1)(n_F-1)a.$

After swapping H and F in $W(F_{uu'}J_{v'v}H) - W(F) - W(J) - W(H)$ we get the following:

$$
\begin{aligned}
&W(H_{vu'}J_{v'u}F) - W(H) - W(J) - W(F)\\
&= (n_F-1)f_J(v^{'}) + (n_J-1)f_F(u) + (n_F-1)f_H(v) + (n_F-1)(n_H-1)a\\
&+ (n_H-1)f_F(u) + (n_J-1)f_H(v) + (n_H-1)f_J(u^{'}).
\end{aligned}
$$

This implies that:

$$
\begin{aligned}
&W(F_{uu'}J_{v'v}H) - W(H_{vu'}J_{v'u}F)\\
&= \Big[(n_F-1)f_J(u^{'}) - (n_F-1)f_J(v^{'})\Big] + \Big[(n_H-1)f_J(v^{'}) - (n_H-1)f_J(u^{'})\Big]\\
&= (n_F-1)\Big[f_J(u^{'}) - f_J(v^{'})\Big] - (n_H-1)\Big[f_J(u^{'}) - f_J(v^{'})\Big]\\
&= (n_F-n_H)\Big[f_J(u^{'}) - f_J(v^{'})\Big] \geq 0.
\end{aligned}
$$

Hence $W(F_{uu'}J_{v'v}H) \geq W(H_{vu'}J_{v'u}F)$. □

Lemma 3.5 *Suppose each of* F, H *and* J *is a connected graph with* $u \in V(F)$, $v, w \in V(H)$ *and* $u^{'}, v^{'} \in V(J)$. *Let* $d(u^{'}, v^{'}) = a$, $d(v, w) = b$. *If*

(i) $f_J(v^{'}) + f_H(w) \geq f_J(u^{'}) + f_H(v)$,

(ii) and $(n_J-1)b \geq (n_H-1)a$,

then $W(F_{uu'}J_{v'v}H) \leq W(J_{v'v}H_{wu}F)$.

Proof. Following from equations (3.1) and (3.2), we have

$$\begin{aligned}
&W(F_{uu'}J_{v'v}H) - W(F) - W(J) - W(H) \\
&= (n_F - 1)f_J(u^{'}) + (n_J - 1)f_F(u) + (n_F - 1)f_H(v) + (n_H - 1)f_F(u) \\
&+ (n_H - 1)(n_F - 1)a + (n_J - 1)f_H(v) + (n_H - 1)f_J(v^{'}),
\end{aligned}$$

$$\begin{aligned}
&W(J_{v'v}H_{wu}F) - W(J) - W(H) - W(F) \\
&= (n_J - 1)f_H(v) + (n_H - 1)f_J(v^{'}) + (n_J - 1)f_F(u) + (n_F - 1)f_J(v^{'}) \\
&+ (n_F - 1)(n_J - 1)b + (n_H - 1)f_F(u) + (n_F - 1)f_H(w)
\end{aligned}$$

and then

$$\begin{aligned}
&W(J_{v'v}H_{wu}F) - W(F_{uu'}J_{v'v}H) \\
&= (n_J - 1)\left[f_F(u) - f_F(u)\right] + (n_F - 1)\left[f_J(v^{'}) + f_H(w) - f_J(u^{'}) - f_H(v)\right] \\
&+ (n_H - 1)\left[f_F(u) - f_F(u)\right] + (n_F - 1)\left[(n_J - 1)b - (n_H - 1)a\right] \\
&= (n_F - 1)\left[f_J(v^{'}) + f_H(w) - f_J(u^{'}) - f_H(v)\right] \\
&+ (n_F - 1)\left[(n_J - 1)b - (n_H - 1)a\right] \geq 0.
\end{aligned}$$

Hence $W(F_{uu'}J_{v'v}H) \leq W(J_{v'v}H_{wu}F)$. □

3.1.1 Minimal Graphs

Definition 3.6 Let C_g be a cycle of length g, and $w, w^{'} \in V(C_g)$ such that $\{w, w^{'}\} \notin E(C_g)$ and $k = d_{C_g}(w, w^{'})$, then we define $B_{n,g,k,l}$ as an n-vertex graph formed from C_g by adding a new path of length $l \leq k$ starting from w ending at $w^{'}$ and then adding $n - g - l + 1$ pendent vertices in w, see Figure 3.1 for $B_{8,5,2,1}$.

Remark 3.7 It should be noted that $k \leq g - k$ since $k = d_{C_g}(w, w^{'})$.

Lemma 3.8 *Let* $A = \{v_1, \ldots, v_m\}$ *be the set of all vertices of degree* 1 *in* $B_{n,g,k,l}$*, for some non-negative integer* m*. Let* $G = B_{n,g,k,l} - v_1 - v_2 - \cdots - v_m$*. If* $z \in V(G)$ *and* $\deg(z) = 3$ *then* $f_G(z) \leq f_G(u)$ *for all* $u \in V(G)$*, with equality if* $\deg(u) = 3$*.*

Proof. Let $w, w^{'} \in V(G)$ such that $w \neq w^{'}$ and $\deg(w) = \deg(w^{'}) = 3$. Let L, K and R be the three segments of length l, k and $g - k$ in G, respectively. Then let B^l, B^k and B^{g-k} be the set of all the vertices in L, K and R, respectively. Each of B^l, B^k and B^{g-k} includes w and $w^{'}$, that is $B^l \cap B^k \cap B^{g-k} = \{w, w^{'}\}$.

Let $C^{'}$ and $C^{''}$ be the two cycles made of vertices in $B^k \cup B^l$ and $B^l \cup B^{g-k}$, respectively. Then for every pair of vertices $u, v \in V(C^{'})$ and $u^{'}, v^{'} \in V(C^{''})$, $f_{C^{'}}(u) = f_{C^{'}}(v)$ and $f_{C^{''}}(u^{'}) = f_{C^{''}}(v^{'})$. Also for every pair of vertices $u \in B^k$ and $v \in B^{g-k}$, the shortest path from u to v passes through w or $w^{'}$. Since $k \geq l$ and $g - k \geq l$, then for all $x \in B^k \cup B^{g-k}$ there exists $x^{'} \in B^l$ such that $d_G(x, w) \geq d_G(x^{'}, w)$ and $d_G(x, w^{'}) \geq d_G(x^{'}, w^{'})$. At least one of the two inequalities is strict if $k > l$ and $g - k > l$. Hence $f_G(z) \leq f_G(z^{'})$ for all $z^{'}$ in G can only hold for some $z \in B^t$, for some $t = l$.

All is left to show is that $f_G(w) = f_G(w^{'}) \leq f_G(y)$ for all $y \in B^l$. But $f_G(w) = f_G(w^{'}) = f_{C^{'}}(w) + f_{C^{''}}(w) - f_{B^l}(w)$, $f_G(y) = f_{C^{'}}(y) + f_{C^{''}}(y) - f_{B^l}(y)$, $f_{C^{'}}(y) = f_{C^{'}}(w)$ and $f_{C^{''}}(y) = f_{C^{''}}(w)$. Then we only need to show that $f_{B^l}(y) \leq f_{B^l}(w)$. Since $f_{B^l}(w) = f_{B^l}(w^{'}) = \sum_{r=1}^{l} r$, $f_{B^l}(y) = \sum_{r=0}^{d_G(y,w)} r + \sum_{r=0}^{d_G(y,w^{'})} r$ and $d_G(y, w) + d_G(y, w^{'}) = l$, then $f_{B^l}(w) \geq f_{B^l}(y)$ and that concludes the proof. ☐

Definition 3.9 $R_{n,g,l}$ is an n-vertex bicyclic graph consisting of exactly two cycles C_g and C_l of lengths g and l, respectively, such that $V(C_g) \cap V(C_l) = \{w\}$, $g \geq l$ and $n - g - l + 1$ pendent vertices attached to the vertex w. In other words w is the only cut vertex of $R_{n,g,l}$, see Figure 3.1 for $R_{9,4,3}$.

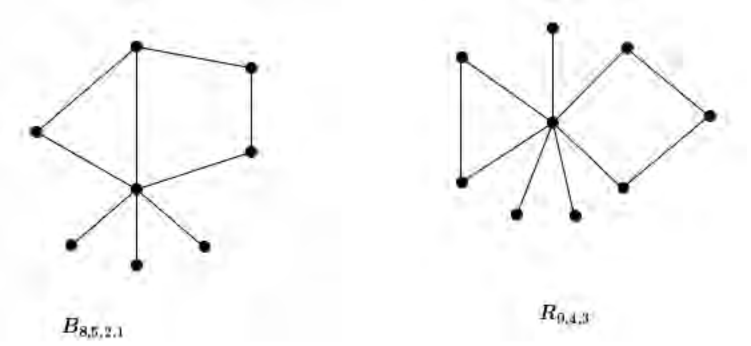

Figure 3.1: $B_{8,5,2,1}$ and $R_{9,4,3}$

The following lemma is a special case of Lemma 3.4 with H being a single vertex.

Lemma 3.10 *Suppose each of F and H is a connected graph with $u \in V(H)$ and $v, w \in V(F)$. Let $G = H_{uv}F$, and $G^{'} = H_{uw}F$, if*

$f_F(v) \geq f_F(w)$ then $W(G) \geq W(G')$.

Lemma 3.3 tells us that a minimal bicyclic graph needs to have at most one cut vertex. To see why this statement is true, let G be a connected bicyclic graph. Suppose that G has at least two cut vertices. Let u and w be two of the cut vertices of G. Then $G = H_{vu}F_{wz}J$, with each of H, F and J a connected graph, $v \in V(H)$, $u, w \in V(F)$ and $z \in V(J)$. By Lemma 3.3, this contradicts the minimality of G. Hence G has at most one cut vertex. Now suppose G has a cut vertex u. Let $A = \{v_1, v_2, \dots, v_m\}$ be the set of all vertices of degree 1 in G. Let $B = G - v_1 - v_2 - \cdots - v_m$. By Lemma 3.10, if G is minimal then $f_B(u) \leq f_B(u')$ for all $u' \in V(B)$. This in conjuction with Lemma 3.8 lead to the conclusion that the minimal bicyclic graph with circumference g has to be either $R_{n,g,l}$ or $B_{n,g,k,l}$. So with that being given we will first derive expressions of $W(R_{n,g,l})$ and $W(B_{n,g,k,l})$ and then determine the values of n, g and l that gives the minimum Wiener index. Then, we compare the minimal $R_{n,g,l}$ with the minimal $B_{n,g,k,l}$.

Lemma 3.11 *Let n, g, and l be integers such that $n \geq g + l - 1$ and $g \geq l \geq 3$.*
(i) If both g and l are odd then

$$\begin{aligned} &W(R_{n,g,l}) \\ &= \frac{g^3 - g}{8} + \frac{l^3 - l}{8} + (n - g - l + 1)^2 + \frac{(g-1)(l-1)(g+l+2)}{4} \\ &+ \frac{(l-1)(n-g-l+1)(l+5)}{4} + \frac{(g-1)(n-g-l+1)(g+5)}{4}. \end{aligned} \tag{3.3}$$

(ii) If g is odd and l is even then

$$\begin{aligned} &W(R_{n,g,l}) \\ &= \frac{g^3 - g}{8} + \frac{l^3}{8} + (n - g - l + 1)^2 + \frac{(g-1)(l^2 + (l-1)(g+1))}{4} \\ &+ \frac{(n-g-l+1)(l^2+4l-4)}{4} + \frac{(g-1)(n-g-l+1)(g+5)}{4}. \end{aligned} \tag{3.4}$$

(iii) If g is even and l is odd then

$$\begin{aligned} &W(R_{n,g,l}) \\ &= \frac{g^3}{8} + \frac{l^3 - l}{8} + (n - g - l + 1)^2 + \frac{(n-g-l+1)(g^2+4g-4)}{4} \\ &+ \frac{(l-1)(g^2 + (g-1)(l+1))}{4} + \frac{(l-1)(n-g-l+1)(l+5)}{4}. \end{aligned} \tag{3.5}$$

(iv) If both g and l are even then

$$\begin{aligned} &W(R_{n,g,l}) \\ &= \frac{g^3}{8} + \frac{l^3}{8} + (n-g-l+1)^2 + \frac{(g-1)l^2}{4} + \frac{(l-1)g^2}{4} \\ &+ (n-g-l+1)\left[\frac{l^2+4l-4}{4}\right] + (n-g-l+1)\left[\frac{g^2+4g-4}{4}\right]. \end{aligned} \tag{3.6}$$

Proof. Let w be the cut vertex of $R_{n,g,l}$, and M the set of vertices in $V(R_{n,g,l})$ that are not in $V(C_g)$ or $V(C_l)$, then

$$\begin{aligned} W(R_{n,g,l}) = W(C_g) + W(C_l) + \sum_{u,v\in M\cup\{w\}} d(u,v) + \sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in V(C_l)\setminus\{w\}}} d(u,v) \\ + \sum_{\substack{u\in V(C_l)\setminus\{w\}\\ v\in M}} d(u,v) + \sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in M}} d(u,v). \end{aligned}$$

In deriving the expression of $W(R_{n,g,l})$, we will consider several cases based on the parity of g and l.

Case (i): both g and l are odd.
Lemmas 2.3 and 2.4 give

$$W(C_g) = \frac{g^3-g}{8},\ W(C_l) = \frac{l^3-l}{8},\ \text{and} \sum_{u,v\in M\cup\{w\}} d(u,v) = (n-g-l+1)^2.$$

Using Lemma 2.1, we get

$$\begin{aligned} \sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in V(C_l)\setminus\{w\}}} d(u,v) &= (g-1)f_{C_l}(w) + (l-1)f_{C_g}(w) \\ &= (g-1)\left[2\sum_{k=1}^{\frac{l-1}{2}} k\right] + (l-1)\left[2\sum_{k=1}^{\frac{g-1}{2}} k\right] \\ &= \frac{(g-1)(l-1)(l+1)}{4} + \frac{(l-1)(g-1)(g+1)}{4} \\ &= \frac{(g-1)(l-1)(g+l+2)}{4}. \end{aligned}$$

Since $d(w,v)=1$ for all $v\in M$, we have

$$\sum_{\substack{u\in V(C_l)\setminus\{w\}\\ v\in M}} d(u,v) = (l-1)\sum_{v\in M} d(w,v) + (n-g-l+1)\sum_{v\in V(C_l)\setminus\{w\}} d(w,v)$$

$$
\begin{aligned}
&= (l-1)(n-g-l+1) + \frac{(n-g-l+1)(l-1)(l+1)}{4}\\
&= \frac{(l-1)(n-g-l+1)(l+5)}{4}
\end{aligned}
$$

and

$$\sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in M}} d(u,v) = \frac{(g-1)(n-g-l+1)(g+5)}{4}.$$

Thus, we have

$$
\begin{aligned}
&W(R_{n,g,l})\\
&= \frac{g^3-g}{8} + \frac{l^3-l}{8} + (n-g-l+1)^2 + \frac{(g-1)(l-1)(g+l+2)}{4}\\
&+ \frac{(l-1)(n-g-l+1)(l+5)}{4} + \frac{(g-1)(n-g-l+1)(g+5)}{4}.
\end{aligned}
$$

Case (ii): g is odd and l is even.
Lemmas 2.3 and 2.4 give

$$W(C_g) = \frac{g^3-g}{8},\ W(C_l) = \frac{l^3}{8}, \text{ and } \sum_{u,v\in M\cup\{w\}} d(u,v) = (n-g-l+1)^2.$$

Using Lemma 2.1, we get

$$
\begin{aligned}
\sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in V(C_l)\setminus\{w\}}} d(u,v) &= (g-1)f_{C_l}(w) + (l-1)f_{C_g}(w)\\
&= (g-1)\left[2\sum_{k=1}^{\frac{l}{2}} k - \frac{l}{2}\right] + (l-1)\left[2\sum_{k=1}^{\frac{g-1}{2}} k\right]\\
&= \frac{(g-1)l^2}{4} + \frac{(l-1)(g-1)(g+1)}{4}\\
&= \frac{(g-1)(l^2+(l-1)(g+1))}{4}.
\end{aligned}
$$

With $d(w,v) = 1$ for all $v \in M$, we have

$$
\begin{aligned}
\sum_{\substack{u\in V(C_l)\setminus\{w\}\\ v\in M}} d(u,v) &= (l-1)\sum_{v\in M} d(w,v) + (n-g-l+1)\sum_{v\in V(C_l)\setminus\{w\}} d(w,v)\\
&= (l-1)(n-g-l+1) + (n-g-l+1)\left[2\sum_{k=1}^{\frac{l}{2}} k - \frac{l}{2}\right]\\
&= (l-1)(n-g-l+1) + \frac{(n-g-l+1)l^2}{4}
\end{aligned}
$$

$$= \frac{(n-g-l+1)(l^2+4l-4)}{4}$$

and

$$\sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in M}} d(u,v) = \frac{(g-1)(n-g-l+1)(g+5)}{4}.$$

Thus, we have

$$\begin{aligned} &W(R_{n,g,l})\\ &= \frac{g^3-g}{8} + \frac{l^3}{8} + (n-g-l+1)^2 + \frac{(g-1)(l^2+(l-1)(g+1))}{4}\\ &+ \frac{(n-g-l+1)(l^2+4l-4)}{4} + \frac{(g-1)(n-g-l+1)(g+5)}{4}. \end{aligned}$$

Case (iii): g is even and l is odd.
Here, we just interchange g and l in case (ii) to get

$$\begin{aligned} &W(R_{n,g,l})\\ &= \frac{g^3}{8} + \frac{l^3-l}{8} + (n-g-l+1)^2 + \frac{(n-g-l+1)(g^2+4g-4)}{4}\\ &+ \frac{(l-1)(g^2+(g-1)(l+1))}{4} + \frac{(l-1)(n-g-l+1)(l+5)}{4}. \end{aligned}$$

Case (iv): both g and l are even.
By similar ways as in previous cases we get

$W(C_g) = \frac{g^3}{8}$, $W(C_l) = \frac{l^3}{8}$, and $\sum_{u,v\in M\cup\{w\}} d(u,v) = (n-g-l+1)^2$,

$$\begin{aligned} \sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in V(C_l)\setminus\{w\}}} d(u,v) &= (g-1)f_{C_l}(w) + (l-1)f_{C_g}(w)\\ &= (g-1)\left[2\sum_{k=1}^{\frac{l}{2}} k - \frac{l}{2}\right] + (l-1)\left[2\sum_{k=1}^{\frac{g}{2}} k - \frac{g}{2}\right]\\ &= \frac{(g-1)l^2}{4} + \frac{(l-1)g^2}{4}, \end{aligned}$$

$$\sum_{\substack{u\in V(C_l)\setminus\{w\}\\ v\in M}} d(u,v) = (l-1)\sum_{v\in M} d(w,v) + (n-g-l+1)\sum_{v\in V(C_l)\setminus\{w\}} d(w,v)$$

$$\begin{aligned}
&= (l-1)(n-g-l+1) + (n-g-l+1)\left[2\sum_{k=1}^{\frac{l}{2}} k - \frac{l}{2}\right] \\
&= (l-1)(n-g-l+1) + (n-g-l+1)\left[\frac{l^2}{4}\right] \\
&= (n-g-l+1)\left[\frac{l^2+4l-4}{4}\right],
\end{aligned}$$

and

$$\begin{aligned}
\sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in M}} d(u,v) &= (g-1)\sum_{v\in M} d(w,v) + (n-g-l+1)\sum_{v\in V(C_g)\setminus\{w\}} d(w,v) \\
&= (g-1)(n-g-l+1) + (n-g-l+1)\left[2\sum_{k=1}^{\frac{g}{2}} k - \frac{g}{2}\right] \\
&= (g-1)(n-g-l+1) + (n-g-l+1)\frac{g^2}{4} \\
&= (n-g-l+1)\left[\frac{g^2+4g-4}{4}\right].
\end{aligned}$$

Thus, we have

$$\begin{aligned}
&W(R_{n,g,l}) \\
&= \frac{g^3}{8} + \frac{l^3}{8} + (n-g-l+1)^2 + \frac{(g-1)l^2}{4} + \frac{(l-1)g^2}{4} \\
&+ (n-g-l+1)\left[\frac{l^2+4l-4}{4}\right] + (n-g-l+1)\left[\frac{g^2+4g-4}{4}\right].
\end{aligned}$$

□

Lemma 3.12 *Let* n*,* g*, and* l *be integers such that* $n \geq g+l-1$ *and* $g \geq l \geq 4$*, then*

$$W(R_{n,g,l}) > W(R_{n,g,l-1}).$$

Proof. We replace l by $l-1$ to obtain $W(R_{n,g,l-1})$ from $W(R_{n,g,l})$. Then we get the following:

(i) If both g and l are odd then Equations 3.3 and 3.4 give

$$\begin{aligned}
&W(R_{n,g,l}) - W(R_{n,g,l-1}) \\
&\qquad = \frac{4(l-3)n-(3l-7)(l+1)}{8}
\end{aligned}$$

$$= \frac{[3(l-3)n - 3(l-3)(l+1)] + [(l-3)n - 2(l+1)]}{8}$$
$$> 0 \quad \textit{since } n > l+1 \textit{ and } l \geq 5.$$

(ii) If g is odd and l is even then Equations 3.3 and 3.4 give

$$W(R_{n,g,l}) - W(R_{n,g,l-1}) = \frac{(l-2)[4n-3l-4]}{8}$$
$$= \frac{(l-2)[3n-3l+n-4]}{8} > 0$$

since $n > l, 4$ and $l \geq 4$.

(iii) If g is even and l is odd then Equations 3.5 and 3.6 give

$$W(R_{n,g,l}) - W(R_{n,g,l-1})$$
$$= \frac{4(l-3)n - (3l-7)(l+1)}{8}$$
$$= \frac{[3(l-3)n - 3(l-3)(l+1)] + [(l-3)n - 2(l+1)]}{8}$$
$$> 0 \quad \textit{since } n > l+1 \textit{ and } l \geq 5.$$

(iv) If both g and l are even then Equations 3.5 and 3.6 give

$$W(R_{n,g,l}) - W(R_{n,g,l-1}) = \frac{(l-2)(4n-3l-4)}{8}$$
$$= \frac{(l-2)[3n-3l+n-4]}{8}$$
$$> 0 \quad \textit{since } n > l, 4 \textit{ and } l \geq 4.$$

Hence $W(R_{n,g,l}) > W(R_{n,g,l-1})$. □

All that is said by Lemma 3.12 is that, reducing the length of the cycle C_l by 1 and adding one more pendent vertex reduces $W(R_{n,g,l})$. With that being given, then if we keep on pulling more and more vertices from the cycle C_l and making them pendent vertices we will reduce $W(R_{n,g,l})$ to $W(R_{n,g,3})$. Hence $R_{n,g,3}$ is minimal among the set of all $R_{n,g,l}$ given that the circumference g is fixed.

Next we derive an expression for $W(B_{n,g,k,l})$.

Lemma 3.13 *Let* n, g, k *and* l *be integers such that* $n \geq g+l-1$, $k \geq l \geq 1$ *and* $k \geq 2$.
(i) If k *is odd,* l *is odd and* g *is even, then*

$$W(B_{n,g,k,l})$$

$$\begin{aligned}
&= \frac{(k+l)^3}{8} + \left[\frac{(l+g-k)^3}{8} - \frac{(l+2)(l+1)l}{6}\right] \\
&+ 2\left[\frac{k-l}{2}\left(\frac{l+g-k}{2}\right)^2 + (l+g-k-1)\cdot\frac{k-l}{4}\cdot\frac{k-l+2}{2}\right. \\
&\qquad\qquad\qquad\qquad\qquad\qquad \left. - \frac{k-l}{2}\cdot\frac{l}{2}\cdot\frac{k+l+4}{2}\right] \\
&+ (l-1)\left(\frac{g}{2}\right)^2 - (k-l+2)\cdot\frac{l-1}{2}\cdot\frac{k+l}{2} - \frac{l(l-1)(l-2)}{3} \\
&+ (n-g-l+1)^2 + (n-g-l+1)\left[\left(\frac{k+l}{2}\right)^2 + k+l-1\right] \\
&+ (n-g-l+1)\left[\left(\frac{l+g-k}{2}\right)^2 - \frac{l}{2}(l+1) + g-k-1\right].
\end{aligned}$$

(ii) If k is odd, l is odd and g is odd, then

$$\begin{aligned}
&W(B_{n,g,k,l}) \\
&= \frac{(k+l)^3}{8} + \left[\frac{(l+g-k)^3-(l+g-k)}{8} - \frac{(l+2)(l+1)l}{6}\right] \\
&+ 2\left[\frac{k-l}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}\right. \\
&\qquad\qquad\qquad \left. + \frac{k-l}{4}\cdot\frac{k-l+2}{2}(g-k-1) - \frac{k-l}{2}\cdot\frac{l}{2}(l+1)\right] \\
&+ (l-1)\cdot\frac{g-1}{2}\cdot\frac{g+1}{2} - (k-l)\cdot\frac{l-1}{2}\cdot\frac{k+l+2}{2} - \frac{l(l-1)(l+1)}{3} \\
&+ (n-g-l+1)^2 + (n-g-l+1)\left[\left(\frac{k+l}{2}\right)^2 + k+l-1\right] \\
&+ (n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2} - \frac{l}{2}(l+1) + g-k-1\right].
\end{aligned}$$

(iii) If k is odd, l is even and g is even, then

$$\begin{aligned}
&W(B_{n,g,k,l}) \\
&= \frac{(k+l)^3-(k+l)}{8} + \left[\frac{(l+g-k)^3-(l+g-k)}{8} - \frac{(l+2)(l+1)l}{6}\right] \\
&+ 2\left[\frac{k-l-1}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}\right. \\
&+ \left.\frac{k-l-1}{4}\cdot\frac{k-l+1}{2}(g-k-l-1)\right] - l(l+1)\cdot\frac{3k-2l-1}{3} + l\left(\frac{g}{2}\right)^2 \\
&+ (n-g-l+1)^2 + (n-g-l+1)\left[\frac{k+l-1}{2}\cdot\frac{k+l+1}{2} + k+l-1\right]
\end{aligned}$$

$$+ (n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}-\frac{l}{2}\,(l+1)\,+g-k-1\right].$$

(iv) If k is even, l is odd and g is odd, then

$$W(B_{n,g,k,l}) = \frac{(g-k+l)^3}{8} + \left[\frac{(l+k)^3-(l+k)}{8}-\frac{(l+2)(l+1)l}{6}\right]$$
$$+2\left[\frac{g-k-l}{2}\cdot\frac{l+k-1}{2}\cdot\frac{l+k+1}{2}\right.$$
$$\left.+\frac{g-k-l}{4}\cdot\frac{g-k-l+2}{2}\,(k-1)-\frac{g-k-l}{2}\cdot\frac{l}{2}\,(l+1)\right]$$
$$+(l-1)\cdot\frac{g-1}{2}\cdot\frac{g+1}{2}-(g-k-l)\cdot\frac{l-1}{2}\cdot\frac{g-k+l+2}{2}-\frac{l(l-1)(l+1)}{3}$$
$$+(n-g-l+1)^2+(n-g-l+1)\left[\left(\frac{g-k+l}{2}\right)^2+g-k+l-1\right]$$
$$+(n-g-l+1)\left[\frac{l+k-1}{2}\cdot\frac{l+k+1}{2}-\frac{l}{2}\,(l+1)+k-1\right].$$

(v) If k is even, l is odd and g is even, then

$$W(B_{n,g,k,l})$$
$$=\frac{(k+l)^3-(k+l)}{8}+\left[\frac{(l+g-k)^3-(l+g-k)}{8}-\frac{(l+2)(l+1)l}{6}\right]$$
$$+2\left[\frac{k-l-1}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}\right.$$
$$\left.+\frac{k-l-1}{4}\cdot\frac{k-l+1}{2}\,(g-k-l-1)\right]$$
$$-l(l+1)\left[\frac{3k-2l-1}{3}\right]+l\left(\frac{g}{2}\right)^2+(n-g-l+1)^2$$
$$+(n-g-l+1)\left[\frac{k+l-1}{2}\cdot\frac{k+l+1}{2}+k+l-1\right]$$
$$+(n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}-\frac{l}{2}\,(l+1)+g-k-1\right].$$

(vi) If k is even, l is even and g is odd, then

$$W(B_{n,g,k,l})$$
$$=\frac{(k+l)^3}{8}+\left[\frac{(l+g-k)^3-(l+g-k)}{8}-\frac{(l+2)(l+1)l}{6}\right]$$
$$+2\left[\frac{k-l}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}+\frac{k-l}{4}\cdot\frac{k-l+2}{2}\,(g-k-l)\right]$$
$$+(l-1)\cdot\frac{g-1}{2}\cdot\frac{g+1}{2}-(k-l)l^2-l(l-1)\cdot\frac{l+1}{3}$$

$$+ (n-g-l+1)^2 + (n-g-l+1)\left[\left(\frac{k+l}{2}\right)^2 + k + l - 1\right]$$
$$+ (n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2} - \frac{l}{2}(l+1) + g - k - 1\right].$$

(vii) If k is odd, l is even and g is odd, then

$$\begin{aligned} &W(B_{n,g,k,l}) \\ &= \frac{(l+g-k)^3}{8} + \left[\frac{(l+k)^3-(l+k)}{8} - \frac{(l+2)(l+1)l}{6}\right] \\ &+ 2\left[\frac{g-k-l}{2}\cdot\frac{l+k-1}{2}\cdot\frac{l+k+1}{2}\right. \\ &\qquad\qquad\qquad \left. + \frac{g-k-l}{4}\cdot\frac{g-k-l+2}{2}(k-l)\right] \\ &+ (l-1)\cdot\frac{g-1}{2}\cdot\frac{g+1}{2} - (g-k-l)l^2 - l(l-1)\cdot\frac{l+1}{3} \\ &+ (n-g-l+1)^2 + (n-g-l+1)\left[\left(\frac{g-k+l}{2}\right)^2 + g - k + l - 1\right] \\ &+ (n-g-l+1)\left[\frac{l+k-1}{2}\cdot\frac{l+k+1}{2} - \frac{l}{2}(l+1) + k - 1\right]. \end{aligned}$$

(viii) If k is even, l is even and g is even, then

$$\begin{aligned} &W(B_{n,g,k,l}) \\ &= \frac{(k+l)^3}{8} + \left[\frac{(l+g-k)^3}{8} - \frac{(l+2)(l+1)l}{6}\right] \\ &+ 2\left[\frac{k-l}{2}\left(\frac{l+g-k}{2}\right)^2 + (l+g-k-1)\cdot\frac{k-l}{4}\cdot\frac{k-l+2}{2}\right. \\ &\left. - \frac{k-l}{2}\cdot\frac{l}{2}\cdot\frac{k+l+4}{2}\right] + (l-1)\left(\frac{g}{2}\right)^2 - (k-l+2)\cdot\frac{l-1}{2}\cdot\frac{k+l}{2} \\ &- \frac{l(l-1)(l-2)}{3} + (n-g-l+1)^2 + (n-g-l+1)\left[\left(\frac{k+l}{2}\right)^2 + k + l - 1\right] \\ &+ (n-g-l+1)\left[\left(\frac{l+g-k}{2}\right)^2 - \frac{l}{2}(l+1) + g - k - 1\right]. \end{aligned}$$

Proof. Let $w, w' \in V(B_{n,g,k,l})$ such that $\deg(w) \geq \deg(w') = 3$. Let L, K and R be the three segments of length l, k and $g-k$, respectively, in $B_{n,g,k,l}$. Then let B^l, B^k, B^{g-k} be the set of all the vertices in L, K, and R, respectively. Each of B^l, B^k and B^{g-k} includes w and w', that is

$B^l \cap B^k \cap B^{g-k} = \{w, w^{'}\}$. Finally let S^{gkl} be the set of all the pendent vertices with their neighbor w included, then

$$W(B_{n,g,k,l}) = W(C_{k+l}) + W(C_{l+g-k}) - \sum_{u,v \in B^l} d(u,v) + \sum_{\substack{u \in B^k \setminus B^l \\ v \in B^{g-k} \setminus B^l}} d(u,v)$$

$$+ W(S_{n-g-l+2}) + \sum_{\substack{u \in S^{gkl} \setminus \{w\} \\ v \in B^k \cup B^l \setminus \{w\}}} d(u,v) + \sum_{\substack{u \in S^{gkl} \setminus \{w\} \\ v \in B^{g-k} \setminus B^l}} d(u,v).$$

As in the case of $W(R_{n,g,l})$, we will consider several cases of l, k *and* g based on their parity.

Case (i): k is odd, l is odd and g is even ($g - k$ odd).
Lemma 2.4 gives

$$W(C_{k+l}) = \frac{(k+l)^3}{8}.$$

Lemma 2.4 and Equation (2.1) combined with the fact that $|B^l| = l+1$, give

$$W(C_{l+g-k}) - \sum_{u,v \in B^l} d(u,v) = \frac{(l+g-k)^3}{8} - \frac{(l+2)(l+1)l}{6}.$$

Now let P be the set of vertices in B^k whose shortest path to some vertices in B^{g-k} passes through L, $P^{'}$ the set of vertices in B^k whose shortest path to vertices in B^{g-k} does not need to pass through L, and $u^{'} \in P$ such that $u^{'}$ is a neighbor of a vertex $x \in P^{'}$, see Figure 3.2. It turned out that $|P \setminus B^l| = 2\left\lfloor \frac{k-l}{2} \right\rfloor$ and $|P^{'}| = l - 1$. From Lemma 2.1 and Equation (2.1) we have,

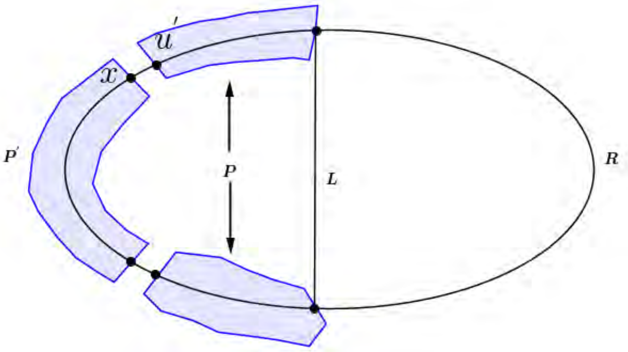

Figure 3.2: P, $P^{'}$, L and R in $B_{n,g,k,l}$

$$
\begin{aligned}
\sum_{\substack{u\in B^k\setminus B^l\\ v\in B^{g-k}\setminus B^l}} d(u,v) = {} & \sum_{\substack{u\in P\\ v\in B^l\cup B^{g-k}}} d(u,v) - \sum_{\substack{u\in P\\ v\in B^l}} d(u,v) + \sum_{\substack{u\in P'\\ v\in B^k\cup B^{g-k}}} d(u,v)\\
& - \sum_{\substack{u\in P\setminus u'\\ v\in P'}} d(u,v) - \sum_{v\in P'} d(u',v) - \sum_{u,v\in P'} d(u,v)
\end{aligned}
$$

which implies that,

$$
\begin{aligned}
& \sum_{\substack{u\in B^k\setminus B^l\\ v\in B^{g-k}\setminus B^l}} d(u,v)\\
& = 2\Bigg[\frac{k-l}{2}\Bigg(2\sum_{j=1}^{\frac{l+g-k}{2}} j - \frac{l+g-k}{2}\Bigg) + (l+g-k-1)\sum_{j=1}^{\frac{k-l}{2}} j\\
& - \Bigg[\frac{k-l}{2}\sum_{j=1}^{l} j + l\sum_{j=1}^{\frac{k-l}{2}} j\Bigg]\Bigg] + (l-1)\Bigg[2\sum_{j=1}^{\frac{g}{2}} j - \frac{g}{2}\Bigg]\\
& - 2\Bigg[\frac{k-l}{2}\sum_{j=1}^{l-1} j + (l-1)\sum_{j=1}^{\frac{k-l}{2}} j\Bigg] - 2\sum_{j=1}^{l-1} j - \frac{2l(l-1)(l-2)}{6}\\
& = 2\Bigg[\frac{k-l}{2}\left(\frac{l+g-k}{2}\left(2+\frac{l+g-k}{2}-1\right) - \frac{l+g-k}{2}\right)\\
& + (l+g-k-1)\cdot\frac{k-l}{4}\left(2+\frac{k-l}{2}-1\right)\\
& - \Bigg[\frac{k-l}{2}\cdot\frac{l}{2}(2+l-1) + \frac{l}{2}\cdot\frac{k-l}{2}\left(2+\frac{k-l}{2}-1\right)\Bigg]\Bigg]\\
& + (l-1)\Bigg[2\sum_{j=1}^{\frac{g}{2}} j - \frac{g}{2}\Bigg] - 2\Bigg[\frac{k-l+2}{2}\sum_{j=1}^{l-1} j + (l-1)\sum_{j=1}^{\frac{k-l}{2}} j\\
& \qquad\qquad + \frac{l(l-1)(l-2)}{6}\Bigg]\\
& = 2\Bigg[\frac{k-l}{2}\left(\frac{l+g-k}{2}\right)^2 + (l+g-k-1)\cdot\frac{k-l}{4}\cdot\frac{k-l+2}{2}\\
& - \frac{k-l}{2}\cdot\frac{l}{2}\cdot\frac{k+l+4}{2}\Bigg] + (l-1)\left[\frac{g}{2}\left(2+\frac{g}{2}-1\right) - \frac{g}{2}\right]\\
& - 2\Bigg[\frac{k-l+2}{2}\cdot\frac{l-1}{2}(2+l-1-1) + (l-1)\cdot\frac{k-l}{4}\cdot
\end{aligned}
$$

$$\left(2+\frac{k-l}{2}-1\right)-\frac{l(l-1)(l-2)}{6}\Bigg]$$

$$\begin{aligned}
&=2\left[\frac{k-l}{2}\left(\frac{l+g-k}{2}\right)^2+(l+g-k-1)\cdot\frac{k-l}{4}\cdot\frac{k-l+2}{2}\right.\\
&\left.-\frac{k-l}{2}\cdot\frac{l}{2}\cdot\frac{k+l+4}{2}\right]+(l-1)\left(\frac{g}{2}\right)^2-(k-l+2)\cdot\frac{l-1}{2}\cdot\frac{k+l}{2}\\
&-\frac{l(l-1)(l-2)}{3}.
\end{aligned}$$

Equation (2.2) gives $W(S_{n-g-l+2})=(n-g-l+1)^2$.

Now we apply Lemma 2.1 to get,

$$\begin{aligned}
&\sum_{\substack{u\in S^{gkl}\smallsetminus\{w\}\\ v\in B^k\cup B^l\smallsetminus\{w\}}} d(u,v)\\
&=(n-g-l+1)\sum_{v\in B^k\cup B^l} d(w,v)+(k+l-1)\sum_{v\in S^{gkl}} d(w,v)\\
&=(n-g-l+1)\left[2\sum_{j=1}^{\frac{k+l}{2}} j-\frac{k+l}{2}\right]+(k+l-1)(n-g-l+1)\\
&=(n-g-l+1)\left[\frac{k+l}{2}\left(2+\frac{k+l}{2}-1\right)-\frac{k+l}{2}\right]\\
&+(k+l-1)(n-g-l+1)\\
&=(n-g-l+1)\left[\left(\frac{k+l}{2}\right)^2+k+l-1\right],
\end{aligned}$$

and

$$\begin{aligned}
&\sum_{\substack{u\in S^{gkl}\smallsetminus\{w\}\\ v\in B^{g-k}\smallsetminus B^l}} d(u,v)\\
&=(n-g-l+1)\sum_{v\in B^l\cup B^{g-k}} d(w,v)+(l+g-k-1)\sum_{v\in S^{gkl}} d(w,v)-\sum_{\substack{u\in B^l\smallsetminus\{w\}\\ v\in S^{gkl}\smallsetminus\{w\}}} d(u,v)\\
&=(n-g-l+1)\left[2\sum_{j=1}^{\frac{l+g-k}{2}} j-\frac{l+g-k}{2}\right]+(l+g-k-1)(n-g-l+1)
\end{aligned}$$

$$
\begin{aligned}
&- \left[(n-g-l+1) \sum_{j=1}^{l} j + l(n-g-l+1) \right] \\
&= (n-g-l+1) \left[\frac{l+g-k}{2} \left(2 + \frac{l+g-k}{2} - 1 \right) - \frac{l+g-k}{2} \right] \\
&+ (l+g-k-1)(n-g-l+1) - \left[(n-g-l+1) \cdot \frac{l}{2} \left(2+l-1 \right) \right. \\
&\hspace{6cm} \left. + l(n-g-l+1) \right] \\
&= (n-g-l+1) \left[\left(\frac{l+g-k}{2} \right)^2 - \frac{l}{2} \left(l+1 \right) + g-k-1 \right].
\end{aligned}
$$

Therefore

$$
\begin{aligned}
&W(B_{n,g,k,l}) \\
&= \frac{(k+l)^3}{8} + \left[\frac{(l+g-k)^3}{8} - \frac{(l+2)(l+1)l}{6} \right] \\
&+ 2 \left[\frac{k-l}{2} \left(\frac{l+g-k}{2} \right)^2 + (l+g-k-1) \cdot \frac{k-l}{4} \cdot \frac{k-l+2}{2} \right. \\
&\hspace{6cm} \left. - \frac{k-l}{2} \cdot \frac{l}{2} \cdot \frac{k+l+4}{2} \right] \\
&+ (l-1) \left(\frac{g}{2} \right)^2 - (k-l+2) \cdot \frac{l-1}{2} \cdot \frac{k+l}{2} - \frac{l(l-1)(l-2)}{3} \\
&+ (n-g-l+1)^2 + (n-g-l+1) \left[\left(\frac{k+l}{2} \right)^2 + k+l-1 \right] \\
&+ (n-g-l+1) \left[\left(\frac{l+g-k}{2} \right)^2 - \frac{l}{2} \left(l+1 \right) + g-k-1 \right].
\end{aligned}
$$

In the following cases we will proceed the same way we did in in case (i).

Case (ii): k is odd, l is odd and g is odd ($g-k$ even).
$W(C_{k+l}) = \dfrac{(k+l)^3}{8}$ and
$W(C_{l+g-k}) - \sum\limits_{u,v \in B^l} d(u,v) = \dfrac{(l+g-k)^3 - (l+g-k)}{8} - \dfrac{(l+2)(l+1)l}{6}$.

$$\sum_{\substack{u\in B^k\setminus B^l\\ v\in B^{g-k}\setminus B^l}} d(u,v) =$$

$$\begin{aligned}
&2\Bigg[\frac{k-l}{2}\Bigg(2\sum_{j=1}^{\frac{l+g-k-1}{2}} j\Bigg) + (l+g-k-1)\sum_{j=1}^{\frac{k-l}{2}} j \\
&-\Bigg(\frac{k-l}{2}\sum_{j=1}^{l} j + l\sum_{j=1}^{\frac{k-l}{2}} j\Bigg)\Bigg] + (l-1)\Bigg[2\sum_{j=1}^{\frac{g-1}{2}} j\Bigg] \\
&-2\Bigg[\frac{k-l}{2}\sum_{j=1}^{l-1} j + (l-1)\sum_{j=1}^{\frac{k-l}{2}} j\Bigg] - 2\sum_{j=1}^{l-1} j - \frac{2l(l-1)(l-2)}{6}
\end{aligned}$$

$$\begin{aligned}
&= 2\bigg[\frac{k-l}{2}\cdot\frac{l+g-k-1}{2}\bigg(2+\frac{l+g-k-1}{2}-1\bigg) \\
&+(l+g-k-1)\cdot\frac{k-l}{4}\bigg(2+\frac{k-l}{2}-1\bigg) \\
&-\bigg(\frac{k-l}{2}\cdot\frac{l}{2}\,(2+l-1) + l\cdot\frac{k-l}{4}\bigg(2+\frac{k-l}{2}-1\bigg)\bigg)\bigg] \\
&+(l-1)\cdot\frac{g-1}{2}\bigg(2+\frac{g-1}{2}-1\bigg) - 2\bigg[\frac{k-l}{2}\cdot\frac{l-1}{2}\cdot(2+l-1-1) \\
&+(l-1)\cdot\frac{k-l}{4}\bigg(2+\frac{k-l}{2}-1\bigg)\bigg] - 2\cdot\frac{l-1}{2}\,(2+l-1-1) \\
&-\frac{2l(l-1)(l-2)}{6}
\end{aligned}$$

$$\begin{aligned}
&= 2\bigg[\frac{k-l}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2} \\
&\qquad\qquad + \frac{k-l}{4}\cdot\frac{k-l+2}{2}\,(g-k-1) - \frac{k-l}{2}\cdot\frac{l}{2}\,(l+1)\bigg] \\
&+(l-1)\cdot\frac{g-1}{2}\cdot\frac{g+1}{2} - (k-l)\cdot\frac{l-1}{2}\cdot\frac{k+l+2}{2} - l(l-1)\cdot\frac{l+1}{3}\ .
\end{aligned}$$

$W(S_{n-g-l+2}) = (n-g-l+1)^2$ and

$$\sum_{\substack{u\in S^{gkl}\setminus\{w\}\\ v\in B^k\cup B^l\setminus\{w\}}} d(u,v) = (n-g-l+1)\left[\left(\frac{k+l}{2}\right)^2 + k+l-1\right].$$

$$\sum_{\substack{u\in S^{gkl}\setminus\{w\}\\ v\in B^{g-k}\setminus B^{l}}} d(u,v) =$$

$$(n-g-l+1)\left[2\sum_{j=1}^{\frac{l+g-k-1}{2}} j\right]+(l+g-k-1)(n-g-l+1)$$
$$-\left[(n-g-l+1)\sum_{j=1}^{l} j+l(n-g-l+1)\right]$$

$$=(n-g-l+1)\cdot\frac{l+g-k-1}{2}\left(2+\frac{l+g-k-1}{2}-1\right)$$
$$+(l+g-k-1)(n-g-l+1)$$
$$-\left[(n-g-l+1)\cdot\frac{l}{2}\,(2+l-1)+l(n-g-l+1)\right]$$
$$=(n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}-\frac{l}{2}\,(l+1)+g-k-1\right].$$

Therefore

$$W(B_{n,g,k,l})$$
$$=\frac{(k+l)^3}{8}+\left[\frac{(l+g-k)^3-(l+g-k)}{8}-\frac{(l+2)(l+1)l}{6}\right]$$
$$+2\left[\frac{k-l}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}\right.$$
$$\left.+\frac{k-l}{4}\cdot\frac{k-l+2}{2}\,(g-k-1)-\frac{k-l}{2}\cdot\frac{l}{2}\,(l+1)\right]$$
$$+(l-1)\cdot\frac{g-1}{2}\cdot\frac{g+1}{2}-(k-l)\cdot\frac{l-1}{2}\cdot\frac{k+l+2}{2}-\frac{l(l-1)(l+1)}{3}$$
$$+(n-g-l+1)^2+(n-g-l+1)\left[\left(\frac{k+l}{2}\right)^2+k+l-1\right]$$
$$+(n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}-\frac{l}{2}\,(l+1)+g-k-1\right].$$

Case (iii): k **is odd,** l **is even and** g **is even (**$g-k$ **odd).**

$W(C_{k+l})=\dfrac{(k+l)^3-(k+l)}{8}$ and

$W(C_{l+g-k})-\displaystyle\sum_{u,v\in B^l} d(u,v)=\dfrac{(l+g-k)^3-(l+g-k)}{8}-\dfrac{(l+2)(l+1)l}{6}.$

$$
\begin{aligned}
&\sum_{\substack{u\in B^{k}\setminus B^{l}\\ v\in B^{g-k}\setminus B^{l}}} d(u,v)\\
&= 2\Bigg[\frac{k-l-1}{2}\left(2\sum_{j=1}^{\frac{l+g-k-1}{2}} j\right)+(l+g-k-1)\sum_{j=1}^{\frac{k-l-1}{2}} j\\
&-\Bigg[\frac{k-l-1}{2}\sum_{j=1}^{l} j+l\sum_{j=1}^{\frac{k-l-1}{2}} j\Bigg]\Bigg]+l\Bigg[2\sum_{j=1}^{\frac{g}{2}} j-\frac{g}{2}\Bigg]\\
&-2\Bigg[\frac{k-l-1}{2}\sum_{j=1}^{l} j+l\sum_{j=1}^{\frac{k-l-1}{2}} j\Bigg]-2\sum_{j=1}^{l} j-\frac{2(l+1)(l)(l-1)}{6}
\end{aligned}
$$

$$
\begin{aligned}
&= 2\Bigg[\frac{k-l-1}{2}\cdot\frac{l+g-k-1}{2}\left(2+\frac{l+g-k-1}{2}-1\right)\\
&+(l+g-k-1)\cdot\frac{k-l-1}{4}\left(2+\frac{k-l-1}{2}-1\right)\\
&-\Bigg[\frac{k-l-1}{2}\cdot\frac{l}{2}(2+l-1)+l\cdot\frac{k-l-1}{4}\left(2+\frac{k-l-1}{2}-1\right)\Bigg]\Bigg]\\
&+l\left[\frac{g}{2}\left(2+\frac{g}{2}-1\right)-\frac{g}{2}\right]\\
&-2\Bigg[\frac{k-l-1}{2}\cdot\frac{l}{2}(2+l-1)+l\cdot\frac{k-l-1}{4}\left(2+\frac{k-l-1}{2}-1\right)\Bigg]\\
&-2\cdot\frac{l}{2}\,(2+l-1)-\frac{2(l+1)l(l-1)}{6}
\end{aligned}
$$

$$
\begin{aligned}
&= 2\Bigg[\frac{k-l-1}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}\\
&\qquad\qquad+\frac{k-l-1}{4}\cdot\frac{k-l+1}{2}\,(g-k-l-1)\Bigg]\\
&-l(l+1)\left[\frac{3k-2l-1}{3}\right]+l\left(\frac{g}{2}\right)^{2}.
\end{aligned}
$$

$$W(S_{n-g-l+2})=(n-g-l+1)^{2},$$

$$\sum_{\substack{u\in S^{gkl}\setminus\{w\}\\ v\in B^{k}\cup B^{l}\setminus\{w\}}} d(u,v)$$

$$
\begin{aligned}
&= (n-g-l+1)\left[2\sum_{j=1}^{\frac{k+l-1}{2}} j\right] + (k+l-1)(n-g-l+1)\\
&= (n-g-l+1)\cdot\frac{k+l-1}{2}\cdot\frac{k+l+1}{2} + (k+l-1)(n-g-l+1)\\
&= (n-g-l+1)\left[\frac{k+l-1}{2}\cdot\frac{k+l+1}{2} + k + l - 1\right]
\end{aligned}
$$

and

$$
\begin{aligned}
&\sum_{\substack{u\in S^{gkl}\setminus\{w\}\\ v\in B^{g-k}\setminus B^{l}}} d(u,v)\\
&= (n-g-l+1)\left[2\sum_{j=1}^{\frac{l+g-k-1}{2}} j\right] + (l+g-k-1)(n-g-l+1)\\
&- \left[(n-g-l+1)\sum_{j=1}^{l} j + l(n-g-l+1)\right]\\
&= (n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2} - \frac{l}{2}\,(l+1) + g - k - 1\right].
\end{aligned}
$$

Therefore

$$
\begin{aligned}
&W(B_{n,g,k,l})\\
&= \frac{(k+l)^3-(k+l)}{8} + \left[\frac{(l+g-k)^3-(l+g-k)}{8} - \frac{(l+2)(l+1)l}{6}\right]\\
&+ 2\left[\frac{k-l-1}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}\right.\\
&+ \left.\frac{k-l-1}{4}\cdot\frac{k-l+1}{2}\,(g-k-l-1)\right] - l(l+1)\cdot\frac{3k-2l-1}{3} + l\left(\frac{g}{2}\right)^2\\
&+ (n-g-l+1)^2 + (n-g-l+1)\left[\frac{k+l-1}{2}\cdot\frac{k+l+1}{2} + k + l - 1\right]\\
&+ (n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2} - \frac{l}{2}\,(l+1) + g - k - 1\right].
\end{aligned}
$$

Case (iv): k is even, l is odd and g is odd ($g-k$ odd).
Here we interchange k and $g-k$ in (ii), that is where there is k we place $g-k$ and vice versa.

$$
W(B_{n,g,k,l}) = \frac{(g-k+l)^3}{8} + \left[\frac{(l+k)^3-(l+k)}{8} - \frac{(l+2)(l+1)l}{6}\right]
$$

$$
\begin{aligned}
&+2\left[\frac{g-k-l}{2}\cdot\frac{l+k-1}{2}\cdot\frac{l+k+1}{2}\right.\\
&\qquad\qquad\left.+\frac{g-k-l}{4}\cdot\frac{g-k-l+2}{2}(k-1)-\frac{g-k-l}{2}\cdot\frac{l}{2}(l+1)\right]\\
&+(l-1)\cdot\frac{g-1}{2}\cdot\frac{g+1}{2}-(g-k-l)\cdot\frac{l-1}{2}\cdot\frac{g-k+l+2}{2}-\frac{l(l-1)(l+1)}{3}\\
&+(n-g-l+1)^2+(n-g-l+1)\left[\left(\frac{g-k+l}{2}\right)^2+g-k+l-1\right]\\
&+(n-g-l+1)\left[\frac{l+k-1}{2}\cdot\frac{l+k+1}{2}-\frac{l}{2}(l+1)+k-1\right].
\end{aligned}
$$

Case (v): k is even, l is odd and g is even ($g-k$ even).

$W(C_{k+l})=\dfrac{(k+l)^3-(k+l)}{8}$ and

$W(C_{l+g-k})-\displaystyle\sum_{u,v\in B^l} d(u,v)=\dfrac{(l+g-k)^3-(l+g-k)}{8}-\dfrac{(l+2)(l+1)l}{6}.$

$$
\begin{aligned}
\sum_{\substack{u\in B^k\setminus B^l\\ v\in B^{g-k}\setminus B^l}} d(u,v)&=2\left[\frac{k-l-1}{2}\left(2\sum_{j=1}^{\frac{l+g-k-1}{2}} j\right)+(l+g-k-1)\sum_{j=1}^{\frac{k-l-1}{2}} j\right.\\
&\quad\left.-\left[\frac{k-l-1}{2}\sum_{j=1}^{l} j+l\sum_{j=1}^{\frac{k-l-1}{2}} j\right]\right]+l\left[2\sum_{j=1}^{\frac{g}{2}} j-\frac{g}{2}\right]\\
&\quad-2\left[\frac{k-l-1}{2}\sum_{j=1}^{l} j+l\sum_{j=1}^{\frac{k-l-1}{2}} j\right]-2\sum_{j=1}^{l} j-\frac{2(l+1)(l)(l-1)}{6}\\
&=2\left[\frac{k-l-1}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}\right.\\
&\qquad\qquad\left.+\frac{k-l-1}{4}\cdot\frac{k-l+1}{2}(g-k-l-1)\right]\\
&\quad-l(l+1)\left[\frac{3k-2l-1}{3}\right]+l\left(\frac{g}{2}\right)^2.
\end{aligned}
$$

$W(S_{n-g-l+2})=(n-g-l+1)^2,$

$$
\sum_{\substack{u\in S^{gkl}\setminus\{w\}\\ v\in B^k\cup B^l\setminus\{w\}}} d(u,v)=(n-g-l+1)\left[2\sum_{j=1}^{\frac{k+l-1}{2}} j\right]+(k+l-1)(n-g-l+1)
$$

$$= (n-g-l+1)\left[\frac{k+l-1}{2}\cdot\frac{k+l+1}{2}+k+l-1\right]$$

and

$$\begin{aligned}
&\sum_{\substack{u\in S^{gkl}\setminus\{w\}\\ v\in B^{g-k}\setminus B^{l}}} d(u,v)\\
&= (n-g-l+1)\left[2\sum_{j=1}^{\frac{l+g-k-1}{2}} j\right]+(l+g-k-1)(n-g-l+1)\\
&-\left[(n-g-l+1)\sum_{j=1}^{l} j + l(n-g-l+1)\right]\\
&= (n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}-\frac{l}{2}\,(l+1)+g-k-1\right].
\end{aligned}$$

Therefore

$$\begin{aligned}
&W(B_{n,g,k,l})\\
&= \frac{(k+l)^3-(k+l)}{8}+\left[\frac{(l+g-k)^3-(l+g-k)}{8}-\frac{(l+2)(l+1)l}{6}\right]\\
&+2\left[\frac{k-l-1}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}\right.\\
&\qquad\qquad\qquad\left.+\frac{k-l-1}{4}\cdot\frac{k-l+1}{2}\,(g-k-l-1)\right]\\
&-l(l+1)\left[\frac{3k-2l-1}{3}\right]+l\left(\frac{g}{2}\right)^2+(n-g-l+1)^2\\
&+(n-g-l+1)\left[\frac{k+l-1}{2}\cdot\frac{k+l+1}{2}+k+l-1\right]\\
&+(n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2}-\frac{l}{2}\,(l+1)+g-k-1\right].
\end{aligned}$$

Case (vi): k is even, l is even and g is odd ($g-k$ odd).
$W(C_{k+l})=\dfrac{(k+l)^3}{8}$ and
$W(C_{l+g-k})-\displaystyle\sum_{u,v\in B^l} d(u,v)=\frac{(l+g-k)^3-(l+g-k)}{8}-\frac{(l+2)(l+1)l}{6}.$

$$\sum_{\substack{u\in B^{k}\setminus B^{l}\\ v\in B^{g-k}\setminus B^{l}}} d(u,v)$$

$$
\begin{aligned}
&= 2 \Bigg[\frac{k-l}{2} \Bigg(2 \sum_{j=1}^{\frac{l+g-k-1}{2}} j \Bigg) + (l+g-k-1) \sum_{j=1}^{\frac{k-l}{2}} j \\
&\qquad - \Bigg[\frac{k-l}{2} \sum_{j=1}^{l} j + l \sum_{j=1}^{\frac{k-l}{2}} j \Bigg] \Bigg] + (l-1) \Bigg[2 \sum_{j=1}^{\frac{g-1}{2}} j \Bigg] \\
&- 2 \Bigg[\frac{k-l}{2} \sum_{j=1}^{l-1} j + (l-1) \sum_{j=1}^{\frac{k-l}{2}} j \Bigg] - 2 \sum_{j=1}^{l-1} j - \frac{2l(l-1)(l-2)}{6} \\
&= 2 \Bigg[\frac{k-l}{2} \cdot \frac{l+g-k-1}{2} \cdot \Bigg(2 + \frac{l+g-k-1}{2} - 1 \Bigg) \\
&+ (l+g-k-1) \cdot \frac{k-l}{4} \Bigg(2 + \frac{k-l}{2} - 1 \Bigg) \\
&- \Bigg[\frac{k-l}{2} \cdot \frac{l}{2} (2+l-1) + l \cdot \frac{k-l}{4} \Bigg(2 + \frac{k-l}{2} - 1 \Bigg) \Bigg] \Bigg] \\
&+ (l-1) \cdot \frac{g-1}{2} \Bigg(2 + \frac{g-1}{2} - 1 \Bigg) \\
&- 2 \Bigg[\frac{k-l}{2} \cdot \frac{l-1}{2} (2+l-1-1) + (l-1) \cdot \frac{k-l}{4} \Bigg(2 + \frac{k-l}{2} - 1 \Bigg) \Bigg] \\
&- 2 \cdot \frac{l-1}{2} (2+l-1-1) - \frac{2l(l-1)(l-2)}{6} \\
&= 2 \Bigg[\frac{k-l}{2} \cdot \frac{l+g-k-1}{2} \cdot \frac{l+g-k+1}{2} + \frac{k-l}{4} \cdot \frac{k-l+2}{2} (g-k-l) \Bigg] \\
&+ (l-1) \cdot \frac{g-1}{2} \cdot \frac{g+1}{2} - (k-l)l^2 - l(l-1) \cdot \frac{l+1}{3} \, .
\end{aligned}
$$

$W(S_{n-g-l+2}) = (n-g-l+1)^2$ and

$$
\begin{aligned}
&\sum_{\substack{u \in S^{gkl} \setminus \{w\} \\ v \in B^k \cup B^l \setminus \{w\}}} d(u,v) \\
&\quad = (n-g-l+1) \Bigg[2 \sum_{j=1}^{\frac{k+l}{2}} j - \frac{k+l}{2} \Bigg] + (k+l-1)(n-g-l+1) \\
&\quad = (n-g-l+1) \Bigg[\left(\frac{k+l}{2} \right)^2 + k + l - 1 \Bigg] .
\end{aligned}
$$

$$
\sum_{\substack{u \in S^{gkl} \setminus \{w\} \\ v \in B^{g-k} \setminus B^l}} d(u,v)
$$

$$
\begin{aligned}
&= (n-g-l+1)\left[2\sum_{j=1}^{\frac{l+g-k-1}{2}} j\right] + (l+g-k-1)(n-g-l+1)\\
&- \left[(n-g-l+1)\sum_{j=1}^{l} j + l(n-g-l+1)\right]\\
&= (n-g-l+1)\cdot\frac{l+g-k-1}{2}\left(2+\frac{l+g-k-1}{2}-1\right)\\
&+ (l+g-k-1)(n-g-l+1)\\
&- \left[(n-g-l+1)\cdot\frac{l}{2}\,(2+l-1) + l(n-g-l+1)\right]\\
&= (n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2} - \frac{l}{2}(l+1)+g-k-1\right].
\end{aligned}
$$

Therefore

$$
\begin{aligned}
&W(B_{n,g,k,l})\\
&= \frac{(k+l)^3}{8} + \left[\frac{(l+g-k)^3-(l+g-k)}{8} - \frac{(l+2)(l+1)l}{6}\right]\\
&+ 2\left[\frac{k-l}{2}\cdot\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2} + \frac{k-l}{4}\cdot\frac{k-l+2}{2}\,(g-k-l)\right]\\
&+ (l-1)\cdot\frac{g-1}{2}\cdot\frac{g+1}{2} - (k-l)l^2 - l(l-1)\cdot\frac{l+1}{3}\\
&+ (n-g-l+1)^2 + (n-g-l+1)\left[\left(\frac{k+l}{2}\right)^2 + k+l-1\right]\\
&+ (n-g-l+1)\left[\frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2} - \frac{l}{2}(l+1)+g-k-1\right].
\end{aligned}
$$

Case (vii): k is odd, l is even and g is odd ($g-k$ even).
Here we interchange k and $g-k$ in (vi) to get

$$
\begin{aligned}
&W(B_{n,g,k,l})\\
&= \frac{(l+g-k)^3}{8} + \left[\frac{(l+k)^3-(l+k)}{8} - \frac{(l+2)(l+1)l}{6}\right]\\
&+ 2\left[\frac{g-k-l}{2}\cdot\frac{l+k-1}{2}\cdot\frac{l+k+1}{2}\right.\\
&\qquad\qquad\qquad\qquad \left. + \frac{g-k-l}{4}\cdot\frac{g-k-l+2}{2}\,(k-l)\right]\\
&+ (l-1)\cdot\frac{g-1}{2}\cdot\frac{g+1}{2} - (g-k-l)l^2 - l(l-1)\cdot\frac{l+1}{3}
\end{aligned}
$$

$$
\begin{aligned}
&+ (n-g-l+1)^2 + (n-g-l+1)\left[\left(\frac{g-k+l}{2}\right)^2 + g-k+l-1\right] \\
&+ (n-g-l+1)\left[\frac{l+k-1}{2}\cdot\frac{l+k+1}{2} - \frac{l}{2}(l+1) + k - 1\right].
\end{aligned}
$$

Case (viii): k is even, l is even and g is even ($g-k$ even).

$W(C_{k+l}) = \dfrac{(k+l)^3}{8}$ and

$W(C_{l+g-k}) - \displaystyle\sum_{u,v\in B^l} d(u,v) = \dfrac{(l+g-k)^3}{8} - \dfrac{(l+2)(l+1)l}{6}$.

$$
\begin{aligned}
&\sum_{\substack{u\in B^k\setminus B^l\\ v\in B^{g-k}\setminus B^l}} d(u,v) \\
&\quad = 2\left[\frac{k-l}{2}\left(2\sum_{j=1}^{\frac{l+g-k}{2}} j - \frac{l+g-k}{2}\right) + (l+g-k-1)\sum_{j=1}^{\frac{k-l}{2}} j\right. \\
&\quad \left. - \left[\frac{k-l}{2}\sum_{j=1}^{l} j + l\sum_{j=1}^{\frac{k-l}{2}} j\right]\right] + (l-1)\left[2\sum_{j=1}^{\frac{g}{2}} j - \frac{g}{2}\right] \\
&\quad - 2\left[\frac{k-l}{2}\sum_{j=1}^{l-1} j + (l-1)\sum_{j=1}^{\frac{k-l}{2}} j\right] - 2\sum_{j=1}^{l-1} j - \frac{2l(l-1)(l-2)}{6} \\
&\quad = 2\left[\frac{k-l}{2}\left(\frac{l+g-k}{2}\right)^2 + (l+g-k-1)\cdot\frac{k-l}{4}\cdot\frac{k-l+2}{2}\right. \\
&\quad \left. - \frac{k-l}{2}\cdot\frac{l}{2}\cdot\frac{k+l+4}{2}\right] + (l-1)\left(\frac{g}{2}\right)^2 - (k-l+2)\cdot\frac{l-1}{2}\cdot\frac{k+l}{2} \\
&\quad - \frac{l(l-1)(l-2)}{3}.
\end{aligned}
$$

$W(S_{n-g-l+2}) = (n-g-l+1)^2$,

$$
\begin{aligned}
&\sum_{\substack{u\in S^{gkl}\setminus\{w\}\\ v\in B^k\cup B^l\setminus\{w\}}} d(u,v) \\
&\quad = (n-g-l+1)\left[2\sum_{j=1}^{\frac{k+l}{2}} j - \frac{k+l}{2}\right] + (k+l-1)(n-g-l+1) \\
&\quad = (n-g-l+1)\left[\left(\frac{k+l}{2}\right)^2 + k+l-1\right]
\end{aligned}
$$

and

$$
\begin{aligned}
&\sum_{\substack{u\in S^{gkl}\setminus\{w\}\\ v\in B^{g-k}\setminus B^{l}}} d(u,v) = \\
&\quad (n-g-l+1)\left[2\sum_{j=1}^{\frac{l+g-k}{2}} j - \frac{l+g-k}{2}\right] + (l+g-k-1)(n-g-l+1) \\
&\quad -\left[(n-g-l+1)\sum_{j=1}^{l} j + l(n-g-l+1)\right] \\
&\quad = (n-g-l+1)\left[\left(\frac{l+g-k}{2}\right)^2 - \frac{l}{2}(l+1) + g-k-1\right].
\end{aligned}
$$

Therefore

$$
\begin{aligned}
&W(B_{n,g,k,l}) \\
&= \frac{(k+l)^3}{8} + \left[\frac{(l+g-k)^3}{8} - \frac{(l+2)(l+1)l}{6}\right] \\
&+2\left[\frac{k-l}{2}\left(\frac{l+g-k}{2}\right)^2 + (l+g-k-1)\cdot\frac{k-l}{4}\cdot\frac{k-l+2}{2}\right. \\
&-\left.\frac{k-l}{2}\cdot\frac{l}{2}\cdot\frac{k+l+4}{2}\right] + (l-1)\left(\frac{g}{2}\right)^2 - (k-l+2)\cdot\frac{l-1}{2}\cdot\frac{k+l}{2} \\
&-\frac{l(l-1)(l-2)}{3} + (n-g-l+1)^2 + (n-g-l+1)\left[\left(\frac{k+l}{2}\right)^2 + k+l-1\right] \\
&+(n-g-l+1)\left[\left(\frac{l+g-k}{2}\right)^2 - \frac{l}{2}(l+1) + g-k-1\right].
\end{aligned}
$$

□

Lemma 3.14 $W(B_{n,g,k,l}) \geq W(B_{n,g,k,l-1})$, *given that* $n \geq 9$ *and* $l \geq 2$.

Proof. In this proof we first focus on the case where $l = 2$, then later on focus on other cases.

(i) For $k = l = g-k = 2$:
We have $W(B_{n,4,2,2}) = n^2 - n - 6$ and $W(B_{n,4,2,1}) = n^2 - 2n - 1$. Then $W(B_{n,4,2,2}) - W(B_{n,4,2,1}) = n - 5 \geq 0,$ *for all* $n \geq 5$. Hence $W(B_{n,4,2,2}) \geq W(B_{n,4,2,1})$ for all $n \geq 9$.

(ii) For $k = l = 2$, $g - k = 3$:
We have $W(B_{n,5,2,2}) = n^2 - 13$ and $W(B_{n,5,2,1}) = n^2 - n - 6$. Then $W(B_{n,5,2,2}) - W(B_{n,5,2,1}) = n - 7 \geq 0$, for all $n \geq 7$. Hence $W(B_{n,5,2,2}) \geq W(B_{n,5,2,1})$, for all $n \geq 9$.

(iii) For $k = g - k = 3$, $l = 2$:
We have $W(B_{n,6,3,2}) = n^2 + n - 20$ and $W(B_{n,6,3,1}) = n^2 - 11$. Then $W(B_{n,6,3,2}) - W(B_{n,6,3,1}) = n - 9 \geq 0$, for all $n \geq 9$. Hence $W(B_{n,6,3,2}) \geq W(B_{n,6,3,1})$, for all $n \geq 9$.

Now, let us check whether our lemma is true for other cases where $3 \leq l \leq k \leq g - k$ or, $l = 2$ and $g - k \geq k \geq 4$.

Let $B = B_{n,g,k,l}$, $y, z \in V(B)$ such that $\deg(z) \geq \deg(y) = 3$ and $z \neq y$. Let L, K and R be the segments in B of length l, k and $g-k$, respectively. Each of L, K and R includes vertices z and y. Furthermore, let w be the vertex in L that is adjacent to z.

We now define a two step transformation from B to $B^{'}$ and then from $B^{'}$ to $B^{''}$ such that $B^{'}$ is obtained from B by merging z and w, to form $z^{'}$ and $B^{''}$ is obtained from $B^{'}$ by attaching a new leaf $z^{''}$ at $z^{'}$, see Figure 3.3. The first step from B to $B^{'}$ results in the decrease in the Wiener index as the vertices are coming closer to each other. The second step from $B^{'}$ to $B^{''}$ results in an increase in the Wiener index, and the distance involving $z^{''}$ is the only increase contributed by this transformation.

To proceed, let $L^{'}$, $K^{'}$ and $R^{'}$ be the segments in $B^{'}$ of length $l - 1$, k, and $g - k$, respectively. And $L^{''}$, $K^{''}$ and $R^{''}$ be segments in $B^{''}$ of length $l - 1$, k and $g - k$, respectively. Again each of $L^{'}$, $K^{'}$, $R^{'}$, $L^{''}$, $K^{''}$ and $R^{''}$ includes the vertices of degree greater than 2.

Now let $u_1 \in V(L)$, $u_2 \in V(R)$ and $u_3 \in V(K)$ such that u_1 is a neighbor of w and $u_1 \neq z$, u_2 and u_3 are neighbors of z.

Let $\Psi = d_B(u_1, u_2) - d_{B'}(u_1, u_2) + d_B(u_1, u_3) - d_{B'}(u_1, u_3)$, then $\Psi = 2$. Let

$$\Phi = \sum_{v \in V(L'') \cup V(K'')} d(z^{''}, v) + \sum_{v \in V(L'') \cup V(R'')} d(z^{''}, v) - \sum_{v \in V(L) \cup V(K)} d(z, v) - \sum_{v \in V(L) \cup V(R)} d(z, v).$$

Since $\sum\limits_{v\in V(L'')} d(z^{''},v) = \sum\limits_{v\in V(L)} d(z,v)$, then

$$\Phi = \sum_{v\in V(B'')\text{ s.t }\deg(v)\neq 1} d(z^{''},v) - \sum_{v\in V(B)\text{ s.t }\deg(v)\neq 1} d(z,v).$$

Finally let

$$\sigma = \sum_{v\in V(B)\setminus\{z\}\ s.t\ \deg(v)\neq 1} d(w,v) - \sum_{v\in V(B')\ s.t\ \deg(v)\neq 1} d(z^{'},v).$$ Since $\sum\limits_{v\in V(L')} d(z^{'},v) = \sum\limits_{v\in V(L)\setminus\{z\}} d(w,v)$, then

$$\begin{aligned}\sigma &= \sum_{v\in V(L)\cup V(K)\setminus\{z\}} d(w,v) + \sum_{v\in V(L)\cup V(R)\setminus\{z\}} d(w,v) - \sum_{v\in V(L')\cup V(K')} d(z^{'},v)\\ &- \sum_{v\in V(L')\cup V(R')} d(z^{'},v)\\ &= \sum_{v\in V(L)\cup V(K)\setminus\{z\}} d(w,v) - \sum_{v\in V(L')\cup V(K')} d(z^{'},v) + \sum_{v\in V(L)\cup V(R)\setminus\{z\}} d(w,v)\\ &- \sum_{v\in V(L')\cup V(R')} d(z^{'},v).\end{aligned}$$

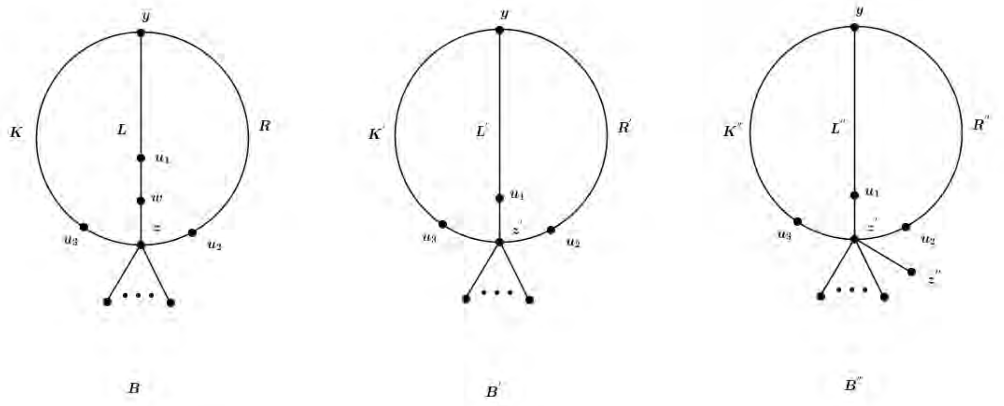

Figure 3.3: Graph transformation in the proof of Lemma 3.14

Since

$$\sum_{v\in V(L)\cup V(K)} d(z,v) = \begin{cases} 2\sum_{j=1}^{\frac{l+k-1}{2}} j & \textit{for } l+k \textit{ odd}\\ 2\sum_{j=1}^{\frac{l+k}{2}} j - \frac{l+k}{2} & \textit{for } l+k \textit{ even}\end{cases}$$

$$= \begin{cases} \frac{l+k-1}{2} \cdot \frac{l+k+1}{2} & \textit{for } l+k \textit{ odd} \\ \left(\frac{l+k}{2}\right)^2 & \textit{for } l+k \textit{ even,} \end{cases}$$

$$\sum_{v \in V(L^{''}) \cup V(K^{''})} d(z^{''}, v) = \begin{cases} \left(\frac{l+k-1}{2}\right)^2 + k + l - 1 & \textit{for } l+k \textit{ odd} \\ \frac{l+k-2}{2} \cdot \frac{l+k}{2} + k + l - 1 & \textit{for } l+k \textit{ even,} \end{cases}$$

$$\sum_{v \in V(L^{''}) \cup V(K^{''})} d(z^{''}, v) - \sum_{v \in V(L) \cup V(K)} d(z, v) = \begin{cases} \frac{l+k-1}{2} & \textit{for } l+k \textit{ odd} \\ \frac{l+k-2}{2} & \textit{for } l+k \textit{ even} \end{cases}$$
$$= \left\lfloor \frac{l+k-1}{2} \right\rfloor$$

and

$$\sum_{v \in V(L^{''}) \cup V(R^{''})} d(z^{''}, v) - \sum_{v \in V(L) \cup V(R)} d(z, v) = \begin{cases} \frac{l+g-k-1}{2} & \textit{for } l+g-k \textit{ odd} \\ \frac{l+g-k-2}{2} & \textit{for } l+g-k \textit{ even} \end{cases}$$
$$= \left\lfloor \frac{l+g-k-1}{2} \right\rfloor$$

we have

$$\Phi = \left\lfloor \frac{l+k-1}{2} \right\rfloor + \left\lfloor \frac{l+g-k-1}{2} \right\rfloor .$$

Since

$$\sum_{v \in V(L) \cup V(K) \setminus \{z\}} d(w, v) = \begin{cases} \frac{l+k-1}{2} \cdot \frac{l+k+1}{2} - 1, & \textit{for } l+k \textit{ odd} \\ \left(\frac{l+k}{2}\right)^2 - 1, & \textit{for } l+k \textit{ even,} \end{cases}$$

$$\sum_{v \in V(L^{'}) \cup V(K^{'})} d(z^{'}, v) = \begin{cases} \left(\frac{l+k-1}{2}\right)^2, & \textit{for } l+k \textit{ odd} \\ \left(\frac{l+k-2}{2}\right)\left(\frac{l+k}{2}\right), & \textit{for } l+k \textit{ even} \end{cases}$$

and

$$\sum_{v \in V(L) \cup V(K) \setminus \{z\}} d(w, v) - \sum_{v \in V(L^{'}) \cup V(K^{'})} d(z^{'}, v) = \left\lfloor \frac{l+k-2}{2} \right\rfloor$$

then

$$\sum_{v\in V(L)\cup V(R)\setminus\{z\}} d(w,v) - \sum_{v\in V(L^{'})\cup V(R^{'})} d(z^{'},v) = \left\lfloor \frac{l+g-k-2}{2} \right\rfloor$$

and

$$\sigma = \left\lfloor \frac{l+k-2}{2} \right\rfloor + \left\lfloor \frac{l+g-k-2}{2} \right\rfloor .$$

Now that $\Psi = 2$, $\Phi = \left\lfloor \frac{l+k-1}{2} \right\rfloor + \left\lfloor \frac{l+g-k-1}{2} \right\rfloor$ and $\sigma = \left\lfloor \frac{l+k-2}{2} \right\rfloor + \left\lfloor \frac{l+g-k-2}{2} \right\rfloor$, then it is clear that $\sigma+\Psi \geq \Phi$. Hence $\Phi - \sigma - \Psi \leq 0$. We next show that $W(B^{''}) - W(B) \leq \Phi - \sigma - \Psi$. Let S be the set of all the vertices of degree 1 in B. Then S is also the set of all the vertices of degree 1 in $B^{'}$ and $S \cup \{z^{''}\}$ is the set of all the vertices of degree 1 in $B^{''}$. Then

$$\begin{aligned}
W(B^{''}) &- W(B)\\
&= W(B^{''}) - W(B^{'}) + W(B^{'}) - W(B)\\
&= \sum_{v\in V(B^{''}-S)} d(z^{''},v) + W(B^{'}) - W(B)\\
&\leq \sum_{v\in V(B^{''}-S)} d(z^{''},v) + \sum_{v\in V(B^{'}-S)} d(z^{'},v) - \sum_{v\in V(B-S-z)} d(w,v)\\
&- \sum_{v\in V(B-S)} d(z,v) + d_{B^{'}}(u_1,u_2) - d_B(u_1,u_2) + d_{B^{'}}(u_1,u_3) - d_B(u_1,u_3)\\
&= \sum_{v\in V(B^{''}-S)} d(z^{''},v) - \sum_{v\in V(B-S)} d(z,v) + \sum_{v\in V(B^{'}-S)} d(z^{'},v)\\
&- \sum_{v\in V(B-S-z)} d(w,v) + d_{B^{'}}(u_1,u_2) - d_B(u_1,u_2) + d_{B^{'}}(u_1,u_3) - d_B(u_1,u_3)\\
&= \Phi - \sigma - \Psi \leq 0.
\end{aligned}$$

Hence $W(B_{n,g,k,l-1}) - W(B_{n,g,k,l}) \leq 0$. □

Iterating Lemma 3.14 as much as possible results in $W(B_{n,g,k,l}) \geq W(B_{n,g,k,1})$ for all n, g, k and l.

Lemma 3.15 $W(B_{n,g,k,1}) > W(B_{n,g,k+1,1})$ *if* $k < g-k-1$, *unless both* k *and* $g-k$ *are even and* $k = g-k-2$.

Proof. After substitution in the expression of $W(B_{n,g,k,1})$ we get the following:

(i) If both k and $g-k$ are odd then

$$\begin{aligned}
&W(B_{n,g,k,1})\\
&=\frac{(k+1)^3}{8}+\frac{(g-k+1)^3}{8}+(k-1)\left[\left(\frac{g-k+1}{2}\right)^2+\frac{k+1}{4}(g-k)\right.\\
&\left.-\frac{k+5}{4}\right]+(n-g)\left[\left(\frac{k+1}{2}\right)^2+\left(\frac{g-k+1}{2}\right)^2+n-2\right]-1,
\end{aligned}$$

$$\begin{aligned}
&W(B_{n,g,k+1,1})\\
&\quad=\frac{(k+2)^3-(k+2)}{8}+\frac{(g-k)^3-(g-k)}{8}+\left(\frac{g}{2}\right)^2\\
&\quad+(k-1)\left[\frac{g-k-1}{2}\cdot\frac{g-k+1}{2}+\frac{k+1}{4}(g-k-3)\right]\\
&\quad+(n-g)\left[\frac{k+1}{2}\cdot\frac{k+3}{2}+\frac{g-k-1}{2}\cdot\frac{g-k+1}{2}+n-2\right]\\
&\quad-2k-1
\end{aligned}$$

and

$$W(B_{n,g,k,1})-W(B_{n,g,k+1,1})=-\frac{3g^2}{8}+\frac{3gk}{4}+\frac{gn}{2}-kn+\frac{k}{2}-\frac{1}{2}.$$

Now let $f(n,g,k)=W(B_{n,g,k,1})-W(B_{n,g,k+1,1})$, then
$\dfrac{\partial f(n,g,k)}{\partial n}=\dfrac{g}{2}-k>0$ since $k<g-k-1$.

The above implies that $f(n,g,k)$ is an increasing function with respect to n. Let $n=g$, the minimum possible value of n. Then

$$\begin{aligned}
f(g,g,k)&=-\frac{3g^2}{8}+\frac{3gk}{4}+\frac{g^2}{2}-kg+\frac{k}{2}-\frac{1}{2}\\
&=\frac{1}{8}(g-2)(g-2k+2)>0\quad\textit{since } g>2k.
\end{aligned}$$

Hence $W(B_{n,g,k,1})>W(B_{n,g,k+1,1})$.

(ii) If k is odd and $g-k$ is even then

$$\begin{aligned}
W(B_{n,g,k,1})&=\frac{(k+1)^3}{8}+\frac{(g-k+1)^3-(g-k+1)}{8}\\
&+(k-1)\left[\frac{g-k}{2}\cdot\frac{g-k+2}{2}+\frac{k+1}{4}(g-k-1)-1\right]\\
&+(n-g)\left[\left(\frac{k+1}{2}\right)^2+\frac{g-k}{2}\cdot\frac{g-k+2}{2}+n-2\right]-1,
\end{aligned}$$

$$\begin{aligned} W(B_{n,g,k+1,1}) &= \frac{(g-k)^3}{8} + \frac{(k+2)^3-(k+2)}{8} \\ &\quad + (g-k-2)\left[\frac{k+1}{2}\cdot\frac{k+3}{2} + \frac{g-k}{4}\cdot k - 1\right] \\ &\quad + (n-g)\left[\left(\frac{g-k}{2}\right)^2 + \frac{k+1}{2}\cdot\frac{k+3}{2} + n - 2\right] - 1. \end{aligned}$$

$$\begin{aligned} f(n,g,k) &= W(B_{n,g,k,1}) - W(B_{n,g,k+1,1}) \\ &= -\frac{3g^2}{8} + \frac{3gk}{4} + \frac{gn}{2} + \frac{g}{4} - kn + \frac{k}{4} - \frac{n}{2} + \frac{1}{8} \end{aligned}$$

and

$$\frac{\partial f(n,g,k)}{\partial n} = \frac{g}{2} - k - \frac{1}{2} = \frac{1}{2}(g-2k-1) > 0 \quad \textit{since } k < g-k-1.$$

The above shows that $f(n,g,k)$ is an increasing function with respect to n, now set $n = g$, the minimum possible value of n. Then

$$\begin{aligned} f(g,g,k) &= -\frac{3g^2}{8} + \frac{3gk}{4} + \frac{g^2}{2} + \frac{g}{4} - kg + \frac{k}{4} - \frac{g}{2} + \frac{1}{8} \\ &= \frac{1}{8}(g-1)(g-2k-1) \geq 0, \end{aligned}$$

with equality if $k = g-k-1$ in which case the two compared graphs are isomorphic. Hence $W(B_{n,g,k,1}) > W(B_{n,g,k+1,1})$.

(iii) If k is even and $g-k$ is odd then

$$\begin{aligned} W(B_{n,g,k,1}) &= \frac{(g-k+1)^3}{8} + \frac{(k+1)^3-(k+1)}{8} \\ &\quad + (g-k-1)\left[\frac{k}{2}\cdot\frac{k+2}{2} + \frac{g-k+1}{4}(k-1) - 1\right] \\ &\quad + (n-g)\left[\left(\frac{g-k+1}{2}\right)^2 + \frac{k}{2}\cdot\frac{k+2}{2} + n - 2\right] - 1, \end{aligned}$$

$$\begin{aligned} W(B_{n,g,k+1,1}) &= \frac{(k+2)^3}{8} + \frac{(g-k)^3-(g-k)}{8} \\ &\quad + k\left[\frac{g-k-1}{2}\cdot\frac{g-k+1}{2} + \frac{k+2}{4}(g-k-2) - 1\right] \end{aligned}$$

$$+ (n-g)\left[\left(\frac{k+2}{2}\right)^2 + \frac{g-k-1}{2}\cdot\frac{g-k+1}{2} + n - 2\right] - 1.$$

$$\begin{aligned} f(n,g,k) &= W(B_{n,g,k,1}) - W(B_{n,g,k+1,1}) \\ &= -\frac{3g^2}{8} + \frac{3gk}{4} + \frac{gn}{2} - kn + \frac{3k}{4} - \frac{n}{2} + \frac{3}{8} \end{aligned}$$

and

$$\begin{aligned} \frac{\partial f(n,g,k)}{\partial n} &= \frac{g}{2} - k - \frac{1}{2} = \frac{1}{2}(g-2k-1) \\ &> 0 \quad \textit{since } g > 2k+1 \quad (k < g-k-1). \end{aligned}$$

The above implies that $f(n,g,k)$ is an increasing function with respect to n. Now set $n = g$, which is the minimum possible value of n. Then

$$\begin{aligned} f(g,g,k) &= \frac{1}{8}(g-3)(g-2k-1) \\ &\geq 0 \quad \textit{(with equality if } k = g-k-1\textit{).} \end{aligned}$$

Hence $W(B_{n,g,k,1}) > W(B_{n,g,k+1,1})$.

(iv) If k is even and $g-k$ is even then

$$\begin{aligned} W(B_{n,g,k,1}) = {} & \frac{(k+1)^3-(k+1)}{8} + \frac{(g-k+1)^3-(g-k+1)}{8} \\ & + (k-2)\left[\frac{g-k}{2}\cdot\frac{g-k+2}{2} + \frac{k}{4}(g-k-2)\right] + \left(\frac{g}{2}\right)^2 \\ & + (n-g)\left[\frac{k}{2}\cdot\frac{k+2}{2} + \frac{g-k}{2}\cdot\frac{g-k+2}{2} + n - 2\right] - 2k + 1, \end{aligned}$$

$$\begin{aligned} W(B_{n,g,k+1,1}) = {} & \frac{(k+2)^3}{8} + \frac{(g-k)^3}{8} \\ & + k\left[\left(\frac{g-k}{2}\right)^2 + \frac{k+2}{4}(g-k-1) - \frac{k+6}{4}\right] \\ & + (n-g)\left[\left(\frac{k+2}{2}\right)^2 + \left(\frac{g-k}{2}\right)^2 + n - 2\right] - 1. \end{aligned}$$

$$f(n,g,k) = W(B_{n,g,k,1}) - W(B_{n,g,k+1,1})$$

$$= -\frac{3g^2}{8} + \frac{3gk}{4} + \frac{gn}{2} + \frac{g}{4} - kn + \frac{k}{2} - n + 1$$

and

$$\begin{aligned}\frac{\partial f(n,g,k)}{\partial n} &= \frac{g}{2} - k - 1 = \frac{1}{2}(g - 2k - 2)\\ &\geq 0 \quad \textit{(with equality if } k = g - k - 2\textit{).}\end{aligned}$$

The above implies that if $k = g - k - 2$, $f(n,g,k)$ will be a constant function with respect to n. Now set $n = g$, the minimum possible value of n and $k = \frac{g-2}{2}$, to get

$$f\left(g, g, \frac{g-2}{2}\right) = \frac{2-g}{4} < 0 \quad \textit{for all } n.$$

All this is saying is that if $k = g - k - 2$ then $B_{n,g,k,1}$ is minimal. Now for $k < g - k - 2$

$$\frac{\partial f(n,g,k)}{\partial n} > 0$$

which shows that $f(n,g,k)$ is an increasing function with respect to n. Now set $n = g$, the minimum possible value of n. Then

$$f(g,g,k) = \frac{1}{8}(g-2)(g-2k-4) > 0 \quad \textit{if } g > 2k + 4.$$

The above implies that $B_{n,g,k+1,1}$ is minimal for $g > 2k+4$. $f(g,g,k) < 0$ for $2k+2 < g < 2k+4$, that is for $g = 2k+3$ and thus $k = g - k - 3$ which is impossible since both k and $g - k$ are even. □

Lemma 3.16 *For $n \geq g + 2$ and $k \leq \dfrac{g-2}{2}$, we have*

$$W(B_{n,g,\frac{g-2}{2},1}), W(B_{n,g,\frac{g-1}{2},1}), W(B_{n,g,\frac{g}{2},1}) \leq W(B_{n,g,2,1}) < W(R_{n,g,3})$$

Proof. After substitution in the formulas of $W(R_{n,g,l})$ and $W(B_{n,g,k,l})$ we get the following

$$W(R_{n,g,3}) = \begin{cases} \frac{g^3-g}{8} + \frac{(g-1)(g+5)(n-g)}{4} + (n-g-2)(n-g+2) + 3 & \textit{for } g \textit{ odd,} \\ \frac{g^3}{8} + \frac{(g^2+4g-4)(n-g)}{4} + (n-g-2)(n-g+2) + 3 & \textit{for } g \textit{ even.} \end{cases}$$

$$W(B_{n,g,2,1}) = \begin{cases} \frac{(g-1)^3}{8} + \frac{g-3}{2} \cdot \frac{g+3}{2} + (n-g)\left[\left(\frac{g-1}{2}\right)^2 + n\right] + 2 & \textit{for } g \textit{ odd,} \\ \frac{(g-1)^3-(g-1)}{8} + (n-g)\left[\frac{g-2}{2} \cdot \frac{g}{2} + n\right] + \left(\frac{g}{2}\right)^2 & \textit{for } g \textit{ even.} \end{cases}$$

Let $f_o(n,g) = W(R_{n,g,3}) - W(B_{n,g,2,1})$ if g is odd and $f_e(n,g) = W(R_{n,g,3}) - W(B_{n,g,2,1})$ if g is even. Then $f_o(n,g) = -\frac{3g^2}{8} + \frac{gn}{2} + g - \frac{3n}{2} - \frac{5}{8}$ and $\frac{\partial f_o(n,g)}{\partial n} = \frac{g}{2} - \frac{3}{2}$. Since there is no such graph as $B_{n,g,k,l}$ with $g \leq 3$ we can assume $g \geq 4$. Hence $\frac{\partial f_o(n,g)}{\partial n} > 0$ for all $g \geq 4$ and for all $n \geq g+2$.

Now it is clear that $f_o(n,g)$ is an increasing function with respect to n, so testing the minimum value of n in $f_o(n,g)$ will tell us whether $f_o(n,g)$ is greater than zero for all the values of n or not. Since the minimum possible value of n is $n = g+2$, then

$$f(g+2,g) = \frac{g^2+4g-29}{8} > 0$$

for all $n \geq g+2 > g \geq 4$.

Now $f_e(n,g) = -\frac{3g^2}{8} + \frac{gn}{2} + \frac{3g}{4} - n - 1$ and $\frac{\partial f_e(n,g)}{\partial n} = \frac{g}{2} - 1$. Reasoning as in the case of $f_o(n,g)$, we have $\frac{\partial f_e(n,g)}{\partial n} > 0$ and $f_e(g+2,g) = \frac{g^2+6g-24}{8} > 0$. Then $f_o(n,g)$, $f_e(n,g) > 0$ for all $n \geq g+2 > g \geq 4$, hence $W(R_{n,g,3}) > W(B_{n,g,2,1})$.

Since $2 \leq k \leq \frac{g-2}{2} < \frac{g-1}{2} < \frac{g}{2}$, then from Lemma 3.15 we can conclude that $W(B_{n,g,\frac{g-2}{2},1}), W(B_{n,g,\frac{g-1}{2},1}), W(B_{n,g,\frac{g}{2},1}) \leq W(B_{n,g,2,1})$. □

Iterating Lemma 3.15 in conjuction with Lemma 3.16 results in the following theorem.

Theorem 3.17 *Among all n-vertex bicyclic graphs with circumference g the following hold. If g is odd, then the minimum Wiener index is reached by $B_{n,g,\frac{g-1}{2},1}$. If both g and $\frac{g}{2}$ are even, then the minimum Wiener index is reached by $B_{n,g,\frac{g}{2},1}$. If g is even and $\frac{g}{2}$ is odd, then the minimum Wiener index is reached by $B_{n,g,\frac{g-2}{2},1}$.*

3.1.2 Maximal Graphs

Let G be a bicyclic graph, if G is maximal i.e if G attains maximum Wiener index then each tree branch in G is a path. This follows from Lemma 3.3. The following lemma is a direct consequence of Lemma 3.10.

Lemma 3.18 *Let G be a connected graph, P_i and P_j be two pendent path subgraphs of G, $v, v^{'} \in V(P_i)$ such that $deg_G(v) > 2$ and $deg_G(v^{'}) = 1$, and $u, u^{'} \in V(P_j)$ such that $deg_G(u) > 2$ and $deg_G(u^{'}) = 1$. Let us further assume that $f_H(v) \geq f_H(u)$, where $H = G - (P_i - v) - (P_j - u)$. If $G^{'}$ is a graph formed from G by removing P_j from u and rejoining it to $v^{'}$ then*

$$W(G^{'}) > W(G).$$

Definition 3.19 Define $D_{n,g,q,h}$ as an n-vertex bicyclic graph consisting of two cycles C_g and C_h joined by a path of length $q - 1$.

Remark 3.20 According to Lemma 3.18, a maximal graph has at most one pendent tree, which has to be a path. The only candidates are $(D_{n,g,q,h})_{vv^{'}}\ (P_i)$ and $(B_{n^{'},g,k,l})_{ww^{'}}(P_j)$ where $n^{'} = g + l - 1$, $v^{'}$ is one end of the path P_i and $w^{'}$ is one end of the path P_j.

Lemma 3.21 *Let G be a connected graph with $z^{'} \in V(G)$. Let C and P be a cycle and a path, with $u, v \in V(C)$, w and z the ends of P. If $u \neq v$ then*

$$W(G_{z^{'}u}C_{vw}P) \leq W(G_{z^{'}z}P_{wv}C).$$

Proof. Let $H = C_{vw}P$, $P^{'}$ be the shortest path from z to u in H and $P^{''}$ a subgraph of H such that $V(P^{''}) = V(H) \setminus V(P^{'})$ and $E(P^{''}) = E(H) \setminus E(P^{'})$. Then $f_H(u) = f_H(P^{'}, u) + f_H(P^{''}, u)$ and $f_H(z) = f_H(P^{'}, z) + f_H(P^{''}, z)$. But $f_H(P^{'}, u) = f_H(P^{'}, z)$, because u and z are the ends of the path $P^{'}$. Since u and v are neighbors of the ends of $P^{'}$ then $f_H(P^{''}, w) = f_H(P^{''}, v) = f_H(P^{''}, u)$ and $f_H(P^{''}, z) = n_{P^{''}} d_P(z, w) + f_H(P^{''}, w)$, where $n_{P^{''}}$ is the total number of vertices in $P^{''}$. Then $f_H(z) = f_H(P^{'}, u) + f_H(P^{''}, u) + n_{P^{''}} d_P(z, w) = f_H(u) + n_{P^{''}} d_P(z, w)$ and $f_H(z) \geq f_H(u)$ since $n_{P^{''}} \geq 1$ and $d_P(z, w) \geq 0$. Hence by Lemma 3.10

$$W(G_{z^{'}u}C_{vw}P) \leq W(G_{z^{'}z}P_{wv}C).$$

□

Lemma 3.21 in conjuction with Remark 3.20 shows that the candidates for the maximum Wiener index are $D_{n,g,q,h}$ and $(B_{n^{'},g,k,l})_{ww^{'}}P_j$, where $n^{'} = g + l - 1$ and $w^{'}$ is one end of the path P_j.

Remark 3.22 Let C and P be a cycle and a path, $w \in V(C)$, x and y the ends of P. Let $H = C_{wx}P$, then the proof of Lemma 3.21 also shows that $f_H(y) \geq f_H(u)$, for any $u \in V(C) - \{w\}$.

The explicit expression of $W(D_{n,g,q,h})$ is available in [2], we provide details here for self-containment. Note that $|V(D_{n,g,q,h})| = |V(C_g)| +$

$|V(P_q)|+|V(C_h)|-2=g+q+h-2$. Let z and $z^{'}$ be the two ends of the graph P_q, then we can write $D_{n,g,q,h}=(C_g)_{wz}(P_q)_{z^{'}w^{'}}(C_h)$, for some $w\in V(C_g)$ and $w^{'}\in V(C_h)$.

$$\begin{aligned}
W(D_{n,g,q,h}) &= \sum_{u,v\in V(D_{n,g,q,h})} d(u,v)\\
&= W(C_g)+W(P_q)+W(C_h)\\
&+ \sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in V(P_q)\setminus\{z\}}} d(u,v) + \sum_{\substack{u\in V(P_q)\setminus\{z^{'}\}\\ v\in V(C_h)\setminus\{w^{'}\}}} d(u,v) + \sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in V(C_h)\setminus\{w^{'}\}}} d(u,v).
\end{aligned}$$

We will be able to find $W(D_{n,g,q,h})$ explicitly by considering several cases based on the parity of g and h.

Case (i): if both g and h are odd.
Lemma 2.4 and Equation 2.1 give
$W(C_g)=\dfrac{g^3-g}{8}$, $W(P_q)=\dfrac{q^3-q}{6}$ and $W(C_h)=\dfrac{h^3-h}{8}$.

Apply Lemma 2.1 to get

$$\begin{aligned}
\sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in V(P_q)\setminus\{z\}}} d(u,v) &= (g-1)\sum_{j=1}^{q-1} j + (q-1)\left(2\sum_{j=1}^{\frac{g-1}{2}} j\right)\\
&= (g-1)\left[\frac{q-1}{2}\left(2(1)+(q-1-1)(1)\right)\right]\\
&+ (q-1)(2)\left[\frac{\frac{g-1}{2}}{2}\left[2(1)+\left(\frac{g-1}{2}-1\right)(1)\right]\right]\\
&= \frac{(g-1)(q-1)}{2}\left[\frac{2q+g+1}{2}\right],
\end{aligned}$$

$$\sum_{\substack{u\in V(P_q)\setminus\{z^{'}\}\\ v\in V(C_h)\setminus\{w^{'}\}}} d(u,v) = \frac{(h-1)(q-1)}{2}\left[\frac{2q+h+1}{2}\right]$$

and

$$\begin{aligned}
&\sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in V(C_h)\setminus\{w^{'}\}}} d(u,v)\\
&= (g-1)\left[\frac{(h-1)(h+1)}{4}+\sum_{j=1}^{h-1}(q-1)\right]+\frac{(h-1)(g-1)(g+1)}{4}
\end{aligned}$$

$$
\begin{aligned}
&= (g-1)\left[\frac{(h-1)(h+1)}{4} + \frac{h-1}{2}(2(q-1)+(h-1-1)(0))\right] \\
&+ \frac{(h-1)(g-1)(g+1)}{4} \\
&= \left[\frac{(g-1)(h-1)}{4}\right](4q+h+g-2).
\end{aligned}
$$

Then

$$
\begin{aligned}
&W(D_{n,g,q,h}) \\
&\quad = \frac{g^3-g}{8} + \frac{q^3-q}{6} + \frac{h^3-h}{8} + \frac{(g-1)(q-1)}{2}\left[\frac{2q+g+1}{2}\right] \\
&\quad + \frac{(h-1)(q-1)}{2}\left[\frac{2q+h+1}{2}\right] + \left[\frac{(g-1)(h-1)}{4}\right](4q+h+g-2).
\end{aligned}
$$

Case (ii): if both g and h are even.

$W(C_g) = \frac{g^3}{8}$, $W(P_q) = \frac{q^3-q}{6}$ and $W(C_h) = \frac{h^3}{8}$.

$$
\begin{aligned}
\sum_{\substack{u\in V(C_g)\smallsetminus\{w\} \\ v\in V(P_q)\smallsetminus\{z\}}} d(u,v) &= (g-1)\sum_{j=1}^{q-1} j + (q-1)\left[2\sum_{j=1}^{\frac{g}{2}} j - \frac{g}{2}\right] \\
&= (g-1)\left[\frac{q-1}{2}(2(1)+(q-1-1)(1))\right] \\
&+ (q-1)\left[2\left[\frac{\frac{g}{2}}{2}\left(2(1)+\left(\frac{g}{2}-1\right)(1)\right)\right] - \frac{g}{2}\right] \\
&= \frac{q-1}{2}\left[(g-1)q + \frac{g^2}{2}\right],
\end{aligned}
$$

$$
\sum_{\substack{u\in V(P_q)\smallsetminus\{z'\} \\ v\in V(C_h)\smallsetminus\{w'\}}} d(u,v) = \frac{q-1}{2}\left[(h-1)q + \frac{h^2}{2}\right]
$$

and

$$
\sum_{\substack{u\in V(C_g)\smallsetminus\{w\} \\ v\in V(C_h)\smallsetminus\{w'\}}} d(u,v) = (g-1)\left[(q-1)(h-1) + \frac{h^2}{4}\right] + \frac{(h-1)g^2}{4}.
$$

Then

$W(D_{n,g,q,h})$

$$= \frac{g^3}{8} + \frac{q^3-q}{6} + \frac{h^3}{8} + \frac{q-1}{2}\left[(g-1)q + \frac{g^2}{2}\right] + \frac{q-1}{2}\left[(h-1)q + \frac{h^2}{2}\right] + (g-1)\left[(q-1)(h-1) + \frac{h^2}{4}\right] + \frac{(h-1)g^2}{4}.$$

Case (iii): if g is even and h is odd.

$W(C_g) = \frac{g^3}{8}$, $W(P_q) = \frac{q^3-q}{6}$ and $W(C_h) = \frac{h^3-h}{8}$.

$$\sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in V(P_q)\setminus\{z\}}} d(u,v) = \frac{q-1}{2}\left[(g-1)q + \frac{g^2}{2}\right],$$

$$\sum_{\substack{u\in V(P_q)\setminus\{z'\}\\ v\in V(C_h)\setminus\{w'\}}} d(u,v) = \frac{(h-1)(q-1)}{2}\left[\frac{2q+h+1}{2}\right]$$

and

$$\sum_{\substack{u\in V(C_g)\setminus\{w\}\\ v\in V(C_h)\setminus\{w'\}}} d(u,v) = \left[\frac{h-1}{4}\right][(g-1)(4q+h-3)+g^2].$$

Then

$$W(D_{n,g,q,h}) = \frac{g^3}{8} + \frac{q^3-q}{6} + \frac{h^3-h}{8} + \frac{(h-1)(q-1)}{2}\left[\frac{2q+h+1}{2}\right] + \frac{q-1}{2}\left[(g-1)q + \frac{g^2}{2}\right] + \left[\frac{h-1}{4}\right][(g-1)(4q+h-3)+g^2].$$

Case (iv): if g is odd and h is even, then we interchange g and h in (iii) to get

$$W(D_{n,g,q,h}) = \frac{g^3-g}{8} + \frac{q^3-q}{6} + \frac{h^3}{8} + \frac{(g-1)(q-1)}{2}\left[\frac{2q+g+1}{2}\right] + \frac{q-1}{2}\left[(h-1)q + \frac{h^2}{2}\right] + \left[\frac{g-1}{4}\right][(h-1)(4q+g-3)+h^2].$$

Lemma 3.23 *$W(D_{n,g,q+1,h-1}) \geq W(D_{n,g,q,h})$ given that $g+q \geq \frac{h+4}{4}$ if h is even, and $g+q \geq \frac{h+1}{4}$ if h is odd. In particular, if $g \geq h$.*

Proof. After substitution in $W(D_{n,g,q,h})$ we get:

(i) If both g and h are odd (g is odd and $h-1$ is even), then

$$W(D_{n,g,q+1,h-1}) = \frac{g^3-g}{8} + \frac{(q+1)^3-(q+1)}{6} + \frac{(h-1)^3}{8}$$

$$
\begin{aligned}
&+\frac{(g-1)q}{2}\left[\frac{2q+g+3}{2}\right]+\frac{q}{2}\left[(h-2)(q+1)+\frac{(h-1)^2}{2}\right]\\
&+\left[\frac{g-1}{4}\right][(h-2)(4q+g+1)+(h-1)^2],
\end{aligned}
$$

$$
\begin{aligned}
&W(D_{n,g,q,h})\\
&=\frac{g^3-g}{8}+\frac{q^3-q}{6}+\frac{h^3-h}{8}+\frac{(g-1)(q-1)}{2}\left[\frac{2q+g+1}{2}\right]\\
&+\frac{(h-1)(q-1)}{2}\left[\frac{2q+h+1}{2}\right]+\left[\frac{(g-1)(h-1)}{4}\right](4q+h+g-2)
\end{aligned}
$$

and

$$
\begin{aligned}
W(D_{n,g,q+1,h-1})-W(D_{n,g,q,h}) &= \frac{(h-1)(4(g+q)-(h+1))}{8}\\
&\geq 0 \quad \textit{if} \quad g+q \geq \frac{h+1}{4}.
\end{aligned}
$$

(ii) If both g and h are even (g is even and $h-1$ is odd), then

$$
\begin{aligned}
W(D_{n,g,q+1,h-1}) &= \frac{g^3}{8}+\frac{(q+1)^3-(q+1)}{6}+\frac{(h-1)^3-(h-1)}{8}\\
&+\frac{q}{2}\left[(g-1)(q+1)+\frac{g^2}{2}\right]+\frac{(h-2)q}{2}\left[\frac{2q+h+2}{2}\right]\\
&+\left[\frac{h-2}{4}\right][(g-1)(4q+h)+g^2],
\end{aligned}
$$

$$
\begin{aligned}
W(D_{n,g,q,h}) &= \frac{g^3}{8}+\frac{q^3-q}{6}+\frac{h^3}{8}+\frac{q-1}{2}\left[(g-1)q+\frac{g^2}{2}\right]\\
&+\frac{q-1}{2}\left[(h-1)q+\frac{h^2}{2}\right]+(g-1)\left[(q-1)(h-1)+\frac{h^2}{4}\right]\\
&+\frac{(h-1)g^2}{4}
\end{aligned}
$$

and

$$
\begin{aligned}
W(D_{n,g,q+1,h-1})-W(D_{n,g,q,h}) &= \frac{(h-2)(4(g+q)-(h+4))}{8}\\
&\geq 0 \quad \textit{if} \quad g+q \geq \frac{h+4}{4}.
\end{aligned}
$$

(iii) If g is even and h is odd (both g and $h-1$ are even), then

$$\begin{aligned}
&W(D_{n,g,q+1,h-1})\\
&\quad= \frac{g^3}{8} + \frac{(q+1)^3-(q+1)}{6} + \frac{(h-1)^3}{8}\\
&\quad+ \frac{q}{2}\left[(g-1)(q+1) + \frac{g^2}{2}\right] + \frac{q}{2}\left[(h-2)(q+1) + \frac{(h-1)^2}{2}\right]\\
&\quad+ (g-1)\left[q(h-2) + \frac{(h-1)^2}{4}\right] + \frac{(h-2)g^2}{4},
\end{aligned}$$

$$\begin{aligned}
W(D_{n,g,q,h}) &= \frac{g^3}{8} + \frac{q^3-q}{6} + \frac{h^3-h}{8} + \frac{(h-1)(q-1)}{2}\left[\frac{2q+h+1}{2}\right]\\
&\quad+ \frac{q-1}{2}\left[(g-1)q + \frac{g^2}{2}\right] + \left[\frac{h-1}{4}\right][(g-1)(4q+h-3)+g^2]
\end{aligned}$$

and

$$\begin{aligned}
W(D_{n,g,q+1,h-1}) - W(D_{n,g,q,h}) &= \frac{(h-1)(4(g+q)-(h+1))}{8}\\
&\geq 0 \quad \textit{if} \quad g+q \geq \frac{h+1}{4}.
\end{aligned}$$

(iv) If g is odd and h is even (both g and $h-1$ are odd), then

$$\begin{aligned}
W(D_{n,g,q+1,h-1}) &= \frac{g^3-g}{8} + \frac{(q+1)^3-(q+1)}{6} + \frac{(h-1)^3-(h-1)}{8}\\
&\quad+ \frac{(g-1)q}{2}\left[\frac{2q+g+3}{2}\right] + \frac{(h-2)q}{2}\left[\frac{2q+h+2}{2}\right]\\
&\quad+ \left[\frac{(g-1)(h-2)}{4}\right](4q+h+g+1),
\end{aligned}$$

$$\begin{aligned}
W(D_{n,g,q,h}) &= \frac{g^3-g}{8} + \frac{q^3-q}{6} + \frac{h^3}{8} + \frac{(g-1)(q-1)}{2}\left[\frac{2q+g+1}{2}\right]\\
&\quad+ \frac{q-1}{2}\left[(h-1)q + \frac{h^2}{2}\right] + \left[\frac{g-1}{4}\right][(h-1)(4q+g-3)+h^2]
\end{aligned}$$

and

$$\begin{aligned}
W(D_{n,g,q+1,h-1}) - W(D_{n,g,q,h}) &= \frac{(h-2)(4(g+q)-(h+4))}{8}\\
&\geq 0 \quad \textit{if} \quad g+q \geq \frac{h+4}{4}.
\end{aligned}$$

□

Iterating Lemma 3.23 as much as possible shows that, if $D_{n,g,q,h}$ is maximal then $h = 3$ since 3 is the smallest possible value of h. The following two lemmas identify the maximal graph if there are no tree branches.

Lemma 3.24 *Let n, g and k be integers such that $n = g + 2 \geq 8$, $k \geq 3$ and $g \geq 6$, then*

$$W(D_{n,g,1,3}) > W(B_{n,g,k,3}).$$

Proof.

(i) If both g and k are odd, then

$$W(D_{n,g,1,3}) = \frac{g^3 - g}{8} + \frac{(g-1)(g+5)}{2} + 3,$$

$$\begin{aligned} W(B_{n,g,k,3}) = {} & \frac{(k+3)^3}{8} + \frac{(g-k+3)^3 - (g-k+3)}{8} \\ & + 2\left[\frac{k-3}{2} \cdot \frac{g-k+2}{2} \cdot \frac{g-k+4}{2}\right. \\ & \left. + \frac{k-3}{4} \cdot \frac{k-1}{2}(g-k-1) - 3(k-3)\right] \\ & + (g-1)\left(\frac{g+1}{2}\right) - 2\left(\frac{k-3}{2}\right)\left(\frac{k+5}{2}\right) - 18 \\ = {} & \frac{g^3}{8} - \frac{g^2k}{8} + \frac{7g^2}{8} + \frac{gk^2}{8} - \frac{gk}{4} - \frac{g}{2} + \frac{k^2}{4} - \frac{k}{8} + \frac{53}{8} \end{aligned}$$

and

$$\begin{aligned} \frac{\partial W(B_{n,g,k,3})}{\partial k} &= -\frac{g^2}{8} + \frac{2gk}{8} - \frac{g}{4} + \frac{2k}{4} - \frac{1}{8} = \frac{-(g^2 + 2g + 1) + 2gk + 4k}{8} \\ &= \frac{-(g+1)(g+1) + 2k(g+2)}{8}. \end{aligned}$$

From the above we can deduce that

$$\frac{\partial W(B_{n,g,k,3})}{\partial k} < 0 \quad \textit{for } k \leq \frac{g-1}{2}.$$

In other words $W(B_{n,g,k,3})$ decreases with increasing k as long as $k \leq \frac{g-1}{2}$. So $W(B_{n,g,k,3})$ will be maximal when $k = 3$ the smallest possible odd value of k. Now

$$\begin{aligned}W(D_{n,g,1,3}) - W(B_{n,g,k,3}) &= \frac{g^2k - 3g^2 - gk^2 + 2gk + 19g - 2k^2 + k - 49}{8}\\ &\geq W(D_{n,g,1,3}) - W(B_{n,g,3,3})\\ &= 2g - 8 > 0 \quad \textit{since } g \geq 6.\end{aligned}$$

(ii) If g is odd and k is even, then

$$W(D_{n,g,1,3}) = \frac{g^3 - g}{8} + \frac{(g-1)(g+5)}{2} + 3,$$

$$\begin{aligned}&W(B_{n,g,k,3})\\ &\quad = \frac{(g-k+3)^3}{8} + \frac{(k+3)^3 - (k+3)}{8}\\ &\quad + 2\left[\frac{g-k-3}{2} \cdot \frac{k+2}{2} \cdot \frac{k+4}{2} + \frac{g-k-3}{4} \cdot \frac{g-k-1}{2}(k-1)\right.\\ &\quad \left. - \left(\frac{g-k-3}{2}\right)(6)\right] + (g-1) \cdot \frac{g+1}{2} - (g-k-3) \cdot \frac{g-k+5}{2} - 18\\ &\quad = \frac{g^3}{8} - \frac{g^2k}{8} + \frac{7g^2}{8} + \frac{gk^2}{8} - \frac{gk}{4} - \frac{5g}{8} + \frac{k^2}{4} + \frac{k}{8} + \frac{53}{8}\end{aligned}$$

and

$$\begin{aligned}\frac{\partial W(B_{n,g,k,3})}{\partial k} &= -\frac{g^2}{8} + \frac{2gk}{8} - \frac{g}{4} + \frac{2k}{4} + \frac{1}{8} = \frac{-(g^2 + 2g - 1) + 2gk + 4k}{8}\\ &= \frac{-(g^2 + 2g - 1) + 2k(g+2)}{8}.\end{aligned}$$

From the above we can deduce that

$$\frac{\partial W(B_{n,g,k,3})}{\partial k} < 0 \quad \textit{when } k \leq \frac{g-1}{2}.$$

The above suggests that $W(B_{n,g,k,3})$ will be maximal when $k = 4$ the smallest possible value of k. Then

$$\begin{aligned}W(D_{n,g,1,3}) - W(B_{n,g,k,3}) &= \frac{g^2k - 3g^2 - gk^2 + 2gk + 20g - 2k^2 - k - 49}{8}\\ &\geq W(D_{n,g,1,3}) - W(B_{n,g,4,3})\\ &= \frac{(g-5)(g+17)}{8} > 0 \quad \textit{since } g \geq 7.\end{aligned}$$

(iii) If g is even and k is odd, then

$$W(D_{n,g,1,3}) = \frac{g^3}{8} + \frac{4(g-1)+g^2}{2} + 3,$$

$$\begin{aligned} W(B_{n,g,k,3}) &= \frac{(k+3)^3}{8} + \frac{(g-k+3)^3}{8} \\ &\quad + 2\left[\frac{k-3}{2}\left(\frac{g-k+3}{2}\right)^2 + (g-k+2)\cdot\frac{k-3}{4}\cdot\frac{k-1}{2}\right. \\ &\quad \left. - \frac{k-3}{2}\cdot\frac{3}{2}\cdot\frac{k+7}{2}\right] + 2\left(\frac{g}{2}\right)^2 - (k-1)\left(\frac{k+3}{2}\right) - 12 \\ &= \frac{g^3}{8} - \frac{g^2k}{8} + \frac{7g^2}{8} + \frac{gk^2}{8} - \frac{gk}{4} - \frac{3g}{8} + \frac{k^2}{4} + \frac{27}{4} \end{aligned}$$

and

$$\begin{aligned} \frac{\partial W(B_{n,g,k,3})}{\partial k} &= -\frac{g^2}{8} + \frac{2gk}{8} - \frac{g}{4} + \frac{2k}{4} = \frac{-(g^2+2g)+2gk+4k}{8} \\ &= \frac{-g(g+2)+2k(g+2)}{8} = \frac{(g+2)(2k-g)}{8}. \end{aligned}$$

From the above we can deduce that

$$\begin{aligned} \frac{\partial W(B_{n,g,k,3})}{\partial k} &< 0 \quad \textit{if } k < \frac{g}{2}, \textit{ and} \\ \frac{\partial W(B_{n,g,k,3})}{\partial k} &= 0 \quad \textit{if } k = \frac{g}{2}. \end{aligned}$$

With the same reasoning as in (ii), $W(B_{n,g,k,3})$ will be maximal when $k = 3$ the smallest possible value of k, hence

$$\begin{aligned} W(D_{n,g,1,3}) - W(B_{n,g,k,3}) &= \frac{g^2k - 3g^2 - gk^2 + 2gk + 19g - 2k^2 - 46}{8} \\ &\geq W(D_{n,g,1,3}) - W(B_{n,g,3,3}) \\ &= 2(g-4) > 0 \quad \textit{since } g \geq 6. \end{aligned}$$

(iv) If both g and k are even, then

$$W(D_{n,g,1,3}) = \frac{g^3}{8} + \frac{4(g-1)+g^2}{2} + 3,$$

$$\begin{aligned} &W(B_{n,g,k,3}) \\ &\quad = \frac{(k+3)^3-(k+3)}{8} + \frac{(g-k+3)^3-(g-k+3)}{8} \end{aligned}$$

$$
\begin{aligned}
&+2\left[\frac{k-4}{2}\cdot\frac{g-k+2}{2}\cdot\frac{g-k+4}{2}+\frac{k-4}{4}\cdot\frac{k-2}{2}(g-k-4)\right]\\
&-4(3k-7)+3\left(\frac{g}{2}\right)^2-10\\
&=\frac{g^3}{8}-\frac{g^2k}{8}+\frac{7g^2}{8}+\frac{gk^2}{8}-\frac{gk}{4}-\frac{3g}{4}+\frac{k^2}{4}+8
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\partial W(B_{n,g,k,3})}{\partial k} &= -\frac{g^2}{8}+\frac{2gk}{8}-\frac{g}{4}+\frac{2k}{4}=\frac{-g^2-2g+2gk+4k}{8}\\
&=\frac{-g(g+2)+2k(g+2)}{8}=\frac{(g+2)(2k-g)}{8}.
\end{aligned}
$$

The above implies that

$$
\begin{aligned}
\frac{\partial W(B_{n,g,k,3})}{\partial k} &< 0 \quad \textit{if } k<\frac{g}{2}, \textit{ and}\\
\frac{\partial W(B_{n,g,k,3})}{\partial k} &= 0 \quad \textit{if } k=\frac{g}{2}.
\end{aligned}
$$

Reasoning as in (i) $W(B_{n,g,k,3})$ will be maximal when $k = 4$, the smallest possible even value of k. Hence

$$
\begin{aligned}
W(D_{n,g,1,3})-W(B_{n,g,k,3}) &= \frac{g^2k-3g^2-gk^2+2gk+22g-2k^2-56}{8}\\
&\geq W(D_{n,g,1,3})-W(B_{n,g,4,3})\\
&=\frac{1}{8}g^2+\frac{7}{4}g-11>0 \quad \textit{since } g\geq 8.
\end{aligned}
$$

Hence $W(D_{n,g,1,3}) > W(B_{n,g,k,3})$.

□

Lemma 3.25 *Let n, g, l, k be integers such that $n = g + l - 1$, $k < \frac{g}{2}$ and $l > 2$, then*

$$W(D_{n,g,l-2,3}) > W(B_{n,g,k,l}).$$

Proof. Suppose $n = g + l - 1$ and $l > 2$. If $l = 3$ then we are done by Lemma 3.24. Suppose $l \geq 4$. Let L be the segment in $B_{n,g,k,l}$ of length l. Let u, v, w, x, $y \in V(B_{n,g,k,l})$ such that $w \neq x$, $\deg(w) = \deg(x) = 3$, u is the neighbor of x in L, v is the neighbor of u that is not x and y is the neighbor of v that is not u.

Now let us define the transformation from $B_{n,g,k,l}$ to $D_{n,g,l-2,3}$ as follows: Remove the edge ux and add the edge uy. One clear observation is that all the vertices in $B_{n,g,k,l} - u$ either stay in the same positions or move further apart from each other. This only contributes to an increase in Wiener index. What is not clear is the contribution of u. To investigate the contribution of u, let $\Phi_B = \sum_{v \in V(B_{n,g,k,l})} d(u,v)$ and $\Phi_D = \sum_{v \in V(D_{n,g,l-2,3})} d(u,v)$. If $\Phi_D - \Phi_B > 0$ then the transformation from $B_{n,g,k,l}$ to $D_{n,g,l-2,3}$ increases the Wiener index and hence $W(D_{n,g,l-2,3}) > W(B_{n,g,k,l})$. Now:

(i) If k is odd, l is odd, and g is odd, then

$$\begin{aligned}
\Phi_D &= 1 + \sum_{j=1}^{l-2} j + 2\sum_{j=1}^{\frac{g-1}{2}} (j + l - 2) \\
&= 1 + \frac{l-2}{2}(2 + l - 2 - 1) + \frac{g-1}{2}\left(2(l-1) + \frac{g-1}{2} - 1\right) \\
&= \frac{l-2}{2}(l-1) + \frac{g-1}{2} \cdot \frac{4l + g - 7}{2} + 1,
\end{aligned}$$

$$\begin{aligned}
\Phi_B &= 2\sum_{j=1}^{\frac{l+k}{2}} j - \frac{l+k}{2} + 2\sum_{j=1}^{\frac{l+g-k-1}{2}} j - \left(\sum_{j=1}^{l-1} j + 1\right) \\
&= \frac{l+k}{2}\left(2 + \frac{l+k}{2} - 1\right) - \frac{l+k}{2} \\
&+ \frac{l+g-k-1}{2}\left(2 + \frac{l+g-k-1}{2} - 1\right) - \frac{l-1}{2}(2 + l - 1 - 1) - 1 \\
&= \left(\frac{l+k}{2}\right)^2 + \frac{l+g-k-1}{2} \cdot \frac{l+g-k+1}{2} - \left(\frac{l-1}{2}\right) l - 1
\end{aligned}$$

and

$$\Phi_D - \Phi_B = \frac{gk + gl - 4g - k^2 + l^2 - 6l + 10}{2}.$$

Let $f(g,k,l) = \Phi_D - \Phi_B$, then

$$\begin{aligned}
\frac{\partial f(g,k,l)}{\partial k} &= \frac{g - 2k}{2} > 0 \quad \textit{for } k < \frac{g}{2} \textit{ and} \\
\frac{\partial f(g,k,l)}{\partial l} &= \frac{g + 2l - 6}{2} > 0 \quad \textit{since } l \geq 3.
\end{aligned}$$

The above partial derivatives suggest that we check for smallest possible values of l and k. The smallest possible values are $l = k = 3$. Since $l \geq 3$ then $g \geq 7$ and $f(g, 3, 3) = g - 4 > 0$, hence we conclude that $\Phi_D - \Phi_B > 0$.

(ii) If k is even, l is even, and g is even, then

$$\begin{aligned}
\Phi_D &= 1 + \sum_{j=1}^{l-2} j + 2\sum_{j=1}^{\frac{g}{2}} (j + l - 2) - \left(\frac{g}{2} + l - 2\right) \\
&= 1 + \frac{l-2}{2}\,(2 + l - 2 - 1) + \frac{g}{2}\left(2(l-1) + \frac{g}{2} - 1\right) - \frac{g}{2} - l + 2 \\
&= \frac{l-2}{2}\,(l-1) + \frac{g}{2}\left(\frac{4l + g - 8}{2}\right) - l + 3,
\end{aligned}$$

$$\begin{aligned}
\Phi_B &= 2\sum_{j=1}^{\frac{k+l}{2}} j - \frac{k+l}{2} + 2\sum_{j=1}^{\frac{l+g-k}{2}} j - \frac{l+g-k}{2} - \left(\sum_{j=1}^{l-1} j + 1\right) \\
&= \left(\frac{l+k}{2}\right)^2 + \left(\frac{l+g-k}{2}\right)^2 - \left(\frac{l-1}{2}\right) l - 1
\end{aligned}$$

and

$$\Phi_D - \Phi_B = \frac{gk + gl - 4g - k^2 + l^2 - 6l + 10}{2}.$$

Then

$$\begin{aligned}
\frac{\partial f(g,k,l)}{\partial k} &= \frac{g - 2k}{2} > 0 \quad \textit{for } k < \frac{g}{2} \textit{ and} \\
\frac{\partial f(g,k,l)}{\partial l} &= \frac{g + 2l - 6}{2} > 0 \quad \textit{since } l \geq 4.
\end{aligned}$$

Reasoning as in (i), with the smallest possible values of l and k being $l = k = 4$. Since $l \geq 4$ then $g \geq 8$ and $f(g, 4, 4) = 2g - 7 > 0$, hence we conclude that $\Phi_D - \Phi_B > 0$.

(iii) If k is even, l is even and g is odd, then

$$\begin{aligned}
\Phi_D &= 1 + \sum_{j=1}^{l-2} j + 2\sum_{j=1}^{\frac{g-1}{2}} (j + l - 2) \\
&= \frac{l-2}{2}\,(l-1) + \frac{g-1}{2}\left(\frac{4l + g - 7}{2}\right) + 1,
\end{aligned}$$

$$\begin{aligned}\Phi_B &= 2\sum_{j=1}^{\frac{k+l}{2}} j - \frac{k+l}{2} + 2\sum_{j=1}^{\frac{l+g-k-1}{2}} j - \left(\sum_{j=1}^{l-1} j + 1\right)\\ &= \left(\frac{k+l}{2}\right)^2 + \frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2} - \left(\frac{l-1}{2}\right) l - 1\end{aligned}$$

and

$$\Phi_D - \Phi_B = \frac{gk + gl - 4g - k^2 + l^2 - 6l + 10}{2}.$$

Then

$$\begin{aligned}\frac{\partial f(g,k,l)}{\partial k} &= \frac{g-2k}{2} > 0 \quad \textit{for } k < \frac{g}{2} \textit{ and}\\ \frac{\partial f(g,k,l)}{\partial l} &= \frac{g+2l-6}{2} > 0 \quad \textit{since } l \geq 4.\end{aligned}$$

Reasoning as in (i), with the smallest possible values of k and l being $l = k = 4$. Since $l \geq 4$ then $g \geq 9$ and $f(g,4,4) = 2g - 7 > 0$, hence we conclude that $\Phi_D - \Phi_B > 0$.

(iv) If k is even, l is odd, and g is even, then

$$\Phi_D = \frac{l-2}{2}(l-1) + \frac{g}{2}\left(\frac{4l+g-8}{2}\right) - l + 3,$$

$$\begin{aligned}&\Phi_B\\ &= 2\sum_{j=1}^{\frac{k+l-1}{2}} j + 2\sum_{j=1}^{\frac{l+g-k-1}{2}} j - \left(\sum_{j=1}^{l-1} j + 1\right)\\ &= \frac{k+l-1}{2}\left(2 + \frac{k+l-1}{2} - 1\right) + \frac{l+g-k-1}{2}\left(2 + \frac{l+g-k-1}{2} - 1\right)\\ &- \left(\frac{l-1}{2}(2 + l - 1 - 1) + 1\right)\\ &= \frac{k+l-1}{2}\cdot\frac{k+l+1}{2} + \frac{l+g-k-1}{2}\cdot\frac{l+g-k+1}{2} - \left(\frac{l-1}{2}\right) l - 1\end{aligned}$$

and

$$\Phi_D - \Phi_B = \frac{gk + gl - 4g - k^2 + l^2 - 6l + 11}{2}.$$

Then

$$\frac{\partial f(g,k,l)}{\partial k} = \frac{g-2k}{2} > 0 \quad \textit{for } k < \frac{g}{2} \textit{ and}$$
$$\frac{\partial f(g,k,l)}{\partial l} = \frac{g+2l-6}{2} > 0 \quad \textit{since } l \geq 3.$$

Reasoning as in (i), with the smallest possible values of k and l being $k = 4$ and $l = 3$. Since $l \geq 3$ then $g \geq 8$ and $f(g,4,3) = \frac{3g-14}{2} > 0$, hence we conclude that $\Phi_D - \Phi_B > 0$.

(v) If k is even, l is odd, and g is odd, then

$$\Phi_D = \frac{l-2}{2}(l-1) + \frac{g-1}{2}\left(\frac{4l+g-7}{2}\right) + 1,$$
$$\Phi_B = \frac{k+l-1}{2} \cdot \frac{k+l+1}{2} + \left(\frac{l+g-k}{2}\right)^2 - \left(\frac{l-1}{2}\right)l - 1$$

and

$$\Phi_D - \Phi_B = \frac{gk + gl - 4g - k^2 + l^2 - 6l + 10}{2}.$$

Then

$$\frac{\partial f(g,k,l)}{\partial k} = \frac{g-2k}{2} > 0 \quad \textit{for } k < \frac{g}{2} \textit{ and}$$
$$\frac{\partial f(g,k,l)}{\partial l} = \frac{g+2l-6}{2} > 0 \quad \textit{since } l \geq 3.$$

Reasoning as in (i), with the smallest possible values of k and l being $k = 4$ and $l = 3$. Since $l \geq 3$ then $g \geq 7$ and $f(g,4,3) = \frac{3g-15}{2} > 0$, hence we conclude that $\Phi_D - \Phi_B > 0$.

(vi) If k is odd, l is even, and g is odd, then

$$\Phi_D = \frac{l-2}{2}(l-1) + \frac{g-1}{2}\left(\frac{4l+g-7}{2}\right) + 1,$$
$$\Phi_B = \frac{k+l-1}{2} \cdot \frac{k+l+1}{2} + \left(\frac{l+g-k}{2}\right)^2 - \left(\frac{l-1}{2}\right)l - 1$$

and

$$\Phi_D - \Phi_B = \frac{gk + gl - 4g - k^2 + l^2 - 6l + 10}{2}.$$

Then

$$\frac{\partial f(g,k,l)}{\partial k} = \frac{g-2k}{2} > 0 \quad \textit{for } k < \frac{g}{2} \textit{ and}$$

$$\frac{\partial f(g,k,l)}{\partial l} = \frac{g+2l-6}{2} > 0 \quad \textit{since } l \geq 4.$$

Reasoning as in (i), with the smallest possible values of k and l being $k = 5$ and $l = 4$. Since $l \geq 4$ then $g \geq 9$ and $f(g,5,4) = \frac{5g-23}{2} > 0$, hence we conclude that $\Phi_D - \Phi_B > 0$.

(vii) If k is odd, l is even, and g is even, then

$$\Phi_D = \frac{l-2}{2}(l-1) + \frac{g}{2}\left(\frac{4l+g-8}{2}\right) - l + 3,$$
$$\Phi_B = \frac{k+l-1}{2} \cdot \frac{k+l+1}{2} + \frac{l+g-k-1}{2} \cdot \frac{l+g-k+1}{2} - \left(\frac{l-1}{2}\right) l - 1$$

and

$$\Phi_D - \Phi_B = \frac{gk+gl-4g-k^2+l^2-6l+11}{2}.$$

Then

$$\frac{\partial f(g,k,l)}{\partial k} = \frac{g-2k}{2} > 0 \textit{ for } k < \frac{g}{2} \textit{ and}$$
$$\frac{\partial f(g,k,l)}{\partial l} = \frac{g+2l-6}{2} > 0, \textit{ since } l \geq 4.$$

Reasoning as in (i), with the smallest possible values of k and l being $k = 5$ and $l = 4$. Since $l \geq 4$ then $g \geq 10$ and $f(g,5,4) = \frac{5g-22}{2} > 0$, hence we conclude that $\Phi_D - \Phi_B > 0$.

(viii) If k is odd, l is odd, and g is even, then

$$\Phi_D = \frac{l-2}{2}(l-1) + \frac{g}{2}\left(\frac{4l+g-8}{2}\right) - l + 3,$$
$$\Phi_B = \left(\frac{k+l}{2}\right)^2 + \left(\frac{l+g-k}{2}\right)^2 - \left(\frac{l-1}{2}\right) l - 1$$

and

$$\Phi_D - \Phi_B = \frac{gk+gl-4g-k^2+l^2-6l+10}{2}.$$

Then

$$\frac{\partial f(g,k,l)}{\partial k} = \frac{g-2k}{2} > 0 \textit{ if } k < \frac{g}{2} \textit{ and}$$

$$\frac{\partial f(g,k,l)}{\partial l} = \frac{g+2l-6}{2} > 0 \text{ since } l \geq 3.$$

Reasoning as in (i), with the smallest possibe values of k and l being $k = l = 3$. Since $l \geq 3$ then $g \geq 6$ and $f(g,3,3) = g - 4 > 0$, hence we can conclude that $\Phi_D - \Phi_B > 0$. Since $\Phi_D - \Phi_B > 0$ in all the cases above then $W(D_{n,g,l-2,3}) > W(B_{n,g,k,l})$. □

Lemma 3.26 *Let g, j, k, l, n and $n^{'}$ be integers such that $n^{'} = g+l-1$, $n = n^{'} + j - 1$, $k \geq l \geq 2$ and $j \geq 2$. Let $w^{'}$ be one end of the path P_j. Then*

$$W(D_{n,g,j+l-3,3}) \geq W((B_{n^{'},g,k,l})_{ww^{'}}P_j), \quad \textit{for all } w \in V(B_{n^{'},g,k,l}).$$

Proof. Let $B = (B_{n^{'},g,k,l})_{ww^{'}}P_j$, L, K and R be segments in $B_{n^{'},g,k,l}$ of length l, k and $g-k$, respectively. Then by Lemma 3.10 in conjuction with the proof of Lemma 3.8, if B is maximal then w is not in L. Suppose w is in L. Since $g-k \geq l$ then by the proof of Lemma 3.8, there exists vertex x in R such that $f_{B_{n^{'},g,k,l}}(w) \leq f_{B_{n^{'},g,k,l}}(x)$. Then by Lemma 3.10 $W(B) \leq W((B_{n^{'},g,k,l})_{x,w^{'}}P_j)$. Hence we conclude that w is not in L for B to be maximal. Let $u, u^{'} \in V(B)$ such that $\deg(u) = 1$ and $u^{'}$ is the neighbor of u. Furthermore, let $v_1, v_2, v_3, v_4, v_5 \in V(L)$ such that $\deg(v_4) = \deg(v_5) = 3$, v_2 and v_3 are the neighbors of v_1, $d_B(v_1, v_4) \leq d_B(v_4, w)$ and $d_B(v_1, v_5) \leq d_B(v_5, w)$, as in Figure 3.4. Note that if L is too short, $\{v_2, v_3\} \cap \{v_4, v_5\}$ may be not empty.

Now let us define a graph transformation from B to $B^{'}$ as follows: Remove v_1 from v_2 and v_3 in B and then attach it to u and $u^{'}$, see Figure 3.4.

It is clear from the transformation that all pairs of vertices in $B - v_1$ either stay in the same distance or move further apart from each other, hence their contribution to the Wiener index either stays unchanged or increases. If there is a decrease in the Wiener index from B to $B^{'}$, it is in the contribution of v_1.

Let P be the shortest path in B from v_1 to $u^{'}$. Without the loss of generality, let us assume that it passes through v_3 and v_5. Let $P^{'}$ be the shortest path in $B^{'}$ from v_3 to v_1. Then the paths P and $P^{'}$ have the same length, hence

$$\sum_{z,z^{'} \in V(P)} d_B(z, z^{'}) = \sum_{z,z^{'} \in V(P^{'})} d_{B^{'}}(z, z^{'}).$$

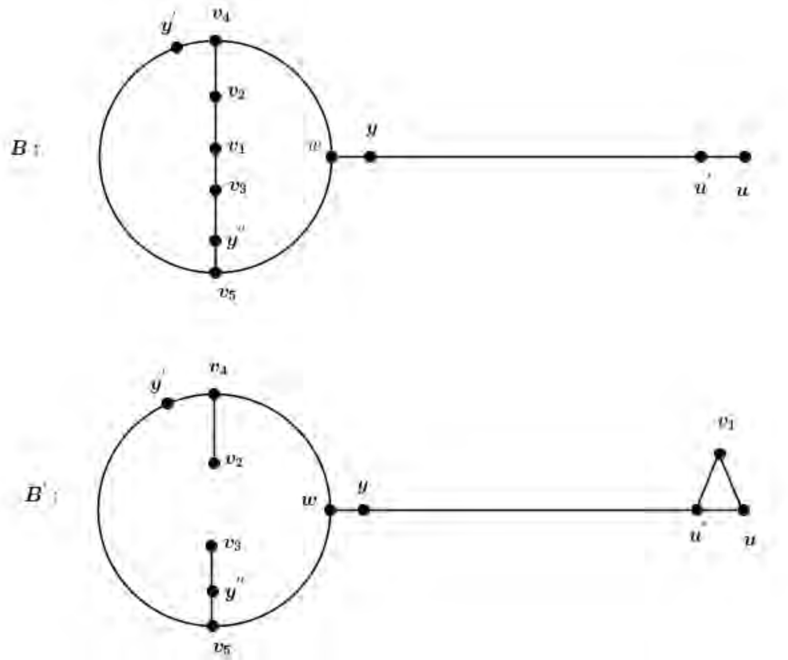

Figure 3.4: Graph transformation from $B = (B_{n',g,k,l})_{ww}P_j$ to B'

Define H to be one of K and R that do not have a vertex from P_j. Since $d_B(v_1, v_4) \leq d_B(v_4, w)$, $d_B(v_1, v_5) \leq d_B(v_5, w)$ and $d_{B'}(w, v_1) \geq 1$, then $d_B(v_1, v) \leq d_{B'}(v_1, v)$ for all $v \in V(H)$. Let P'' be the path from v_2 to w in B that passes through v_4 but not v_5 and P^* be the same path P'' but in B'. Since $d_{B'}(v_1, w) \geq 1$, $d_B(v_4, v_5) \leq d_{B'}(v_4, v_5)$ and all the vertices in L and R form a cycle then $f_B(P'' - w, v_1) = f_{P''}(w)$. Let $y \in V(P_j)$ such that y is the neighbor of w', then

$$f_B(P'' - w - v_2, v_1) \leq f_B(P'' - w - v_2, y) \leq f_{B'}(P^* - w - v_2, v_1).$$

Hence $f_B(B - u - v_2, v_1) \leq f_{B'}(B' - u - v_2, v_1)$. Let $y' \in V(H)$ such that y' is the neighbor of v_4. Since $d_B(v_1, v_4) \leq d_B(v_4, w)$, $d_B(v_1, v_5) \leq d_B(v_5, w)$ and $d_{B'}(v_1, w) \geq 1$ then

$$d_B(u, v_1) = d_{B'}(v_2, v_1) + 1 \leq d_{B'}(v_2, v_1) + d_{B'}(v_1, y') - d_B(v_1, y').$$

Hence we conclude that $f_B(v_1) \leq f_{B'}(v_1)$ and $W(B) \leq W(B')$. If $l = 2$ then we are done since $D_{n,g,j-1,3} = B'$. Suppose that $l \geq 3$. Then we define a two step transformation from B' to B'' and from B'' to $D_{n,g,j+l-3,3}$ as follows: Let y'' be the neighbor of v_5 in L. Let B'' be formed from B' by removing the edge $y''v_5$ and adding the edge $y''v_2$. Then $D_{n,g,j+l-3,3}$ is formed from B'' by removing the edge yw' and adding the edge yv_3. Then by Lemmas 3.18 and 3.21 we have

$$W(B') \leq W(B'') \leq W(D_{n,g,j+l-3,3})$$

hence $W(D_{n,g,j+l-3,3}) \geq W(B = (B_{n',g,k,l})_{ww'}P_j)$. $\square$

Lemmas 3.24, 3.25 and 3.26 gives the following theorem. Note that since $l = 1$, then $n^{'} = g$.

Theorem 3.27 *There are only two candidates for the maximum Wiener index with circumference g and they are $D_{n,g,n-g-1,3}$ and $(B_{g,g,k,1})_{ww'}P_{n-g+1}$, where $w^{'}$ is one end of the path P_{n-g+1}.*

3.2 Fixed Size of the Core

Definition 3.28 Let G be a connected graph, we call a core of G the maximal subgraph of G that has no vertex of degree less than 2.

In the previous section, graph transformations were carefully made with the circumference kept fixed. In this section, we make sure that graph transformations keep the size of the core fixed. In other words whatever the graph transformation is doing in a particular graph, the number of vertices and edges in the core must remain the same. In the rest of this thesis whenever we say the size of the core is m, we mean that the number of edges of the core is equal to m.

As much as the preceding section was about keeping the circumference fixed, there are some lemmas and theorems that can still be used in this section e.g Lemmas 3.18 and 3.25 since the graph transformations used in those lemmas kept the core fixed too. Also from Lemma 3.18 we concluded that the maximal bicyclic graph with fixed circumference is either $(D_{n,g,q,h})_{ww'}(P_i)$ or $(B_{n',g,k,l})_{zz'}(P_j)$ with n not neccessarily equal to $n^{'}$ and i not neccessarily equal to j, but here the case is different, the graphs being compared should have the same size of the core.

Before we start with lemmas and theorems of this section, we highlight that the maximal bicyclic graph with n vertices and m size of the core is either $(D_{m-1,g',q,h})_{ww'}(P_{n-m+2})$ or $(B_{m-1,g,k,l})_{zw'}(P_{n-m+2})$, where $w^{'}$ is an end of a path P_{n-m+2}. This follows from Lemma 3.18.

Lemma 3.29 *Let each of F, H and J be a connected graph with $u \in V(F)$, $v \in V(H)$ and $w \in V(J)$. If $W(H) \geq W(J)$, $f_H(v) \geq f_J(w)$ and $n_H \geq n_J$ then $W(F_{uv}H) \geq W(F_{uw}J)$.*

Proof.

$$\begin{aligned} W(F_{uv}H) &= W(F) + W(H) + n_F f_H(v) + n_H f_F(u) \\ &\geq W(F) + W(J) + n_F f_J(w) + n_J f_F(u) = W(F_{uw}J). \end{aligned}$$

□

Lemma 3.30 *Let $C = C_n$ and $H = (C_3)_{ww'} P_{n-2}$, where n is a natural number greater than or equal to 3, $w \in V(C_3)$ and w' is an end of P_{n-2}. Let $u \in V(C)$ and $v \in V(H)$.*

(i) If $\deg(v) = 1$ then $f_C(u) \leq f_H(v)$.

(ii) If v is not in P_{n-2} then $f_C(u) \leq f_H(v)$.

Proof.

(i)

$$f_C(u) = \begin{cases} 2\sum_{r=1}^{\frac{n-1}{2}} r & \text{if } n \text{ is odd} \\ 2\sum_{r=1}^{\frac{n}{2}} r - \dfrac{n}{2} & \text{if } n \text{ is even} \end{cases} = \begin{cases} \frac{n-1}{2} \cdot \frac{n+1}{2} & \text{if } n \text{ is odd} \\ \left(\frac{n}{2}\right)^2 & \text{if } n \text{ is even.} \end{cases}$$

$$f_H(v) = \sum_{r=1}^{n-3} r + 2(n-2) = \frac{n+1}{2}(n-2).$$

Then

$$f_H(v) - f_C(u) = \begin{cases} \frac{(n-3)(n+1)}{4} & \text{if } n \text{ is odd} \\ \frac{n^2-2n-4}{4} & \text{if } n \text{ is even.} \end{cases}$$

Since $n \geq 3$ then $f_H(v) - f_C(u) \geq 0$ and hence $f_H(v) \geq f_C(u)$.

(ii) $f_H(v) = 1 + \sum_{r=1}^{n-2} r = 1 + \dfrac{(n-2)(n-1)}{2}$, and

$$f_H(v) - f_C(u) = \begin{cases} \frac{(n-3)^2}{4}, & \text{if } n \text{ is odd} \\ \frac{(n-4)(n-2)}{4}, & \text{if } n \text{ is even.} \end{cases}$$

Since $n \geq 3$, if n is even then $n \geq 4$. Then $f_H(v) - f_C(u) \geq 0$. Hence $f_H(v) \geq f_C(u)$.

□

The following lemma is about graphs with no pendent tree.

Lemma 3.31 *Let g be the circumference of a graph $B_{n,g,k,l}$. If $k \geq 3$ and $n = g + l - 1$ then $W(D_{n,l+g-k,k-2,3}) \geq W(B_{n,g,k,l})$.*

Proof. Let $B = B_{n,g,k,l}$, L, K and R be segments in B of length l, k and $g-k$, respectively. Let $x, y \in V(B)$ such that $x \neq y$ and $\deg(x) = \deg(y) = 3$. Furthermore, let $u, v, z \in V(K)$ such that u is the neighbor of y, v is the neighbor of u that is not y and z is the neighbor of v that is not u.

Now let us define a graph transformation from B to B' as follows: Remove the edge uy in B and then add the edge uz. Then $B' = D_{n,l+g-k,k-2,3}$. It should be noted that

$$\sum_{w,w' \in V(B-u)} d_B(w,w') \leq \sum_{w,w' \in V(B'-u)} d_{B'}(w,w'),$$

since all pairs of vertices in $B-u$ moved further apart from each other or stay at the same distance, when we move from B to B'. Now, we will compare the contributions of u in $W(B)$ and $W(B')$. To proceed let

$$\Phi_B(k) = \sum_{w \in V(B)} d(u,w) \quad \text{and} \quad \Phi_{B'}(k) = \sum_{w \in V(B')} d(u,w).$$

If $\Phi_{B'}(k) - \Phi_B(k) \geq 0$ then the lemma is true.

(i) If k is odd, l is odd and g is odd, then

$$\begin{aligned}
\Phi_{B'}(k) &= 1 + \sum_{j=1}^{k-2} j + 2\sum_{j=1}^{\frac{l+g-k-1}{2}} (j+k-2) \\
&= \frac{k-2}{2}(k-1) + \frac{l+g-k-1}{2} \cdot \frac{l+g+3k-7}{2} + 1,
\end{aligned}$$

$$\begin{aligned}
\Phi_B(k) &= 2\sum_{j=1}^{\frac{k+l}{2}} j - \frac{k+l}{2} + 2\sum_{j=1}^{\frac{l+g-k-1}{2}} (j+1) - \sum_{j=1}^{l}(j+1) \\
&= \left(\frac{k+l}{2}\right)^2 + \frac{l+g-k-1}{2} \cdot \frac{l+g-k+5}{2} - \frac{l}{2}(l+3)
\end{aligned}$$

and

$$\Phi_{B'}(k) - \Phi_B(k) = \frac{4gk - 12g - 3k^2 + 2kl + 2k + l^2 - 6l + 20}{4}.$$

Let $f(g,k,l) = \Phi_{B'}(k) - \Phi_B(k)$. To show that $f(g,k,l) \geq 0$, we notice that $g \geq k+2$ and

$$\begin{aligned} f(g,k,l) &= \frac{(4k-12)g-(3k-8)(k+2)+(l-3)^2+2kl-5}{4} \\ &= \frac{(k-4)g+(3k-8)g-(3k-8)(k+2)+(l-3)^2+2kl-5}{4} \geq 0. \end{aligned}$$

Note that for the case where $k = 3$ we have $f(7,3,3) = 2$ and $f(7,3,1) = 0$, since $k = 3 \implies l \leq 3$ and $g \geq 7$.

(ii) If k is odd, l is even and g is even, then

$$\Phi_{B'}(k) = \frac{k-2}{2}(k-1) + \frac{l+g-k-1}{2} \cdot \frac{l+g+3k-7}{2} + 1.$$

Let us first look at the case of $k = l+1$:

$$\begin{aligned} \Phi_B(l+1) &= 2\sum_{j=1}^{\frac{k+l-1}{2}} j + 2\sum_{j=1}^{\frac{g}{2}} j - \frac{g}{2} - \left(1 + \sum_{j=1}^{l} j\right) \\ &= \frac{k+l-1}{2} \cdot \frac{k+l+1}{2} + \left(\frac{g}{2}\right)^2 - \frac{l}{2}(l+1) - 1 \\ &= \frac{l(2l+2)}{2} + \frac{g^2}{4} - \frac{l(l+1)}{2} - 1 \end{aligned}$$

and

$$\begin{aligned} f(g,l+1,l) &= \frac{2gl-3g-6l+8}{2} = \frac{g(2l-3)-6l+8}{2} \\ &> 0 \quad \textit{since } l \geq 2 \textit{ and } g \geq 5. \end{aligned}$$

Now, we consider the case where $k > l+1$

$$\begin{aligned} \Phi_B(k) &= 2\sum_{j=1}^{\frac{k+l-1}{2}} j + 2\sum_{j=1}^{\frac{l+g-k-1}{2}} (j+1) - \sum_{j=1}^{l}(j+1) \\ &= \frac{k+l-1}{2} \cdot \frac{k+l+1}{2} + \frac{l+g-k-1}{2} \cdot \frac{l+g-k+5}{2} - \frac{l}{2}(l+3) \end{aligned}$$

and

$$\begin{aligned} f(g,k,l) &= \frac{4gk-12g-3k^2+2kl+2k+l^2-6l+21}{4} \\ &= \frac{(4k-12)g-(3k-8)(k+2)+(l-3)^2+2kl-4}{4} \\ &= \frac{(k-4)g+(3k-8)g-(3k-8)(k+2)+(l-3)^2+2kl-4}{4} \end{aligned}$$

$$> 0 \quad \textit{since } l \geq 2 \implies k \geq 5.$$

(iii) If k is even, l is odd and g is even, then

$$\Phi_{B'}(k) = \frac{k-2}{2}(k-1) + \frac{l+g-k-1}{2} \cdot \frac{l+g+3k-7}{2} + 1,$$

$$\begin{aligned}
\Phi_B(l+1) &= 2\sum_{j=1}^{\frac{k+l-1}{2}} j + 2\sum_{j=1}^{\frac{g}{2}} j - \frac{g}{2} - \left(1 + \sum_{j=1}^{l} j\right) \\
&= \frac{k+l-1}{2} \cdot \frac{k+l+1}{2} + \left(\frac{g}{2}\right)^2 - \frac{l}{2}(l+1) - 1 \\
&= \frac{l(2l+2)}{2} + \frac{g^2}{4} - \frac{l(l+1)}{2} - 1
\end{aligned}$$

and

$$\begin{aligned}
f(g, l+1, l) &= \frac{2gl - 3g - 6l + 8}{2} = \frac{g(2l-3) - 6l + 8}{2} \\
&> 0 \quad \textit{since } l \geq 3 \textit{ and } g \geq 8.
\end{aligned}$$

We need to take a note that, in this case we can't have $l = 1$ since $k = l + 1$ needs to be greater or equal to 3, so we only consider the case where $l \geq 3$.

For $k > l + 1$ we have

$$\begin{aligned}
\Phi_B(k) &= 2\sum_{j=1}^{\frac{k+l-1}{2}} j + 2\sum_{j=1}^{\frac{l+g-k-1}{2}} (j+1) - \sum_{j=1}^{l} (j+1) \\
&= \frac{k+l-1}{2} \cdot \frac{k+l+1}{2} + \frac{l+g-k-1}{2} \cdot \frac{l+g-k+5}{2} - \frac{l}{2}(l+3)
\end{aligned}$$

and

$$\begin{aligned}
f(g,k,l) &= \frac{(k-4)g + (3k-8)g - (3k-8)(k+2) + (l-3)^2 + 2kl - 4}{4} \\
&> 0 \quad \textit{since } k \geq 4 \textit{ (} k \geq 3 \textit{ but } k \textit{ is even)}
\end{aligned}$$

(iv) If k is even, l is even and g is odd, then

$$\Phi_{B'}(k) = \frac{k-2}{2}(k-1) + \frac{l+g-k-1}{2} \cdot \frac{l+g+3k-7}{2} + 1,$$

$$
\begin{aligned}
\Phi_B(k) &= 2\sum_{j=1}^{\frac{k+l}{2}} j - \frac{k+l}{2} + 2\sum_{j=1}^{\frac{l+g-k-1}{2}} (j+1) - \sum_{j=1}^{l}(j+1) \\
&= \left(\frac{k+l}{2}\right)^2 + \frac{l+g-k-1}{2}\cdot\frac{l+g-k+5}{2} - \frac{l}{2}(l+3)
\end{aligned}
$$

and

$$
\begin{aligned}
f(g,k,l) &= \frac{4gk-12g-3k^2+2kl+2k+l^2-6l+20}{4} \\
&= \frac{(k-4)g+(3k-8)g-(3k-8)(k+2)+(l-3)^2+2kl-5}{4} \\
&> 0 \quad \textbf{\textit{since }} k \geq 4 \textbf{\textit{ (}} k \textbf{\textit{ is even and }} k \geq 3\textbf{\textit{).}}
\end{aligned}
$$

(v) If k is odd, l is odd and g is even, then

$$
\begin{aligned}
\Phi_{B'}(k) &= 1 + \sum_{j=1}^{k-2} j + 2\sum_{j=1}^{\frac{l+g-k}{2}} (j+k-2) - \left(\frac{l+g-k}{2} + k - 2\right) \\
&= 1 + \frac{k-2}{2}(2+k-2-1) + \frac{l+g-k}{2}\left(2(k-1) + \frac{l+g-k}{2} - 1\right) \\
&\quad - \left(\frac{l+g-k}{2} + k - 2\right) \\
&= \frac{k-2}{2}(k-3) + \frac{l+g-k}{2}\cdot\frac{l+g+3k-8}{2} + 1,
\end{aligned}
$$

$$
\begin{aligned}
\Phi_B(k) &= 2\sum_{j=1}^{\frac{k+l}{2}} j - \frac{k+l}{2} + 2\sum_{j=1}^{\frac{l+g-k}{2}} (j+1) - \left(\frac{l+g-k}{2} + 1\right) - \sum_{j=1}^{l}(j+1) \\
&= \frac{k+l}{2}\left(2 + \frac{k+l}{2} - 1\right) - \frac{k+l}{2} + \frac{l+g-k}{2}\left(2(2) + \frac{l+g-k}{2} - 1\right) \\
&\quad - \left(\frac{l+g-k}{2}\right) - 1 - \frac{l}{2}(2(2)+l-1) \\
&= \left(\frac{k+l}{2}\right)^2 + \frac{l+g-k}{2}\cdot\frac{l+g-k+4}{2} - \frac{l}{2}(l+3) - 1
\end{aligned}
$$

and

$$
\begin{aligned}
f(g,k,l) &= \frac{4gk-12g-3k^2+2kl+2k+l^2-6l+20}{4} \\
&= \frac{(k-4)g+(3k-8)g-(3k-8)(k+2)+(l-3)^2+2kl-5}{4}
\end{aligned}
$$

$$\begin{cases} > 0 & \textit{for } k > 4 \\ = 2 & \text{for } k = 3 \text{ and } l = 3 \\ = 0 & \textit{for } k = 3 \textit{ and } l = 1. \end{cases}$$

(vi) If k is even, l is even and g is even, then

$$\Phi_{B'}(k) = \frac{k-2}{2}(k-3) + \frac{l+g-k}{2} \cdot \frac{l+g+3k-8}{2} + 1,$$

$$\begin{aligned} \Phi_B(k) &= 2\sum_{j=1}^{\frac{k+l}{2}} j - \frac{k+l}{2} + 2\sum_{j=1}^{\frac{l+g-k}{2}} (j+1) - \left(\frac{l+g-k}{2} + 1\right) - \sum_{j=1}^{l} (j+1) \\ &= \left(\frac{k+l}{2}\right)^2 + \frac{l+g-k}{2} \cdot \frac{l+g-k+4}{2} - \frac{l}{2}(l+3) - 1 \end{aligned}$$

and

$$\begin{aligned} f(g,k,l) &= \frac{(k-4)g + (3k-8)g - (3k-8)(k+2) + (l-3)^2 + 2kl - 5}{4} \\ &> 0 \quad \textit{since } k \geq 4 \textit{ (} k \textit{ is even and } k \geq 3\textit{).} \end{aligned}$$

(vii) If k is odd, l is even and g is odd, then

$$\Phi_{B'}(k) = \frac{k-2}{2}(k-3) + \frac{l+g-k}{2} \cdot \frac{l+g+3k-8}{2} + 1,$$

$$\begin{aligned} \Phi_B(l+1) &= 2\sum_{j=1}^{\frac{k+l-1}{2}} j + 2\sum_{j=1}^{\frac{g-1}{2}} j - \left(1 + \sum_{j=1}^{l} j\right) \\ &= \frac{k+l-1}{2} \cdot \frac{k+l+1}{2} + \frac{g-1}{2} \cdot \frac{g+1}{2} - \frac{l}{2}(l+1) - 1 \\ &= \frac{l(2l+2)}{2} + \frac{g-1}{2} \cdot \frac{g+1}{2} - \frac{l}{2}(l+1) - 1 \end{aligned}$$

and

$$f(g, l+1, l) = \frac{(g-3)(2l-3)}{2} > 0 \quad \textit{since } l \geq 2 \textit{ (} l \textit{ is even).}$$

For $k > l+1$ we have

$$\Phi_B(k) = 2\sum_{j=1}^{\frac{k+l-1}{2}} j + 2\sum_{j=1}^{\frac{l+g-k}{2}} (j+1) - \left(\frac{l+g-k}{2} + 1\right) - \sum_{j=1}^{l} (j+1)$$

$$
\begin{aligned}
&= \frac{k+l-1}{2}\cdot\frac{k+l+1}{2} + \frac{l+g-k}{2}\cdot\frac{l+g-k+4}{2}\\
&- \frac{l}{2}(l+3) - 1
\end{aligned}
$$

and

$$
\begin{aligned}
f(g,k,l) &= \frac{4gk-12g-3k^2+2kl+2k+l^2-6l+21}{4}\\
&= \frac{(k-4)g+(3k-8)g-(3k-8)(k+2)+(l-3)^2+2kl-4}{4}\\
&> 0 \quad \textit{since } k \geq 5 \textit{ (} k \textit{ is odd, } l \textit{ is even and } k > l+1 \geq 3\textit{).}
\end{aligned}
$$

(viii) If k is even, l is odd and g is odd, then

$$
\Phi_{B'}(k) = \frac{k-2}{2}(k-3) + \frac{l+g-k}{2}\cdot\frac{l+g+3k-8}{2} + 1,
$$

$$
\begin{aligned}
\Phi_B(l+1) &= 2\sum_{j=1}^{\frac{k+l-1}{2}} j + 2\sum_{j=1}^{\frac{g-1}{2}} j - \left(1+\sum_{j=1}^{l} j\right)\\
&= \frac{k+l-1}{2}\cdot\frac{k+l+1}{2} + \frac{g-1}{2}\cdot\frac{g+1}{2} - \frac{l}{2}(l+1) - 1\\
&= \frac{l(2l+2)}{2} + \frac{g-1}{2}\cdot\frac{g+1}{2} - \frac{l}{2}(l+1) - 1
\end{aligned}
$$

and

$$
\begin{aligned}
f(g,l+1,l) &= \frac{(g-3)(2l-3)}{2}\\
&> 0 \quad \textit{since } l \geq 3 \textit{ (} k = l+1 \textit{ is even and } k \geq 3\textit{).}
\end{aligned}
$$

For $k > l+1$ we have

$$
\begin{aligned}
\Phi_B(k) &= 2\sum_{j=1}^{\frac{k+l-1}{2}} j + 2\sum_{j=1}^{\frac{l+g-k}{2}} (j+1) - \left(\frac{l+g-k}{2}+1\right) - \sum_{j=1}^{l}(j+1)\\
&= \frac{k+l-1}{2}\cdot\frac{k+l+1}{2} + \frac{l+g-k}{2}\cdot\frac{l+g-k+4}{2}\\
&- \frac{l}{2}(l+3) - 1
\end{aligned}
$$

and

$$
f(g,k,l) = \frac{4gk-12g-3k^2+2kl+2k+l^2-6l+21}{4}
$$

$$= \frac{(k-4)g + (3k-8)g - (3k-8)(k+2) + (l-3)^2 + 2kl - 4}{4}$$
$$> 0 \quad \textit{since } k \geq 4 \textit{ (} k \geq 3 \textit{ and } k \textit{ is even).}$$

All the cases show that $f(g,k,l) = \Phi_{B'}(k) - \Phi_B(k) \geq 0$, hence we conclude that

$$W(D_{n,l+g-k,q=k-2,3}) \geq W(B_{n,g,k,l}).$$

$\square$

Remark 3.32 We follow the proof of Lemma 3.31 to show that $W(B_{n,g,k,l}) \leq W(D_{n,l+k,g-k-2,3})$ by choosing u, v and z to be in R not in K.

Lemma 3.33 *Suppose we keep all the definitions and transformations in the proof of Lemma 3.31, that is* $B = B_{n,g,k,l}$, L, K *and* R *are segments in* B *of length* l, k *and* $g-k$, *respectively.* $x, y \in V(B)$ *such that* $x \neq y$ *and* $\deg(x) = \deg(y) = 3$. $u, v, z \in V(K)$ *such that* u *is the neighbor of* y, v *is the neighbor of* u *that is not* y *and* z *is the neighbor of* v *that is not* u. $B^{'}$ *is formed from* B *as follows: Remove the edge* uy *in* B *and then add the edge* uz. *Furthermore, let* $z^{'} \in V(B)$ *such that* $f_B(z^{'}) \geq f_B(v^{'})$ *for all* $v^{'} \in V(B)$. *Then* $f_B(z^{'}), f_{B'}(z^{'}) \leq f_{B'}(u)$.

Proof. In the proof of Lemma 3.8, we showed that $z^{'}$ is not in L, so $z^{'}$ is either in K or R. Let us assume that $z^{'}$ is in K. If $z^{'} = u$ then the proof of Lemma 3.31 shows that $f_{B'}(u) \geq f_B(u)$. Let C be the cycle in $B^{'}$ made of vertices in R and L, P be the shortest path from $z^{'}$ to x in $B^{'}$ and $P^{'}$ be the path from $z^{'}$ to u that passes through v.

Suppose $z^{'} = v$ then $f_{B'}(u) = f_{B'}(z^{'})$, since $d_{B'}(u,v) = d_{B'}(u,z) = d_{B'}(v,z) = 1$. If the shortest path in B, from $z^{'}$ to a vertex $v^{'} \in V(B)$ does not pass through y then $d_B(z^{'},v^{'}) = d_{B'}(z^{'},v^{'})$. If the shortest path passes through y then $d_B(z^{'},x) + d_B(x,v^{'}) \geq d_B(z^{'},y) + d_B(y,v^{'})$. But $d_{B'}(z^{'},x) + d_{B'}(x,v^{'}) \geq d_B(z^{'},x) + d_B(x,v^{'})$, with equality only if the shortest path in B from $z^{'}$ to x does not pass through y. Hence $d_{B'}(z^{'},v^{'}) \geq d_B(z^{'},v^{'})$ and $f_{B'}(u) = f_{B'}(z^{'}) \geq f_B(z^{'})$.

Suppose $z^{'} \notin \{u,v\}$. Since the shortest path from u to all vertices $v^{'} \in V(C) \cup V(P)$ in $B^{'}$ passes through $z^{'}$ then $d_{B'}(u,v^{'}) > d_{B'}(z^{'},v^{'})$. Let $z^{''}$ be the neighbor of $z^{'}$ such that $z^{''} \in V(P)$. Since $d_{B'}(z^{'},z^{''}) = 1$, $d_{B'}(u,z^{''}) = d_{B'}(u,z^{'}) + 1$ and $d_{B'}(z^{'},u) = d_{B'}(z^{'},v)$ then $f_{B'}(P^{'} \cup z^{''},u) = f_{B'}(P^{'} \cup z^{''},z^{'}) + 1$. Hence $f_{B'}(u) > f_{B'}(z^{'})$. Since the transformation can only keep or increase distances between pairs of vertices in $B-u$ we have $f_{B'}(B^{'}-u,z^{'}) \geq f_B(B-u,z^{'})$. If the shortest path in B from $z^{'}$ to u passes through y then $d_{B'}(z^{'},u) \geq d_B(z^{'},u)$. If the shortest path does not pass through y then $d_B(z^{'},u) = d_{B'}(z^{'},u) + 1$. Then $f_{B'}(B^{'}-u,z^{'})+d_{B'}(z^{'},u)+1 \geq f_B(B-u,z^{'})+d_B(z^{'},u)$ that is $f_{B'}(z^{'})+1 \geq f_B(z^{'})$. But $f_{B'}(u) > f_{B'}(z^{'})$, hence $f_{B'}(u) \geq f_{B'}(z^{'}) + 1 \geq f_B(z^{'})$. If $z^{'}$ is in R and not in K then let u, v and z to be in R and follow the same procedure. □

Theorem 3.34 *Among all bicyclic graphs with n vertices and m size of the core, there is only one bicyclic graph that maximizes the Wiener index and that is $(D_{m-1,3,q,3})_{ww'}P_{n-m+2}$, where w is vertex in C_3 that is not in P_{n-m+2} and $w^{'}$ is an end of a path P_{n-m+2}.*

Proof. Let G be a connected graph with n vertices and core size m. If G is maximal then by Lemma 3.18 G has at most one pendent tree and that needs to be the path P_{n-m+2}, since m is the core size of G. Then $G = (B_{m-1,g,k,m-g})_{vw'}P_{n-m+2}$ or $G = (D_{m-1,i,q',h})_{v_1w'}P_{n-m+2}$, where v is a vertex in $B_{m-1,g,k,m-g}$, $w^{'}$ is an end of P_{n-m+2} and $v_1 \in V(C_h)$ with v_1 not in the path $P_{q'}$. Lemmas 2.5, 3.29 and 3.30 show that $W((D_{m-1,i,q',h})_{v_1w'}P_{n-m+2}) \leq W((D_{m-1,i,q'+h-3,3})_{v_2w'}P_{n-m+2}) \leq W((D_{m-1,3,q'+h+i-6,3})_{v_3w'}P_{n-m+2})$, where $v_2 \in V(C_3) \setminus V(P_{q'+h-3})$, $v_3 \in V(C_3) \setminus V(P_{q'+h+i-6})$.

Let $B = B_{m-1,g,k,m-g}$ and $B^{'} = D_{m-1,i,q',3}$. Lemma 3.31 shows that $W(B) \leq W(B^{'})$ with $q^{'} = k-2$ or $q^{'} = g-k-2$. But Lemma 3.33 says that there exists $u \in V(B^{'})$ such that $f_{B'}(u) \geq f_B(u^{'})$ for all $u^{'} \in V(B)$. Then by Lemma 3.29 $W(B_{u'w'}P_{n-m+2}) \leq W(B^{'}_{uw'}P_{n-m+2})$. Since $W(B_{u'w'}P_{n-m+2}) \leq W(B^{'}_{uw'}P_{n-m+2}) = W((D_{m-1,i,q',3})_{uw'}P_{n-m+2}) \leq W((D_{m-1,3,q'+i-3,3})_{uw'}P_{n-m+2})$ then $G = (D_{m-1,3,q,3})_{ww'}P_{n-m+2}$, where w is a vertex in C_3 that is not in P_{n-m+2}. □

4 Graphs with fixed Segment Sequence

Definition 4.1 A segment of a graph G is either a path whose end vertices have degree 1 or at least 3 in G and all the internal vertices have degree 2 in G, or a cycle where all the vertices have degree 2 in G except possibly one. The lengths of all the segments of G in a non-increasing order form its segment sequence.

Initially, we were hoping to study Wiener index of bicyclic graphs with fixed segment sequence. To be more precise, we wanted to find extremal bicyclic graph(s) among all bicyclic graphs given the segment sequence. We did not reach that goal, but we encounter interesting results along the way as presented in this chapter. The results presented in this chapter do not apply only to bicyclic graphs but to graphs in general.

Lemma 4.2 *Let G be a connected graph, $u^{'},v^{'}\in V(G)$ such that $d_G(u^{'},v^{'})\geq 3$. If $G^{'}$ is formed from G by merging $u^{'}$ and $v^{'}$ then*

$$W(G) > W(G^{'}).$$

Proof. Let w be the vertex obtained by merging $u^{'}$ and $v^{'}$, P_{uv} be a shortest path from u to v in G. then

$$\begin{aligned}
&W(G)\\
&=\sum_{u,v\in V(G)} d_G(u,v) = d_G(u^{'},v^{'}) + \sum_{\substack{u,v\in V(G)\\ \{u,v\}\neq\{u^{'},v^{'}\}}} d_G(u,v) > \sum_{\substack{u,v\in V(G)\\ \{u,v\}\neq\{u^{'},v^{'}\}}} d_G(u,v)\\
&=\sum_{\substack{v\in V(G)\\ v\neq v^{'}}} d_G(u^{'},v) + \sum_{\substack{v\in V(G)\\ v\neq u^{'}}} d_G(v,v^{'}) + \sum_{\substack{u,v\in V(G)\\ u,v\notin\{u^{'},v^{'}\}}} d_G(u,v)\\
&\geq \sum_{\substack{v\in V(G)\\ v\neq v^{'}}} \min\{d_G(u^{'},v), d_G(v,v^{'})\}
\end{aligned}$$

$$
\begin{aligned}
&+ \sum_{\substack{v\in V(G)\\ v\neq u'}} \min\{d(v,v'), d(v,u')\} + \sum_{\substack{u,v\in V(G)\\ u,v\notin\{u',v'\}}} d_G(u,v)\\
&= \sum_{v\in V(G')} d_{G'}(w,v) + \sum_{v\in V(G')} d_{G'}(w,v) + \sum_{\substack{u,v\in V(G)\\ u,v\notin\{u',v'\}}} d_G(u,v)\\
&> \sum_{v\in V(G')} d_{G'}(w,v) + \sum_{\substack{u,v\in V(G)\\ u,v\notin\{u',v'\}}} d_G(u,v)\\
&= \sum_{v\in V(G')} d_{G'}(w,v)\\
&+ \sum_{\substack{u,v\in V(G)\\ u,v\notin\{u',v'\}}} \min\Big(\{d_G(u,u') + d_G(u',v), d_G(u,v') + d_G(v',v)\}\cup\\
&\qquad\qquad \{l(P) : P\in P_G(u,v) \text{ and } u',v'\notin V(P)\}\Big)\\
&\geq \sum_{v\in V(G')} d_{G'}(w,v)\\
&+ \sum_{\substack{u,v\in V(G')\\ u,v\neq w}} \min\{\{d_{G'}(u,w) + d_{G'}(w,v)\}\cup\{l(P) : P\in P_{G'}(u,v) \text{ and } w\notin V(P)\}\}\\
&= \sum_{u,v\in V(G')} d_{G'}(u,v) = W(G').
\end{aligned}
$$

□

The transformation in Lemma 4.2 reduces the number of vertices. And when passing from G to G' no pair of vertices get further apart.

4.1 Graphs of Long Segments

In this section we study the set of graphs with all segments of length at least 3.

Theorem 4.3 *Let G be a connected graph whose segments are all of length at least 3. If G has minimum Wiener index among all graphs with the same segment sequence as G, then it satisfies the following:*

(i) G has no vertex of degree 1.

(ii) G has at most 1 cut vertex.

(iii) For all vertices $u\in V(G)$, if u is not a cut vertex then $\deg(u) = 2$.

Proof. Let G be the connected graph whose segments are all of length at least 3. Suppose G is minimal.

Claim (i): G has no vertex of degree 1.

Suppose there exists a vertex v in G with $\deg(v) = 1$, then there exists a vertex $v^{'}$ closest to v with $\deg(v^{'}) \neq 2$ in G. Then the path $P \in P_G(v, v^{'})$ is a segment in G and $l(P) \geq 3$. A segment of a graph G is either a path whose end vertices have degree 1 or at least 3 in G and all the internal vertices have degree 2 in G, or a cycle where all the vertices have degree 2 in G except possibly one. Applying Lemma 4.2 by merging v and $v^{'}$ we get $G^{'}$ with the same segment sequence as G and $W(G^{'}) < W(G)$, which contradicts the minimality of G. Hence G has no vertex of degree 1.

Claim (ii): G has at most 1 cut vertex.

Suppose G has more than 1 cut vertex. Then $G = H_{uu^{'}} J_{v^{'}v} F$ for some connected graphs H, J and F. By choosing J to be maximal (such that the only cut vertices of G in H and F are u and v, respectively), we can assume that $\deg(u)$, $\deg(v) \geq 3$. If $d_G(u, v) = 1$ or 2 then G has segment of length less than 3. But all the segments in G are of length at least 3. So, $d_G(u, v) \geq 3$. Now we can apply Lemma 4.2 by merging u and v to get a graph $G^{'}$ with $W(G^{'}) < W(G)$, which contradicts the minimality of G. Hence G must have at most one cut vertex.

Claim (iii): For all vertices $u \in V(G)$, if u is not a cut vertex then $\deg(u) = 2$.

Suppose G has no vertex of degree 1, has at most 1 cut vertex and at least 2 vertices of degree at least 3. Let v be a vertex in G with $\deg(v) \geq 3$. Consider the vertex $v^{'}$ closest to v in G with $\deg(v^{'}) \geq 3$. Then $d_G(v, v^{'}) \geq 3$, because all the segments in G are of length at least 3. Now apply Lemma 4.2 by merging v and $v^{'}$ to get graph $G^{'}$ with the same segment sequence as G and $W(G^{'}) < W(G)$, which contradicts the minimality of G. Hence G must have at most 1 vertex of degree at least 3. Since G has no vertex of degree 1, then G has no pendent path. Since each of the vertices of degree 2 in G are contained in a segment in G, then the cut vertex is of degree greater than 2. G has at most one cut vertex and at most one vertex of degree at least 3, hence the only vertex of degree at least 3 is a cut vertex in G and all the other vertices are of degree 2. □

Definition 4.4 Let $D = (l_1, l_2, ..., l_m)$ be a segment sequence of a graph G such that all the segments in G are of length at least 3 $(l_1, l_2, ..., l_m \geq$

3). Let C_{l_1}, C_{l_2}, …, C_{l_m} be cycles of lengths l_1, l_2, …, l_m, respectively. Define $F(D)$ as a graph obtained from cycles C_{l_1}, C_{l_2},…, C_{l_m} by choosing a vertex in each cycle and merging all these vertices to a single vertex. Then $F(D)$ has a segment sequence D.

We will need the following lemma to obtain a characterisation of minimal graphs with given number of segments.

Lemma 4.5 *Let $D = (l_1, l_2, \ldots, l_i, \ldots, l_j, \ldots, l_m)$ be a non-increasing sequence of natural numbers such that $l_k \geq 3$ for all $1 \leq k \leq m$ and $m > 1$ and $l_i - l_j \geq 2$ for some $1 \leq i < j \leq m$. Define $D' = (l_1, l_2, \ldots, l_{i-1}, l_i - 1, l_{i+1}, \ldots, l_{j-1}, l_j + 1, l_{j+1}, \ldots, l_m)$. Then*

(i) $W(F(D)) < W(F(D'))$ if l_i and l_j are odd and $l_i - l_j = 2$,

(ii) otherwise $W(F(D)) > W(F(D'))$.

Proof. Let L_i and L_j denote the sets of vertices in the segments in $F(D)$ corresponding to l_i and l_j (each of the sets L_i and L_j includes the cut vertex), respectively. Let w be the cut vertex of $F(D)$ and $H = \{w\} \cup \{v \in V(F(D)),\ \text{s.t}\ v \notin L_i \cup L_j\}$ then

$$\begin{aligned}
W(F(D)) &= \sum_{\{u,v\} \in V(F(D))} d(u,v) \\
&= \sum_{\{u,v\} \in L_i} d(u,v) + \sum_{\{u,v\} \in L_j} d(u,v) + \sum_{\{u,v\} \in H} d(u,v) \\
&+ \sum_{\substack{u \in L_i \setminus w \\ v \in L_j \setminus w}} d(u,v) + \sum_{\substack{u \in L_i \setminus w \\ v \in H \setminus w}} d(u,v) + \sum_{\substack{u \in L_j \setminus w \\ v \in H \setminus w}} d(u,v).
\end{aligned}$$

We first determine each term then combine them later.
(i) If both l_i and l_j are odd then Lemma 2.4 gives
$\sum_{\{u,v\} \in L_i} d(u,v) = \frac{l_i^3 - l_i}{8}$ and $\sum_{\{u,v\} \in L_j} d(u,v) = \frac{l_j^3 - l_j}{8}$.

$$\begin{aligned}
\sum_{\substack{u \in L_i \setminus w \\ v \in L_j \setminus w}} d(u,v) &= (l_i - 1) \sum_{v \in L_j} d(w,v) + (l_j - 1) \sum_{v \in L_i} d(w,v) \\
&= (l_i - 1) \left[2 \sum_{k=1}^{\frac{l_j - 1}{2}} k \right] + (l_j - 1) \left[2 \sum_{k=1}^{\frac{l_i - 1}{2}} k \right] \\
&= (l_i - 1) \cdot \frac{l_j - 1}{2} \left[2(1) + \frac{l_j - 1}{2} - 1 \right]
\end{aligned}$$

$$\begin{aligned}
&+ (l_j - 1) \cdot \frac{l_i - 1}{2} \left[2 + \frac{l_i - 1}{2} - 1 \right] \\
&= \frac{(l_i - 1)(l_j - 1)(l_i + l_j + 2)}{4}.
\end{aligned}$$

$$\begin{aligned}
\sum_{\substack{u \in L_i \setminus w \\ v \in H \setminus w}} d(u,v) &= (n_H - 1) \sum_{v \in L_i} d(w,v) + (l_i - 1) \sum_{v \in H} d(w,v) \\
&= (n_H - 1) \cdot \frac{l_i - 1}{2} \cdot \frac{l_i + 1}{2} + (l_i - 1) \sum_{v \in H} d(w,v)
\end{aligned}$$

and

$$\begin{aligned}
\sum_{\substack{u \in L_j \setminus w \\ v \in H \setminus w}} d(u,v) &= (n_H - 1) \sum_{v \in L_j} d(w,v) + (l_j - 1) \sum_{v \in H} d(w,v) \\
&= (n_H - 1) \cdot \frac{l_j - 1}{2} \cdot \frac{l_j + 1}{2} + (l_j - 1) \sum_{v \in H} d(w,v).
\end{aligned}$$

Therefore

$$\begin{aligned}
W(F(D)) = \frac{l_i^3 - l_i}{8} + \frac{l_j^3 - l_j}{8} + \frac{(l_i - 1)(l_j - 1)(l_i + l_j + 2)}{4} + \sum_{\{u,v\} \in H} d(u,v) \\
+ (n_H - 1) \cdot \frac{l_i - 1}{2} \cdot \frac{l_i + 1}{2} + (l_i - 1) \sum_{v \in H} d(w,v) \\
+ (n_H - 1) \cdot \frac{l_j - 1}{2} \cdot \frac{l_j + 1}{2} + (l_j - 1) \sum_{v \in H} d(w,v).
\end{aligned}$$

We now determine $W(F(D^{'}))$. If both l_i and l_j are odd then $l_i - 1$ and $l_j + 1$ are even. Let $L_i^{'}$ and $L_j^{'}$ denote the sets of vertices in the segments in $F(D^{'})$ corresponding to $l_i - 1$ and $l_j + 1$ (each of the sets $L_i^{'}$ and $L_j^{'}$ includes the cut vertex), respectively. Then

$$\begin{aligned}
W(F(D^{'})) &= \sum_{\{u,v\} \in V(F(D'))} d(u,v) \\
&= \sum_{\{u,v\} \in L_i^{'}} d(u,v) + \sum_{\{u,v\} \in L_j^{'}} d(u,v) + \sum_{\{u,v\} \in H} d(u,v) \\
&+ \sum_{\substack{u \in L_i^{'} \setminus w \\ v \in L_j^{'} \setminus w}} d(u,v) + \sum_{\substack{u \in L_i^{'} \setminus w \\ v \in H \setminus w}} d(u,v) + \sum_{\substack{u \in L_j^{'} \setminus w \\ v \in H \setminus w}} d(u,v).
\end{aligned}$$

Lemma 2.4 gives
$\displaystyle\sum_{\{u,v\}\in L_i'} d(u,v) = \frac{(l_i-1)^3}{8}$ and $\displaystyle\sum_{\{u,v\}\in L_j'} d(u,v) = \frac{(l_j+1)^3}{8}$.

$$\begin{aligned}
\sum_{\substack{u\in L_i'\setminus w\\ v\in L_j'\setminus w}} d(u,v) &= (l_i-2)\sum_{v\in L_j'} d(w,v) + l_j \sum_{v\in L_i'} d(w,v)\\
&= (l_i-2)\left[2\sum_{k=1}^{\frac{l_j+1}{2}} k - \frac{l_j+1}{2}\right] + l_j\left[2\sum_{k=1}^{\frac{l_i-1}{2}} k - \frac{l_i-1}{2}\right]\\
&= (l_i-2)\left(\frac{l_j+1}{2}\right)^2 + l_j\left(\frac{l_i-1}{2}\right)^2.
\end{aligned}$$

$$\begin{aligned}
\sum_{\substack{u\in L_i'\setminus w\\ v\in H\setminus w}} d(u,v) &= (n_H-1)\sum_{u\in L_i'} d(w,v) + (l_i-2)\sum_{v\in H} d(w,v)\\
&= (n_H-1)\left[2\sum_{k=1}^{\frac{l_i-1}{2}} k - \frac{l_i-1}{2}\right] + (l_i-2)\sum_{v\in H} d(w,v)\\
&= (n_H-1)\left(\frac{l_i-1}{2}\right)^2 + (l_i-2)\sum_{v\in H} d(w,v)\\
&= (n_H-1)\left(\frac{l_i-1}{2}\right)^2 + (l_i-2)\sum_{v\in H} d(w,v).
\end{aligned}$$

$$\begin{aligned}
\sum_{\substack{u\in L_j'\setminus w\\ v\in H\setminus w}} d(u,v) &= (n_H-1)\sum_{u\in L_j'} d(w,v) + (l_j)\sum_{v\in H} d(w,v)\\
&= (n_H-1)\left[2\sum_{k=1}^{\frac{l_j+1}{2}} k - \frac{l_j+1}{2}\right] + (l_j)\sum_{v\in H} d(w,v)\\
&= (n_H-1)\left(\frac{l_j+1}{2}\right)^2 + (l_j)\sum_{v\in H} d(w,v)\\
&= (n_H-1)\left(\frac{l_j+1}{2}\right)^2 + (l_j)\sum_{v\in H} d(w,v).
\end{aligned}$$

Therefore

$$\begin{aligned}
&W(F(D^{'}))\\
&= \frac{(l_i-1)^3}{8} + \frac{(l_j+1)^3}{8} + \sum_{\{u,v\}\in H} d(u,v) + (l_i-2)\left(\frac{l_j+1}{2}\right)^2 + l_j\left(\frac{l_i-1}{2}\right)^2\\
&+ (n_H-1)\left(\frac{l_i-1}{2}\right)^2 + (l_i-2)\sum_{v\in H} d(w,v) + (n_H-1)\left(\frac{l_j+1}{2}\right)^2\\
&+ l_j\sum_{v\in H} d(w,v)
\end{aligned}$$

and

$$\begin{aligned}
W(F(D)) - W(F(D^{'})) &= \frac{l_i^2 + 4l_in_H + 4l_j + 16 - (l_j^2 + (4l_j+8)n_H + 12l_i)}{8}\\
&\begin{cases} > 0 \text{ if } l_i > l_j + 2,\\ < 0 \text{ otherwise.}\end{cases}
\end{aligned}$$

(ii) If both l_i and l_j are even, then

$$\sum_{\{u,v\}\in L_i} d(u,v) = \frac{l_i^3}{8} \text{ and } \sum_{\{u,v\}\in L_j} d(u,v) = \frac{l_j^3}{8}.$$

$$\begin{aligned}
\sum_{\substack{u\in L_i\smallsetminus w\\ u\in L_j\smallsetminus w}} d(u,v) &= (l_i-1)\sum_{v\in V(l_j)} d(w,v) + (l_j-1)\sum_{v\in V(l_i)} d(w,v)\\
&= (l_i-1)\left[2\sum_{k=1}^{\frac{l_j}{2}} k - \frac{l_j}{2}\right] + (l_j-1)\left[2\sum_{k=1}^{\frac{l_i}{2}} k - \frac{l_i}{2}\right]\\
&= (l_i-1)\left(\frac{l_j}{2}\right)^2 + (l_j-1)\left(\frac{l_i}{2}\right)^2.
\end{aligned}$$

$$\begin{aligned}
\sum_{\substack{u\in L_i\smallsetminus w\\ v\in H\smallsetminus w}} d(u,v) &= (n_H-1)\sum_{u\in L_i} d(w,v) + (l_i-1)\sum_{v\in H} d(w,v)\\
&= (n_H-1)\left(\frac{l_i}{2}\right)^2 + (l_i-1)\sum_{v\in H} d(w,v),
\end{aligned}$$

and

$$\sum_{\substack{u\in L_j\smallsetminus w\\ v\in H\smallsetminus w}} d(u,v) = (n_H-1)\sum_{v\in L_j} d(w,v) + (l_j-1)\sum_{v\in H} d(w,v)$$

$$= (n_H - 1)\left(\frac{l_j}{2}\right)^2 + (l_j - 1)\sum_{v\in H} d(w,v).$$

Therefore

$$\begin{aligned}
&W(F(D))\\
&= \frac{l_i^3}{8} + \frac{l_j^3}{8} + \sum_{\{u,v\}\in H} d(u,v) + (l_i - 1)\left(\frac{l_j}{2}\right)^2 + (l_j - 1)\left(\frac{l_i}{2}\right)^2 + (n_H - 1)\left(\frac{l_i}{2}\right)^2\\
&+ (l_i - 1)\sum_{v\in H} d(w,v) + (n_H - 1)\left(\frac{l_j}{2}\right)^2 + (l_j - 1)\sum_{v\in H} d(w,v).
\end{aligned}$$

If both l_i and l_j are even then $l_i - 1$ and $l_j + 1$ are odd. Hence

$$\sum_{\{u,v\}\in L_i'} d(u,v) = \frac{(l_i-1)^3 - (l_i - 1)}{8} = \frac{(l_i-2)(l_i-1)l_i}{8},$$

$$\sum_{\{u,v\}\in L_j'} d(u,v) = \frac{(l_j+1)^3 - (l_j + 1)}{8} = \frac{(l_j)(l_j+1)(l_j+2)}{8} \text{ and}$$

$$\begin{aligned}
\sum_{\substack{u\in L_i'\setminus w\\ u\in L_j'\setminus w}} d(u,v) &= (l_i - 2)\sum_{v\in L_j'} d(w,v) + (l_j)\sum_{v\in L_i'} d(w,v)\\
&= (l_i - 2)\left[2\sum_{k=1}^{\frac{l_j}{2}} k\right] + l_j\left[2\sum_{k=1}^{\frac{l_i-2}{2}} k\right]\\
&= (l_i - 2)\cdot\frac{l_j}{2}\left[2(1) + \frac{l_j}{2} - 1\right] + l_j\cdot\frac{l_i-2}{2}\left[2 + \frac{l_i-2}{2} - 1\right]\\
&= \frac{(l_i-2)(l_j)(l_i+l_j+2)}{4}.
\end{aligned}$$

$$\begin{aligned}
\sum_{\substack{u\in L_i'\setminus w\\ v\in H\setminus w}} d(u,v) &= (n_H - 1)\sum_{u\in L_i'} d(w,v) + (l_i - 2)\sum_{v\in H} d(w,v)\\
&= (n_H - 1)\cdot\frac{l_i-2}{2}\cdot\frac{l_i}{2} + (l_i - 2)\sum_{v\in H} d(w,v)
\end{aligned}$$

and

$$\sum_{\substack{u\in L_j'\setminus w\\ v\in H\setminus w}} d(u,v) = (n_H - 1)\sum_{v\in L_j'} d(w,v) + l_j\sum_{v\in H} d(w,v)$$

$$= (n_H - 1) \cdot \frac{l_j}{2} \cdot \frac{l_j + 2}{2} + l_j \sum_{v \in H} d(w, v).$$

Therefore

$$\begin{aligned}
&W(F(D^{'})) \\
&\quad = \frac{(l_i - 2)(l_i - 1)(l_i)}{8} + \frac{l_j(l_j + 1)(l_j + 2)}{8} + \sum_{\{u,v\} \in H} d(u, v) \\
&\quad + \frac{(l_i - 2)(l_j)(l_i + l_j + 2)}{4} + (n_H - 1) \cdot \frac{l_i - 2}{2} \cdot \frac{l_i}{2} + (l_i - 2) \sum_{v \in V(H)} d(w, v) \\
&\quad + (n_H - 1) \cdot \frac{l_j}{2} \cdot \frac{l_j + 2}{2} + l_j \sum_{v \in H} d(w, v).
\end{aligned}$$

and

$$\begin{aligned}
W(F(D)) - W(F(D^{'})) &= \frac{l_i^2 + 4l_i n_H + 10l_j - (l_j^2 + 4l_j n_H + 6l_i)}{8} \\
&\begin{cases} > 0 \text{ if } l_i \geq l_j + 2, \\ \leq 0 \text{ otherwise.} \end{cases}
\end{aligned}$$

(iii) If l_i is odd and l_j is even, then

$$\sum_{\{u,v\} \in L_i} d(u, v) = \frac{l_i^3 - l_i}{8}, \quad \sum_{\{u,v\} \in L_j} d(u, v) = \frac{l_j^3}{8},$$

$$\begin{aligned}
\sum_{\substack{u \in L_i \setminus w \\ u \in L_j \setminus w}} d(u, v) &= (l_i - 1) \sum_{v \in V(l_j)} d(w, v) + (l_j - 1) \sum_{v \in V(l_i)} d(w, v) \\
&= (l_i - 1) \left(\frac{l_j}{2}\right)^2 + (l_j - 1) \cdot \frac{l_i - 1}{2} \cdot \frac{l_i + 1}{2} \\
&= \frac{(l_i - 1)(l_i l_j - l_i + l_j^2 + l_j - 1)}{4},
\end{aligned}$$

$$\begin{aligned}
\sum_{\substack{u \in L_i \setminus w \\ v \in H \setminus w}} d(u, v) &= (n_H - 1) \sum_{u \in L_i} d(w, v) + (l_i - 1) \sum_{v \in H} d(w, v) \\
&= (n_H - 1) \cdot \frac{l_i - 1}{2} \cdot \frac{l_i + 1}{2} + (l_i - 1) \sum_{v \in H} d(w, v),
\end{aligned}$$

and

$$\sum_{\substack{u \in L_j \setminus w \\ v \in H \setminus w}} d(u, v) = (n_H - 1) \sum_{v \in L_j} d(w, v) + (l_j - 1) \sum_{v \in H} d(w, v)$$

$$= (n_H - 1)\left(\frac{l_j}{2}\right)^2 + (l_j - 1)\sum_{v\in H} d(w,v).$$

Therefore

$$\begin{aligned}
&W(F(D))\\
&\quad = \frac{l_i^3 - l_i}{8} + \frac{l_j^3}{8} + \sum_{\{u,v\}\in H} d(u,v) + \frac{(l_i-1)(l_il_j - l_i + l_j^2 + l_j - 1)}{4}\\
&\quad + (n_H - 1)\cdot\frac{l_i - 1}{2}\cdot\frac{l_i+1}{2} + (l_i - 1)\sum_{v\in H} d(w,v) + (n_H - 1)\left(\frac{l_j}{2}\right)^2\\
&\quad + (l_j - 1)\sum_{v\in H} d(w,v).
\end{aligned}$$

If l_i is odd and l_j is even, then $l_i - 1$ is even and $l_j + 1$ is odd. To get $W(F(D'))$ we first interchange l_i and l_j in $W(F(D))$ then replace l_i with $l_i - 1$ and l_j with $l_j + 1$, hence

$$\begin{aligned}
&W(F(D'))\\
&\quad = \frac{(l_i-1)^3}{8} + \frac{l_j(l_j+1)(l_j+2)}{8} + \sum_{\{u,v\}\in H} d(u,v)\\
&\quad + \frac{l_j((l_i-1)(l_j+1) - l_j + (l_i-1)^2 + l_i - 3)}{4} + (n_H - 1)\left(\frac{l_i - 1}{2}\right)^2\\
&\quad + (l_i - 2)\sum_{v\in H} d(w,v) + (n_H - 1)\cdot\frac{l_j}{2}\cdot\frac{l_j+2}{2} + l_j\sum_{v\in H} d(w,v)
\end{aligned}$$

and

$$\begin{aligned}
W(F(D)) - W(F(D')) &= \frac{(l_i - l_j - 1)(l_i + l_j + 4n_H - 7)}{8}\\
&\begin{cases} > 0 \text{ if } l_i > l_j + 1,\\ \leq 0 \text{ otherwise.}\end{cases}
\end{aligned}$$

(iv) If l_i is even and l_j is odd, then interchanging l_i and l_j in $W(F(D))$ of (iii) gives

$$\begin{aligned}
&W(F(D))\\
&\quad = \frac{l_i^3}{8} + \frac{l_j^3 - l_j}{8} + \sum_{\{u,v\}\in H} d(u,v) + \frac{(l_j-1)(l_jl_i - l_j + l_i^2 + l_i - 1)}{4}
\end{aligned}$$

$$+ (n_H - 1)\left(\frac{l_i}{2}\right)^2 + (l_i - 1)\sum_{v\in H} d(w,v) + (n_H - 1)\cdot \frac{l_j - 1}{2}\cdot\frac{l_j+1}{2}$$
$$+ (l_j - 1)\sum_{v\in H} d(w,v).$$

If we replace l_i with $l_i - 1$ and l_j with $l_j + 1$ in $W(F(D))$ of (iii) we get

$$\begin{aligned} &W(F(D'))\\ &\quad= \frac{(l_i-2)(l_i-1)l_i}{8} + \frac{(l_j+1)^3}{8} + \sum_{\{u,v\}\in H} d(u,v)\\ &\quad+ \frac{(l_i-2)((l_i-1)(l_j+1) - l_i + (l_j+1)^2 + l_j + 1)}{4}\\ &\quad+ (n_H-1)\cdot\frac{l_i-2}{2}\cdot\frac{l_i}{2} + (l_i-2)\sum_{v\in H} d(w,v) + (n_H-1)\left(\frac{l_j+1}{2}\right)^2\\ &\quad+ l_j\sum_{v\in H} d(w,v). \end{aligned}$$

and

$$W(F(D)) - W(F(D')) = \frac{(l_i - l_j - 1)(l_i + l_j + 4n_H - 9)}{8}$$
$$\begin{cases} > 0 \text{ if } l_i > l_j + 1,\\ \leq 0 \text{ otherwise.}\end{cases}$$

□

Remark 4.6 As a consequence of Lemma 4.5, a minimal graph with given number of segments and have segments all of length at least 3 cannot have two segments of same even length, that is $l_i = l_j$. Because then replacing the two segments with two new segments of length $l_i - 1$ and $l_j + 1$ would reduce Wiener index.

Iterate Lemma 4.5 as much as possible to get the following theorem. Note that iterating Lemma 4.5 in a graph does not change the size of that graph.

Theorem 4.7 *Among all graphs of size m, number of segments s and all segments of length at least 3, $F(D)$ has the minimum Wiener index for some $D = (l_1, l_2, \ldots, l_s)$ where* $\begin{cases} |l_i - l_j| \in \{0,2\} & \text{if } l_i \text{ and } l_j \text{ are odd,}\\ |l_i - l_j| = 1 & \text{if } l_i \text{ or } l_j \text{ is even.}\end{cases}$

Note that Theorem 4.7 provides full characterization of the minimal graphs it describes.

4.2 Graphs of Short Segments

In this section we study graphs with segments all of length less than or equal to 2.

Lemma 4.8 *Let G be a connected graph with segment sequence $D = (1, 1, \ldots, 1)$, u and $v \in V(G)$ such that*

- *(i)* $d(u, v) = 3$
- *(ii)* $\deg(u) \neq 1$ *or* $\deg(v) \neq 1$.

If $G^{'}$ is the graph formed from G by merging u and v then

$$W(G) > W(G^{'}).$$

The proof of Lemma 4.8 looks the same as that of Lemma 4.2. Also because of condition (ii), G and $G^{'}$ in Lemma 4.8 have the same segment sequence.

Lemma 4.9 *Let H be a connected graph with m edges and segment sequence $D = (1, 1, \ldots, 1)$. If H is minimal then $diam(H) \leq 2$.*

Proof. Suppose that Lemma 4.8 cannot be applied to H. In other words there are no two vertices that can be merged, then either:

- (i) $d_H(u, v) < 3$ for all $u, v \in V(H)$ or
- (ii) There exists $u, v \in V(H)$ such that $d_H(u, v) = 3$ and $\deg(u) = \deg(v) = 1$.

If (i) holds, we are done. If (ii) holds then $H = P_{wu^{'}} K_{v^{'}z} P^{'}$, where each of P and $P^{'}$ is a $2-$vertex path and K some connected graph. Without loss of generality let $u \in V(P)$ and $v \in V(P^{'})$. If K has a vertex y that is neither adjacent to $u^{'}$ nor $v^{'}$, then merge u, y and v.

Otherwise each vertex in K is adjacent to either $u^{'}$ or $v^{'}$. Let $N^{u^{'}}$ be the set of all vertices $w^{'}$ in H such that $w^{'}$ is adjacent to $u^{'}$ and $\deg(w^{'}) = 1$. If $\deg(u^{'}) - |N^{u^{'}}| = 2$, then there exists $x, x^{'} \in V(K)$ such that x is adjacent to both $u^{'}$ and $x^{'}$ with $x^{'}$ not adjacent to $u^{'}$. Since $x^{'}$ is adjacent to $v^{'}$, $d_H(u^{'}, v^{'}) = 1$ and H has segment sequence $D = (1, \ldots, 1)$, we must have $d_H(x^{'}, u^{'}) = 2$, $d_H(x^{'}, u) = 3$, $\deg(u) = 1$ and $\deg(x^{'}) \geq 3$. Then merge $x^{'}$ and u as in Lemma 4.8. If $\deg(u^{'}) - |N^{u^{'}}| \neq 2$, then we can safely apply Lemma 3.3 by removing the edge $\{u^{'}, w^{'}\}$ in H and adding the edge $\{v^{'}, w^{'}\}$, for all $w^{'}$ in $N^{u^{'}}$. All the cases lead to $diam(H) \leq 2$ if H is minimal. $\square$

Lemma 4.10 ***[10, Proposition 2]*** *Let H and F be two graphs such that they are both*

- *connected,*
- *of diameter 2,*
- *have the same number of vertices and*
- *have the same number of edges.*

Then $W(H) = W(F)$.

Proof. Let $|V(H)| = |V(F)| = n, |E(H)| = |E(F)| = m$, then

$$\begin{aligned} W(F) &= \sum_{u,v\in V(F)} d(u,v) = \sum_{\substack{u,v\in V(F)\\ d(u,v)=2}} 2 + \sum_{\substack{u,v\in V(F)\\ d(u,v)=1}} 1 \\ &= 2(\tbinom{n}{2} - |E(F)|) + |E(F)| = 2(\tbinom{n}{2} - m) + m \\ &= 2(\tbinom{n}{2} - |E(H)|) + |E(H)| = \sum_{\substack{u,v\in V(H)\\ d(u,v)=2}} 2 + \sum_{\substack{u,v\in V(H)\\ d(u,v)=1}} 1 \\ &= W(H). \end{aligned}$$

□

Definition 4.11 Define G_m as a connected graph with m edges such that for $m \leq 6$, $G_0 = S_1$, $G_1 = S_2$, G_2 is undefined, $G_3 = S_4$, $G_4 = S_5$, $G_5 = S_6$ and $G_6 = K_4$. For $m \geq 7$, G_m is constructed as follows: Let n be such that $\binom{n-1}{2} < m \leq \binom{n}{2}$. Then $n \geq 4$.

- If $m - \binom{n-1}{2} = 2$, then remove the edge between u and v in K_{n-1} and add three edges zu, zv, zx for some vertex x of K_{n-1} that is not in {u,v}, see Figure 4.1.

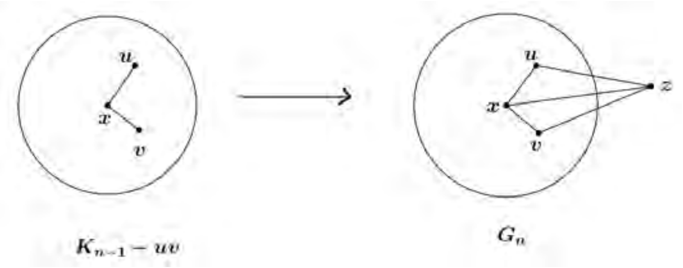

Figure 4.1: Transform $K_{n-1} - uv$ to G_n

- If $m - \binom{n-1}{2} \neq 2$ then G_n is obtained by joining a new vertex to $m - \binom{n-1}{2}$ vertices of K_{n-1}.

Note that for any m, G_m has a vertex that is adjacent to all other vertices in G_m. For $m \leq 6$, this can be seen by inspection. For $m > 6$, the vertex x in Figure 4.1 is one example of such vertex and any vertex of the K_{n-1} part works for the other case.

Theorem 4.12 *Among all graphs with m edges and segment sequence $D = (1, \dots, 1)$, G_m has the minimum Wiener index.*

Proof. Let G be of m edges and segment sequence $D = (1, \dots, 1)$. Suppose G has the minimum Wiener index, then by Lemma 4.9 $diam(G) \leq 2$. If $diam(G) \leq 1$, we are done since $G = K_{n_G} = G_m$ for $m = \binom{n_G}{2}$. Otherwise $diam(G) = 2$. So $W(G) = m + 2\left(\binom{n_G}{2} - m\right)$, while $W(G_m) = m + 2\left(\binom{n}{2} - m\right)$ for some n with $\binom{n-1}{2} < m \leq \binom{n}{2}$. All we need to prove is that $n \leq n_G$. Suppose that $n > n_G$, then $n - 1 \geq n_G$. Then the maximum edge that G can have is $\binom{n_G}{2} \leq \binom{n-1}{2} < m$ which is a contradicts the fact that G has m edges. □

Remark 4.13 Among all graphs with m edges G_m has minimum Wiener index. To prove this claim one can use Lemma 4.2 combined with ideas used in the proof of Theorem 4.12.

Definition 4.14 For any natural number $m \geq 3$, $K_{2,m}$ is defined as the graph obtained from $(m + 1)-$vertex star S_{m+1} by adding a new vertex and join it to all m leaves of S_{m+1}. $K_{2,m}$ has segment sequence $D = (2, 2, \dots, 2)$.

Theorem 4.15 *Among all graphs with m segments and segment sequence $D = (2, 2, \dots, 2)$, the minimum Wiener index is reached by $K_{2,m}$.*

Proof. Let G be a graph with m segments and segment sequence $D = (2, 2, \dots, 2)$. For any two vertices $u \neq v$ of G that have degree 2, $d_G(u, v) \geq 2$. For any vertices x, y, z in a segment of G with ends x and z, $d_G(x, y) = d_G(y, z) = 1$. So $W(G) \geq 2\binom{m}{2} + 2m = W(K_{2,m})$. □

Now, we are ready for the cases where the graph may have segments of length 2 and 1 at the same time.

Definition 4.16 For any natural numbers m and l, we define $D(m, l) = (2, \dots, 2, 1, \dots, 1)$, where 2 repeats m times and 1 repeats l times.

Definition 4.17 Let m and l be two natural numbers. Let $x \in V(G_l)$ such that $N_{G_l}(x) = V(G_l - x)$. Let $y \in N_{G_l}(x)$ of maximum degree.

We define $G_{m,l}$ to be the graph obtained by adding m segments of length 2 to G_l by merging one end with x and the other end to y, see Figure 4.2 for example. Unless $m = 1$ and $l < 6$, $G_{m,l}$ has the segment sequence $D(m, l)$. So, let us redefine $G_{m,l}$ for $m = 1$ and $l < 6$ as follows: let $P = P' = P_2$, $H = C_3$, $R = S_4$ with $v \in V(R)$ and $\deg(v) = 1$. Then $G_{1,1}$ does not exist, since there is no graph corresponding to $D(1, 1)$. $G_{1,2} = P_{u'v}R$, $G_{1,3} = P_{u'u}H_{ww'}P'$ with $u \neq w$. $G_{1,4}$ is obtained by removing an edge uv in K_4 and attaching a new vertex z in u. Let $x \in V(G_{1,4})$ such that $\deg(x) = 3$, then $G_{1,5} = P_{u'x}G_{1,4}$, see Figure 4.3.

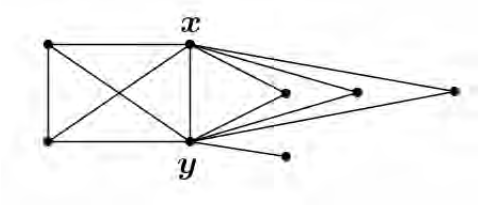

Figure 4.2: $G_{3,7}$

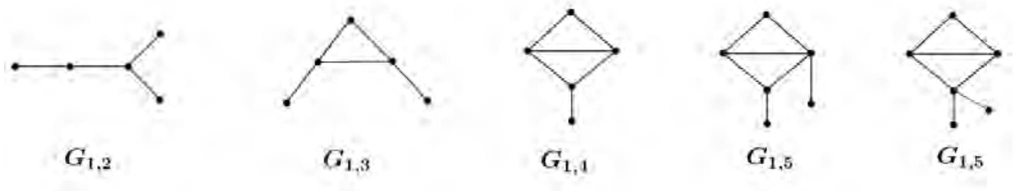

Figure 4.3: $G_{1,2}$, $G_{1,3}$, $G_{1,4}$ and $G_{1,5}$

Note that there are two graphs corresponding to $G_{1,5}$, but they have the same Wiener index.

Theorem 4.18 *Let* $\mathbb{N}$ *be the set of natural numbers. For any* $(m, l) \in \mathbb{N} \times \mathbb{N} - \{(1, 1), (1, 2)\}$, $G_{m,l}$ *has the minimum Wiener index.*

Proof. For $(m, l) \in \{(1, 3), (1, 4), (1, 5)\}$ check Figure 4.4 for graphs and their Wiener indices. For the rest of the proof, we assume that $(m, l) \in \mathbb{N} \times \mathbb{N} - \{(1, 1), (1, 2), (1, 3), (1, 4), (1, 5)\}$. Let G be a graph with segment sequence $D(m, l)$. Let $A = \{v_1, \ldots, v_m\}$ be the set of vertices of degree 2 in G. Then

$$\sum_{u,v \in A} d_G(u, v) \geq 2m.$$

Let B be the set of vertices of G that is an end of segment of length 2, then

$$\sum_{u\in A, v\in B} d_G(u,v) \geq m(1+1) = 2m.$$

Let $G^{'} = G - v_1 - v_2 - \cdots - v_m$, then $G^{'}$ has l edges. Then remark 4.13 assures that $W(G^{'}) \geq W(G_l)$. Hence $W(G) \geq 2m + 2m + W(G_l) = W(G_{m,l})$. $\square$

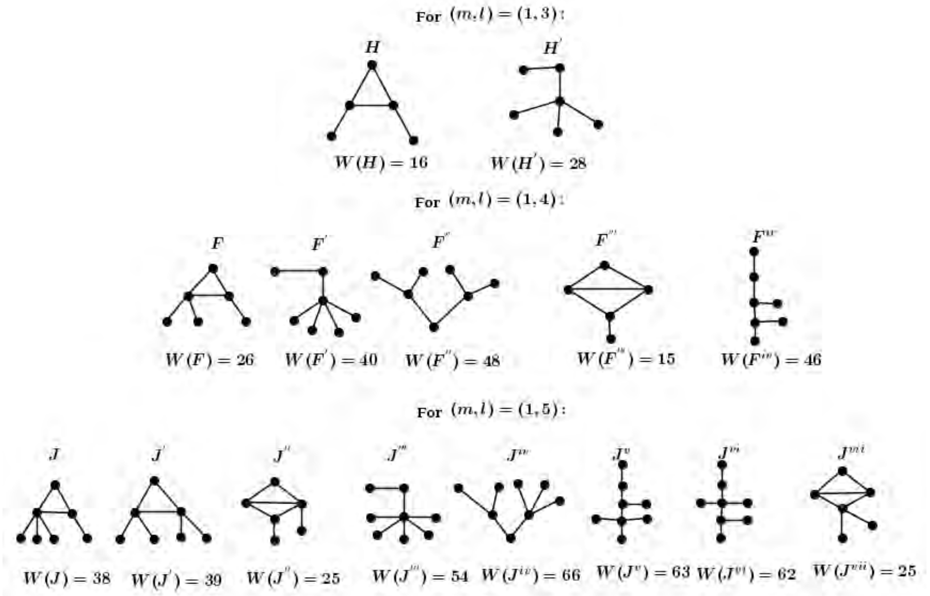

Figure 4.4: Graphs corresponding to $(m,l) \in \{(1,3),(1,4),(m,l) = (1,5)\}$

5 Conclusions

In this thesis we found extremal bicyclic graphs under each of the following conditions: The circumference is fixed and the size of the core is fixed. We also found extremal graphs given the segment sequence.

We first studied the Wiener index of bicyclic graphs with circumference g and order n. It turned out from Theorem 3.17 that, among all bicyclic graphs with circumference g and order n, the Wiener index is minimized by $B_{n,g,\frac{g-1}{2},1}$ if g is odd, $B_{n,g,\frac{g-2}{2},1}$ if g is even and $\frac{g}{2}$ is odd and $B_{n,g,\frac{g}{2},1}$ if both g and $\frac{g}{2}$ are even. While Theorem 3.27 provides two candidates for the maximum Wiener index, among all bicyclic graphs with circumference g and order n. And the candidates are $D_{n,g,n-g-1,3}$ and $(B_{g,g,k,1})_{w'w}P_{n-g+1}$, where w is an end of a path P_{n-g+1}.

We then studied Wiener index of bicyclic graphs with core size m and order n. We found in Theorem 3.34 that, among all bicyclic graphs with core size m and order n, $(D_{m-1,3,q,3})_{ww'}P_{n-m+2}$ maximizes Wiener index, with $w \in V(C_3)$, w not in P_{n-m+2} and $w^{'}$ an end of a path P_{n-m+2}. The case of the minimum Wiener index had not been examined.

Finally, we studied graphs with fixed segment sequence, where we found in Theorem 4.3 that, among all graphs with the same segment sequence and all segments of length at least 3, the graph that minimizes Wiener index has all of its segments ending in one vertex. However if we fix the total number of edges and the total number of segments but allow the length of segments to change then, by Theorem 4.7, among all graphs of size m, number of segments s and all segments of length at least 3, $F(D)$ has the minimum Wiener index, for some

$$D = (l_1, l_2, \ldots, l_s), \text{ where } \begin{cases} |l_i - l_j| \in \{0, 2\} & \text{if both } l_i \text{ and } l_j \text{ are odd,} \\ |l_i - l_j| = 1 & \text{if } l_i \text{ or } l_j \text{ is even.} \end{cases}$$

According to Theorem 4.12, we can conclude that, among all graphs with m edges and segment sequence $D = (1, \ldots, 1)$, G_m attains minimum Wiener index. For large m, most of the time, G_m is obtained by removing some edges adjacent to a given vertex of a complete graph. While Theorem 4.15 shows that, in the set of all graphs with m segments and segment sequence $D = (2, \ldots, 2)$, the minimum Wiener index is reached by $K_{2,m}$. $K_{2,m}$ can be obtained by adding edges to join all leaves of a $(m + 1)$-vertex star S_{m+1} to a new vertex. Let $\mathbb{N}$ be the set of natural numbers. Then Theorem 4.18 shows that, for any $(m, l) \in \mathbb{N} \times \mathbb{N} - \{(1, 1), (1, 2)\}$, $G_{m,l}$ has the minimum Wiener index. $G_{m,l}$ is obtained by merging a vertex of largest degree of $K_{2,m}$ with a vertex of largest degree in G_l. The case for the graphs with the mix of segments of length less than 3 and segments of length greater than or equal to 3 have not been examined. Also the case of the maximum Wiener index have not been examined.

Theorem 3.34 in conjuction with Lemma 3.21 shows that, among all bicyclic graphs of order n, $D_{n,3,n-4,3}$ maximizes Wiener index. This confirms the conjecture that arose in [2] about maximal bicyclic graph of size m.

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